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Presto 4.18 User's Guide

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Computational Solid Mechanics and Structural Dynamics Department
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Abstract

Presto is a Lagrangian, three-dimensional explicit, transient dynamics code that is used to analyze solids subjected to large, suddenly applied loads. The code is designed for a parallel computing environment and for problems with large deformations, nonlinear material behavior, and contact. Presto also has a versatile element library that incorporates both continuum elements and structural elements. This user's guide describes the input for Presto that gives users access to all the current functionality in the code. The environment in which Presto is built allows it to be coupled with other engineering analysis codes. Using a concept called *scope*, the input structure reflects the fact that Presto can be used in a coupled environment. The user's guide describes how scope is implemented from the outermost to the innermost scopes. Within a given scope, the descriptions of input commands are grouped based on functionality of the code. For example, all material input command lines are described in a chapter of the user's guide for all the material models that can be used in Presto.

Acknowledgments

This document is the result of the collective effort of a number of individuals. The current development team responsible for Adagio and Presto, the SIERRA Solid Mechanics codes, includes Nathan K. Crane, Jason D. Hales, Martin W. Heinstein, Alex J. Lindblad, David J. Littlewood, Kendall H. Pierson, Vicki L. Porter, Nathaniel S. Roehrig, Timothy R. Shelton, Gregory D. Sjaardema, Benjamin W. Spencer, and Jesse D. Thomas. This document is written and maintained by this team.

Outside the core development team, there are number of other individuals who have contributed to this manual. Nicole L. Breivik, J. Franklin Dempsey, Jeffery D. Gruda, and Chi S. (David) Lo have provided valuable input from the user community as Presto and Adagio Product Managers.

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Presto 4.18 Release Notes

Following is a list of new features and syntax changes made to Presto since the 4.16 release.

Material Model Documentation

Documentation has been added for a number of material models. These include Thermoelastic (Section 4.2.2), Neo-Hookean (Section 4.2.3), Power Law Creep (Section 4.2.12), K&C Concrete (Section 4.2.14), Low Density Foam (Section 4.2.16), and Wire Mesh (Section 4.2.18).

Linear Shell

A fully linear shell element is available. See Section 5.2.4.

New Methods for Defining Beam/Shell Offset

Shell offset can now be defined based on a mesh variable, and beam offset can now be defined in the global coordinate system either directly in the input file or by a mesh variable. See Sections 5.2.4 and 5.2.6.

New Syntax for SPH and other Particle Formulations

New syntax is required for SPH (now Particle) sections. The `SPH SECTION` command block has been replaced with the more general `PARTICLE SECTION` command block, which supports multiple particle method formulations. See Section 5.2.11.

Peridynamics

Presto now includes an implementation of peridynamics, a nonlocal formulation of continuum mechanics. Peridynamics may be applied to a wide variety of problems but is generally best suited for problems such as crack formation and fracture. Peridynamics may be applied to blocks of sphere elements through the use of a `PERIDYNAMICS SECTION` (see Section 5.2.13). For an overview of peridynamic theory and basic guidelines for setting up peridynamic analyses, see Section 9.3.

Point Mass for Rigid Bodies

Mass may now be added to a rigid body at a user-specified location. See Section 5.3.1.

Element Disconnection For Shells

The element disconnection method for handling failure with element death is now available for shell elements. See Section 5.5.4.6.

New Syntax for Element to Particle Conversion

New syntax is required for element to particle conversion. The `CONVERT TO PARTICLES WITH SECTION` command line has been replaced by the `PARTICLE CONVERSION` command block to allow for more options. See Section 5.5.4.7.

Element to Multiple Particle Conversion

It is now possible to convert a single element into multiple particles using element death. See Section 5.5.4.7

Initialization of Variables with Weibull Distribution

Field variables can be initialized with a spatially varying random variable conforming to the Weibull probability distribution function. See Section 6.2.4.

MPCs for Volumetric Constraints

The capability to use MPCs for tied contact has been extended to allow for volumetric constraints between slave nodes and the nodes on an enclosing surface. This is primarily intended to be used to constrain volumes of void elements to an enclosing solid. See Section 6.10.8.

Time-Period Dependent Friction Models

Friction models can now be switched between time periods using the new `TIME VARIANT` friction model with Dash contact. See Section 7.11.14.

Changes in Contact Interaction Definition for Particle Blocks

Several changes have occurred in the way Dash contact defines the default interactions for particle elements. These changes make the use of particles and particle conversion in contact more intuitive. See Section 7.18.

Hourglass Energy by Block

The hourglass energy sums are now available on each block as global variables. See Section 8.2.1.8.

Output Synchronization

The results, restart, heartbeat, and history output can be synchronized with databases of the same type in other regions and output from coupled applications. See Sections 8.2.1.16, 8.3.10, 8.4.10, and 8.5.12.

User Output Data Filtering

Frequency based data filters can now be automatically computed off of nodal and element quantities. See Section 8.2.2.6.

Surface Normal Data Transfer

The `VARIABLE INTERPOLATION` command block may now be used to transfer only component of a variable normal to a surface. See Section 8.7.

Global Energy Reporting

Options for global energy reporting have been introduced to adjust accuracy and performance. See Section 8.8.

Global Rigid Body Variable Output

The default global rigid body variable output may now be modified. See Section 8.8.

RVE Usage Enhancements

A representative volume element (RVE) with nonmatching opposing surfaces can be used by including a block of membranes surrounding the RVE. This membrane block is required to have matching opposing surfaces and must be tied to the underlying RVE. See Section 9.1.

Presto 4.18 Known Issues

Section 3.4.1.2: When using explicit control modes, the Lanczos and power method time step estimators can not yet be used with problems that have contact, rigid bodies, blocks in the fine mesh that are not controlled by the coarse mesh, or coarse elements that contain no fine nodes.

Section 5.2.12: Superelements are not compatible with several modeling capabilities. They cannot be used with element death. They cannot be used with node-based, power method, or Lanczos critical time step estimation methods. They are also not compatible with some preconditioners (such as FETI) for implicit solutions.

Section 6.3.2.2: If a prescribed displacement with the `CYLINDRICAL AXIS` option is applied to nodes that fall on the axis, it will have no effect. Separate boundary conditions should be applied to those nodes to fix them in the plane normal to the axis.

Section 6.3.3.2: If a prescribed velocity with the `CYLINDRICAL AXIS` option is applied to nodes that fall on the axis, it will have no effect. Separate boundary conditions should be applied to those nodes to fix them in the plane normal to the axis.

Section 7.12.1: Attempting to use `GLOBAL SEARCH INCREMENT` with a value greater than 1, especially in a problem that contains shells and/or restart, will, in most cases, cause code failure. A `GLOBAL SEARCH INCREMENT` value greater than 1 will, under the best circumstances, give only a marginal improvement in speed.

Section 8.4: User defined variables (see Section 10.2.4) are not currently supported with heartbeat output.

Section 9.2: Currently, the J-Integral evaluation capability is based on assumptions of elastostatics and a stationary crack, and is only implemented for uniform gradient hex elements.

Chapter 1

Introduction

This document is a user's guide for the code Presto. Presto is a three-dimensional transient dynamics code with a versatile element library, nonlinear material models, large deformation capabilities, and contact. It is built on the SIERRA Framework [1, 2]. SIERRA provides a data management framework in a parallel computing environment that allows the addition of capabilities in a modular fashion. Contact capabilities are parallel and scalable.

The *Presto 4.18 User's Guide* provides information about the functionality in Presto and the command structure required to access this functionality in a user input file. This document is divided into chapters based primarily on functionality. For example, the command structure related to the use of various element types is grouped in one chapter; descriptions of material models are grouped in another chapter.

The input and usage of Presto is similar to that of the code Adagio [3]. Adagio is a three-dimensional quasi-static code with a versatile element library, nonlinear material models, large deformation capabilities, and contact. Adagio, like Presto, is built on the SIERRA Framework [1]. Contact capabilities for Adagio are also parallel and scalable. A significant feature of Adagio is that it offers a multilevel, nonlinear iterative solver.

Because of the similarities in input and usage between Presto and Adagio, the user's guides for the two codes are structured in the same manner and share common material. (Once you have mastered the input structure for one code, it will be easy to master the syntax structure for the other code.) To maintain the commonality between the two user's guides, we have used a variety of techniques. For example, references to Adagio may be found in the Presto user's guide and vice versa, and the chapter order across the two guides is the same.

On the other hand, each of the two user's guides is expressly tailored to the features of the specific code and documents the particular functionality for that code. For example, though both Presto and Adagio have contact functionality, the content of the chapter on contact in the two guides differs.

Important references for both Adagio and Presto are given in the references section at the end of this chapter. Adagio was preceded by the codes JAC and JAS3D; JAC is described in Reference 4; JAS3D is described in Reference 5. Presto was preceded by the code Pronto3D. Pronto3D is described in References 6 and 7. Some of the fundamental nonlinear technology used by both Presto and Adagio are described in References 8, 9, and 10. Currently, both Presto and Adagio

use the Exodus II database and the XDMF database; Exodus II is more commonly used than XDMF. (Other options may be added in the future.) The Exodus II database format is described in Reference 11, and the XDMF database format is described in Reference 12. Important information about contact is provided in the reference document for ACME [13]. ACME is a third-party library for contact.

One of the key concepts for the command structure in the input file is a concept referred to as *scope*. A detailed explanation of scope is provided in Section 1.2. Most of the command lines in Chapter 2 are related to a certain scope rather than to some particular functionality.

1.1 Document Overview

This document describes how to create an input file for Presto. Highlights of the document contents are as follows:

- Chapter 1 presents the overall structure of the input file, including conventions for the command descriptions, style guidelines for file preparation, and naming conventions for input files that reference the Exodus II database [11]. The chapter also gives an example of the general structure of an input file that employs the concept of scope.

- Chapter 2 explains some of the commands that are general to various applications based on the SIERRA Framework. These commands let you define scopes, functions, and coordinate systems, and they let you set up some of the main time control parameters (begin time, end time, time blocks) for your analysis. (Time control and time step control are discussed in more detail in Chapter 3.) Other capabilities documented in this chapter are available for calculating element distortion and for activating and deactivating functionality at different times throughout an analysis.

- Chapter 3 describes how to set the start time, end time, and time blocks for an analysis. This chapter also discusses various options for controlling the critical time step in Presto.

- Chapter 4 describes material models that can be used in conjunction with the elements in Presto and Adagio. Most of the material models have an interface that allows the models to be used by the elements in both codes. Even though a material model can be used by both codes, it may be that the use of the material model is better suited for one code rather than for the other code. For example, a material model set up to characterize behavior over a long time would be better suited for use in Adagio than in Presto. If a material model is better suited for one of the two codes, this information will be noted for the material model. In some cases, a material model may only be included in one of the two user's guides. Chapter 4 also discusses the application of temperature to a mesh and the computation of thermal strains (isotropic and anisotropic).

- Chapter 5 lists the elements in Presto and Adagio and describes how to set up commands to use the various options for the elements. Most elements can be used in either Presto or Adagio. If an element is available in one code but not the other, this information will

be noted for the element. In some cases, an element may only be included in one of the two user's guides. For example, Presto has a special element implementation referred to as smoothed particle hydrodynamics (SPH). The Presto user's guide contains a section on SPH, but the Adagio user's guide does not. Chapter 5 also includes descriptions of the commands for mass property calculations, element death, and mesh rebalancing. Two "element-like" capabilities are discussed in Chapter 5—rigid bodies and torsional springs.

- Chapter 6 documents how to use kinematic boundary conditions, force boundary conditions, initial conditions, and specialized boundary conditions.
- Chapter 7 discusses how to define interactions of contact surfaces.
- Chapter 8 details the various options for obtaining output.
- Chapter 9 documents special modeling techniques.
- Chapter 10 provides an overview of the user subroutine functionality.
- Appendix A provides a sample input file from an analysis of 16 lead spheres being crushed together inside a steel box. This problem emphasizes large deformation and contact.
- Appendix B lists all the permissible Presto input lines in their proper scope.
- The index allows you to find information about command blocks and command lines. In general, single-level entries identify the page where the command syntax appears, with discussion following soon thereafter—on the same page or on a subsequent page. Page ranges are not provided in this index. Some entries consist of two or more levels. Such entries are typically based on context, including such information as the command blocks in which a command line appears, the location of the discussion related to a particular command line, and tips on usage. The PDF version of this document contains hyperlinked entries from the page numbers listed in the index to the text in the body of the document.

Note that all references cited within the text of each chapter are listed at the end of the respective chapters rather than in a separate references chapter. The reference sections in the chapters are not necessarily edited so that they are specific to Adagio or Presto. Some chapters will have exactly the same set of references (even if not all are cited for a particular user's guide), and some chapters will have the references tailored to the specific user's guide.

1.2 Overall Input Structure

Presto is one of many mechanics codes built on the SIERRA Framework. The SIERRA Framework provides the capability to perform multiphysics analyses by coupling together SIERRA codes appropriate for the mechanics of interest. Input files may be set up for analyses using only Presto, or they may be set up to couple Presto and one or more other SIERRA analysis codes. For example, you might run Adagio to compute a stress state, and then use the results of this analysis as initial conditions for a Presto analysis. For a multiphysics analysis using Presto and Adagio, the time-step control, the mesh-related definitions, and the boundary conditions for both Presto and Adagio will all be in the same input file. Therefore, the input for Presto reflects the fact that it could be part of a multiphysics analysis. (Note that not all codes built on the SIERRA Framework can be coupled. Consult with the authors of this document to learn about the codes that can be coupled with Presto.)

To create files defining multiphysics analyses, the input files use a concept called "scope." Scope is used to group similar commands; a scope can be nested inside another scope. The broadest scope in the input file is the SIERRA scope. The SIERRA scope contains information that can be shared among different physics. Examples of physics information that can be shared are definitions of functions and materials. Thus, in our above example of a coupled Presto/Adagio multiphysics analysis, both Adagio and Presto could reference functions to define such things as time histories for boundary conditions or stress-strain curves. Some of the functions could even be shared by these two applications. Both Presto and Adagio could also share information about materials.

Within the SIERRA scope are two other important scopes: the procedure scope and the region scope. The region is nested inside the procedure, and the procedure is nested inside the SIERRA scope. The procedure scope controls the overall analysis from the start time to the end time; the region scope controls a single time step. For a multiphysics analysis, the SIERRA scope could contain several different procedures and several different regions.

Inside the procedure scope (but outside of the region scope) are commands that set the start time and the end time for the analysis.

Inside the region scope for Presto are such things as definitions for boundary conditions and contact. In a multiphysics analysis, there would be more than one region. In our Presto/Adagio example, there would be both a Presto region and an Adagio region, each within its respective procedures. The definitions for boundary conditions and contact and the mesh specification for Presto would appear in the Presto region; the definitions for boundary conditions and contact and the mesh specification for Adagio would appear in the Adagio region.

The input for Presto consists of command blocks and command lines. The command blocks define a scope. These command blocks group command lines or other command blocks that share a similar functionality. A command block will begin with an input line that has the word "begin"; the command block will end with an input line that has the word "end". The SIERRA scope, for example, is defined by a command block that begins with an input line of the following form:

```
BEGIN SIERRA my_problem
```

The two character strings `BEGIN` and `SIERRA` are the key words for this command block. An input line defining a command block or a command line will have one or more key words. The string

`my_problem` is a user-specified name for this SIERRA scope. The SIERRA scope is terminated by an input line of the following form:

```
END SIERRA my_problem
```

In the above input line, `END` and `SIERRA` are the key words to end this command block. The SIERRA scope can also be terminated simply by using the following key word:

```
END
```

The above abbreviated command line will be discussed in more detail in later chapters. There are similar input lines used to define the procedure and region scopes. Boundary conditions are another example where a scope is defined. A particular instance of a boundary condition for a prescribed displacement boundary condition is defined with a command block. The command block for the boundary condition begins with an input line of the form:

```
BEGIN PRESCRIBED DISPLACEMENT
```

and ends with an input line of either of the following forms:

```
END PRESCRIBED DISPLACEMENT
```

```
END
```

Command lines appear within the command blocks. The command lines typically have the form `keyword = value`, where `value` can be a real, an integer, or a string. In the previous example of the prescribed displacement boundary condition, there would be command lines inside the command block that are used to set various values. For example, the boundary condition might apply to all nodes in node set 10, in which case there would be a command line of the following form:

```
NODE SET = nodelist_10
```

If the prescribed displacement were to be applied along a given component direction, there would be a command line of this form:

```
COMPONENT = X
```

The form above would specify that the prescribed displacement would be in the x-direction. Finally, if the displacement magnitude is described by a time history function with the name `cosine_curve`, there would be a command line of this form:

```
FUNCTION = cosine_curve
```

The command block for the boundary condition with the appropriate command lines would appear as follows:

```
BEGIN PRESCRIBED DISPLACEMENT
  NODE SET = nodelist_10
  COMPONENT = X
  FUNCTION = cosine_curve
END PRESCRIBED DISPLACEMENT
```

It is possible to have a command line with the same key words appearing in different scopes. For example, we might have a command line identified by the word `TYPE` in two or more different

scopes. The command line would perform different functions based on the scope in which it appeared, and the associated value could be different in the two locations.

The input lines are read by a parser that searches for recognizable key words. If the key words in an input line are not in the list of key words used by Presto to describe command blocks and command lines, the parser will generate an error. A set of key words defining a command line or command block for Presto that is not in the correct scope will also cause a parser error. For example, the key words `STEP INTERVAL` define a valid command line in the scope of the `TIME CONTROL` command block. However, if this command line was to appear in the scope of one of the boundary conditions, it would not be in the proper scope, and the parser would generate an error. Once the parser has an input line with any recognizable key words in the proper scope, a method can be called that will handle the input line.

There is an initial parsing phase that checks only the parser syntax. If the parser encounters a command line it cannot parse within a certain scope, the parser will indicate it cannot recognize the command line and will list the various command lines that can appear within that scope. The initial parsing phase will catch errors such as the one described in the previous paragraph (a command line in the wrong scope). It will also catch misspelled key words. The initial parsing does not catch some other types of errors, however. If you have specified a value on a command line that is out of a specified range for that command line, the initial parsing will not catch this error. If you have some combination of command lines within a command block that is not allowed, the initial parsing will not catch this error. These other errors are caught after the initial parsing phase and are handled one error at a time.

1.3 Conventions for Command Descriptions

The conventions below are used to describe the input commands for Presto. A number of the individual command lines discussed in the text appear on several text lines. In the text of this document, the continuation symbols that are used to continue lines in an actual input file (`\#` and `\$`, Section 1.4.2) are not used for those instances where the description of the command line appears on several text lines. The description of command lines will clearly indicate all the key words, delimiters, and values that constitute a complete command line. As an example, the `DEFINE POINT` command line (Section 2.1.6) is presented in the text as follows:

```
DEFINE POINT <string>point_name WITH COORDINATES
     <real>value_1 <real>value_2 <real>value_3
```

If the `DEFINE POINT` command line were used as a command line in an input file and spread over two input lines, it would appear, with actual values, as follows:

```
DEFINE POINT center WITH COORDINATES \#
  10.0 144.0 296.0
```

In the above example, the `\#` symbol implies the first line is continued onto the second line.

1.3.1 Key Words

The key word or key words for a command are shown in uppercase letters. For actual input, you can use all uppercase letters for the key words, all lowercase letters for the key words, or some combination of uppercase and lowercase letters for the key words.

1.3.2 User-Specified Input

The input that you supply is typically shown in lowercase letters. (Occasionally, uppercase letters may be used for user input for purposes of clarity or in examples.) The user-supplied input may be a real number, an integer, a string, or a string list. For the command descriptions, a type appears before the user input. The type (real, integer, string, string list) description is enclosed by angle brackets, `<>`, and precedes the user-supplied input. For example:

```
<real>value
```

indicates that the quantity `value` is a real number. For the description of an input command, you would see the following:

```
FUNCTION = <string>function_name
```

Your input would be

```
FUNCTION = my_name
```

if you have specified a function name called `my_name`.

Valid user input consists of the following:

`<integer>`	Integer data is a single integer number.
`<real>`	Real data is a single real number. It may be formatted with the usual conventions, such as `1234.56` or `1.23456e+03`.
`<string>`	String data is a single string.
`<string list>`	A string list consists of multiple strings separated by white space, a comma, a tab, or white space combined with a comma or a tab.

1.3.3 Optional Input

Anything in an input line that is enclosed by square brackets, [ ], represents optional input within the line. Note, however, that this convention is not used to identify optional input lines. Any command line that is optional (in its entirety) will be described as such within the text.

1.3.4 Default Values

A value enclosed by parentheses, (), appearing after the user input denotes the default value. For example:

```
SCALE FACTOR = <real>scale_factor(1.0)
```

implies the default value for `scale_factor` is 1.0. Any value you specify will overwrite the default.

For your actual input file, you may simply omit a command line if you want to use the default value associated with the command line. For example, there is a `TIME STEP SCALE FACTOR` command line used to set one of the time control parameters; the parameter for this command line has a default value of 1.0. If you want to use the default value of 1.0 for this parameter, you do not have to include the `TIME STEP SCALE FACTOR` command line in the `TIME CONTROL` command block.

1.3.5 Multiple Options for Values

Quantities separated by the `|` symbol indicate that one and only one of the possible choices must be selected. For example:

```
EXPANSION RADIUS = <string>SPHERICAL|CYLINDRICAL
```

implies that expansion radius must be defined as `SPHERICAL` or `CYLINDRICAL`. One of the values must appear. This convention also applies to some of the command options within a begin/end block. For example:

```
SURFACE = <string>surface_name|
     NODE SET = <string>nodelist_name
```

in a command block specifies that either a surface or a node set must be specified.

Quantities separated by the / symbol can appear in any combination, but any one quantity in the sequence can appear only once. For example,

```
COMPONENTS = <string>X/Y/Z
```

implies that components can equal any combination of X, Y, and Z. Any value (X or Y or Z) can appear at most once, and at least one value of X, Y, or Z must appear. Some examples of valid expressions in this case are as follows:

```
COMPONENTS = Z

COMPONENTS = Z X

COMPONENTS = Y X Z

COMPONENTS = Z Y X
```

An example of an invalid expression would be the following:

```
COMPONENTS = Y Y Z
```

1.3.6 Known Issues and Warnings

Where there are known issues with the code, these are documented in the following manner:

Known Issue: A description of the known issue with the code would be provided here.

Similarly, warnings regarding usage of code features that are not defective, but must be used with care because of their nature, are documented as follows:

Warning: A description of the warning related to the usage of a code feature would be provided here.

1.4 Style Guidelines

This section gives information that will affect the overall organization and appearance of your input file. It also contains recommendations that will help you construct input files that are readable and easy to proof.

1.4.1 Comments

A comment is anything between the `#` symbol or the `$` symbol and the end-of-line. If the first non-blank character in a line is a `#` or `$`, the entire line is a comment line. You can also place a `#` or `$` (preceded by a blank space) after the last character in an input line used to define a command block or command line.

1.4.2 Continuation Lines

An input line can be continued by placing a `\#` pair of characters (or `\$`) at the end of the line. The following line is then taken to be a continuation of the preceding line that was terminated by the `\#` or `\$`. Note that everything after the line-continuation pair of characters is discarded, including the end-of-line.

1.4.3 Case

Almost all the character strings in the input lines are case insensitive. For example, the `BEGIN SIERRA` key words could appear as one of the following:

```
BEGIN SIERRA
begin sierra
Begin Sierra
```

You could specify a `SIERRA` command block with:

```
BEGIN SIERRA BEAM
```

and terminate the command block with this input line:

```
END SIERRA beam
```

Case is important only for file name specifications. If you have defined a restart file with uppercase and lowercase letters and want to use this file for a restart, the file name you use to request this restart file must exactly match the original definition you chose.

1.4.4 Commas and Tabs

Commas and tabs in input lines are ignored.

1.4.5 Blank Spaces

We highly recommend that everything be separated by blank spaces. For example, a command line of the form

```
node set = nodelist_10
```

is recommended over the following forms:

```
node set= nodelist_10
```

```
node set =nodelist_10
```

Both of the above two lines are correct, but it is easier to check the first form (the equal sign surrounded by blank space) in a large input file.

The parser will accept the following line:

```
BEGIN SIERRABEAM
```

However, it is harder to check this line for the correct spelling of the key words and the intended SIERRA scope name than this line:

```
BEGIN SIERRA BEAM
```

It is possible to introduce hard-to-detect errors because of the way in which the blank spaces are handled by the command parser. Suppose you type

```
begin definition for functions my_func
```

rather than the following correct form:

```
begin definition for function my_func
```

For the incorrect form of this command line (in which `functions` is used rather than `function`), the parser will generate a string name of

```
s my_func
```

for the function name rather than the following expected name:

```
my_func
```

If you attempt to use a function named `my_func`, the parser will generate an error because the list of function names will include `s my_func` but not `my_func`.

1.4.6 General Format of the Command Lines

In general, command lines have the following form:

```
keyword = value
```

This pattern is not always followed, but it describes the vast majority of the command lines.

1.4.7 Delimiters

The delimiter used throughout this document is "=" (the equal sign). Typically, but not always, the = separates key words from input values in a command line. Consider the following command line:

```
COMPONENTS = X
```

Here, the key word `COMPONENTS` is separated from its value, a string in this case, by the =. Some command lines do allow for other delimiters. The use of these alternate delimiters is not consistent, however, throughout the various command lines. (This lack of consistency has the potential for introducing errors in this document as well as in your input.) The = provides a strong visual cue for separating key words from values. By using the = as a delimiter, it is much easier to proof your input file. It also makes it easier to do "cut and paste" operations. If you accidentally delete =, it is much easier to detect than accidentally removing part of one of the other delimiters that could be used.

1.4.8 Order of Commands

There are no requirements for ordering the commands. Both the input sequence:

```
BEGIN PRESCRIBED DISPLACEMENT
  NODE SET = nodelist_10
  COMPONENT = X
  FUNCTION = cosine_curve
END PRESCRIBED DISPLACEMENT
```

and the input sequence:

```
BEGIN PRESCRIBED DISPLACEMENT
  FUNCTION = cosine_curve
  COMPONENT = X
  NODE SET = nodelist_10
END PRESCRIBED DISPLACEMENT
```

are valid, and they produce the same result. Remember, that command lines and command blocks must appear in the proper scope.

1.4.9 Abbreviated END Specifications

It is possible to terminate a command block without including the key word or key words that identify the block. You could define a specific instance of the prescribed displacement boundary condition with:

```
BEGIN PRESCRIBED DISPLACEMENT
```

and terminate it simply with:

```
END
```

as opposed to the following specification:

```
END PRESCRIBED DISPLACEMENT
```

Both the short termination (`END` only) and the long termination (`END` followed by identification, or name, of the command block) are valid. It is recommended that the long termination be used for any command block that becomes large. The `RESULTS OUTPUT` command block described in later chapters can become fairly lengthy, so this is probably a good place to use the long termination. For most boundary conditions, the command block will typically consist of five lines. In such cases, the short termination can be used. Using the long termination for the larger command blocks will make it easier to proof your input files. If you use the long termination, the text following the `END` key word must exactly match the text following the `BEGIN` key word. You could not have `BEGIN PRESCRIBED DISPLACEMENT` paired with an `END PRESCRIBED DISPL` to define the beginning and ending of a command block.

1.4.10 Indentation

When constructing an input file, it is useful, but not required, to indent a scope that is nested inside another scope. Command lines within a command block should also be indented in relation to the lines defining the command block. This will make it easier to construct the input file with everything in the correct scope and with all the command blocks in the correct structure.

1.4.11 Including Files

External text files containing input commands can be included at any point in the Presto input file using the `INCLUDEFILE` command. This command can be used in any context in the input file. To use this command, simply use the command `INCLUDEFILE` followed by the name of the file to be included. For example, the command:

```
INCLUDEFILE displacement_history.i
```

would include the `displacement_history.i` as if the contents of that file were places in the position that it is included in the input file. The included file is contained in the standard echo of the input that is provided at the beginning of the log file.

1.5 Naming Conventions Associated with the Exodus II Database

When the mesh file has an Exodus II format, there are three basic conventions that apply to user input for various command lines. First, for a mesh file with the Exodus II format, the Exodus II side set is referenced as a surface. In SIERRA, a surface consists of element faces plus all the nodes and edges associated with these faces. A surface definition can be used not only to select a group of faces but also to select a group of edges or a group of nodes that are associated with those faces. In the case of boundary conditions, a surface definition can be used not only to apply boundary conditions that typically use surface specifications (pressure) but also to apply boundary conditions for what are referred to as nodal boundary conditions (fixed displacement components). For nodal boundary conditions that use the surface specification, all the nodes associated with the faces on a specific surface will have this boundary condition applied to them. The specification for a surface identifier in the following chapters is `surface_name`. It typically has the form `surface_integerid`, where `integerid` is the integer identifier for the surface. If the side set identifier is 125, the value of `surface_name` would be `surface_125`. It is also possible to generate an alias for the side set[1] and use this for `surface_name`. If `surface_125` is aliased to `outer_skin`, then `surface_name` becomes `outer_skin` in the actual input line. It is also possible to name a surface in some mesh generation programs and that name can be used in the input file.

Second, for a mesh file with the Exodus II format, the Exodus II node set is still referenced as a node set. A node set can be used only for cases where a group of nodes needs to be defined. The specification for a node set identifier in the following chapters is `nodelist_name`. It typically has the form `nodelist_integerid`, where `integerid` is the integer identifier for the node set. If the node set number is 225, the value of `nodelist_name` would be `nodelist_225`. It is also possible to generate an alias for the node set and use this for `nodelist_name`. If `nodelist_225` is aliased to `inner_skin`, then `nodelist_name` becomes `inner_skin` in the actual input line. It is also possible to name a nodelist in some mesh generation programs and that name can be used in the input file.

Third, an element block is referenced as a block. The specification for an element block identifier in the following chapters is `block_name`. It typically has the form `block_integerid`, where `integerid` is the integer identifier for the block. If the element block number is 300, the value of `block_name` would be `block_300`. It is also possible to generate an alias for the block and use this for `block_name`. If `block_300` is aliased to `big_chunk`, then `block_name` becomes `big_chunk` in the actual input line. It is also possible to name an element block in some mesh generation programs and that name can be used in the input file.

A group of elements can also be used to select other mesh entities. In SIERRA, a block consists of elements plus all the faces, edges, and nodes associated with the elements. The block and surface concepts are similar in that both have associated derived quantities. Chapters 6 and 7 show how this concept of derived quantities is used in the input command structure.

[1] See the `ALIAS` command in Section 5.1.2

1.6 Major Scope Definitions for an Input File

The typical input file will have the structure shown below. The major scopes—SIERRA, procedure, and region—are delineated with input lines for command blocks. Comment lines are included that indicate some of the key scopes that will appear within the major scopes. Note the indentation used for this example.

```
BEGIN SIERRA <string>some_name
  #
  # All command blocks and command lines in the SIERRA
  # scope appear here. The PROCEDURE PRESTO command
  # block is the beginning of the next scope.
  #
  # function definitions
  # material descriptions
  # description of mesh file
  #
  BEGIN PRESTO PROCEDURE <string>procedure_name
    #
    # time step control
    #
    BEGIN PRESTO REGION <string>region_name
      #
      # All command blocks and command lines in the
      # region scope appear here
      #
      # specification for output of result
      # specification for restart
      # boundary conditions
      # definition of contact
      #
    END [PRESTO REGION <string>region_name]
  END [PRESTO PROCEDURE <string>procedure_name]
END [SIERRA <string>some_name]
```

1.7 Input/Output Files

The primary user input to Presto is the input file introduced in this chapter. Throughout this document, we explain how to construct a valid input file. It is important to be aware that Presto also processes a number of other types of input files and produces a variety of output files. These additional files are also discussed in this document where applicable. Figure 1.1 presents a simple schematic diagram of the various input and output files in Presto. Both Adagio and Presto use the same file structure. Therefore, in Figure 1.1, we indicate that the code (graphically represented by the central cylinder) can be either Presto or Adagio.

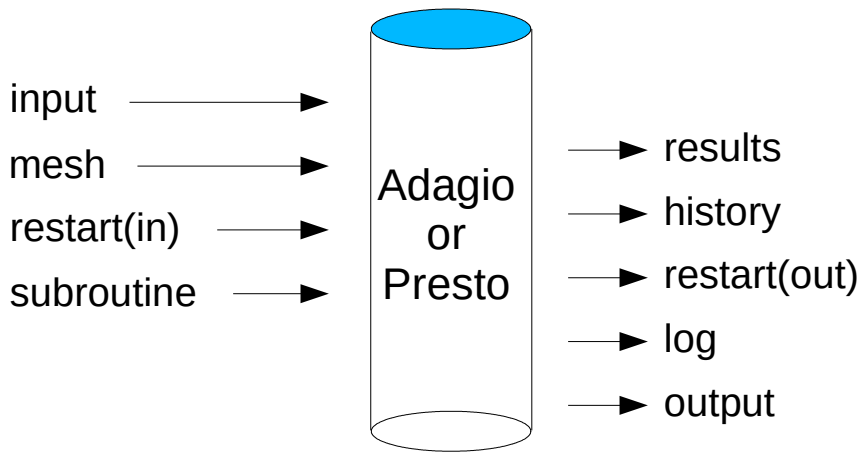

Figure 1.1: Input/output files

As shown in Figure 1.1, Presto uses the input file, mesh files, restart files, and user subroutine files. The input file, which is required, is a set of valid Presto command lines. Another required input is a mesh file, which provides a description of the finite element mesh for the object being analyzed. Restart and user subroutine files are optional inputs. The restart functionality lets you break an analysis from the start time to the termination time into a sequence of runs. The files generated by the restart functionality contain a complete state description for a problem at various analysis times, which we will refer to as restart times. You can restart Presto at any of these restart times because the complete state description is known (see Chapter 8). The user subroutine files let you build and incorporate specialized functionality into Presto (Chapter 10).

As also shown in Figure 1.1, Presto can generate a number of files. These include results files, history files, restart files, a log file, and an output file. Typically, only the log file and the output file are produced automatically. Generation of the other types of files is based on user settings in the input file for the particular kinds of output desired. Results files provide the values of global variables, element variables, and node variables at specified times (see Chapter 8). History files will also provide values of global variables, element variables, and node variables at specified times (see Chapter 8). History files are set up to provide a specific value at a specific node, for example, whereas results files provide a nodal value for large subsets of nodes or, more typically, all nodes. History files provide a much more limited set of information than results files. As noted above, restart files can be generated at various analysis times. The log file contains a variety of

information such as the Presto version number, a listing of the input file, initialization information, some model information (mass, critical time steps for element blocks, etc.), and information at various time steps. At every n^{th} step, where n is user selected, the log file gives the current analysis time; the current time step; the kinetic, internal, and external energies; the error in the energy; and computing time information. You can monitor step information in the log file to gain information about how your analysis is progressing. The output file contains error information.

1.8 Obtaining Support

Support for all SIERRA Mechanics codes, including Presto, can be obtained by contacting the SIERRA Mechanics user support hotline by email at sierra-help@sandia.gov, or by telephone at (505)845-1234.

1.9 References

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Chapter 2

General Commands

The commands described in this section appear in the SIERRA or procedure scope or control general functionality in Presto.

2.1 SIERRA Scope

These commands are used to set up some of the fundamentals of the Presto input. The commands are physics independent, or at least can be shared between physics. The commands lie in the SIERRA scope, not in the procedure or region scope.

2.1.1 SIERRA Command Block

```
BEGIN SIERRA <string>name
  #
  # All other command blocks and command lines
  # appear within the SIERRA scope defined by
  # begin/end sierra.
  #
END [SIERRA <string>name]
```

All input commands must occur within a `SIERRA` command block. The syntax for beginning the command block is:

```
BEGIN SIERRA <string>name
```

and for terminating the command block is as follows:

```
END [SIERRA <string>name]
```

In these input lines, `name` is a name for the `SIERRA` command block. All other commands for the analysis must be within this command block structure. The name for the `SIERRA` command block is often a descriptive name that identifies the analysis. The name is not currently used anywhere else in the file and is completely arbitrary.

2.1.2 Title

```
TITLE <string list>title
```

To permit a fuller description of the analysis, the input has a `TITLE` command line for the analysis, where `title` is a text description of the analysis. The title is transferred to the results file.

2.1.3 Restart Control

The restart capability in Presto allows a user to run an analysis up to a certain time, stop the analysis at this time, and then restart the analysis from this time. Restart can be used to break a long-running analysis into several smaller runs so that the user can examine intermediate results before proceeding with the next step. Restart can also be used in case of abnormal termination. If a restart file has been written at various intervals throughout the analysis up to the point where the abnormal termination has occurred, you can pick a restart time before the abnormal termination and restart the problem from there. Thus, users do not have to go back to the beginning of the analysis, but can continue the analysis at some time well into the analysis. With the restart capability, you will generate a sequence of restart runs. Each run can have its own set of restart, results, and history files.

When using the restart capability, you can reset a number of the parameters in the input file. However, not all parameters can be reset. Users should exercise care in resetting parameters in the input file for a restart. You will want to change parameters if you have encountered an abnormal termination. You may want to change certain parameters, hourglass control for example, to see whether you can prevent the abnormal termination and continue the analysis past the abnormal termination time you had previously encountered.

The use of the restart capability involves commands in **both the SIERRA scope and the region scope**. One of two restart command lines, `RESTART` or `RESTART TIME`, appears in the SIERRA scope. A command block in the region scope, the `RESTART DATA` command block, specifies restart file names and the frequency at which the restart files will be written. The `RESTART DATA` command block is described in Section 8.5. This section gives a brief discussion of the command lines that appear in the SIERRA scope. For a full discussion of all the command lines used for restart, consult Chapter 8. The use of some of the command lines in the `RESTART DATA` command block depends on the command line, either `RESTART` or `RESTART TIME`, you select in the SIERRA scope.

If you specify a time from a specific restart file for the restart, you will use the `RESTART TIME` command line described in Section 2.1.3.1. If you select the automatic restart option, you will use the `RESTART` command line described in Section 2.1.3.2. The command lines for both of these methods are in the **SIERRA scope**. All other commands for restart are in the **region scope** in the `RESTART DATA` command block.

For restarts specified with a restart time from a specific restart file, you will have to be concerned about overwriting information in existing files. The issue of overwriting information is discussed in Chapter 8. In general, you will want to have a restart file (or files in the case of parallel runs)

for each run in a sequence of runs you create with the restart option. You will want to preserve all restart files you have written prior to any given run in a sequence of restart runs. The easiest way to preserve prior restart information is with the use of the `RESTART` command line. How you preserve previous restart information is discussed in detail in Chapter 8.

The amount of data written at a restart time is quite large. The restart data written at a given time is a complete description of the state for the problem at that time. The restart data includes not only information such as displacement, velocity, and acceleration, but also information such as element stresses and all the state variables for the material model associated with each element.

2.1.3.1 Restart Time

```
RESTART TIME = <real>restart_time
```

The `RESTART TIME` command line is used to specify a time from a specific restart file for the restart run. This restart option will pick the restart time on the restart file that is closest to the user-specified time on the `RESTART TIME` command line. If the user specifies a restart time greater than the last time written to a restart file, then the last time written to the restart file is picked as the restart time. Use of this command line can result in previous restart information being overwritten. To prevent the overwriting of existing restart files, you can specify both an input restart file and an output restart file (and rename the results and history files) for the various restarts. The use of the `RESTART TIME` command line requires the user to be more active in the management of the file names to prevent the overwriting of restart, results, and history files. The automatic restart feature (e.g., the `RESTART` command line in Section 2.1.3.2) prevents the overwriting of restart, results, and history files. See Section 8.5 for a full discussion of implementing the restart capability.

2.1.3.2 Automatic Restart

```
RESTART = AUTOMATIC
```

The `RESTART` command line automatically selects for restart the last restart time written to the last restart file. The automatic restart feature lets the user restart runs with minimal changes to the input file. The only quantity that must be changed to move from one restart to another is the termination time. The `RESTART` command line manages the restart files so as not to write over any previous restart files. It also manages the results and history files so as not to write over any previous results or history files. See Section 8.5 for a full discussion of implementing the restart capability.

2.1.4 User Subroutine Identification

```
USER SUBROUTINE FILE = <string>file_name
```

This command line is a part of a set of commands that are used to implement the user subroutine functionality. The string `file_name` identifies the name of the file that contains the FORTRAN code of one or more user subroutines.

To understand how this command line is used, see Chapter 10.

2.1.5 Functions

```
BEGIN DEFINITION FOR FUNCTION <string>function_name
  TYPE = <string>CONSTANT|PIECEWISE LINEAR|PIECEWISE CONSTANT|
    ANALYTIC
  ABSCISSA = <string>abscissa_label
    [scale = <real>abscissa_scale(1.0)]
    [offset = <real>abscissa_offset(0.0)]
  ORDINATE = <string>ordinate_label
    [scale = <real>ordinate_scale(1.0)]
    [offset = <real>ordinate_offset(0.0)]
  X SCALE = <real>x_scale(1.0)
  X OFFSET = <real>x_offset(0.0)
  Y SCALE = <real>y_scale(1.0)
  Y OFFSET = <real>y_offset(0.0)
  BEGIN VALUES
    <real>x_1   <real>y_1
    <real>x_2   <real>y_2
    ...
    <real>x_n   <real>y_n
  END [VALUES]
  AT DISCONTINUITY EVALUATE TO <string>LEFT|RIGHT(LEFT)
  EVALUATE EXPRESSION = <string>analytic_expression1;
    analytic_expression2; ...
  DEBUG = ON|OFF(OFF)
END [DEFINITION FOR FUNCTION <string>function_name]
```

A number of Presto features are driven by a user-defined description of the dependence of one variable on another. For instance, the prescribed displacement boundary condition requires the definition of a time-versus-displacement relation, and the thermal strain computations require the definition of a thermal-strain-versus-temperature relation. SIERRA provides a general method of defining these relations as functions using the `DEFINITION FOR FUNCTION` command block, as shown above.

There is no limit to the number of functions that can be defined. All function definitions must appear within the SIERRA scope.

A description of the various parts of the `DEFINITION FOR FUNCTION` command block follows:

- The string `function_name` is a user-selected name for the function that is unique to the function definitions within the input file. This name is used to refer to this function in other locations in the input file.
- The `TYPE` command line has four options to define the type of function. The value of this string can be `CONSTANT`, `PIECEWISE LINEAR`, `PIECEWISE CONSTANT`, or `ANALYTIC`.

- The `ABSCISSA` command line provides a descriptive label for the independent variable (x-axis) with the string `abscissa_label`. This command line is optional. The user can optionally add a scale factor and/or an offset which has the following effect: $abscissa_{scaled} = scale * (abscissa + offset)$.

- The `ORDINATE command` line provides a descriptive label for the dependent variable (y-axis) with the string `ordinate_label`. This command line is optional. The user can also optionally add a scale factor and/or an offset which has the following effect: $ordinate_{scaled} = scale * (ordinate + offset)$.

- The `X SCALE` command line sets the scale factor value for the abscissa and has the same effect as if the optional `SCALE` command were used in the `ABSCISSA` command line.

- The `X OFFSET` command line sets the offset value for the abscissa and has the same effect as if the optional `OFFSET` command were used in the `ABSCISSA` command line.

- The `Y SCALE` command line sets the scale factor value for the ordinate and has the same effect as if the optional `SCALE` command were used in the `ORDINATE` command line.

- The `Y OFFSET` command line sets the offset value for the ordinate and has the same effect as if the optional `OFFSET` command were used in the `ORDINATE` command line.

- The `DEBUG command` line prints functions to the log file if they were scaled and/or offset. This command line is optional. The generated function function name is the original function name concatenated with `_with_scale_and_offset_applied`. The generated function is a valid function and could be placed into the input file and used.

- The `VALUES` command block consists of the real value pairs (`x_1`,`y_1`) through (`x_n`, `x_n`), which describe the function. This command block must be used if the value on the `TYPE` command line is `CONSTANT`, `PIECEWISE LINEAR`, or `PIECEWISE CONSTANT`. For a `CONSTANT` function, only one value is needed. For a `PIECEWISE LINEAR` or `PIECEWISE CONSTANT` function, the values are (x, y) pairs of data that describe the function. The values are nested inside the `VALUES` command block.

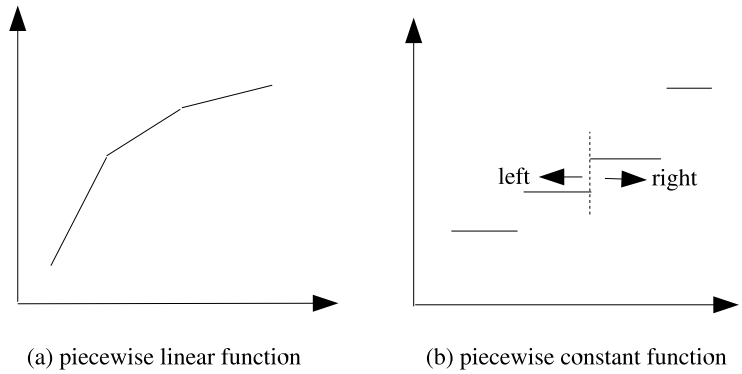

Figure 2.1: Piecewise linear and piecewise constant functions

A PIECEWISE LINEAR function performs linear interpolations between the provided value pairs; a PIECEWISE CONSTANT function is constant valued between provided value pairs. Figure 2.1 (a) shows an example of a piecewise linear function, and Figure 2.1 (b) shows an example of a piecewise constant function.

For functions that are based on tabular values, such as the PIECEWISE LINEAR and PIECEWISE CONSTANT functions, there is a possibility that the function may be evaluated for abscissa values that fall outside the range of the tabulated values. If the abscissa for which the function is to be evaluated is lower than the lowest tabulated abscissa, the function returns the ordinate corresponding to the smallest tabulated abscissa. Likewise, if the function is evaluated for an abscissa higher than the highest tabulated abscissa, the function returns the ordinate corresponding to the highest tabulated abscissa. For example, consider the following function:

```
begin definition for function my_func
  type = piecewise linear
  begin values
    5.0  0.0
    10.0 50000.0
  end values
end definition for function my_func
```

For values less than 5, this function returns 0, and for values greater than 10, it returns 50000.

- For a piecewise constant function, a constant valued segment ends on the left hand side of an abscissa value and a new constant value segment begins on the right hand side of the same abscissa value. (This transition from one constant value to another is indicated by the dotted line in Figure 2.1 (b).) When the value of the function is to be evaluated at a discontinuity, where there two potential values for the ordinate, the default behavior is to use the ordinate from the value pair that has the lower-valued abscissa, or in other words, to use the value on the left hand side of the discontinuity. The AT DISCONTINUITY EVALUATE TO command line can be used to override this default behavior at an abscissa with two ordinate values. The command line can have a value of either LEFT or RIGHT. If LEFT (the default) is specified, the ordinate value to the left of the abscissa is used; if RIGHT is specified, the ordinate value to the right of the abscissa is used.

- The EVALUATE EXPRESSION command line consists of one or more user-supplied algebraic expressions. This command line must be used if the value on the TYPE command line is ANALYTIC. See the rules and options for composing algebraic expressions discussed below.

Importantly, a DEFINITION FOR FUNCTION command block cannot contain both a VALUES command block and an EVALUATE EXPRESSION command line.

Rules and options for composing algebraic expressions. If you choose to use the EVALUATE EXPRESSION command line, you will need to write the algebraic expressions. The algebraic expressions are written using a C-like format. Each algebraic expression is terminated by a semicolon(;). The entire set of algebraic expressions, whether a single expression or several, is enclosed in a single set of double quotes(" ").

An expression is evaluated with `x` as the independent variable. We first provide several simple examples and then list the options available in the algebraic expressions.

Example: Return `sin(x)` as the value of the function.

```
begin definition for function fred
  type is analytic
  evaluate expression is ``sin(x);''
end definition for function fred
```

In this example, the commented out table is equivalent to the evaluated expression:

```
begin definition for function pressure
  type is analytic
  evaluate expression is ``x <= 0.0 ? 0.0 : (x < 0.5 ? x*200.0
    : 100.0);''
    #     begin values
    #       0.0      0.0
    #       0.5    100.0
    #       1.0    100.0
    #     end values
end definition for function pressure
```

The following functionality is currently implemented for the expressions:

Operators

```
+ - * / == != > < >= <= ! & | && || ? :
```

Parentheses

```
()
```

Math functions

```
abs(x), absolute value of x
mod(x, y), modulus of x|y
ipart(x), integer part of x
fpart(x), fractional part of x
```

Power functions

```
pow(x, y), x to the y power
pow10(x), x to the 10 power
sqrt(x), square root of x
```

Trigonometric functions

```
acos(x), arccosine of x
asin(x), arcsine of x
atan(x), arctangent of x
atan2(y, x), arctangent of y/x, signs of x and y
  determine quadrant (see atan2 man page)
cos(x), cosine of x
cosh(x), hyperbolic cosine of x
sin(x), sine of x
sinh(x), hyperbolic sine of x
tan(x), tangent of x
tanh(x), hyperbolic tangent of x
```

Logarithm functions

```
log(x), natural logarithm of x
ln(x), natural logarithm of x
log10(x), the base 10 logarithm of x
exp(x), e to the x power
```

Rounding functions

```
ceil(x), smallest integral value not less than x
floor(x), largest integral value not greater than x
```

Random functions

```
rand(), random number between 0.0 and 1.0, not including 1.0
randomize(), random number between 0.0 and 1.0, not
  including 1.0
srand(x), seeds the random number generator
```

Conversion functions

```
deg(x), converts radians to degrees
rad(x), converts degrees to radians
recttopolr(x, y), magnitude of vector x, y
recttopola(x, y), angle of vector x, y
poltorectx(r, theta), x coordinate of angle theta at
  distance r
poltorecty(r, theta), y coordinate of angle theta at
  distance r
```

Constants. There are two predefined constants that may be used in an expression. These two constants are `e` and `pi`.

e = e = 2.7182818284...
pi = π = 3.1415926535...

2.1.6 Axes, Directions, and Points

```
DEFINE POINT <string>point_name WITH COORDINATES
  <real>value_1 <real>value_2 <real>value_3
DEFINE DIRECTION <string>direction_name WITH VECTOR
  <real>value_1 <real>value_2 <real>value_3
DEFINE AXIS <string>axis_name WITH POINT
  <string>point_1 POINT <string>point_2
DEFINE AXIS <string>axis_name WITH POINT
  <string>point DIRECTION <string>direction
```

A number of Presto features require the definition of geometric entities. For instance, the prescribed displacement boundary condition requires a direction definition, and the cylindrical velocity initial condition requires an axis definition. Currently, Presto input permits the definition of points, directions, and axes. Definition of these geometric entities occurs in the SIERRA scope.

The `DEFINE POINT` command line is used to define a point:

```
DEFINE POINT <string>point_name WITH COORDINATES
  <real>value_1 <real>value_2 <real>value_3
```

where

- The string `point_name` is a name for this point. This name must be unique to all other points defined in the input file.
- The real values `value_1`, `value_2`, and `value_3` are the x, y, and z coordinates of the point.

The `DEFINE DIRECTION` command line is used to define a direction:

```
DEFINE DIRECTION <string>direction_name WITH VECTOR
  <real>value_1 <real>value_2 <real>value_3
```

where

- The string `direction_name` is a name for this direction. This name must be unique to all other directions defined in the input file.
- The real values `value_1`, `value_2`, and `value_3` are the x, y, and z magnitudes of the direction vector.

There are two command lines that can be used to define an axis. The first `DEFINE AXIS` command line uses two points:

```
DEFINE AXIS <string>axis_name WITH POINT
  <string>point_1 POINT <string>point_2
```

where

- The string `axis_name` is a name for this axis. This name must be unique to all other axes defined in the input file.
- The strings `point_1` and `point_2` are the names for two points defined in the input file via a `DEFINE POINT` command line.

The second `DEFINE AXIS` command line uses a point and a direction:

```
DEFINE AXIS <string>axis_name WITH POINT
  <string>point DIRECTION <string>direction
```

where

- The string `axis_name` is a name for this axis. This name must be unique to all other axes defined in the input file.
- The string `point` is the name of a point defined in the input file via a `DEFINE POINT` command line.
- The string `direction` is the name of a direction defined in the input file via a `DEFINE DIRECTION` command line.

2.1.7 Orientation

```
BEGIN ORIENTATION <string>orientation_name
  SYSTEM = <string>RECTANGULAR|Z RECTANGULAR|CYLINDRICAL|
    SPHERICAL(RECTANGULAR)
  #
  POINT A = <real>global_ax <real>global_ay <real>global_az
  POINT B = <real>global_bx <real>global_by <real>global_bz
  #
  ROTATION ABOUT <integer> 1|2|3(2) = <real>theta(0.0)
END [ORIENTATION <string>orientation_name]
```

The `ORIENTATION` command block is currently used in Presto to define a local *co-rotational* coordinate system at each shell element centroid for output of shell in-plane stresses and strains. Each `BEGIN SHELL SECTION` command block has an orientation that generates this local coordinate system for each element in the associated element blocks. The generated local coordinate system rotates with the shell element, thus making it *co-rotational*.

Stresses and strains for shell elements are computed in the shell element's local coordinate system, which typically varies from one element to the next, and can be seen in Figure 2.2. The local **R** axis of element 1 does not align with the local **R** axis of element 2. Thus without the use of an orientation to rotate the local coordinate system in to a consistent coordinate system, stress and strain results would be difficult to decipher. The use of an orientation generates a transformation matrix from a shell element's local **R**, **S**, **T** coordinate system to the final coordinate system, **R**′, **S**′, **T**′, by use of orientation and element-specific basis vectors and a rotation about an axis, all defined below.

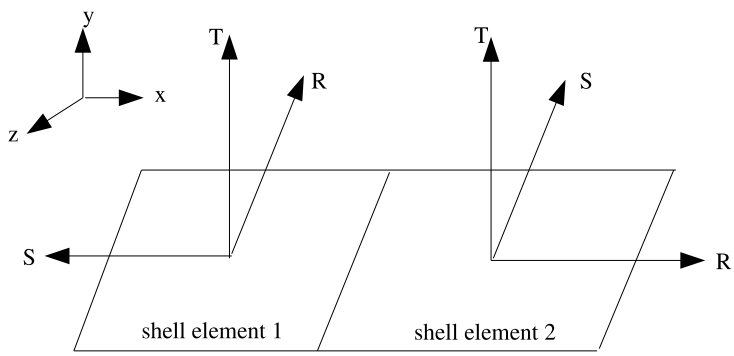

Figure 2.2: Adjacent shell elements with nonaligned local coordinate systems

There are four orientation systems available in Presto to better align the stress and strain output of shell elements. These orientations are defined via the optional `SYSTEM` command line within the `ORIENTATION` command block and are: `RECTANGULAR`, `Z_RECTANGULAR`, `CYLINDRICAL` and `SPHERICAL` with the default being `RECTANGULAR`. If the `ORIENTATION` command line within a `SHELL SECTION` block is not used, the default orientation is a `RECTANGULAR` system with axes aligned with the global X,Y and Z axes.

Each of the four systems produces a unique set of bases vectors, $\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3$, computed using the centroid of the shell element and the two required inputs, `POINT A` and `POINT B`. These four methods of computing $\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3$ are described below.

- `RECTANGULAR`: `POINT A` defines a point, P_A, in the local coordinate system of the shell element that lies in the direction of the the first basis vector, $\mathbf{g}_1$, from the centroid, C with local coordinate of $(0, 0, 0)$, see Figure 2.3. Thus, the vector from the centroid of the element to point P_A is defined as $\mathbf{p}_A = P_A - C$. Similarly, a vector from the centroid to point P_B, defined via `POINT B`, can be computed as $\mathbf{p}_B = P_B - C$. Using these two vectors, the rectangular basis vectors are defined as: $\mathbf{g}_1 = \frac{\mathbf{p}_A}{\|\mathbf{p}_A\|}$, $\mathbf{g}_3 = \frac{\mathbf{g}_1 \times \mathbf{p}_B}{\|\mathbf{g}_1 \times \mathbf{p}_B\|}$, $\mathbf{g}_2 = \frac{\mathbf{g}_3 \times \mathbf{g}_1}{\|\mathbf{g}_3 \times \mathbf{g}_1\|}$.

- `Z RECTANGULAR`: This set of basis vectors is defined very similarly to the `RECTANGULAR` system, however point P_A now defines a point that lies in the direction of the third basis vector, $\mathbf{g}_3$ from the centroid of the element, see Figure 2.4. Using the same definition for $\mathbf{p}_A$

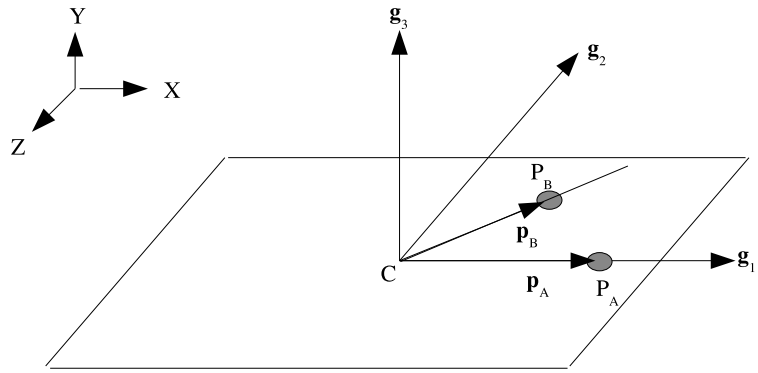

Figure 2.3: Rectangular coordinate system

and $\mathbf{p}_B$ as above we can define the three basis vectors as: $\mathbf{g}_3 = \frac{\mathbf{p}_A}{\|\mathbf{p}_A\|}$, $\mathbf{g}_2 = \frac{\mathbf{g}_3 \times \mathbf{p}_B}{\|\mathbf{g}_3 \times \mathbf{p}_B\|}$, $\mathbf{g}_1 = \frac{\mathbf{g}_2 \times \mathbf{g}_3}{\|\mathbf{g}_2 \times \mathbf{g}_3\|}$.

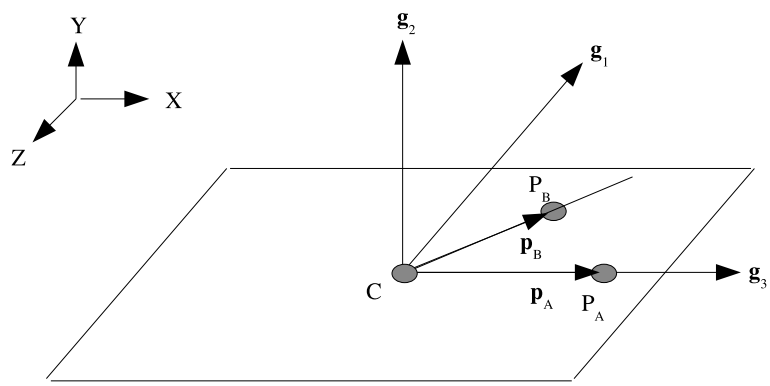

Figure 2.4: Z-Rectangular coordinate system.

- `CYLINDRICAL`: `POINT A`, P_A, and `POINT B`, P_B, define the direction of the third basis vector, $\mathbf{g}_3$ such that $\mathbf{g}_3 = \frac{P_B - P_A}{\|P_B - P_A\|}$, as seen in Figure 2.5. Defining a vector, $\mathbf{v}$, from P_A to the centroid of the element, C in the global coordinate system, the second basis vector, $\mathbf{g}_2$ is defined as: $\mathbf{g}_2 = \frac{\mathbf{v} \times \mathbf{g}_3}{\|\mathbf{v} \times \mathbf{g}_3\|}$. Therefore the first basis vector is defined as $\mathbf{g}_1 = \frac{\mathbf{g}_2 \times \mathbf{g}_3}{\|\mathbf{g}_2 \times \mathbf{g}_3\|}$.

- `SPHERICAL`: The point P_A, from the `POINT A` command line, defines the center of a sphere. The point P_B, from the `POINT B` command line, defines a polar axis for the sphere. (See Figure 2.6.) The first basis vector is defined by the vector that passes from P_A to the centroid, C in the global coordinate system, of the element: $\mathbf{g}_1 = \frac{C - P_A}{\|C - P_A\|}$. The third basis vector is parallel to the vector from P_A to P_B such that $\mathbf{g}_3 = \frac{P_B - P_A}{\|P_B - P_A\|}$. From these two vector, the

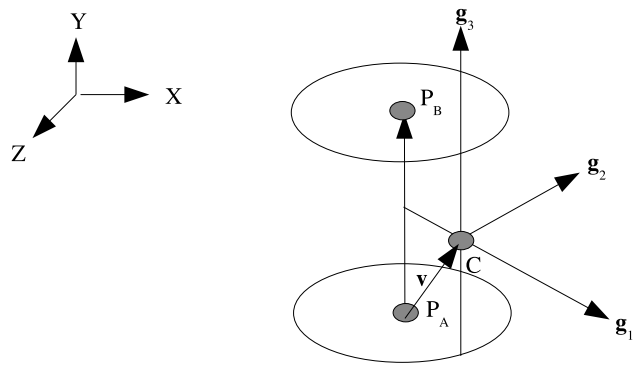

Figure 2.5: Cylindrical coordinate system.

second basis vector is defined as $\mathbf{g}_2 = \frac{\mathbf{g}_3 \times \mathbf{g}_1}{\|\mathbf{g}_3 \times \mathbf{g}_1\|}$. If $\mathbf{g}_1$ and $\mathbf{g}_3$ are collinear, the second basis vector is taken to be the normal of the element, $\mathbf{T}$, and the third basis is $\mathbf{g}_3 = \frac{\mathbf{g}_1 \times \mathbf{g}_2}{\|\mathbf{g}_1 \times \mathbf{g}_2\|}$.

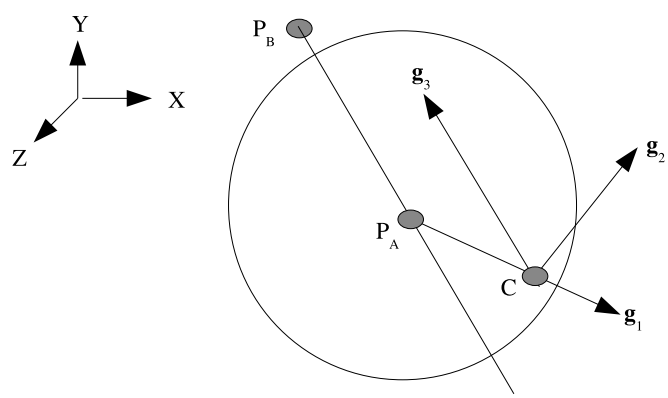

Figure 2.6: Spherical coordinate system.

It is possible, using the `ROTATION ABOUT` command line, to specify an angle and an axis to rotate the basis vectors, $\mathbf{g}_1$, $\mathbf{g}_2$ and $\mathbf{g}_3$ about in order to produce a second set of basis vectors, $\mathbf{g}'_1$, $\mathbf{g}'_2$ and $\mathbf{g}'_3$, that are then used to compute the final transformation matrix. The syntax for this command is as follows: `ROTATION ABOUT 1|2|3(2) = <real>theta(0.0)`

Where the 1,2,3 refers to which basis vector the rotation will occur about. The default value is 2 with an angle theta of 0.0, thus implying a rotation of 0.0 radians about $\mathbf{g}_2$. How $\mathbf{g}'_1$, $\mathbf{g}'_2$ and $\mathbf{g}'_3$ are computed for each of the three cases is described below. In each case, the second order rotation

tensor, $\mathbf{Q}$, is defined as:

$$\mathbf{Q} = \begin{bmatrix} 2(q_0^2 + q_1^2) - 1 & 2(q_1q_2 - q_0q_3) & 2(q_1q_3 - q_0q_3) \\ 2(q_1q_2 + q_0q_3) & 2(q_o^2 + q_2^2) - 1 & 2(q_2q_3 - q_0q_1) \\ 2(q_1q_3 - q_0q_2) & 2(q_2q_3 + q_0q_1) & 2(q_0^2 + q_3^2) - 1 \end{bmatrix}$$

Where: $q_0 = cos(\frac{\theta}{2})$, $q_1 = a_1 sin(\frac{\theta}{2})$, $q_2 = a_2 sin(\frac{\theta}{2})$, and $q_3 = a_3 sin(\frac{\theta}{2})$, where the vector $\mathbf{a} = [a_1, a_2, a_3]$ is the basis vector we are rotating about.

- Rotation about $\mathbf{g}_1$ (`ROTATION ABOUT 1`): The prime set of basis vectors are defined as: $\mathbf{g}'_1 = \mathbf{Q}\mathbf{g}_3$, $\mathbf{g}'_2 = \mathbf{Q}\mathbf{g}_2$, $\mathbf{g}'_3 = -\mathbf{g}_1$. Which can graphically be seen in Figure 2.7

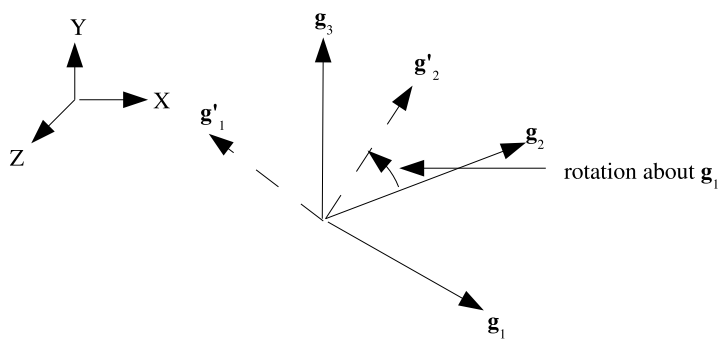

Figure 2.7: Rotation about 1

- Rotation about $\mathbf{g}_2$ (`ROTATION ABOUT 2`), default: The prime set of basis vectors are defined as: $\mathbf{g}'_1 = \mathbf{Q}\mathbf{g}_1$, $\mathbf{g}'_2 = \mathbf{Q}\mathbf{g}_3$, $\mathbf{g}'_3 = -\mathbf{g}_2$.

- Rotation about $\mathbf{g}_3$ (`ROTATION ABOUT 3`): The prime set of basis vectors are defined as: $\mathbf{g}'_1 = \mathbf{Q}\mathbf{g}_2$, $\mathbf{g}'_2 = \mathbf{Q}\mathbf{g}_1$, $\mathbf{g}'_3 = -\mathbf{g}_3$.

The next step is to project $\mathbf{g}'_1$ onto the shell face as follows: $\mathbf{R}' = \mathbf{g}'_1 - (\mathbf{g}'_1 \cdot \mathbf{T})\mathbf{T}$, which defines a rotated $\mathbf{R}$ vector. If $\mathbf{R}'$ is perpendicular to the face of the element, we then redefine $\mathbf{R}'$ to be: $\mathbf{R}' = \mathbf{g}'_2 - (\mathbf{g}'_2 \cdot \mathbf{T})\mathbf{T}$, the projection of $\mathbf{g}'_2$ onto the element face. Once we have $\mathbf{R}'$ we can define $\mathbf{S}'$ as $\frac{\mathbf{T}\times\mathbf{R}'}{\|\mathbf{T}\times\mathbf{R}'\|}$. Hence, the final transformation matrix taking local stress and strain (in the $\mathbf{R}$, $\mathbf{S}$ coordinate system) to the $\mathbf{R}'$, $\mathbf{S}'$ coordinate system is:

$$\mathbf{Q}' = \begin{bmatrix} \mathbf{R}\cdot\mathbf{R}' & \mathbf{R}\cdot\mathbf{S}' & 0 \\ \mathbf{S}\cdot\mathbf{R}' & \mathbf{S}\cdot\mathbf{S}' & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

2.1.8 Coordinate System Block Command

```
BEGIN COORDINATE SYSTEM <string>coordinate_system_name
  TYPE = <string>RECTANGULAR|CYLINDRICAL|SPHERICAL (RECTANGULAR)
  #
  ORIGIN = <string>origin_point_name
  VECTOR = <string>z_vector_point_name
  POINT = <string>x_vector_point_name
  ORIGIN NODE = <string>origin_nodelist_name
  VECTOR NODE = <string>z_vector_nodelist_name
  POINT NODE = <string> x_vector_nodelist_name
  #
END [COORDINATE SYSTEM <string>coordinate_system_name]
```

The `COORDINATE SYSTEM` command block is used to define a local coordinate system for transforming a stress tensor from components in the global xyz coordinate system to the local system for output. This command block cannot be used for in-plane stresses and strains of shell elements because the shell integration point stresses and strains are computed in a local element system that varies element to element and rotates with the element. For output of shell stresses, the `BEGIN ORIENTATION` command must be used as explained in the previous section.

The `COORDINATE SYSTEM` block is also used to define a local coordinate system on the elements of a block for use in a representative volume analysis. In these analyses, elements of each representative volume will be aligned with the local system defined on the parent element.

A local element coordinate system may be defined using points defined in the input file with the `DEFINE POINT` command or using nodelists in the mesh file that contain exactly one node each. By using nodes in the mesh file, the defined coordinate system may translate and rotate during the analysis.

The `TYPE` command line allows three options for constructing a local coordinate system: `RECTANGULAR`, `CYLINDRICAL`, and `SPHERICAL`. The type defaults to `RECTANGULAR` if the `TYPE` command line is not present.

- `RECTANGULAR`: The command line `ORIGIN` or `ORIGIN NODE` specifies the origin of the local Cartesian coordinate system. The local Z' axis is a vector from the origin to the point given in the `VECTOR` of `VECTOR NODE` command. The local X' axis is the component of the vector from the origin to the `POINT` or `POINT NODE` that is orthogonal to the Z' axis. Finally, the local Y' axis is obtained from the cross product of Z' and X'.

- `CYLINDRICAL`: The command line `ORIGIN` or `ORIGIN NODE` specifies one point on the axis of the cylinder. The local Z' axis, the axis of the cylinder, is a vector from the origin to the point given in the `VECTOR` or `VECTOR NODE` command. The local X' axis is constructed as the vector normal to the cylindrical axis and passing through the location at which the local system is desired. Depending on the context, this local point may be a node, an element centroid, or an element integration point. If this local point lies on the Z' axis, then the point defined by the `POINT` or `POINT NODE` command is instead used to define the X' axis.

Finally, the Y' axis is obtained from the cross product of Z' and X'. Thus at the desired point not on the cylinder axis, the X' axis is through the cylinder thickness, Y' is tangent to the cylinder, and Z' is parallel to the cylinder axis.

- `SPHERICAL`: The command line `ORIGIN` or `ORIGIN NODE` specifies the location of the center of the sphere. The local X' axis is constructed as the vector from the center through the location at which the local system is desired. Depending on the context, this local point may be a node, an element centroid, or an element integration point. The local Z' axis is the component of the vector from the origin to the point given in the `VECTOR` or `VECTOR NODE` command that is normal to the X' axis. If this Z' is parallel the X' axis, then the Z' axis is defined along the vector from the point defined in `POINT` or `POINT NODE` to the origin. Finally, the Y' axis is obtained from the cross product of Z' and X'. Thus at a desired point, the X' axis is through the sphere thickness and the Y' and Z' axes lie in the tangent plane.

2.1.9 Define Coordinate System Line Command

```
DEFINE COORDINATE SYSTEM <string>coord_sys_name <string>coord_sys_type
  WITH POINT <string>point_1 POINT <string>point_2
  POINT <string>point_3
```

The line command `DEFINE COORDINATE SYSTEM` can also be used to define the axis directions of a local coordinate system to be located at nodes, element centroids, or element integration points. In this command

- The string `coord_sys_name` is a name for this coordinate system. This name must be unique to all other coordinate systems defined in the input file.
- The string `coord_sys_type` states the type of the coordinate system to be used. Three options are allowed for constructing a local coordinate system: `RECTANGULAR`, `CYLINDRICAL`, and `SPHERICAL`.
- The strings `point_1`, `point_2`, and `point_3` are the names for three points defined in the input file via `DEFINE POINT` command lines. These three points are used to define two of the coordinate system axes as described below for the different types of systems.

For a rectangular system, the local Z' axis is parallel to the vector from the `point_1` to `point_2`. The local X' axis is the component of the vector from `point_1` to `point_3` that is orthogonal to the Z' axis. Finally, the local Y' axis is obtained from the cross product of Z' and X'.

Likewise, for a cylindrical system, the local Z' axis is parallel to the vector from the `point_1` to `point_2` and defines the axis of the cylinder. The local X' axis is constructed as the vector normal to the cylindrical axis and passing through the location at which the local system is desired. This local point may be a node, an element centroid, or an element integration point. If this local point lies on the Z' axis, then the point `point_3` is instead used to define the X' axis. Finally, the Y' axis is obtained from the cross product of Z' and X'. Thus at the desired point not on the cylinder axis,

the X' axis is through the cylinder thickness, Y' is tangent to the cylinder, and Z' is parallel to the cylinder axis.

For a spherical system, `point_1` specifies the center of a sphere. The local X' axis is constructed as the vector from `point_1` through the location at which the local system is desired. This local point may be a node, an element centroid, or an element integration point. The local Z' axis is the component of the vector from the `point_1` to `point_3` that is normal to the X' axis. If this Z' is parallel the X' axis, then `point_3` is used instead. Finally, the Y' axis is obtained from the cross product of Z' and X'. Thus at a desired point, the X' axis is through the sphere thickness and the Y' and Z' axes lie in the tangent plane.

2.2 Procedure and Region

The Presto procedure scope is nested within the SIERRA scope, and the Presto region scope is nested within the procedure scope (see Section 1.2 for more information about scope). To create the scopes for the Presto procedure and Presto region, use the following commands:

```
BEGIN PRESTO PROCEDURE <string>presto_procedure_name

  PRINT BANNER INTERVAL = <integer>print_banner_interval(MAX_INT)

  #
  # TIME CONTROL command block
  #
  BEGIN PRESTO REGION <string>presto_region_name
    #
    # command blocks and command lines that appear in the
    # region scope
    #
  END [PRESTO REGION <string>presto_region_name]
END [PRESTO PROCEDURE <string>presto_procedure_name]
```

The `TIME CONTROL` command block also appears within the `PRESTO PROCEDURE` command block but outside of the `PRESTO REGION` command block. These three command blocks (procedure, time control, and region) are discussed below.

The `PRINT BANNER INTERVAL` line command sets the number of PRESTO output lines to print before re-printing the column headings. The default value is set to the maximum allowed integer value. This means that the banner will be printed to the log file one time by default.

Many command blocks and command lines fall within the region scope. These command blocks and command lines are described in other sections of this document.

2.2.1 Procedure

The analysis time, from the initial time to the termination time, is controlled within the procedure scope defined by the `PRESTO PROCEDURE` command block. The command block begins with an input line of the form:

```
BEGIN PRESTO PROCEDURE <string>presto_procedure_name
```

and is terminated with an input line of the following form:

```
END [PRESTO PROCEDURE <string>presto_procedure_name]
```

The string `presto_procedure_name` is the name for the Presto procedure.

2.2.2 Time Control

Within the procedure scope, there is a `TIME CONTROL` command block. This command block lets the user set the initial time and the termination time for an analysis. This block also allows the user to control the size of the time step.

Because Presto is an explicit, transient dynamics code, it must run at a time step that is less than the critical time for the problem at any given instant. Typically, this global critical time step is based on a critical time step estimate calculated for each element. With the `TIME CONTROL` command block, the user can set an initial time step, scale the element-based time step estimate, and control the growth of the element-based estimate for the critical time step.

In addition to the element-based method for estimating the critical time step, Presto offers other methods for estimating the critical time step. One approach for estimating the critical time step is to calculate the maximum eigenvalue for the model. There are two methods for calculating the maximum eigenvalue: the Lanczos method and the power method. A second approach for estimating the critical time step is to use a node-based method. The command blocks for implementing these various methods (maximum eigenvalue calculation and node-based) are in the region scope. There is also a mass-scaling technique that will influence the magnitude of the critical time step. If you use the mass-scaling technique, you must use the node-based method to obtain a critical time step estimate.

The estimation of the time step is a key part of any Presto analysis. Time step determination and control is discussed in detail in Chapter 3 of this document. The `TIME CONTROL` command block with its associated command lines are described in detail in Chapter 3. Consult Chapter 3 to determine how to specify command lines associated with the `TIME CONTROL` command block and how the `TIME CONTROL` command block fits into the overall scheme for time step control in Presto. Also see Chapter 3 to learn about the other methods for estimating the critical time step and the mass-scaling technique.

2.2.3 Region

Individual time steps are controlled within the region scope. The region scope is defined by a `PRESTO REGION` command block that begins with an input line of the form

```
BEGIN PRESTO REGION <string>presto_region_name
```

and is terminated with an input line of the following form:

```
END [PRESTO REGION <string>presto_region_name]
```

The string `presto_region_name` is the name for the Presto region.

The region, as indicated previously, determines what happens at each time step. In the procedure, we set the begin time and end time for the analysis. Time is incremented in the region. It is in the region where we set information about what occurs at various time steps. The output of results, for example, is set by command blocks in the region. If we want results output at certain times or certain steps in the analysis, this information is set in command blocks in the region. The region also contains command blocks for the boundary conditions. A boundary condition can have a

time-varying component. The region determines the value of the component for the current time step.

Two of the major types of command blocks, those for results output and boundary conditions, have already been mentioned. Other major types of command blocks in the region are those for restart control and contact. The region is also where the user selects the analysis model (finite element mesh).

The region makes use of information in the procedure and the SIERRA scope. For example, the specific element type used for an element block in the analysis model is defined in the SIERRA scope. This information about the element type is collected into an analysis model. The region then references this analysis model. As another example, the boundary condition command blocks can reference a function. The function will be defined in the SIERRA scope.

2.3 Use Finite Element Model

```
USE FINITE ELEMENT MODEL <string>model_name
```

The model specification occurs within the region scope. To specify the model (finite element mesh), use this command line. The string `model_name` must match a name used in a `FINITE ELEMENT MODEL` command block described in Section 5.1. If one of these command blocks uses the name `penetrator` in the command-block line and this is the model we wish to use in the region scope, then we would enter the command line as follows:

```
USE FINITE ELEMENT MODEL penetrator
```

2.4 Element Distortion Metrics

Presto can compute a number of element distortion metrics useful for assessing the quality of the solution as the mesh evolves over time. These metrics are computed as element variables, and can be used for output or as criteria for element death, just like any other element variable. The solution quality generally deteriorates as elements approach inversion, and if they do invert, the analysis aborts. The distortion metrics measure how close an element is to inversion. For all metrics a value of 1.0 is an ideal element and a value of 0.0 is a degenerate element. The following distortion metrics are available:

- `NODAL_JACOBIAN_RATIO` is currently available only for 8 node hexahedra. This metric evaluates the Jacobian function at each node of each element, and then computes the nodal Jacobian ratio as the smallest nodal Jacobian divided by the largest nodal Jacobian. An element having right angles between all adjacent edges has a nodal Jacobian ratio of 1.0. A negative nodal Jacobian ratio indicates that the element is becoming either convex or locally inverted. See Figure 2.8 for examples of quadrilateral elements with positive, zero, and negative nodal Jacobian ratios. The element calculations on poorly shaped elements (those with negative nodal Jacobian ratios) will generally be less accurate than those on well shaped elements (those with positive nodal Jacobian ratios). In addition, contact surfaces may become tangled and non-physical if elements start to invert.

- `ASPECT_RATIO` is available only for tetrahedral elements. A perfect equilateral tetrahedron has an aspect ratio of 1.0. A degenerate zero-volume tetrahedron has an aspect ratio of zero. An inverted tetrahedron has a negative aspect ratio. A very thin element can have a very small aspect ratio.

- `SOLID_ANGLE` computes the minimum or maximum angle between edges of an element as compared to optimal angles. The optimal solid angle for tetrahedra and triangles is 60 degrees; for hexahedra and quadrilaterals, it is 90 degrees. This error metric is 1.0 for an element in which all angles are optimal. Severely distorted or twisted elements have values of this metric near 0.0, and it is negative for inverted elements. This metric is 0 for degenerate elements. The `SOLID ANGLE` metric functions with hex, tet, triangle, and quad elements.

- `PERIMETER_RATIO` measures the the ratio of the deformed perimeter of an element to the undeformed perimeter of the element. This metric initially has a value of 1.0, and assumes values either greater than or lower than 1 as the mesh deforms. The `PERIMETER_RATIO` metric only works with triangle and quad elements.

- `DIAGONAL_RATIO` measures the the ratio of the deformed max diagonal of an element to the undeformed max diagonal of the element. This metric initially has a value of 1.0, and assumes values either greater than or lower than 1 as the mesh deforms. The `DIAGONAL_RATIO` metric only works with hex and quad elements.

The results from any of these distortion metrics can be requested by specifying an `ELEMENT VARIABLES` command line (Section 8.2.1.4) in the `RESULTS OUTPUT` command block (Section 8.2.1) for each metric for which the results are of interest. For example, to request the

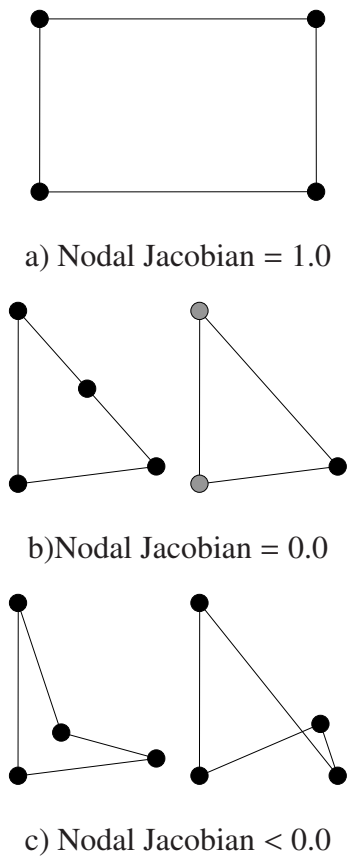

Figure 2.8: Examples of elements with varying nodal Jacobians

`ASPECT_RATIO` metric to be output as an element variable named `aspect` in the results output file, the following syntax can be included in a `RESULTS OUTPUT` command block:

```
ELEMENT ASPECT_RATIO as aspect
```

The distortion metrics can also be used for element death (Section 5.5). For example, to kill all elements in which the value of the `SOLID_ANGLE` metric is less than 0.2, the following line can be used in an `ELEMENT DEATH` command block:

```
CRITERION IS ELEMENT VALUE OF SOLID_ANGLE < 0.2
```

For more information about the use of element variables for element death, see Section 5.5.2.2.

2.5 Activation/Deactivation of Functionality

```
ACTIVE PERIODS = <string list>period_names
INACTIVE PERIODS = <string list>period_names
```

The `ACTIVE PERIODS` or `INACTIVE PERIODS` command line can be used to activate or deactivate functionality in the code at various points during an analysis. This functionality can include such things as boundary conditions, element blocks, and user subroutines. Command blocks that support this capability are documented accordingly in the sections of this manual where they are described.

In the command line, the string list `period_names` is a list of the time periods defined in `TIME STEPPING BLOCK` command blocks (see Section 3.1) during which the particular functionality is considered to be active. Each such `period_name` must match a name used in a `TIME STEPPING BLOCK` command block, e.g., `time_block_name`. Each defined time period runs from that period's start time to the next period's start time.

Only one of `ACTIVE PERIODS` or `INACTIVE PERIODS` can be used in any given command block. If the `ACTIVE PERIODS` command line is present, the functionality will be treated as active for all of the named periods, and inactive for any time periods that are not listed. If the `INACTIVE PERIODS` command line is present, the functionality will be treated as inactive for all of the named periods and active for any period not listed. If neither of these command lines is present, by default the functionality is active during all time periods.

2.6 Error Recovery

```
ERROR TOLERANCE = ON|OFF (ON)
```

This command controls how aggressively Presto will attempt to recover from a non-physical or ill-defined condition and continue with the analysis.

Under the default setting of `ON`, the code may invoke methods to keep the analysis moving forward despite the presence of non-physical or ambiguous conditions. For example, if the contact algorithm determines that a facet is potentially in two contact surfaces (an ambiguous condition), Presto will assign the facet to one of the surfaces and continue with the analysis. A second example pertains to SPH particles: if the deformation gradient of an SPH particle is inverted, the particle will be ignored rather than causing the analysis to terminate. Non-physical and ambiguous conditions will generally result in a warning message being printed.

If `ERROR TOLERANCE` is `OFF`, Presto will terminate an analysis in the presence of ambiguous or non-physical conditions. This may make it easier for an analyst to address non-fatal but potentially problematic issues.

2.7 Manual Job Control

The output of a running job can be controlled externally through the use of "shutdown" and "control" files. This mechanism allows for additional output of restart, results, history, and/or heartbeat data to be requested, as well as an optional graceful shutdown of the job.

A graceful shutdown is requested by inserting a "shutdown" file in the working directory of a running Presto job. The name of this file can be any of the following:

```
sierra.shutdown
<application_name>.shutdown
<base_name>.shutdown
```

If the `<application_name>.shutdown` variant is used, `<application_name>` is the name of the Sierra application being run. For example, `presto.shutdown` would be used to shut down Presto. If the `<base_name>.shutdown` variant is used, `<base_name>` is the basename of the input file. For example, if the input file name is `my_analysis.i`, then the shutdown file would be `my_analysis.shutdown`.

If the code detects the existence of a shutdown file, it will dump an output step to any open restart, results, history, or heartbeat file and then gracefully terminate the job. An entry will be written to the log file specifying that a shutdown file was detected and the file will be deleted. The contents of the file are not important; the shutdown file is only checked for existence.

The control file capability is provided to give more control over output and execution than is possible with the shutdown file. The name of the control file is the same as that of the shutdown file except that the filename suffix is `.control` instead of `.shutdown`. The contents of the file consist of a single line, and are case insensitive. The syntax is:

```
DUMP [RESTART] [RESULTS] [HISTORY] [HEARTBEAT] [STEP] [TIME]
  [STOP|ABORT|SHUTDOWN|CONTINUE]
```

The optional strings `RESTART`, `RESULTS`, `HISTORY`, `HEARTBEAT`, `STEP`, and `TIME` are used to specify the type of output that is written before an action is taken. If any output blocks of the specified type were defined in the input file for the model, output will be written to the files. The `STEP` and `TIME` options result in the last step and time being written to the log file. Multiple output types may be requested. If no output type is requested, all types of output specified in the input file will be written.

In addition to controlling the type of output that occurs, the `.control` file also specifies whether the job should be terminated or allowed to continue. If `STOP`, `ABORT`, or `SHUTDOWN` is specified at the end of the line, the job will be gracefully terminated. If `CONTINUE` is specified or no option is specified, the job will continue.

Several examples of the contents of continue files are shown below. The following examples all result in output being written to all types of output file and the job continuing:

```
dump
```

```
dump continue
dump restart results history heartbeat step continue
```

In both of the following examples, the current step and time will be written to the the log file, but no additional output will be written and the job will continue:

```
dump step
dump time continue
```

This example would result in a write to all output types and a graceful shutdown:

```
dump stop
```

In the following example, no output would be written to any files, but the current step and time would be written to the log file before a graceful shutdown:

```
dump step abort
```

An alternate abbreviated syntax is also supported. The abbreviated commands are shown below along with the full commands to which they are mapped:

```
sw1          dump restart shutdown
sw2          dump step continue
sw3          dump restart continue
sw4          dump results continue
```

If either the shutdown or control files are used, a message is output to the log file listing the name of that file, and in the case of the control file, the contents of that file. The control or shutdown file is then deleted.

Chapter 3

Time Step Control in Presto

This chapter discusses time control in Presto. We begin with a broad overview of time control in Presto and then describe the options that are available to users for time control.

The user initiates time control in Presto by setting a start time and a termination time for an analysis. The analysis is typically carried out with a large number of time steps, with each time step being much smaller than the analysis time. Because Presto is an explicit, transient dynamics code, a time step must be less than some critical value. Presto has a number of methods for computing an estimate for the critical time step. These methods are discussed in detail in this chapter.

The primary time control uses a `TIME CONTROL` command block that appears in the procedure scope. Use of the `TIME CONTROL` command block gives the user, by default, access to an element-based method for estimating the critical time step. The user can access three other methods for estimating the critical time step by using specific command blocks that are placed in the region scope. These other methods tend to give better (larger) estimates for the critical time step. In addition, Presto has a technique for adjusting the time step that is known as mass scaling.

Section 3.1 describes the `TIME CONTROL` command block. In Section 3.2 we discuss the other methods for estimating the critical time step. One approach for improving this estimate is to compute the maximum eigenvalue for a problem. Two methods for computing the maximum eigenvalue are available in Presto: the Lanczos method and the power method. Section 3.2.1 discusses the Lanczos method; Section 3.2.1.5 describes the command block required to implement the Lanczos method. Section 3.2.2 discusses the power method; Section 3.2.2.5 describes the command block required to implement the power method. Another approach for improving the time step estimate relies on a node-based estimate. Section 3.2.3 discusses the node-based method; Section 3.2.3.1 describes the command block required to implement the node-based method. You should read the introductory material for the maximum eigenvalue calculation methods and the node-based method and understand this material thoroughly before you attempt to use these methods. Although these other methods give larger time step estimates than the element-based method, they may not result in a net reduction of central processor unit (CPU) time for an analysis unless they are used properly. In those sections dealing with these other methods, we discuss how to use these methods in a cost-effective manner. Finally, in Section 3.2.3 we describe the technique of mass scaling. Mass scaling is a much different approach for adjusting the time step when compared

to the methods (element-, node-, maximum eigenvalue-based) we have just been discussing. The command block for mass scaling is in the region scope. Importantly, the mass-scaling technique requires that the node-based method of estimating the critical time step also be used.

3.1 Procedure Time Control

As indicated previously, the primary time control in Presto uses a `TIME CONTROL` command block in the procedure scope. The user sets the start time and the termination time for the analysis in the `TIME CONTROL` command block. For reference purposes, the general layout of the command block is as follows:

```
BEGIN TIME CONTROL
  BEGIN TIME STEPPING BLOCK <string>time_block_name
    START TIME = <real>start_time_value
    BEGIN PARAMETERS FOR PRESTO REGION <string>region_name
      INITIAL TIME STEP = <real>initial_time_step_value
      TIME STEP SCALE FACTOR =
        <real>time_step_scale_factor(1.0)
      TIME STEP INCREASE FACTOR =
        <real>time_step_increase_factor(1.1)
      STEP INTERVAL = <integer>nsteps(100)
      USER TIME STEP = <real>time_step
    END [PARAMETERS FOR PRESTO REGION <string>region_name]
  END [TIME STEPPING BLOCK <string>time_block_name]
  # Second TIME STEPPING BLOCK command block
  # would be placed here, as applicable.
  #
  # Additional TIME STEPPING BLOCK command blocks
  # would be placed here, as applicable.
  #
  # Last TIME STEPPING BLOCK command block
  # would be placed here, as applicable.
  #
  TERMINATION TIME = <real>termination_time
END [TIME CONTROL]
```

The analysis time, as demonstrated above, can be subdivided into a number of time blocks, i.e., `TIME STEPPING BLOCK` command blocks. If the total analysis time is from time 0 to time T and there are three blocks, then the first block is defined from time 0 to time t_1, the second block is defined from time t_1 to time t_2, and the third block is defined from time t_2 to time T. (The times t_1 and t_2 are set by the user.) If we sum all the times for each block, the sum will be T. The different time periods defined by each block can be referenced so that we can turn certain functionality on or off throughout an analysis. For example, we may want to have a certain boundary condition turned off during our first time period and activated for the second time period. (Most analyses require

only one block.) Use the `ACTIVE PERIODS` or `INACTIVE PERIODS` command lines described in Section 2.5 to activate and deactivate functionality during specific time blocks.

By default, Presto relies on the element-based critical time step estimate. At every time step, an element-based calculation is performed to determine a critical time step. You have some control over the actual time step that is used by employing one of two techniques. We discuss these two techniques in the following paragraphs. The specific command lines for using these techniques are described in Section 3.1.1.

With the first technique, you can set an initial time step that is smaller than the element-based critical time step estimate. Presto will start the analysis by using your initial time step value instead of the element-based critical time step estimate (as long as your value is less than the element-based critical time step estimate). You can then control the rate at which the time step increases from your initial value. This technique is employed by using the `TIME STEP INCREASE FACTOR` command line as follows:

- If you set a time step increase factor equal to 1, then the initial value you specified will be used throughout the analysis (provided that the initial time step is never smaller than the element-based critical time step estimate throughout the computations).
- If you set a time step increase factor to some value greater than 1, the time step will grow (from the initial value) at each time step until it reaches the value of the element-based critical time step estimate. From then on, the element-based critical time step estimate will essentially control the time step.

With the second technique, you can manipulate the element-based estimate with either a scale factor or a time step increase factor. This technique is employed by using the `TIME STEP SCALE FACTOR` command line or the `TIME STEP INCREASE FACTOR` command line as follows:

- The element-based estimate for the critical time step is usually smaller than some maximum theoretical value for your model. It may therefore be possible to scale the element-based critical time step estimate by some factor greater than 1. (Your scaled value must remain below the theoretical maximum limit, however. We discuss ways to obtain a critical time step close to the theoretical maximum in later sections of this chapter.)
- If there are stability problems with a particular problem, it may be necessary to scale the element-based estimate with a factor less than 1.
- You can also control the rate at which the time step can increase for an analysis. By specifying a time step increase factor, you can limit the increase in the size of the time step so that it does not increase too rapidly from one step to the next. For certain problems, the element-based critical time step estimate may increase rapidly from one step to the next. Limiting the increase in the size of the time step may enable some problems to run in a more stable fashion.

The `USER TIME STEP` command can be used to explicitly set the integration time step, overriding the critical time step computed by any time step estimation methods. This command can be used to force the analysis to integrate at any specified time step, even a super-critical one.

Warning: The `TIME STEP SCALE FACTOR` and `USER TIME STEP` commands both provide the ability to force the code to take a time step larger than the stability limit, and as such, should be used with caution. If the time step specified with either of these commands is too large, the time integration will add energy to the system, causing the analysis to go unstable and ultimately fail.

Now that we have presented an overview of the functionality in the `TIME CONTROL` command block, we will discuss the actual command lines.

3.1.1 Command Blocks for Time Control and Time Stepping

```
BEGIN TIME CONTROL
  BEGIN TIME STEPPING BLOCK <string>time_block_name
    START TIME = <real>start_time_value
    BEGIN PARAMETERS FOR PRESTO REGION <string>region_name
      #
      # Time control parameters specific to PRESTO
      # are set in this command block.
      #
    END [PARAMETERS FOR PRESTO REGION <string>region_name]
  END [TIME STEPPING BLOCK <string>time_block_name]
  TERMINATION TIME = <real>termination_time
END [TIME CONTROL]
```

Presto time control resides in a `TIME CONTROL` command block. The command block begins with an input line of the form

```
BEGIN TIME CONTROL
```

and terminates with an input line of the following form:

```
END [TIME CONTROL]
```

Within the `TIME CONTROL` command block, a number of `TIME STEPPING BLOCK` command blocks can be defined. Each `TIME STEPPING BLOCK` command block contains the time at which the time stepping starts and a number of parameters that set time-related values for the analysis. Each `TIME STEPPING BLOCK` command block terminates at the start time of the following command block. The start times for the `TIME STEPPING BLOCK` command blocks must be in increasing order. Otherwise, an error will be generated by Presto. (The example in Section 3.1.6 shows the overall structure of the `TIME CONTROL` command block.)

In the above input lines, the values are as follows:

- The string `time_block_name` is a name for the `TIME STEPPING BLOCK` command block. This name must be unique to each command block of this type. The string `time_block_name` can be referenced in an `ACTIVE PERIODS` or `INACTIVE PERIODS` command line to activate and deactivate functionality (see Section 2.5).

- The real value `start_time_value` is the start time for this `TIME STEPPING BLOCK` command block. Values set in this block apply from the start time for this block until the next start time or the termination time. The start time may be negative.

- The string `region_name` is the name of the Presto region affected by the parameters (see Section 2.2).

The termination time for the analysis is given by the following command line:

```
TERMINATION TIME = <real>termination_time
```

Here, `termination_time` is the time at which the analysis will stop. The `TERMINATION TIME` command line appears inside the `TIME CONTROL` command block but outside of any `TIME STEPPING BLOCK` command block.

The `TERMINATION TIME` command line can appear before the first `TIME STEPPING BLOCK` command block or after the last `TIME STEPPING BLOCK` command block. Note that it is permissible to have `TIME STEPPING BLOCK` command blocks with start times after the termination time; in this case, those command blocks that have start times after the termination time are not executed. Only one `TERMINATION TIME` command line can appear in the `TIME CONTROL` command block. If more than one of these command lines appears, Presto gives an error.

Nested inside the `TIME STEPPING BLOCK` command block is a `PARAMETERS FOR PRESTO REGION` command block containing parameters that control the time stepping.

```
BEGIN PARAMETERS FOR PRESTO REGION <string>region_name
  INITIAL TIME STEP = <real>initial_time_step_value
  TIME STEP SCALE FACTOR = <real>time_step_scale_factor(1.0)
  TIME STEP INCREASE FACTOR =
    <real>time_step_increase_factor(1.1)
  STEP INTERVAL = <integer>nsteps(100)
END [PARAMETERS FOR PRESTO REGION <string>region_name]
```

These parameters are specific to a Presto analysis.

The command block begins with an input line of the form

```
BEGIN PARAMETERS FOR PRESTO REGION <string>region_name
```

and is terminated with an input line of the following form:

```
END [PARAMETERS FOR PRESTO REGION <string>region_name]
```

As noted previously, the string `region_name` is the name of the Presto region affected by the parameters. The command lines nested inside the `PARAMETERS FOR PRESTO REGION` command block are described next. It should be noted that certain of these command lines will be ignored when either of the maximum-eigenvalue methods or the node-based method is used to estimate the critical time step. The discussions of the command blocks associated with these methods indicate whether or not these command lines are pertinent.

3.1.2 Initial Time Step

```
INITIAL TIME STEP = <real>initial_time_step_value
```

By default, Presto computes a critical time step for the analysis and uses this value as the initial time step. To directly specify a different initial time step, use the `INITIAL TIME STEP` command line, where `initial_time_step_value` is the size of the initial time step. This command line is only valid if it is in the first `TIME STEPPING BLOCK` command block in the problem.

The value for the initial time step will overwrite the calculated value for the critical time step. If you specify an initial time step that is larger than the critical time step, the time step is set to the value of the calculated critical time step.

3.1.3 Time Step Scale Factor

```
TIME STEP SCALE FACTOR = <real>time_step_scale_factor(1.0)
```

During the element computations, Presto computes a minimum time step required for stability of the computation (the critical time step). Using the `TIME STEP SCALE FACTOR` command line, you can provide a scale factor to modify the critical time step. Note that a value greater than 1.0 for `time_step_scale_factor` will cause the time step to be greater than the computed critical time step, and thus the problem may become unstable. By default, the scale factor is 1.0.

3.1.4 Time Step Increase Factor

```
TIME STEP INCREASE FACTOR =
  <real>time_step_increase_factor(1.1)
```

During an analysis, the computed critical time step may change as elements deform, are killed, and so forth. By using the `TIME STEP INCREASE FACTOR` command line, you can limit the amount that the time step can increase between two adjacent time steps. The value `time_step_increase_factor` is a factor that multiplies the previous time step. The current time step can be no larger than the product of the previous time step and the scale factor.

Note that an increase factor less than 1.0 will cause the time step to continuously decrease. The default value for this factor is 1.1, i.e., a time step cannot be more than 1.1 times the previous step.

3.1.5 Step Interval

```
STEP INTERVAL = <integer>nsteps(100)
```

Presto can output data about the current time step, the current internal and external energy, and the kinetic energy throughout an analysis. The `STEP INTERVAL` command line controls the frequency

of this output, where `nsteps` is the number of time steps between output. The default value for `nsteps` is 100.

The output at any given step (read from left to right) is

- step number,
- time,
- time step,
- global element identifier for element controlling time step
- kinetic energy,
- internal energy,
- external energy (work done on boundary),
- error in energy balance,
- hour glass energy
- cpu time, and
- wall clock time.

The time is at the current time, step n, and the time increment is the previous time step increment from step $n-1$ to step n.

The error in the energy balance is computed from the following relation:

```
energy balance error = (kinetic energy + internal energy
  - external energy) / external energy * 100
```

The above expression gives a percent error for the energy balance.

3.1.6 Example

The following is a simple example of a `TIME CONTROL` command block:

```
BEGIN TIME CONTROL
  BEGIN TIME STEPPING BLOCK p1
    START TIME = 0.0
    BEGIN PARAMETERS FOR PRESTO REGION presto_region
      INITIAL TIME STEP = 1.0e-6
      STEP INTERVAL = 50
    END
```

```
  END
  BEGIN TIME STEPPING BLOCK p2
    START TIME = 0.5e-3
    BEGIN PARAMETERS FOR PRESTO REGION presto_region
      TIME STEP SCALE FACTOR = 0.9
      TIME STEP INCREASE FACTOR = 1.5
      STEP INTERVAL = 10
    END
  END
  TERMINATION TIME = 1.0e-3
END
```

The first `TIME STEPPING BLOCK`, `p1`, begins at time 0.0, the initial start time, and terminates at time 0.5×10^{-3}. The second `TIME STEPPING BLOCK`, `p2`, begins at time 0.5×10^{-3} and terminates at time 1.0×10^{-3}, which is the time listed on the `TERMINATION TIME` command line. The `TIME STEPPING BLOCK` names `p1` and `p2` can be referenced by the `ACTIVE PERIODS` or `INACTIVE PERIODS` command lines as described in Section 2.5 to activate and deactivate functionality.

3.2 Other Critical Time Step Methods

Currently, there are four methods for calculating a critical time step for Presto. First, there is the traditional element-based method. We know that, in general, the element-based time step in Presto can give a fairly conservative estimate for the time step. Second, there is a node-based method for giving a critical time step estimate. Depending on the problem, the node-based method may or may not give an estimate for the critical time step that approaches the theoretical maximum value for a particular model. Although the node-based method can give a larger critical time step estimate than the element-based method, the node-based estimate may still be significantly lower than the maximum theoretical time step for a problem. Finally, there are two methods that use an estimate for the maximum eigenvalue to obtain an estimate for the critical time step. From the maximum eigenvalue, it is possible to derive the theoretical maximum critical time step for a problem via the formula

$$\Delta t_{crit} = 2.0/\sqrt{\theta_{max}}, \tag{3.1}$$

where Δt_{crit} is the critical time step and θ_{max} is the maximum eigenvalue. The two methods employed in Presto to give an estimate for the maximum eigenvalue are the Lanczos method and the power method. The Lanczos method can give an accurate estimate of the maximum eigenvalue for a problem using a very small number of Lanczos vectors compared to the total number of degrees of freedom in a problem. The power method uses a simple iterative process to obtain an estimate for the maximum eigenvalue. The power method is not as powerful a mathematical technique as the Lanczos method for obtaining a maximum eigenvalue estimate. However, it does present another viable option for obtaining a maximum eigenvalue estimate for certain problems and has therefore been included as another method for obtaining the maximum eigenvalue estimate.

The use of a critical time step from the node-based method or a method based on the maximum eigenvalue estimate is desirable because the larger critical time steps produced by these methods (compared to the element-based method) reduce CPU time. Both methods, however, are not cost effective if they are called every time step to give a critical time step estimate. The cost of doing one node-based estimate or one maximum eigenvalue estimate for the critical time step will not offset the cost benefit of the increase to the critical time step (compared to the element-based time step estimate) over a single time step. Hence, there must be some scheme for

- calling these methods only periodically throughout a calculation and
- maintaining a larger estimate (than the element-based estimate) for the critical time step in between these calls

if we are to gain a net benefit from the increase in the critical time step these methods can produce.

If you want to use the maximum eigenvalue estimate for calculating the critical time step and your problem has long periods with a relatively stable time step estimate, the Lanczos method for calculating the maximum eigenvalue will be the preferred method to use. If you have a problem for which the changes in the time step should be monitored more frequently, the power method will be better suited for this problem than the Lanczos method. The preferred use for each of these

two different eigenvalue methods will become obvious as you read the background material for these two methods in Section 3.2.1 and Section 3.2.2. Both the Lanczos method and the power method require the use of a variety of control parameters. For some of these control parameters, techniques have been devised to automatically calculate values for these parameters in what should be a robust and reliable method for a wide range of problems. Other parameters are defaulted to values that will optimize the use of a particular eigenvalue calculation method (Lanczos method or power method) with the type of problems that best suit the method that is employed. The default values for these control parameters may change as we gain more experience in using the Lanczos method and the power method.

Detailed discussions of the Lanczos method, the power method, and the node-based method follow. There are many similarities in the implementation of the Lanczos method and the power method.

3.2.1 Lanczos Method

The Lanczos method, as implemented in Presto, is outlined here so that certain aspects of it can be referenced in subsequent parts of this chapter. In the following set of equations, $\mathbf{K}_T$ is a tangent stiffness matrix, $\mathbf{M}$ is the mass matrix, and $\mathbf{r}_0$ is an arbitrary starting vector.

$$
\begin{aligned}
&\textit{Initialize}\\
&\quad \mathbf{q}_0 = \mathbf{0}\\
&\quad \beta = ([\mathbf{r}_0]^T \mathbf{M}^{-1} \mathbf{r}_0)^{1/2}\\
&\quad \mathbf{q}_1 = \mathbf{r}_0/\beta_1\\
&\quad \mathbf{p}_1 = \mathbf{M}^{-1}\mathbf{q}_1\\
&\textit{for } j = 1, n\\
&\quad \bar{\mathbf{r}}_j = \mathbf{K}_T \mathbf{p}_j\\
&\quad \hat{\mathbf{r}}_j = \bar{\mathbf{r}}_j - \mathbf{q}_{j-1}\beta_j\\
&\quad \alpha_j = [\mathbf{q}_j]^T \mathbf{M}^{-1} \hat{\mathbf{r}}_j = [\mathbf{p}_j]^T \hat{\mathbf{r}}_j\\
&\quad \mathbf{r}_j = \hat{\mathbf{r}}_j - q_j \alpha_j\\
&\quad \hat{\mathbf{p}}_j = \mathbf{M}^{-1}\mathbf{r}_j\\
&\quad \beta_{j+1} = ([\mathbf{r}_j]^T \mathbf{M}^{-1} \mathbf{r}_j)^{1/2} = ([\bar{\mathbf{p}}_j]^T \mathbf{r}_j)^{1/2}\\
&\quad \textit{if enough vectors, terminate loop}\\
&\quad \mathbf{q}_{j+1} = \mathbf{r}_j/\beta_{j+1}\\
&\quad \mathbf{p}_{j+1} = \bar{\mathbf{p}}_j/\beta_{j+1}\\
&\textit{end}
\end{aligned}
$$

The details for this form of the Lanczos method are described in Reference 1. Notice that the Lanczos method is an iterative method. If we use the Lanczos method in a code like Presto to compute the maximum eigenvalue for a particular finite element model, the number of iterations

required to give a good estimate for the maximum eigenvalue will depend on the size of the finite element model (the number of nodes and elements), the types of elements in the model, and the material types and material properties used in the model.

The maximum eigenvalue for a particular finite element model gives us the largest estimate we can obtain for the critical time step. Hence, the time step estimate derived from the maximum eigenvalue is our "best" estimate for the critical time step. The estimate for the critical time step based on the maximum eigenvalue can be significantly larger than an element-based time step estimate. However, computing the critical time step (for a given time step) with the Lanczos method is more expensive than computing the critical time step with element-based calculations. Over one time step, it is not possible to recoup the cost of the Lanczos calculations with the increase in the size of the time step over the element-based estimate. Using the Lanczos method for estimating the critical time step in an explicit, transient dynamics code requires a methodology that effectively addresses the computational costs. The following sections outline a cost-effective approach to using the Lanczos method in an explicit, transient dynamics code.

3.2.1.1 Lanczos Method with Constant Time Steps

To explain how to use the Lanczos method in a cost-efficient manner, we must first establish the computational cost of using the Lanczos method. As indicated previously, computing the maximum eigenvalue for a finite element model requires some number of iterations (each iteration in the Lanczos method produces a Lanczos vector) to obtain a good estimate for the maximum eigenvalue. The cost of an iteration (Lanczos vector) is approximately the cost of an internal force calculation. Notice, in preceding equations for the Lanczos method, that the Lanczos method requires the product of the tangent stiffness matrix $\mathbf{K}_T$ with a vector $\mathbf{p}$. In Presto, we do not construct a tangent stiffness matrix. Instead, we simply provide the vector $\mathbf{p}$ for the internal force calculations. The internal force calculations give us the desired matrix $\times$ vector product of $\mathbf{K}_T\mathbf{p}$.

Over a given time step, the cost of an internal force calculation is the major computational cost. (This assumes no contact. The addition of contact introduces another computationally expensive process into a time step. For our initial discussion, we ignore the cost of contact.) In order to use the Lanczos method to get a critical time step estimate, one has to call the Lanczos method for some given time step. If the Lanczos method made n iterations to get a good estimate for the maximum eigenvalue, then the overall cost of the time step would be approximately $n + 1$ times the cost of the internal force calculation. The cost of the time step would be the n internal force calculations for Lanczos and the actual internal force calculation to advance the time step. If n is 20 (a minimum for typical problems), the cost of the time step becomes 21 times the cost of the internal force calculation. The critical time step estimate based on the maximum eigenvalue would have to be at least 21 times greater than the element-based critical time step to recoup the cost of the maximum eigenvalue calculation. A typical value for the critical time step estimate based on the maximum value is more in the range of 1.1 to 2.0 times the element-based critical time step estimate. Obviously, the Lanczos method is much too expensive to call at every time step for a critical time step estimate.

To explain how the Lanczos method can effectively be used in an explicit, transient dynamics code, we begin with a simple case study. In this case study, we compute the critical time step using

the Lanczos method at some time step and then assume that this critical time step value remains constant for a subsequent number of time steps, n_L. We only call the Lanczos method once during the n_L time steps. (In reality, the critical time step in an explicit, transient dynamics code like Presto changes with each time step. We address this issue of the changing time step when we present the details for using the Lanczos method in a cost-effective manner.) For this case study, we also assume that the computational cost of an element-based estimate for the critical time step is part of the cost of an internal force calculation. The cost of the element-based time step estimate is a small part of the overall internal force calculations. Finally, for our initial discussion, we assume no contact. We address the issue of contact further in the discussion.

Assume that the Lanczos method computes a global estimate for the critical time step of Δt_L, which is the value to be used for n_L time steps. At the end of the n_L time steps, the analysis time for the code has been incremented by an amount ΔT, which is computed simply as

$$\Delta T = n_L \Delta t_L \,. \tag{3.2}$$

If the element-based estimate for the time step is Δt_e and the number of time steps required to increment the analysis time by ΔT is n_e, then, for the element-based time step, we have

$$\Delta T = n_e \Delta t_e \,. \tag{3.3}$$

Because the Lanczos estimate for the critical time step is larger than the element-based estimate, we know that $n_e > n_L$. Let us define the ratio r as

$$r = \Delta t_L / \Delta t_e = n_e / n_L \,. \tag{3.4}$$

The ratio r is greater than 1.

Now that we have determined the relation between the number of steps required for a Lanczos-based critical time step estimate versus the element-based critical time step estimate to achieve the same analysis time increment, let us examine the computational costs for these two cases in terms of CPU time. Designate the CPU cost for a time step as Δt_{IF}. If the number of Lanczos vectors required to obtain the critical time step estimate is N_L, then the total computational cost of the Lanczos method and the n_L time steps is

$$n_L \Delta t_{IF} + N_L \Delta t_{IF} \,. \tag{3.5}$$

If we use the element-based method, the total computational cost is

$$n_e \Delta t_{IF} \,. \tag{3.6}$$

Recall that we have chosen n_L and n_e so that we have the same analysis time increment ΔT even though we have different critical time steps. Now, we must determine the point at which the computational cost for the Lanczos-based critical time step calculations is the same as the cost for the element-based critical time step calculations. This is simply the point at which

$$n_e \Delta t_{IF} = n_L \Delta t_{IF} + N_L \Delta t_{IF} \,. \tag{3.7}$$

If we rearrange the above equation to eliminate Δt_{IF} and make use of the ratio r, then we obtain

$$n_e = \frac{N_L}{1 - 1/r} \,. \tag{3.8}$$

Consider the case of $r = 1.25$ and $N_L = 20$. When $n_L = 80$ and $n_e = 100$, the above equations show that the calculations with the Lanczos-based critical time step and the calculations with the element-based time step give the same analysis time for the same computational expense. If we use the Lanczos-based critical time step Δt_L for more than eighty iterations, then the Lanczos-based approach becomes cost effective. Our above equations have established the "break-even" point at which it becomes cost effective to use the Lanczos method to reduce computational costs by overcoming the initial cost of the Lanczos calculations with the larger critical time step.

We can build on what we have done thus far to account for contact. Suppose that the computational cost of contact over a time step is some multiple m of the computational cost of the internal force calculation Δt_{IF}. Then the point at which the computational cost for the Lanczos-based calculations is the same as the computational cost for the element-based calculations is

$$(1 + m) n_L \Delta t_{IF} + N_L \Delta t_{IF} = (1 + m) n_e \Delta t_{IF} \,. \tag{3.9}$$

For the case with contact,

$$n_e = \frac{N_L}{(1 + m)(1 - 1/r)} \,. \tag{3.10}$$

Again, consider the case of $r = 1.25$ and $N_L = 20$. Assume the computational cost of contact calculations is the same as an internal force calculation ($m = 1$). For these values, the break-even point is $n_L = 40$ and $n_e = 50$. The added computational cost of the contact calculations results in reaching the break-even point with a smaller number of iterations when compared to the case with no contact.

The above derivations let us calculate a break-even point based on our assumptions of a constant critical time step. Considering that a typical analysis will run for tens of thousands of time steps, something on the order of 100 steps represents a reasonable number of steps to recoup the cost of the Lanczos calculations. Whether or not the cost of the Lanczos calculations can be recouped in something on the order of 100 calculations depends heavily upon N_L. If N_L is sufficiently small, we can recoup the cost of the Lanczos calculations in a reasonable number of steps.

Some computational studies indicate that N_L is in an acceptable range for many problems. The Lanczos method computes a good estimate for the maximum eigenvalue with a small number of Lanczos vectors, N_L, compared to the number of degrees of freedom in a problem. Some component studies show that, for a problem with between 250,000 and 350,000 degrees of freedom, one can obtain a good estimate for the maximum eigenvalue with only twenty Lanczos vectors. A large-scale study of a model involving 1.7 million nodes (5.1 million degrees of freedom) showed

that only forty-five Lanczos vectors were required to obtain a good estimate of the maximum eigenvalue. These examples demonstrate that the number of Lanczos vectors required for a good maximum eigenvalue estimate is very small when compared to the number of degrees of freedom for a problem. When N_L is in the range of twenty to forty-five, Equations 3.7 and 3.10 show that, with an increase in the time step on the order of 1.2 to 1.25, we can recoup the cost of the Lanczos method in a reasonable number of time steps.

Now that we have determined we can recoup the cost of the Lanczos calculations in a reasonable number of time steps, let us look at the issue of reusing a Lanczos-based estimate in some manner.

3.2.1.2 Controls for Lanczos Method

As indicated in the above discussion, the Lanczos method can be used in a cost-effective manner in an explicit, transient dynamics code if a Lanczos calculation can be performed and the Lanczos-based estimate for the critical time step can be reused in some way over a number of subsequent time steps. This section presents an approach for reusing a Lanczos-based estimate over a number of time steps so that we maintain a critical time step estimate that is close to the theoretical maximum value in between the calls to the Lanczos method. The approach discussed here makes use of the element-based critical time step estimate at each time step.

We start our approach with a Lanczos calculation to determine the maximum eigenvalue. The Lanczos method converges to the maximum eigenvalue from below, which means that the method underestimates the maximum eigenvalue. Because the critical time step depends on the inverse of the maximum eigenvalue, we overestimate the critical time step. It is necessary, therefore, to scale back the critical time step estimate from the Lanczos method so that the calculations in the explicit time-stepping scheme do not become unstable. Our approach for determining a scaled-back value for the maximum critical time step makes use of the element-based time step estimate. Again, let Δt_L be the critical time step estimate from the Lanczos method and Δt_e be the critical time step estimate from the element-based calculations. The scaled-back estimate for the critical time step, Δt_s, is computed from the equation

$$\Delta t_s = \Delta t_e + f_s(\Delta t_L - \Delta t_e), \tag{3.11}$$

where f_s is a scale factor. (A reasonable value for f_s ranges from 0.9 to 0.95 for our problems.) This value of f_s puts Δt_s close to and slightly less than a theoretical maximum critical time step.

Once Δt_s is determined, the ratio

$$t_r = \Delta t_s / \Delta t_e \tag{3.12}$$

is computed. This ratio is then used to scale subsequent element-based estimates for the critical time step. If $\Delta t_{e(n)}$ is the nth element-based critical time step after the time step where the Lanczos calculations are performed, then the nth time step after the Lanczos calculations, $\Delta t_{(n)}$, is simply

$$\Delta t_{(n)} = t_r \Delta t_{e(n)}. \tag{3.13}$$

The ratio t_r is used until the next call to the Lanczos method. The next call to the Lanczos method is controlled by one of two mechanisms. With the first mechanism, the user can set the frequency with which the Lanczos method is called. The user can set a parameter so that the Lanczos method is called only once every n time steps. This number remains fixed throughout an analysis. With the second mechanism, the user can control when the Lanczos method is called based on changes in the element-based critical time step. For this second mechanism, the change in the element-based critical time step estimate is tracked. Suppose the element-based critical time step at the time the Lanczos method was called is Δt_e. At the nth step after the call to the Lanczos method, the element-based critical time step is $\Delta t_{e(n)}$. If the value

$$\Delta t_{lim} = \frac{|\Delta t_{e(n)} - \Delta t_e|}{\Delta t_e} \tag{3.14}$$

is greater than some limit set by the user, then the Lanczos method will be called. If there is a small, monotonic change in the element-based critical time step over a large number of time steps, this second mechanism will result in the Lanczos method being called. Or if there is a large, monotonic change in the element-based critical time step over a few time steps, the Lanczos method will also be called.

These two mechanisms for calling the Lanczos method can be used together. For example, suppose the second mechanism (the mechanism based on a change in the element-based time step) results in a call to the Lanczos method. This resets the counter for the first mechanism (the mechanism using a set number of time steps between calls to the Lanczos method).

This approach for reusing a Lanczos-based time step estimate has been implemented in Presto, and it has been used for a number of studies. One of the component studies, as indicated previously, used the same scale factor for $n_L = 1700$ iterations. The break-even point for this problem is $n_e = 45$ time steps (not accounting for contact, which was a part of the component modeling). For this particular problem, the extended use of the Lanczos estimate reduced the computational cost to 56% of what it would have been with the element-based time step.

Not all problems will lend themselves to reusing one Lanczos-based estimate for thousands of time steps. However, if it is possible to use the Lanczos-based estimate for two to three times the number of time steps required to reach the break-even point, we begin to see a noticeable reduction in the total number of time steps required for a problem.

3.2.1.3 Scale Factor for Lanczos Method

When the Lanczos method is called for a given time step, it must appear that the calculations are using the constant tangent stiffness matrix $\mathbf{K}_T$ for all iterations. As indicated previously, we use the internal force calculations to generate the product $\mathbf{K}_T\mathbf{p}_j$ (for the jth iteration) in the Lanczos calculations. Any vector $\mathbf{p}_j$, as calculated by the Lanczos method, may be such that it represents large-strain behavior and moves the internal force calculations into a nonlinear regime. It is necessary to scale the $\mathbf{p}_j$ vectors so that the internal force calculations are in a small-strain regime, which makes it appear that we are working with a constant tangent stiffness matrix. The vectors $\mathbf{p}_j$ must be scaled so that they represent velocities associated with small strain. When properly scaled

vectors are sent to the internal force calculation, the internal force calculation effectively becomes a matrix × vector product with a constant tangent stiffness matrix for all iterations during a given call to the Lanczos method.

The scale factor for the $\mathbf{p}_j$ vectors, which we will designate as v_{sf}, must not be too small, as this will create round-off problems and give a bad estimate for the critical time step. If the scale factor is too large, we violate the above restriction of a constant tangent stiffness matrix.

There are two approaches for controlling the scale factor when the Lanczos method is used to compute the maximum eigenvalue. These approaches are discussed in Section 3.2.1.5.

3.2.1.4 Accuracy of Eigenvalue Estimate

Every time a new Lanczos vector is computed, we obtain an additional eigenvalue for our model and, in general, a better estimate for the maximum eigenvalue (and hence a better estimate for the critical time step). The Lanczos method can compute a good value for the maximum eigenvalue with a very small number of total computed eigenvalues compared to the number of degrees of freedom in a problem. There are examples, as previously indicated, of problems with 250,000 to 350,000 degrees of freedom where we have obtained a good estimate of the critical time step with twenty eigenvalues. In one problem with 5.1 million degrees of freedom, we obtained a good estimate of the critical time step with forty-five eigenvalues.

A user could, in theory, determine a reasonable number of eigenvalues necessary for obtaining a good estimate of the maximum eigenvalue based on the above information on model size and the number of eigenvalues required for a good maximum eigenvalue estimate. The user could test the validity of the choice of the number of eigenvalues by increasing the number of eigenvalues slightly and comparing the maximum eigenvalue estimate obtained with the larger number of eigenvalues to the original maximum eigenvalue estimate obtained with the smaller number of eigenvalues. If the change in the two maximum eigenvalue estimates (larger versus smaller total number of eigenvalues) is small, then the original estimate for the number of eigenvalues is reasonably accurate.

As an alternative to directly specifying the number of eigenvalues to be computed, a convergence tolerance could be set on the change in the magnitude of the maximum eigenvalue as additional eigenvalues (Lanczos vectors) are computed. Let θ_{max_n} be the maximum eigenvalue calculated corresponding to n eigenvalues (Lanczos vectors), and let θ_{max_n+1} be the maximum eigenvalue corresponding to $n + 1$ eigenvalues (Lanczos vectors). The eigenvalues would be computed until

$$\frac{|\ \theta_{max_n+1} - \theta_{max_n}\ |}{\theta_{max_n+1}} \tag{3.15}$$

is less than some tolerance. (We will now refer to the value of Equation (3.15) as the *convergence measure*.) If we calculate the convergence measure for a sequence of maximum eigenvalues computed by the Lanczos method, we will not necessarily see a monotonic decrease in the convergence measure for all time. Typically, the convergence measure will initially show a monotonically decreasing value for an increasing n, and then the convergence measure will show a monotonically increasing value for an increasing n. (The phase in which the convergence measure increases is usually very small, on the order of one to two iterations.) After the phase in which the convergence

measure monotonically increases, there is then a phase in which the convergence measure begins a long (over many iterations) monotonic decrease. This behavior (decrease of the convergence measure, slight increase, then long monotonic decrease) is typical of Krylov methods, of which the Lanczos method is one. Using the convergence measure to determine the number of eigenvalues to be computed for a problem is a reasonable option, but some care must be taken in setting the tolerance for the convergence measure.

Both of the techniques just discussed are offered as a way to set the maximum number of eigenvalues required to obtain an accurate eigenvalue estimate for a model. These techniques are discussed further in Section 3.2.1.5.

3.2.1.5 Lanczos Parameters Command Block

```
BEGIN LANCZOS PARAMETERS <string>lanczos_name
  STARTING VECTOR = <string>STRETCH_X|STRETCH_Y|STRETCH_Z|
    ISOTHERMAL(ISOTHERMAL)
  INCREASE OVER STEPS = <integer>incr_int(5)
  NUMBER EIGENVALUES = <integer>num_eig(150)
  EIGENVALUE CONVERGENCE TOLERANCE = <real>converge_tol(0.5e-3)
  SMALL STRAIN = <real>small_strain(1.0e-3)
  VECTOR SCALE = <real>vec_scale(1.0e-5)
  SCALE FACTOR = <real>time_scale(0.9)
  UPDATE ON TIME STEP CHANGE = <real>tstep_change(0.10)
  UPDATE STEP INTERVAL = <integer>step_int(500)
END [LANCZOS PARAMETERS <string>lanczos_name]
```

If you use the Lanczos method to compute a critical time step, there should be only one `LANCZOS PARAMETERS` command block, and it should appear in the region. If you have a `LANCZOS PARAMETERS` command block, you should not specify a `NODE BASED TIME STEP PARAMETERS` or a `POWER METHODS PARAMETERS` command block. If you use the Lanczos method to compute the critical time step, the time step increase factor (default or user-specified) will be used to control the increase in the time step estimate; the time step scale factor (default or user-specified) will not be used. These factors are specified in the `PARAMETERS FOR PRESTO REGION` portion of a `TIME STEPPING BLOCK` in the `TIME CONTROL` command block.

The Lanczos method requires some type of starting vector. This is determined by the `STARTING VECTOR` command line. The various options available for this command line will generate a displacement vector that stretches your model in the x-, y-, or z-direction, or in all three directions (x, y, and z) at once. (`STRETCH_X` stretches the model in the x-direction, `STRETCH_Y` stretches the model in the y-direction, `STRETCH_Z` stretches the model in the z-direction, and `ISOTHERMAL` stretches the model in all three directions at once.) The displacement vector then serves as a basis for generating the starting vector r_0 in the initialization phase of the Lanczos method. The Lanczos method appears to be fairly insensitive to the choice of a starting vector. The default starting vector is the `ISOTHERMAL` option. You may encounter cases where the use of one of the other options for a starting vector—`STRETCH_X`, `STRETCH_Y`, or `STRETCH_Z`—may result in a slight increase in accuracy for the critical time step estimate for a given number of eigenvalues. These other options

(STRETCH_X, STRETCH_Y, and STRETCH_Z) are offered for these special cases.

The INCREASE OVER STEPS command line determines how many steps, i.e., incr_int, are used to transition from an element-based critical time step estimate to the Lanczos-based estimate at the beginning of an analysis. The user may want to increase from the element-based estimate to the Lanczos-based estimate over a number of time steps if the difference between these two estimates is large. The value of incr_int for this command line defaults to 5.

As indicated in Section 3.2.1.4, some number of eigenvalues must be computed by the Lanczos method to obtain a good estimate for the maximum eigenvalue for a given finite element model. As one option, the user can simply specify the number of eigenvalues to be computed by the Lanczos method by using the NUMBER EIGENVALUES command line. The default value for num_eig in this command line is 150. As an alternative, the user can specify a tolerance on the convergence measure defined in Equation (3.15). The tolerance is set with the EIGENVALUE CONVERGENCE TOLERANCE command line. The default value for the convergence tolerance, converge_tol, is 0.5×10^{-3}. (This default value may change in the future as we gain more experience with the Lanczos method.)

By default, the convergence measure (with the default value of 0.5×10^{-3}) is used to determine the number of eigenvalues to be computed. If neither the EIGENVALUE CONVERGENCE TOLERANCE command line nor the NUMBER EIGENVALUES command line appears in the LANCZOS PARAMETERS command block, then the convergence measure will be used to determine the number of eigenvalues. If the EIGENVALUE CONVERGENCE TOLERANCE command line appears in the command block with a specified tolerance other than the default value, then the number of eigenvalues computed will be determined by the convergence measure and the user-specified tolerance. If the NUMBER EIGENVALUES command line appears in the LANCZOS PARAMETERS command block, then the user-defined number of eigenvalues will be used to set the number of eigenvalues computed by the Lanczos method.

The recommended technique for determining the number of eigenvalues is to use the convergence measure option with the default tolerance. If you use this technique, neither the NUMBER EIGENVALUES command line nor the EIGENVALUE CONVERGENCE TOLERANCE command line should be included in the LANCZOS PARAMETERS command block.

As indicated in Section 3.2.1.3, it is necessary to scale one of the vectors (with a scale factor v_{sf}) in the Lanczos calculations so that it appears we are always working with a constant tangent stiffness each time we call the Lanczos method. There are two approaches for determining the scale factor. With the first approach, the user can specify the value of a small strain for a particular model by using the SMALL STRAIN command line. (As long as the internal force calculation inside the Lanczos method is working with a vector that approximates small-strain behavior, it will appear that we are working with a constant tangent stiffness inside the Lanczos method.) The value for v_{sf} is then computed based on your specification for what constitutes a small strain in the model. (The default value for small_strain is 1.0×10^{-3}.) With the second approach for determining the scale factor, the user can specify a value for v_{sf} directly by using the VECTOR SCALE command line. The default value for v_{sf}, the vec_scale parameter in that command line, is 1.0×10^{-5}. A number of tests have established that this value for the scale factor, 1.0×10^{-5}, works well for a range of models encountered at Sandia National Laboratories. If the user wants to use the option of directly specifying the scale factor, it is possible to determine whether a particular scale factor

is suitable for a particular problem. Take a scale factor v_{sf}, plus values on either side of it, say, $0.9 \times v_{sf}$ and $1.1 \times v_{sf}$. If all three of these scale factor values produce almost the same estimate for the critical time step for a particular model, then the value for v_{sf} meets the criterion for an acceptable scale factor.

By default, the small-strain approach (with the default value of 1.0×10^{-3}) is used to determine a scale factor. If neither the `SMALL STRAIN` command line nor the `VECTOR SCALE` command line appears in the `LANCZOS PARAMETERS` command block, then the small-strain value will be used to calculate the scale factor. If the `SMALL STRAIN` command line appears in the command block with any value other than the default value *and* the `VECTOR SCALE` command line does not appear in the command block, then the vector scale will be determined by the user-specified value for the small strain. If the `VECTOR SCALE` command line does appear in the `LANCZOS PARAMETERS` command block, then the vector scale will be determined by the user-specified value for the vector scale.

The recommended way of determining the scale factor is to use the small-strain approach with the default small-strain value. If you follow this advice, neither the `SMALL STRAIN` command line nor the `VECTOR SCALE` command line should be included in the `LANCZOS PARAMETERS` command block.

As indicated previously, the scale factor must not be too small, as this will create round-off problems and give a bad estimate for the critical time step. If the scale factor is too large, we violate the above restriction of a constant tangent stiffness matrix.

The `SCALE FACTOR` command line sets the factor f_s in Equation (3.11). The value for f_s, i.e., `time_scale`, is set to 0.9. More experience with the Lanczos method will help us determine whether a slightly larger value of f_s can be used as a default.

The `UPDATE ON TIME STEP CHANGE` command line sets the value for Δt_{lim} in Equation (3.14). If the change in the element-based critical time step estimate as given by Equation (3.14) exceeds the value for Δt_{lim}, then the Lanczos method is called for a new estimate for the critical time step. The default value for Δt_{lim}, i.e., `tstep_change`, is 0.10.

The `UPDATE STEP INTERVAL` command line sets the number of step intervals at which the Lanczos method is called. If `step_int` is set to 1000, the Lanczos method will be called every one thousand steps to compute an estimate for the critical time step. (The default value of `step_int` is 500.) This control mechanism interacts with the control established by the `UPDATE ON TIME STEP CHANGE` command line. Suppose we have set `step_int` to 1000, and we have computed 800 steps since the last call to the Lanczos method. If Δt_{lim} has been set to 0.15 and we exceed this value at step 800, then the change in the element-based time step will result in the Lanczos method being called. The counter for keeping track of the number of step intervals since the last Lanczos computation will be reset to zero. The next call to the Lanczos method will occur again in one thousand steps, unless we again exceed the change in the element-based time step.

3.2.2 Power Method

The power method is a simple iterative technique that gives an estimate for the maximum eigenvalue. Consider the following form of the eigenvalue problem, which is useful for our explicit transient dynamics problem.

$$\mathbf{K}_T\mathbf{x}_i - \theta_i\mathbf{M}\mathbf{x}_i = 0 \tag{3.16}$$

Reformulate the problem as

$$[\mathbf{M}]^{-1}\mathbf{K}_T\mathbf{x}_i - \theta_i\mathbf{x}_i = 0\,. \tag{3.17}$$

Denote the matrix product $\mathbf{M}^{-1}\mathbf{K}_T$ as the matrix operator $\mathbf{A}$. The eigenvalue problem is now

$$\mathbf{A}\mathbf{x}_i - \theta_i\mathbf{x}_i = 0\,. \tag{3.18}$$

The maximum eigenvalue for the problem in Equation (3.18) can be computed with the following iterative process:

$$\begin{aligned}
&\textit{for } i = 1, n\\
&\quad \mathbf{x}_i = \mathbf{A}\mathbf{x}_{i-1}\\
&\quad \mathbf{x}_i = \mathbf{x}_i / \parallel \mathbf{x}_i \parallel\\
&\quad \theta_i = [\mathbf{x}_i]^T\mathbf{A}\mathbf{x}_i\\
&\textit{end}
\end{aligned}$$

The value θ_i is the ith estimate for the maximum eigenvalue. As n increases, the power method should yield a more accurate estimate for the maximum eigenvalue. So, just as with the Lanczos method, the power method must iterate at some given time step to obtain an estimate for the maximum eigenvalue at that time step. The details for the above form of the power method are described in Reference 2.

Like the Lanczos method, the power method requires the use of an internal force calculation. The power method, however, is somewhat simpler than the Lanczos method. The power method requires that one vector and one scalar be computed. The Lanczos method requires the computation of five vectors and two scalars. Further, the power method yields a direct estimate for the maximum eigenvalue, whereas the Lanczos method requires that the maximum eigenvalue be extracted from a tridiagonal matrix.

If the sequence of eigenvalues for an analysis problem is

$$\mid \lambda_1 \mid > \mid \lambda_2 \mid \geq \cdots \geq \mid \lambda_n \mid, \tag{3.19}$$

then the rate of convergence to the maximum eigenvalue depends on the ratio

$$\frac{\mid \lambda_1 \mid}{\mid \lambda_2 \mid}. \tag{3.20}$$

Depending on the magnitudes of $\mid \lambda_1 \mid$ and $\mid \lambda_2 \mid$, the rate of convergence could be rather slow. The power method, for a given problem, may not converge to as accurate an estimate for the maximum eigenvalue as quickly as the Lanczos method. We should be careful, however, in how

we interpret this convergence property for the power method. For many of our problems, we probably have a large number of eigenvalues clustered just below the maximum eigenvalue. The power method may give a reasonable estimate for the maximum eigenvalue in a relatively small number of iterations. The power method may converge quickly to some eigenvalue estimate that is just below the maximum eigenvalue. Convergence to the maximum eigenvalue, in terms of accuracy to many digits, might then be very slow. However, one would still have an adequate estimate for the maximum eigenvalue to set a value for the critical time step.

One of the advantages of the power method is that we can use the last value for $\mathbf{x}_i$ from a previous call to the power method as a starting vector for our current call to the power method and converge quickly (for some problems) to an accurate estimate for the maximum eigenvalue. Consider the following scenario. We make an initial call to the power method using some arbitrary $\mathbf{x}_0$ starting vector. We obtain a good estimate for the maximum eigenvalue after n iterations. After some number of time steps, we again call the power method and we use $\mathbf{x}_n$ from the previous call to the power method as our current starting vector. Because we are solving nonlinear problems, the matrix operator, $\mathbf{A}$, has most likely changed from the time when we made the initial call to the power method. If the changes in the matrix operator are small, then $\mathbf{x}_n$ should be an excellent choice for the starting vector, and we should converge quickly to a good estimate for the maximum eigenvalue. This behavior, quick convergence to a good eigenvalue estimate using a prior value of $\mathbf{x}_n$ as a starting vector, has been observed in some sample problems. We discuss this issue of restarting the power method using a previous $\mathbf{x}_n$ in more detail in Section 3.2.2.1.

Obtaining a cost-effective and user-friendly implementation of the power method requires addressing the same issues discussed above for an automated implementation of the Lanczos method. First, we must determine some scheme to call the power method on an intermittent basis so that it is cost effective. The control mechanism for calling the Lanczos method on an intermittent basis can also be used for the power method. Second, the $\mathbf{x}$ vector must be scaled appropriately before it is used in the internal force calculations. (For the Lanczos method, we must scale the vector $\mathbf{p}$.) Finally, we need to terminate the power method. A tolerance on the value in Equation (3.15) can be set to terminate the method. (Setting a tolerance on Equation (3.15) is the same approach used for the Lanczos method.)

3.2.2.1 Power Method with Constant Time Steps

The cost of making one iteration for the power method is approximately the cost of an internal force calculation. As indicated previously, the cost of one iteration for the Lanczos method (the calculation of a Lanczos vector) is also approximately the cost of an internal force calculation. Therefore, the equations developed in Section 3.2.1.1 are also applicable for determining when the power method can be used in a cost-effective manner. Recall that the equation

$$n_e = \frac{N_L}{1 - 1/r} \tag{3.21}$$

in Section 3.2.1.1 gives the number of time steps for the break-even point at which it becomes cost effective for the case of no contact to use the Lanczos method to reduce computational costs by overcoming the initial cost of the Lanczos calculations with the larger critical time step. In the

above equation, N_L is the number of Lanczos iterations, and r is the ratio of the Lanczos-based critical time to the element-based time step estimate. This equation is directly applicable to the power method because the cost of one iteration in the power method is similar to the cost of one iteration in the Lanczos method. (The variable N_L becomes the number of iterations for the power method.)

Now let us return to the scenario in Section 3.2.2 where we look at restarting the power method with the last value for $\mathbf{x}_i$ from a previous call to the power method. We make an initial call to the power method using some arbitrary $\mathbf{x}_0$ starting vector. We obtain a good estimate for the maximum eigenvalue after n iterations. Our estimate for the critical time step based on the maximum eigenvalue gives us a value of 1.25 for r. After some number of time steps, we again call the power method, and we use $\mathbf{x}_n$ from the previous call to the power method as our current starting vector. In our second call to the power method, the power method converges to a good estimate for the maximum eigenvalue in two iterations. The break-even point where we recoup the cost of the power method (in our second call) is ten time steps. If the power method converges to a good estimate for the maximum eigenvalue in three iterations, then the break-even point where we recoup the cost of the power method (in our second call) is fifteen time steps. There are some problems where we can obtain a good estimate for the maximum eigenvalue in two or three iterations when we use the last value for $\mathbf{x}_n$ from a previous call to the power method as our starting vector for the current call to the power method. For the case where we can converge to a good estimate for the maximum eigenvalue in two or three iterations, we can easily call the power method once every forty or fifty time steps and use the power method to improve the time step estimate in a cost-effective manner. Over a time span of forty or fifty time steps, matrix operator $\mathbf{A}$, as defined in Equation (3.18) may change by only a small amount for a large class of problems. If matrix operator $\mathbf{A}$ changes by a small amount, then using the last value of $\mathbf{x}_n$ from a previous call to the power method provides an excellent starting vector and gives us quick convergence. This ability of the power method to converge quickly by using previous information makes it a viable scheme for calculating the maximum eigenvalue and producing a critical time step estimate.

For a problem with contact, the equations derived for the Lanczos method (with contact) in Section 3.2.1.1 are also applicable to the power method. For the power method, as in the case of the Lanczos method, the added computational cost of the contact calculations results in reaching a break-even point with a smaller number of iterations when compared to a case where there is no contact.

3.2.2.2 Controls for Power Method

Using the power method is similar to using the Lanczos method in that we must be able to perform a power method calculation and reuse the power method estimate for the critical time step in some way over a number of subsequent time steps. The approach for reusing a power method estimate for the critical time step over a number of time steps is the same as the approach for reusing a Lanczos-based estimate over a number of time steps as described in Section 3.2.1.2. The approach discussed in Section 3.2.1.2 presents a way to reuse a maximum eigenvalue time step estimate over a number of time steps so that we maintain a critical time step estimate that is close to the theoretical maximum value in between the calls to the maximum eigenvalue calculations. The

approach discussed in in Section 3.2.1.2 makes use of the element-based critical time step estimate at each time step.

3.2.2.3 Scale Factor for Power Method

When the power method is called for a given time step, it must appear that the calculations are using a constant matrix operator, $\mathbf{A}$, for all iterations. The $\mathbf{A}$ operator is the product of the inverse of the mass matrix $\mathbf{M}^{-1}$ and the tangent stiffness matrix $\mathbf{K}_T$ for the problem. The mass matrix is a constant. Therefore, we must assure that we are working with what is effectively a constant tangent stiffness matrix for all iterations during a call to the power method. This is the same requirement that we encounter in the Lanczos method (see Section 3.2.1.3). For the power method, we use the internal force calculations to generate the product $\mathbf{A}\mathbf{x}_i$ by first computing the internal forces using $\mathbf{x}_i$, which gives us the product $\mathbf{K}_T\mathbf{x}_i$, and then multiplying the internal force results by the inverse of the mass matrix. Any vector $\mathbf{x}_i$, as calculated by the power method, may be such that it represents large-strain behavior and moves the internal force calculations into a nonlinear regime. It is necessary to scale the $\mathbf{x}_i$ vectors so that the internal force calculations are in a small-strain regime, which makes it appear that we are working with a constant tangent stiffness matrix. The vectors $\mathbf{x}_i$ must be scaled so that they represent velocities associated with small-strain calculations. When properly scaled vectors are sent to the internal force calculation, the internal force calculation becomes a matrix $\times$ vector product with a constant tangent stiffness matrix for all iterations during a given call to the power method.

The scale factor for the $\mathbf{x}_i$ vectors, which we will designate as v_{sf}, must not be too small, as this will create round-off problems and give a bad estimate for the critical time step. If the scale factor is too large, we violate the above restriction of a constant tangent stiffness matrix.

There are two approaches for controlling the scale factor when the power method is used to compute the maximum eigenvalue. These approaches are discussed in Section 3.2.2.5.

3.2.2.4 Accuracy of Eigenvalue Estimate

To use the power method efficiently, it is best not to specify a set number of iterations for every instance when the power method is called. Instead, some tolerance should be set on the convergence measure defined in Equation (3.15). The initial call to the power method may take a significant number of iterations to produce a good estimate for the maximum eigenvalue. On subsequent calls to the power method, the number of iterations to converge to a good estimate for the maximum eigenvalue should be quite small when we use previous values of $\mathbf{x}$ as a starting vector.

For the power method, we rely on the convergence measure defined by Equation (3.15) to control the number of iterations. The user can set an upper limit on the number of iterations for the power method. Control of the number of iterations for the power method is discussed in more detail in Section 3.2.2.5.

3.2.2.5 Power Method Parameters Command Block

```
BEGIN POWER METHOD PARAMETERS <string>powermethod_name
  STARTING VECTOR = <string>STRETCH_X|STRETCH_Y|STRETCH_Z|
    ISOTHERMAL(ISOTHERMAL)
  INCREASE OVER STEPS = <integer>incr_int(5)
  NUMBER ITERATIONS = <integer>num_iter(150)
  EIGENVALUE CONVERGENCE TOLERANCE =
    <real>converge_tol(0.5e-3)
  SMALL STRAIN = <real>small_strain(1.0e-3)
  VECTOR SCALE = <real>vec_scale(1.0e-5)
  SCALE FACTOR = <real>time_scale(0.9)
  UPDATE ON TIME STEP CHANGE = <real>tstep_change(0.10)
  UPDATE STEP INTERVAL = <integer>step_int(50)
END [POWER METHOD PARAMETERS <string>powermethod_name]
```

If you use the power method to compute a critical time step, there should be only one `POWER METHOD PARAMETERS` command block, and it should appear in the region. If you have a `POWER METHOD PARAMETERS` command block, you should not specify a command block for the node-based method or the Lanczos method. If you use the power method to compute the critical time step, the time step increase factor (default or user-specified) set in the `TIME CONTROL` command block will be used to control the increase in the time step estimate; the time step scale factor (default or user-specified) set in the `TIME CONTROL` command block will not be used. These factors are specified in the `PARAMETERS FOR PRESTO REGION` portion of a `TIME STEPPING BLOCK` in the `TIME CONTROL` command block.

The power method requires some type of starting vector. This is determined by the `STARTING VECTOR` command line. The various options available in this command line will generate a displacement vector that stretches your model in the x-, y-, or z-direction, or in all three directions (x, y, and z) at once. (`STRETCH_X` stretches the model in the x-direction, `STRETCH_Y` stretches the model in the y-direction, `STRETCH_Z` stretches the model in the z-direction, and `ISOTHERMAL` stretches the model in all three directions at once.) The displacement vector then serves as a basis for generating the starting vector x_0 in the initialization phase of the Lanczos method. The default starting vector is the `ISOTHERMAL` option. You may encounter cases where use of one of the other options for a starting vector—`STRETCH_X`, `STRETCH_Y`, or `STRETCH_Z`—may result in a slight increase in accuracy for the critical time step estimate for a given number of iterations. These other options (`STRETCH_X`, `STRETCH_Y`, and `STRETCH_Z`) are offered for these special cases.

The `INCREASE OVER STEPS` command line determines how many steps, `incr_int`, are used to transition from an element-based critical time step estimate to the power method estimate at the beginning of an analysis. The user may want to increase from the element-based estimate to the power method estimate over a number of time steps if the difference between these two estimates is large. The value of `incr_int` defaults to 5.

As indicated in Section 3.2.2.4, some number of iterations are required by the power method to obtain a good estimate for the maximum eigenvalue for a given model. The number of iterations is controlled by the tolerance set for the convergence measure given in Equation (3.15). The tolerance

is set with the EIGENVALUE CONVERGENCE TOLERANCE command line. The default value for the convergence tolerance, converge_tol is 0.5×10^{-3}. (This default value may change in the future as we gain more experience with the power method.)

The user can set an upper limit on the number of iterations for the power method by using the NUMBER ITERATIONS command line. If the number of iterations in the power method exceeds the value set by num_iter, then the power method is terminated. Otherwise, the iterative process in the power method is terminated by the tolerance set on the convergence measure. The default value for num_iter is 150.

As indicated in Section 3.2.2.3, it is necessary to scale the vectors $\mathbf{x}_i$ (with a scale factor v_{sf}) in the power method calculations so that it appears we are always working with a constant tangent stiffness each time we call the power method. There are two approaches for determining the scale factor. With the first approach, the user can specify the value of a small strain for a particular model by using the SMALL STRAIN command line. (As long as the internal force calculation inside the power method is working with a vector that approximates small-strain behavior, it will appear that we are working with a constant tangent stiffness inside the power method.) The value for v_{sf} is then computed based on your specification for what constitutes a small strain in the model. (The default value for small_strain is 1.0×10^{-3}.) With the second approach for determining the scale factor, the user can specify a value for v_{sf} directly by using the VECTOR SCALE command line. The default value for v_{sf}, the vec_scale parameter in that command line, is 1.0×10^{-5}. A number of tests have established that this value for the scale factor, 1.0×10^{-5}, works well for a range of models encountered at Sandia National Laboratories. If the user wants to use the option of directly specifying the scale factor, it is possible to determine whether a particular scale factor is suitable for a particular problem. Take a scale factor v_{sf}, plus values on either side of it, say, $0.9 \times v_{sf}$ and $1.1 \times v_{sf}$. If all three of these scale factor values produce almost the same estimate for the critical time step for a particular model, then the value for v_{sf} meets the criterion for an acceptable scale factor.

By default, the small-strain approach (with the default value of 1.0×10^{-3}) is used to determine a scale factor. If neither the SMALL STRAIN command line nor the VECTOR SCALE command line appears in the POWER METHOD PARAMETERS command block, then the default small-strain value will be used to calculate the scale factor. If the SMALL STRAIN command appears in the command block with any value other than the default value *and* the VECTOR SCALE command line does not appear in the command block, then the vector scale will be determined by the user-specified value for the small strain. If the VECTOR SCALE command line does appear in the POWER METHOD PARAMETERS command block, then the vector scale will be determined by the user-specified value for the vector scale.

The recommended way of determining the scale factor is to use the small-strain approach with the default small-strain value. Thus, if you follow this advice, neither the SMALL STRAIN command line nor the VECTOR SCALE command line should be included in the POWER METHOD PARAMETERS command block.

As indicated previously, the scale factor must not be too small, as this will create round-off problems and give a bad estimate for the critical time step. If the scale factor is too large, we violate the above restriction of a constant tangent stiffness matrix.

The `SCALE FACTOR` command line sets the factor f_s in Equation (3.11). The value for f_s, i.e., `time_scale` is set to 0.9. More experience with the power method will help us determine whether a slightly larger value of f_s can be used as a default.

The `UPDATE ON TIME STEP CHANGE` command line sets the value for Δt_{lim} in Equation (3.14). If the change in the element-based critical time step estimate as given by Equation (3.14) exceeds the value for Δt_{lim}, then the power method is called for a new estimate for the critical time step. The default value for Δt_{lim}, i.e., `tstep_change`, is 0.10.

The `UPDATE STEP INTERVAL` command line sets the number of step intervals at which the power method is called. If `step_int` is set to 40, the power method will be called every forty steps to compute an estimate for the critical time step. (The default value of `step_int` is 50.) This control mechanism interacts with the control established by the `UPDATE ON TIME STEP CHANGE` command line. Suppose we have set `step_int` to 40, and we have computed thirty-five steps since the last call to the power method. If Δt_{lim} has been set to 0.15 and we exceed this value at step 35, then the change in the element-based time step will result in the power method being called. The counter for keeping track of the number of step intervals since the last power method computation will be reset to zero. The next call to the power method will then occur again in forty steps, unless we again exceed the change in the element-based time step.

3.2.3 Node-Based Method

Now that we have developed schemes to make the Lanczos method and power method cost-effective tools for estimation of the critical time step, let us examine the node-based scheme.

The node-based method in Presto will give an estimate for the critical time step that is greater than or equal to the element-based estimate. It may or may not give an estimate for the time step that is close to the maximum value associated with the maximum eigenvalue for the problem. In general, we assume the node-based method will give us an estimate larger than the element-based estimate, but not significantly larger.

If the node-based scheme is used to determine the critical time step for a block of uniform elements (all the same material), then the estimate from the node-based method will be the same as that for the element-based estimate. The node-based estimate begins to diverge from (become larger than) the element-based estimate as the differences in aspect ratios of the elements attached to a node become larger. We can assume, therefore, that if the stiffest part of our structure has a relatively uniform mesh, the node-based method will not give a significantly larger estimate than the element-based method.

The node-based method costs only a fraction of an internal force calculation. However, the node-based method makes use of element time step estimates. Therefore, in order to do the node-based method, one must also do the element-based method. The cost of the node-based method is in addition to the element-based method. The modest increase in the critical step estimate from the node-based method is unlikely to offset the added cost of the node-based method.

To make the node-based method cost-effective, we can use the same methodology that is employed for the Lanczos method. Let t_b be the estimate for the critical time step from the node-based

method. We define the ratio of the node-based estimate to the element-based estimate as

$$t_r = \frac{\Delta t_b}{\Delta t_e}. \tag{3.22}$$

This ratio is then used to scale subsequent element-based estimates for the critical time step. If $\Delta t_{e(n)}$ is the nth element-based critical time step after the time step where the node-based calculations are performed, then the nth time step after the node-based calculations, $\Delta t_{(n)}$, is simply

$$\Delta t_{(n)} = t_r \Delta t_{e(n)}. \tag{3.23}$$

The ratio t_r is used until the next call to the node-based method. The next call to the node-based method is controlled by one of two mechanisms described in the Lanczos discussion. The node-based method is called after a set number of times or a significant change in the element-based estimate for the critical time step.

3.2.3.1 Node-Based Parameters Command Block

```
BEGIN NODE BASED TIME STEP PARAMETERS <string>nbased_name
  INCREMENT INTERVAL = <integer>incr_int(5)
  STEP INTERVAL = <integer>step_int(1)
  TIME STEP LIMIT = <real>step_lim(0.10)
END [NODE BASED TIME STEP PARAMETERS <string>nbased_name]
```

If you use the node-based method to compute a critical time step, there should be only one `NODE BASED TIME STEP PARAMETERS` command block, and it should appear in the region. If you use the node-based method to compute the critical time step, you should set the time step scale factor to 1.0 and the time step increase factor to a large number (5.0 is an acceptable value for the time step increase factor). These factors are specified in the `PARAMETERS FOR PRESTO REGION` portion of a `TIME STEPPING BLOCK` in the `TIME CONTROL` command block. If you have a `NODE BASED TIME STEP PARAMETERS` command block, you should not specify a `LANCZOS PARAMETERS` command block.

The `INCREMENT INTERVAL` command line determines how many steps, `incr_int`, are used to transition from an element-based critical time step estimate to the node-based estimate at the beginning of an analysis. The user may want to increase from the element-based estimate to the node-based estimate over a number of time steps if the difference between these two estimates is large. The value of `incr_int` defaults to 0 so the node based time step is used immediately at the beginning of the analysis.

The `STEP INTERVAL` command line sets the number of step intervals at which the node-based method is called. If `step_int` is set to 1000, the node-based method will be called every one thousand steps to compute an estimate for the critical time step. (The default value of `step_int` is 1.) Increasing the step interval can improve performance, but depending on the problem could run the risk of sending the time step super-critical. This control mechanism interacts with the control established by the `TIME STEP LIMIT` command line. Suppose we have set `step_int` to

1000, and we have computed 800 steps since the last call to the node-based method. If Δt_{lim} has been set to 0.15 and we exceed this value at step 800, then the change in the element-based time step will result in the node-based method being called. The counter for keeping track of the number of step intervals since the last node-based computation will be reset to zero. The next call to the node-based method will occur again in one thousand steps, unless we again exceed the change in the element-based time step.

The `TIME STEP LIMIT` command line sets the value for Δt_{lim} in Equation (3.14). If the change in the element-based critical time step estimate as given by Equation (3.14) exceeds the value for Δt_{lim}, then the node-based method is called for a new estimate for the critical time step. The default value for Δt_{lim}, i.e., `step_lim`, is 0.10.

3.3 Mass Scaling

3.3.1 What is Mass Scaling?

Mass scaling allows for arbitrarily increasing the mass of certain nodes in order to increase the global estimate for the critical time step. The nodes where the mass is increased must be associated with those elements that have the minimum time step. By increasing the mass at any node for an element, we have effectively raised the critical time step estimate for that element.

Note that mass scaling does not adjust the value for the density used in the element calculations. Mass scaling only adjusts the mass at the nodes. The net effect of the mass scaling makes it appear, however, as if we have modified the density of selected elements (even though no adjustment has been made to element densities).

Warning: Use of mass scaling will introduce error into your analysis. The amount of error incurred is unbounded and can be unpredictable. It is entirely up to the analyst to decide whether mass scaling can be used in a way that does not distort the results of interest.

Mass scaling can be useful in a number of circumstances, as listed below. However, in all of these circumstances, error will be introduced into the calculations. The user must be extremely careful not to introduce excessive error.

- Quasi-static or rigid-body motion: If the model or part of a model is undergoing what is basically quasi-static or rigid-body motion, then adding mass may have little effect on the end result.
- Disparate sizes in element geometry: A model may contain elements for some portion of the model that are much smaller than the majority of elements in the rest of the model. For example, a model might include screws or gears that are modeled in detail. The elements for the screw threads or gear teeth could be much smaller than elements in other portions of the model. If the dynamics of these parts modeled with small elements (compared to the rest of

the mesh) are relatively unimportant, adding mass to them might not affect the quantities of interest.

- Increasing time step for “unimportant" sections of the mesh: For some problems, you may not want part of the mesh to control the time step. Consider a car-crash problem in which the bumper is the first part to strike an object. The crumpling of the bumper could greatly reduce the time step in some elements of the bumper, and these elements would control the time step for the problem. At a later time in the analysis, the effect of the bumper on the overall crash dynamics may not be significant. Mass scaling could be applied to ensure that this now noncritical part (the bumper) is no longer controlling the global time step.

3.3.2 Mass Scaling Command Block

```
BEGIN MASS SCALING
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list> nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  TARGET TIME STEP = <real>target_time_step
  ALLOWABLE MASS INCREASE RATIO = <real>mass_increase_ratio
  #
  # additional command
  ACTIVE PERIODS = <string list>periods
  INACTIVE PERIODS = <string list>periods
END MASS SCALING
```

The `MASS SCALING` command block controls mass scaling for a specified set of nodes. This command block contains one or more command lines to specify the node set. It also contains two command lines that determine how the actual mass scaling will be applied to the nodes in the node set. In addition to the command lines in the two command groups, there are two additional command lines: `ACTIVE PERIODS` and `INACTIVE PERIODS`. These command lines are used to activate or deactivate the mass scaling for specified time periods.

Multiple `MASS SCALING` command blocks can exist to apply different criteria to different portions of the mesh at different times. For any given set of `MASS SCALING` command blocks, mass will only be added to a node if doing so will allow increasing the global time step. The amount of artificial mass added to a node will vary in time as the mesh deforms and moves. The added mass computation is recomputed every time the node-based time step estimate is recomputed.

NOTE: Mass scaling must be used in conjunction with the node-based time step estimation method.

See the preceding sections for a description of the node-based method for estimating the critical time step.

Following are descriptions of the different command groups:

3.3.3 Node Set Commands

The `node set commands` portion of the `MASS SCALING` command block specifies the nodes associated with the boundary condition. This portion of the command block can include some combination of the following lines:

```
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list> nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes for mass scaling. There must be at least one `NODE SET`, `SURFACE`, `BLOCK`, or `INCLUDE ALL BLOCKS` command line in the command block.

3.3.3.1 Mass Scaling Commands

The `MASS SCALING` command block may contain either a

```
TARGET TIME STEP = <real>target_time_step
```

command line or an

```
ALLOWABLE MASS INCREASE RATIO = <real>mass_increase_ratio
```

command line, or both of these command lines can appear in the input block.

The `TARGET TIME STEP` command lines sets the maximum time step for a set of nodes. The parameter `target_time_step` is the maximum time step for all the nodes specified in the command block.

The `ALLOWABLE MASS INCREASE RATIO` command line sets an upper limit on the mass scaling at a node. The value specified for `mass_increase_ratio` limits the ratio of the mass at a node, as set by mass scaling, to the original mass at the node. (The original mass of the node is determined only by the element contributions.) This ratio must be a factor greater than or equal to 1. If m_s is the scaled mass at a node and m_0 is the original mass at the node due only to element contributions, then the ratio $m_s \div m_0$ will not exceed the value of `mass_increase_ratio`.

Mass scaling will add mass to nodes until the target time step is reached, the mass added to some node reaches the allowable mass increase ratio, or the current set of nodes no longer controls the

global analysis time step.

The amount of mass added due to mass scaling is stored in the nodal variable `mass_scaling_added_mass`. This variable can be output and post-processed to determine how much mass is being added at a given time. See Section 8.2.1 regarding the output of nodal variables to a results file.

3.3.3.2 Additional Commands

The `ACTIVE PERIODS` or `INACTIVE PERIODS` command lines can optionally appear in the `MASS SCALING` command block:

```
ACTIVE PERIODS = <string list>periods
INACTIVE PERIODS = <string list>periods
```

These command lines determine when mass scaling is active. See Section 2.5 for more information about these command lines.

3.4 Explicit Control Modes

Presto provides an algorithm known as "explicit control modes" that uses a coarse mesh overlaying the actual problem mesh, referred to as the reference mesh. The name "control modes" comes from the implicit multigrid solution algorithm in Adagio with that name. The explicit control modes algorithm uses the coarse and reference meshes together to enable a potentially significant increase in the critical time step in explicit dynamic calculations. Reference 3 provides an in-depth discussion of this algorithm.

Warning: Explicit Control Modes is a new and experimental analysis technique. While it has been shown to be an extremely useful technique on some problems, it has not undergone rigorous testing. It also does not interoperate with some features, such as rigid bodies.

In the explicit dynamic algorithm, the nodal accelerations are computed by dividing the residual (external force minus internal force) by the nodal mass. In the explicit control modes algorithm, the reference mesh residual is mapped to the coarse mesh, and accelerations are computed on the coarse mesh. These accelerations are then interpolated back to the reference mesh. The portion of the residual with higher frequency content that cannot be represented by the basis functions of the coarse mesh is left on the reference mesh, and is used to compute an acceleration that is added to the acceleration that is interpolated from the coarse mesh.

By computing the acceleration on the coarse mesh, the explicit control modes algorithm allows for the critical time step to be computed based on the size of the coarse mesh rather than the size of the reference mesh. A critical time step is estimated based on the coarse mesh, and mass scaling is applied to the high frequency component of the acceleration that is computed on the reference

mesh. While some error is introduced due to this mass scaling, this error only applies to the high frequency part of the response, which is often well beyond the frequency range of interest. This is in contrast to traditional mass scaling, which affects the full spectrum of structural response.

The choice of the degree of refinement in the coarse and reference meshes has a large influence on the effectiveness of the explicit control modes algorithm. The reference mesh should be created to give a discretization that is appropriate to capture the geometry of the problem with sufficient refinement to adequately represent gradients in the discretized solution. The coarse mesh should completely overlay the reference mesh, and it should be coarser than the reference mesh at every location in the model. All coarse elements need not contain elements in the reference mesh, so it is possible to use a coarse mesh that extends significantly beyond the domain of the reference mesh.

To maximize solution efficiency by increasing the critical time step, the coarse mesh should be significantly coarser than the reference mesh. The code user has the freedom to create a coarse mesh that gives an acceptable critical time step without using an excessively crude discretization. It is important to remember that the reference mesh controls the spatial discretization, while the coarse mesh controls the temporal discretization of the model.

To use explicit control modes, the user should set up the reference mesh file and the input file as usual, except that the following additional items must be provided:

- A coarse mesh must be generated, as discussed above. The coarse mesh must be in a separate file from the reference mesh, which is the real model.
- A second `FINITE ELEMENT MODEL` command block must be provided in addition to the standard definition for the reference finite element model in the input file. This command block is set up exactly as it normally would be (see Section 5.1), except that the mesh file referenced is the coarse mesh instead of the reference mesh. Although the coarse mesh does not use any material models, each block in the coarse mesh must still be assigned a material model.
- A `CONTROL MODES REGION` command block must appear alongside the standard `PRESTO REGION` command block within the `PRESTO PROCEDURE` command block. The presence of the `CONTROL MODES REGION` command block instructs Presto to use the explicit control modes algorithm. The `CONTROL MODES REGION` command block is documented in Section 3.4.1. It contains the same commands used within the standard `PRESTO REGION` command block, except that the commands in the `CONTROL MODES REGION` command block are used to control the control modes algorithm and the boundary conditions on the coarse mesh.

3.4.1 Control Modes Region

```
BEGIN CONTROL MODES REGION
  #
  # model setup
  USE FINITE ELEMENT MODEL <string>model_name
  CONTROL BLOCKS [WITH <string>coarse_block] =
```

```
    <string list>control_blocks
  #
  # time step control
  TIME STEP RATIO SCALING = <real>cm_time_scale(1.0)
  TIME STEP RATIO FUNCTION = <string>cm_time_func
  LANCZOS TIME STEP INTERVAL = <integer>lanczos_interval
  POWER METHOD TIME STEP INTERVAL = <integer>pm_interval
  #
  # mass scaling
  HIGH FREQUENCY MASS SCALING = <real>cm_mass_scale(1.0)
  #
  # stiffness damping
  HIGH FREQUENCY STIFFNESS DAMPING COEFFICIENT =
    <real>cm_stiff_damp(0.0)
  #
  # kinematic boundary condition commands
  BEGIN FIXED DISPLACEMENT
    #
    # Parameters for fixed displacement
    #
  END [FIXED DISPLACEMENT]
  #
  # output commands
  BEGIN RESULTS OUTPUT <string> results_name
    #
    # Parameters for results output
    #
  END RESULTS OUTPUT <string> results_name
END [CONTROL MODES REGION]
```

The `CONTROL MODES REGION` command block controls the behavior of the control modes algorithm, and is placed alongside a standard `PRESTO REGION` command block within the `PRESTO PROCEDURE` scope. With the exception of the `CONTROL BLOCKS` command line, all the commands that can be used in this block are standard commands that appear in the Presto region. These commands have the same meaning in either context; they simply apply to the coarse mesh or to the reference mesh, depending on the region block in which they appear. Sections 3.4.1.1 through 3.4.1.3 describe the components of the `CONTROL MODES REGION` command block.

3.4.1.1 Model Setup Commands

```
USE FINITE ELEMENT MODEL <string>model_name
CONTROL BLOCKS [WITH <string>coarse_block] =
  <string list>control_blocks
```

The command lines listed above must appear in the `CONTROL MODES REGION` command block if explicit control modes is used. The `USE FINITE ELEMENT MODEL` command line should refer-

ence the finite element model for the coarse mesh. This command line is used in the same way that the command line is used for the reference mesh (see Section 2.3).

The `CONTROL BLOCKS` command line provides a list of blocks in the reference mesh that will be controlled by the coarse mesh. The block names are listed using the standard method of referencing mesh entities (see Section 1.5). For example, the block with an ID of 1 would be listed as `block_1` in this command. Multiple `CONTROL BLOCKS` command lines may be used.

The `CONTROL BLOCKS` command line does not require the coarse blocks used to control the fine blocks to be listed. In the following example, blocks 10 and 11 are controlled by the coarse mesh, but the element blocks in the coarse mesh that control those blocks are not listed:

```
CONTROL BLOCKS = block_10 block_11
```

If the `CONTROL BLOCKS` command line is used in this manner, the search for fine nodes contained within coarse elements will be conducted for all elements in the coarse mesh. The coarse block used to control a given set of fine blocks can optionally be specified by using the `CONTROL BLOCKS WITH coarse_block` variant of the command. For example, the command:

```
CONTROL BLOCKS WITH block_1 = block_10 block_11
```

would use block 1 on the coarse mesh to control blocks 10 and 11 on the fine mesh. This variant of the command is necessary when the coarse blocks overlap. It removes any ambiguity about which coarse elements control which fine nodes. This is particularly useful for contact problems where the fine block on one side of an interface should be controlled by one block, and the fine block on the other side of the interface should be controlled by a different block. Only one coarse block can be listed in a given instance of this command, so if there are multiple coarse blocks, they must be listed in separate commands.

3.4.1.2 Time Step Control Commands

```
TIME STEP RATIO SCALING = <real>cm_time_scale(1.0)
TIME STEP RATIO FUNCTION = <string>cm_time_func
LANCZOS TIME STEP INTERVAL = <integer>lanczos_interval
POWER METHOD TIME STEP INTERVAL = <integer>pm_interval
```

The control modes algorithm computes a node-based time step for the coarse mesh at each time step, and uses this as the default time step. This time step is typically much larger than the critical time step for the fine mesh.

The `TIME STEP RATIO SCALING` and `TIME STEP RATIO FUNCTION` command lines allow the user to control the time step used with explicit control modes. The `TIME STEP RATIO SCALING` command is used to specify a scale factor `cm_time_scale`, which has a default value of 1.0. The `TIME STEP RATIO FUNCTION` command is used to specify a function `cm_time_func` that is used to control the scale factor as a function of time. At any given time, a scale factor, f_{ts}, is computed by multiplying `cm_time_scale` by the current value of the function. Both of these commands are optional and one can be used without the other.

The time step Δt, is computed as a function of f_{ts}, as well as of the time step of the fine mesh, Δt_f

and the time step of the coarse mesh, Δt_c.

$$\Delta t = \Delta t_f + f_{ts}(\Delta t_c - \Delta t_f) \tag{3.24}$$

Thus, if the scale factor is zero, the time step of the fine mesh is used, and if it is one, the time step of the coarse mesh is used.

The nodal time step estimator for the coarse mesh typically works well on problems where the fine mesh overlaid by the coarse mesh is essentially isotropic. In cases where it is not, such as when there are significant voids covered by the coarse mesh, the nodal time step can be non-conservative, resulting in stability problems. The time step control command lines described above can be used to manually scale down the time step in such scenarios.

Alternatively, the Lanczos or power method global time step estimators can be applied to the coarse mesh to give an improved estimate of the stability limit. These are invoked using the `LANCZOS TIME STEP INTERVAL` or `POWER METHOD TIME STEP INTERVAL` command lines, respectively. Only one of these command lines can be used at a time, and both commands specify an interval at which the global time step estimate is calculated. When the global time step estimate is calculated, a ratio of the global estimate to the nodal estimate is calculated, and this ratio is used to scale the nodal estimate in subsequent time steps in which the global estimate is not computed.

Experience has shown that the time step predicted by the global time step estimators is typically slightly higher than the actual stability limit. For this reason, it is recommended that a scale factor of 0.9 be used in conjunction with these estimators. This can be set using the `TIME STEP SCALE FACTOR` command line in the `TIME CONTROL` block as described in Section 3.1.

Known Issue: The Lanczos and power method time step estimators can not yet be used with problems that have contact, rigid bodies, blocks in the fine mesh that are not controlled by the coarse mesh, or coarse elements that contain no fine nodes.

3.4.1.3 Mass Scaling Commands

```
HIGH FREQUENCY MASS SCALING = <real>cm_mass_scale(1.0)
```

The `HIGH FREQUENCY MASS SCALING` command line allows the user to control the mass scaling applied to the high frequency component of the response. The mass scaling factor required to stably integrate the high frequency response at the time step being used is computed at every node on the fine mesh. The parameter `cm_mass_scale` that can optionally be supplied with this command line is applied as a multiplier to that mass scaling. If that mass scaling (multiplied by `cm_mass_scale`) is greater than 1.0, then the scaled mass is used at that node. If not, the original nodal mass is used.

It may be useful for some models to use this command line to set `cm_mass_scale` to a value greater than 1.0 to stabilize the high frequency response. Experience has shown, however, that this is rarely needed, so it is recommended that this command line not be used in most cases.

3.4.1.4 Damping Commands

```
HIGH FREQUENCY STIFFNESS DAMPING COEFFICIENT =
  <real>cm_stiff_damp(0.0)
```

The `HIGH FREQUENCY STIFFNESS DAMPING COEFFICIENT` command is used to apply stiffness-proportional damping on the high frequency portion of the response in explicit control modes. This may help reduce high frequency noise in problems that have abrupt loading such as that caused by contact. The default value of `cm_stiff_damp` is 0.0. The value specified for `cm_stiff_damp` can be between 0 and 1. It is recommended that small values (around 0.001) be specified if this option is used.

3.4.1.5 Kinematic Boundary Condition Commands

```
BEGIN FIXED DISPLACEMENT
  #
  # Parameters for fixed displacement
  #
END FIXED DISPLACEMENT
```

All types of kinematic boundary conditions can be applied to the coarse mesh. This is done by inserting a kinematic boundary condition command block in the `CONTROL MODES REGION` command block. The mesh entity (node set, surface, or block) to which the boundary condition is applied must exist on the coarse mesh.

This capability is potentially useful to ensure better enforcement of kinematic boundary conditions on the fine mesh by applying the same type of boundary condition on the portion of the coarse mesh that overlays the portion of the fine mesh to which boundary conditions are applied. For example, if there is a node set on the fine mesh that has a fixed displacement boundary condition, a node set can be created on the coarse mesh that covers the same physical domain. The same fixed displacement boundary condition could then be applied to the coarse mesh.

Although the capability to enforce boundary conditions on the coarse mesh is provided, it is not necessary to do so. It is also often very difficult to create a node set on the coarse mesh that matches the discretization of the node set on the fine mesh. Users are advised to initially prescribe kinematic boundary conditions only on the fine mesh and only prescribe boundary conditions on the coarse if the initial results appear questionable.

3.4.1.6 Output Commands

```
BEGIN RESULTS OUTPUT <string> results_name
  #
  # Parameters for results output
  #
END RESULTS OUTPUT <string> results_name
```

Variables can be output from the coarse mesh just as they can from the fine mesh with explicit control modes. Because the actual results of interest for the model all reside on the fine mesh, it is typically not necessary to output results on the coarse mesh, but this can be helpful for debugging purposes.

The syntax for the results output for the coarse mesh is identical to that used for output from the fine mesh, and is documented in Section 8.2. The only thing that differentiates the `RESULTS OUTPUT` command block for the coarse mesh from that of the fine mesh is that the results output block for the coarse mesh is put in the `CONTROL MODES REGION` command block instead of in the `PRESTO REGION` command block. The output files for the coarse and fine mesh must be different from each other, so different output file names must be used within the output blocks for the coarse and fine meshes.

One of the most useful variables to output from the coarse mesh is the nodal `timestep`. This variable is similar in nature to the element `timestep`, which exists on the fine mesh, but is a nodal rather than an element variable, and exists on the coarse mesh. It reports the critical time step calculated for each node on the coarse mesh. If the coarse time step is higher than expected, the output from `nodal_time_step` can be examined to see which region of the coarse mesh is controlling the time step.

Central difference time integration is performed on the coarse mesh in addition to the fine mesh, so the `displacement`, `velocity`, and `acceleration` variables can be requested for visualization on the coarse mesh.

3.5 References

1. Hughes, T. J. R. *The Finite Element Method:Linear Static and Dynamic Finite Element Analysis*. Englewood Cliffs, NJ: Prentice-Hall, Inc., 1987.

2. Golub, G. H., and C. F. Van Loan *Matrix Computations, Third Edition*. Baltimore, MD: The John Hopkins University Press, 1996.

3. Spencer, B. W., M. W. Heinstein, J. D. Hales, K. H. Pierson and J. R. Overfelt. *Multi-Length Scale Algorithms for Failure Modeling in Solid Mechanics*, SAND2008-6499. Albuquerque, NM: Sandia National Laboratories, October 2008.

Chapter 4

Materials

This chapter describes material models that can be used in conjunction with the elements in Presto and Adagio. Most of the material models have an interface that allows them to be used by the elements in both codes. Even though a material model can be used by both codes, usage of the model may be better suited for the type of problems solved by one code rather than the type of problems solved by the other code. For example, a material model that was built to characterize behavior over a long time would be better suited for use in Adagio than in Presto. If a particular material model is better suited for one code rather than the other, this usage information is provided in the description of that model.

The material models described in this chapter are, in general, applicable to solid elements. The structural elements, such as shells and beams, have a much more limited set of material models. Chapter 5 describes the element library, including which material models are available for the various elements. The introduction to Chapter 5 summarizes all the element types in Presto and Adagio. For each element type, a list of available material models is provided.

When using the nonlinear material models, you may want to output state variables that are associated with these models. See Section 8.9.2 to learn how to output the state variables for the various nonlinear material models.

Most material models for solid elements are available in two libraries. The newer library is the LAME library [17], but it is not the default. The line command to activate the LAME material library for a particular section is described in Section 5.2.1.

General Model Form. `PROPERTY SPECIFICATION FOR MATERIAL` command blocks appear in the SIERRA scope in the general form shown below.

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  #
  # Command lines and command blocks for material
  # models appear in this scope.
  #
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

PROPERTY SPECIFICATION FOR MATERIAL command blocks are physics independent in the sense that the information in them can be shared by more than one application. For example, some of the PROPERTY SPECIFICATION FOR MATERIAL command blocks contain density information that can be shared among several applications.

The command block begins with the line:

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
```

and terminates with the line:

```
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

Here, the string mat_name is a user-specified name for the command block. This name is typically descriptive of the material being modeled, e.g., aluminum_t6061.

Within a PROPERTY SPECIFICATION FOR MATERIAL command block, there will be other command blocks and possibly other general material command lines that are used to describe particular material models. The general material command lines, if present, are listed first, followed by one or more material-model command blocks. The general material command lines may be used to specify the density of the material, the Biot's coefficient, and the application of temperatures and thermal strains to two- or three-dimensional elements. Each material-model command block follows the naming convention of PARAMETERS FOR MODEL model_name, where model_name identifies a particular material model, such as elastic, elastic-plastic, or orthotropic crush. Each such command block contains all the parameters needed to describe a particular material model.

As noted above, more than one material-model command block can appear within a PROPERTY SPECIFICATION FOR MATERIAL command block. Suppose we have a PROPERTY SPECIFICATION FOR MATERIAL command block called steel. It would be possible to have two material-model command blocks within this command block. One of the material-model command blocks would provide an elastic model for steel; the other material-model command block would provide an elastic-plastic model for steel. The general form of a PROPERTY SPECIFICATION FOR MATERIAL command block would be as follows:

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  #
  # General material command lines
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_coefficient_value
  #
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL <string>model_name1
    #
    # Parameters for material model model_name1
  END PARAMETERS FOR MODEL <string>model_name1
  #
  BEGIN PARAMETERS FOR MODEL <string> model_name2
    #
    # Parameters for material model model_name2
  END PARAMETERS FOR MODEL <string> model_name2
  #
  # Additional model command blocks if required
  #
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

In the above general form for a `PROPERTY SPECIFICATION FOR MATERIAL` command block, the string `model_name1` could be `ELASTIC` and the string `model_name2` could be `ORTHOTROPIC CRUSH`. Typically, however, only one material model would be desired for a given block, and the `PROPERTY SPECIFICATION FOR MATERIAL` command block would have only one `PARAMETERS FOR MODEL` command block. A particular material model may only appear once within a given `PROPERTY SPECIFICATION FOR MATERIAL` command block.

Although multiple material models can be defined for one material within a `PROPERTY SPECIFICATION FOR MATERIAL` command block, only one material model is actually used for a given element block during an analysis. The ability to define multiple constitutive models for one material is provided as a convenience to enable the user to easily switch between models. The material name and the model name are both referenced when material models are assigned to element blocks within the `FINITE ELEMENT MODEL` command block, which is described in Section 5.1.

This chapter is organized to correspond to the general form presented for the `PROPERTY SPECIFICATION FOR MATERIAL` command block. Section 4.1 discusses the `DENSITY` command line, the `BIOTS COEFFICIENT` command line, and the command lines used for thermal strains, and also explains how temperatures and thermal strains are applied. Section 4.2 describes each of the material models that are shared by Presto and Adagio. References applicable for both

Presto and Adagio are listed in Section 4.4.

As indicated in the introductory material, not all the material models available are applicable to all the element types. As one example, there is a one-dimensional elastic material model that is used for a truss element but is not applicable to solid elements such as hexahedra or tetrahedra. For this particular example, the specific material-model usage is hidden from the user. If the user specifies a linear elastic material model for a truss, the one-dimensional elastic material model is used. If the user specifies a linear elastic material model for a hexahedron, a full three-dimensional elastic material model is used. As another example, the energy-dependent material models available in Presto cannot be used for a one-dimensional element such as a truss. The energy-dependent material models can only be used for solid elements such as hexahedra and tetrahedra. (Chapter 5 indicates what material models are available for which element models.)

For each material model, the parameters needed to describe that model are listed in the section pertinent to that particular model. Solid models with elastic constants require only two elastic constants. These two constants are then used to generate all the elastic constants for the model. For example, if the user specifies Young's modulus and Poisson's ratio, then the shear modulus, bulk modulus, and lambda are calculated. If the shear modulus and lambda are specified, then Young's modulus, Poisson's ratio, and the bulk modulus are calculated.

The various nonlinear material models have state variables. See Section 8.9.2 to learn how to output the state variables for the nonlinear material models.

Note that only brief descriptions of the material models are presented in this chapter. For a detailed description of the various material models, you will need to consult a variety of references. Specific references are identified for most of the material models shared by Presto and Adagio.

4.1 General Material Commands

A PROPERTY SPECIFICATION FOR MATERIAL command block for a particular material may include additional command lines that are applicable to all the material models specified within the command block. These command lines related to density, to Biot's coefficient, and to thermal strain behavior are discussed, respectively, in Section 4.1.1, Section 4.1.2, and Section 4.1.3.

4.1.1 Density Command

```
DENSITY = <real>density_value
```

This command line specifies the density of the material described in a PROPERTY SPECIFICATION FOR MATERIAL command block. The units of the input parameter density_value are specified as mass per unit volume.

As previously explained, a PROPERTY SPECIFICATION FOR MATERIAL command block can contain one or more PARAMETERS FOR MODEL command blocks. The specified density_value for the material will be used with all of the models described in these PARAMETERS FOR MODEL command blocks.

4.1.2 Biot's Coefficient Command

```
BIOTS COEFFICIENT = <real>biots_value
```

This command line specifies the Biot's coefficient of the material. Biot's coefficient is used with the pore pressure capability. See Section 6.8 for more information on pore pressure. If not given, the value defaults to 1.0. This parameter is unitless.

As previously explained, a PROPERTY SPECIFICATION FOR MATERIAL command block can contain one or more PARAMETERS FOR MODEL command blocks. The specified biots_value for the material will be used with all of the models described in these PARAMETERS FOR MODEL command blocks.

4.1.3 Thermal Strain Behavior

Isotropic and orthotropic thermal strains may be defined for use by material models listed in a PROPERTY SPECIFICATION FOR MATERIAL command block. Section 4.1.3.1 describes the command lines that are used to define the thermal strain behavior. These command lines must be used in conjunction with other command blocks outside of a PROPERTY SPECIFICATION FOR MATERIAL command block for the calculations of thermal strains to be activated. Section 4.1.3.2 explains the process for activating thermal strains.

4.1.3.1 Defining Thermal Strains

```
THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION =
  <string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
  <string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
  <string>thermal_strain_z_function
```

A `PROPERTY SPECIFICATION FOR MATERIAL` command block may include command lines that define thermal strain behavior. It is possible to specify either an isotropic thermal-strain field using the command line `THERMAL STRAIN FUNCTION` or an orthotropic thermal-strain field using the command lines `THERMAL STRAIN X FUNCTION`, `THERMAL STRAIN Y FUNCTION`, and `THERMAL STRAIN Z FUNCTION`. For any of these command lines, the user supplies a thermal strain function (via a `DEFINITION FOR FUNCTION` command block), which defines the thermal strain as a function of temperature. The computed thermal strain is then subtracted from the strain passed to the material model.

A thermal strain can be applied to any two-dimensional or three-dimensional element, regardless of material type. For a three-dimensional element such as a hexahedron or tetrahedron, the thermal strains are applied to the strain in the global XYZ coordinate system. For the isotropic case, the thermal strains are the same in the X-direction, the Y-direction, and the Z-direction. For the anisotropic case, the thermal strains can be different in each of the three global directions—X, Y, and Z. For a two-dimensional element, shell or membrane, the thermal strain corresponding to the `THERMAL STRAIN X FUNCTION` command line is applied to the strain in the shell (or membrane) r-direction. (Reference Section 5.2.4 for a discussion of the shell rst coordinate system.) The thermal strain corresponding to the `THERMAL STRAIN Y FUNCTION` command line is applied to the strain in the shell (or membrane) s-direction. For two-dimensional elements, the current implementation of orthotropic thermal strains is limited, for practical purposes, to special cases—flat sheets of uniform shell elements lying in one of the global planes, e.g., XY, YZ, or ZX. The current orthotropic thermal-strain capability has limited use for shells and membranes in the current release of the code. Tying the orthotropic thermal-strain functionality to the shell orientation functionality (Section 5.2.4) in the future will provide much more useful orthotropic thermal-strain functionality for two-dimensional elements.

If an isotropic thermal-strain field is to be applied, the `THERMAL STRAIN FUNCTION` command line is placed in the `PROPERTY SPECIFICATION FOR MATERIAL` command block, outside of the specifications of any material models in the block. Such placement is necessary because the isotropic thermal strain is a general material property, not a property that is specific to any particular constitutive model, such as `ELASTIC` or `ELASTIC-PLASTIC`. The input value of `thermal_strain_function` is the name of the function that defines thermal strain as a function of temperature for the material model described in this particular `PROPERTY SPECIFICATION FOR MATERIAL` command block. The function is defined within the SIERRA scope using a `DEFINITION FOR FUNCTION` command block. For more information on how to set the input to compute thermal strains and how to apply temperatures, see Section 4.1.3.2.

The specification of an orthotropic thermal-strain field requires that all three of the `THERMAL STRAIN X FUNCTION`, `THERMAL STRAIN Y FUNCTION`, and `THERMAL STRAIN Z FUNCTION` command lines be placed in the `PROPERTY SPECIFICATION FOR MATERIAL` command block. All three command lines must be provided, even when there is no thermal strain in one or more directions. The values of `thermal_strain_x_function`, `thermal_strain_y_function`, and `thermal_strain_z_function` are the names of the functions for thermal strains in the X-direction, the Y-direction, and the Z-direction, respectively. These functions are defined within the SIERRA scope using `DEFINITION FOR FUNCTION` command blocks. To specify that there should be no thermal strain in a given direction, use a function that always evaluates to zero for that direction.

The `THERMAL STRAIN FUNCTION` command line and the `THERMAL STRAIN X FUNCTION`, `THERMAL STRAIN Y FUNCTION`, and `THERMAL STRAIN Z FUNCTION` command lines are not used for several of the material models, as discussed in Section 4.1.3.2. Note that specification of a thermal strain is identified in the descriptions of the material models in Section 4.2 by the notation "`thermal strain option`".

4.1.3.2 Activating Thermal Strains

Presto has the capability to compute thermal strains on three-dimensional continuum and two-dimensional (shell, membrane) elements. Three things are required to activate thermal strains:

- First, one or more thermal strain functions (strain as a function of temperature) must be defined. Each thermal strain function is defined with a `DEFINITION FOR FUNCTION` command block. (This function is the standard function definition that appears in the SIERRA scope.) The thermal strain function gives the total thermal strain associated with a given temperature. It is the change in thermal strain with the change in temperature that gives rise to thermal stresses in a body.

- Second, the material models used by blocks that experience thermal strain must have their thermal strain behavior defined. The command lines for defining isotropic and orthotropic thermal strain are described in Section 4.1.3.1. Materials with isotropic thermal strain use the `THERMAL STRAIN FUNCTION` command line, while those with orthotropic thermal strain must define thermal strain in all three directions using the `THERMAL STRAIN X FUNCTION`, `THERMAL STRAIN Y FUNCTION`, and `THERMAL STRAIN Z FUNCTION` command lines. These inputs can be used with all material models with the exception of the following: elastic three-dimensional orthotropic, elastic laminate, Mooney-Rivlin, NLVE three-dimensional orthotropic, Swanson, and viscoelastic Swanson. These models require their own model-specific inputs to define thermal strain and must not use these standard commands. Information for defining thermal strains is provided in the individual descriptions of these models in Section 4.2.

- Third, a temperature field must be applied to the affected blocks. The command block to specify the application of temperatures is `PRESCRIBED TEMPERATURE`, which is implemented as a standard boundary condition. A description of the `PRESCRIBED TEMPERATURE` command block is given in Section 6.7.

Whenever a temperature field is applied, the temperature is prescribed at the nodes, but thermal strain is computed based on element temperature. Element temperatures are obtained by averaging the temperatures of the nodes connected to a given element. Thermal strains are applied in rate form, so the thermal strain in an element is relative to the thermal strain at the initial temperature. Thus, the initial temperature is the stress-free temperature. If desired, a different stress-free temperature can be used by prescribing the initial temperature with the `INITIAL CONDITION` command block as described in Section 6.2.

4.2 Material Models

This section contains descriptions of the material models that are shared by Presto and Adagio.

4.2.1 Elastic Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL ELASTIC
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
  END [PARAMETERS FOR MODEL ELASTIC]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

An elastic material model is used to describe simple linear elastic behavior of materials. This model is generally valid for small deformations.

The command block for an elastic material starts with the line:

```
BEGIN PARAMETERS FOR MODEL ELASTIC
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL ELASTIC]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.
- The Biot's coefficient of the material is defined with the `BIOTS COEFFICIENT` command line.

- The `thermal strain option` is used to define thermal strains. See Section 4.1.3.1 and Section 4.1.3.2 for further information on defining and activating thermal strains.
- Any two of the following elastic constants are required:
  - Young's modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson's ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.

There are no output variables available for the elastic model. For information about the elastic model, consult Reference 1.

4.2.2 Thermoelastic Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL THERMOELASTIC
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    YOUNGS MODULUS FUNCTION = <string>ym_function_name
    POISSONS RATIO FUNCTION = <string>pr_function_name
  END [PARAMETERS FOR MODEL THERMOELASTIC]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The thermoelastic material model is used to describe the temperature-dependent linear elastic behavior of materials. This model is generally valid for small deformations.

The command block for a thermoelastic material starts with the line:

```
BEGIN PARAMETERS FOR MODEL THERMOELASTIC
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL THERMOELASTIC]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.
- The Biot's coefficient of the material is defined with the `BIOTS COEFFICIENT` command line.
- The `thermal strain option` is used to define thermal strains. See Section 4.1.3.1 and Section 4.1.3.2 for further information on defining and activating thermal strains.

- Any two of the following elastic constants are required:
    - Young's modulus is defined with the `YOUNGS MODULUS` command line.
    - Poisson's ratio is defined with the `POISSONS RATIO` command line.
    - The bulk modulus is defined with the `BULK MODULUS` command line.
    - The shear modulus is defined with the `SHEAR MODULUS` command line.
    - Lambda is defined with the `LAMBDA` command line.
- The `YOUNGS MODULUS FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope that describes a scale factor on Young's modulus as a function of temperature.
- The `POISSONS RATIO FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope that describes a scale factor on Poisson's ratio as a function of temperature.

There are no output variables available for the thermoelastic model. For information about the thermoelastic model, consult Reference 1.

4.2.3 Neo-Hookean Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL NEO_HOOKEAN
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
  END [PARAMETERS FOR MODEL NEO_HOOKEAN]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The neo-Hookean material model is used to describe linear elastic behavior of materials. Unlike the elastic model, this model is valid for both large and small deformations. The neo-Hookean model uses a strain energy density, which makes it a hyperelastic constitutive model. This feature makes it applicable to finite strains. Currently the neo-Hookean model, as implemented in LAME, does not support thermal strains.

The command block for a neo-Hookean material starts with the line:

```
BEGIN PARAMETERS FOR MODEL NEO_HOOKEAN
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL NEO_HOOKEAN]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.
- The Biot's coefficient of the material is defined with the `BIOTS COEFFICIENT` command line.

- The `thermal strain option` is used to define thermal strains. See Section 4.1.3.1 and Section 4.1.3.2 for further information on defining and activating thermal strains.

- Any two of the following elastic constants are required:

  - Young's modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson's ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.

There are no output variables available for the neo-Hookean model. For information about the neo-Hookean model, consult Reference 5.

4.2.4 Elastic Fracture Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL ELASTIC_FRACTURE
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    MAX STRESS = <real>max_stress
    CRITICAL CRACK OPENING STRAIN = <real>critical_strain
  END [PARAMETERS FOR MODEL ELASTIC_FRACTURE]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

An elastic fracture material is a simple failure model that is based on linear elastic behavior. The model uses a maximum-principal-stress failure criterion. The stress decays isotropically based on the component of strain parallel to the maximum principal stress. The value of the component of strain over which the stress is decayed to zero is a user-defined parameter for the model. This strain parameter can be adjusted so that failure is mesh independent.

The command block for an elastic fracture material starts with the line:

```
BEGIN PARAMETERS FOR MODEL ELASTIC_FRACTURE
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL ELASTIC_FRACTURE]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.
- The Biot's coefficient of the material is defined with the `BIOTS COEFFICIENT` command line.

- The `thermal strain option` is used to define thermal strains. See Section 4.1.3.1 and Section 4.1.3.2 for further information on defining and activating thermal strains.
- Any two of the following elastic constants are required:
  - Young's modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson's ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.
- The maximum principal stress at which failure occurs is defined with the `MAX STRESS` command line.
- The component of strain over which the stress decays to zero is defined with the `CRITICAL CRACK OPENING STRAIN` command line. This component of strain is aligned with the maximum-principal-stress direction at failure.

Output variables available for this model are listed in Table 8.20.

4.2.5 Elastic-Plastic Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL ELASTIC_PLASTIC
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    YIELD STRESS = <real>yield_stress
    HARDENING MODULUS = <real>hardening_modulus
    BETA = <real>beta_parameter(1.0)
  END [PARAMETERS FOR MODEL ELASTIC_PLASTIC]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The elastic-plastic linear hardening models are used to model materials, typically metals, that undergoing plastic deformation at finite strains. Linear hardening generally refers to the shape of a uniaxial stress-strain curve where the stress increases linearly with the plastic, or permanent, strain. In a three-dimensional framework, hardening is the law that governs how the yield surface grows in stress space. If the yield surface grows uniformly in stress space, the hardening is referred to as isotropic hardening. When `BETA` is 1.0, we have only isotropic hardening.

Because the linear hardening model is relatively simple to integrate, the model also has the ability to define a yield surface that not only grows, or hardens, but also moves in stress space. This ability is known as kinematic hardening. When `BETA` is 0.0, we have only kinematic hardening. The elastic-plastic linear hardening model allows for isotropic hardening, kinematic hardening, or a combination of the two.

The command block for an elastic-plastic material starts with the line:

```
BEGIN PARAMETERS FOR MODEL ELASTIC_PLASTIC
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL ELASTIC_PLASTIC]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.
- The Biot's coefficient of the material is defined with the `BIOTS COEFFICIENT` command line.
- The `thermal strain option` is used to define thermal strains. See Section 4.1.3.1 and Section 4.1.3.2 for further information on defining and activating thermal strains.
- Any two of the following elastic constants are required:
  - Young's modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson's ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.
- The yield stress is defined with the `YIELD STRESS` command line.
- The hardening modulus is defined with the `HARDENING MODULUS` command line.
- The beta parameter is defined with the `BETA command` line.

Output variables available for this model are listed in Table 8.21. For information about the elastic-plastic model, consult Reference 1.

4.2.6 Elastic-Plastic Power-Law Hardening Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL EP_POWER_HARD
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    YIELD STRESS = <real>yield_stress
    HARDENING CONSTANT = <real>hardening_constant
    HARDENING EXPONENT = <real>hardening_exponent
    LUDERS STRAIN = <real>luders_strain
  END [PARAMETERS FOR MODEL EP_POWER_HARD]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

A power-law hardening model for elastic-plastic materials is used for modeling metal plasticity up to finite strains. The power-law hardening model, as opposed to the linear hardening model, has a power law fit for the uniaxial stress-strain curve that has the stress increase as the plastic strain raised to some power. The power-law hardening model also has the ability to model materials that exhibit Luder's strains after yield. Due to the more complicated yield behavior, the power-law hardening model can only be used with isotropic hardening.

The command block for an elastic-plastic power-law hardening material starts with the line:

```
BEGIN PARAMETERS FOR MODEL EP_POWER_HARD
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL EP_POWER_HARD]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.

- The Biot's coefficient of the material is defined with the `BIOTS COEFFICIENT` command line.
- The `thermal strain option` is used to define thermal strains. See Section 4.1.3.1 and Section 4.1.3.2 for further information on specifying and applying thermal strains and temperatures.
- Any two of the following elastic constants are required:
  - Young's modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson's ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.
- The yield stress is defined with the `YIELD STRESS` command line.
- The hardening constant is defined with the `HARDENING CONSTANT` command line.
- The hardening exponent is defined with the `HARDENING EXPONENT` command line.
- The Luder's strain is defined with the `LUDERS STRAIN` command line.

Output variables available for this model are listed in Table 8.22. For information about the elastic-plastic power-law hardening model, consult Reference 1.

4.2.7 Ductile Fracture Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL DUCTILE_FRACTURE
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    YIELD STRESS = <real>yield_stress
    HARDENING CONSTANT = <real>hardening_constant
    HARDENING EXPONENT = <real>hardening_exponent
    LUDERS STRAIN <real>luders_strain
    CRITICAL TEARING PARAMETER = <real>crit_tearing
    CRITICAL CRACK OPENING STRAIN = <real>critical_strain
  END [PARAMETERS FOR MODEL DUCTILE_FRACTURE]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

This model is identical to the elastic-plastic power-law hardening model with the addition of a failure criterion and a post-failure isotropic decay of the stress to zero within the constitutive model. The point at which failure occurs is defined by a critical tearing parameter. The critical tearing parameter t_p is related to the plastic strain at failure ε_f by the evolution integral

$$t_p = \int_0^{\varepsilon_f} \langle \frac{2\sigma_{\max}}{3\,(\sigma_{\max} - \sigma_m)} \rangle^4 \, d\varepsilon_p \,. \tag{4.1}$$

In Equation (4.1), $\sigma_{\max}$ is the maximum principal stress, and σ_m is the mean stress. The quantity in the angle brackets, the expression

$$\frac{2\sigma_{\max}}{3\,(\sigma_{\max} - \sigma_m)} \,, \tag{4.2}$$

is nonzero only if it evaluates to a positive value. This quantity is set to zero if it has a negative value.

The stress decays isotropically based on the component of strain parallel to the maximum principal stress. The value of the component of strain over which the stress is decayed to zero is a user-defined parameter for the model. This strain parameter can be adjusted so that failure is mesh independent.

The command block for an elastic-plastic power-law hardening material with failure starts with the line:

```
BEGIN PARAMETERS FOR MODEL DUCTILE_FRACTURE
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL DUCTILE_FRACTURE]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.
- The Biot's coefficient of the material is defined with the `BIOTS COEFFICIENT` command line.
- The `thermal strain option` is used to define thermal strains. See Section 4.1.3.1 and Section 4.1.3.2 for further information on defining and activating thermal strains and temperatures.
- Any two of the following elastic constants are required:
  - Young's modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson's ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.
- The yield stress is defined with the `YIELD STRESS` command line.
- The hardening constant is defined with the `HARDENING CONSTANT` command line.
- The hardening exponent is defined with the `HARDENING EXPONENT` command line.
- The Luder's strain is defined with the `LUDERS STRAIN` command line.
- The critical tearing parameter is defined with the `CRITICAL TEARING PARAMETER` command line.
- The component of strain over which the stress decays to zero is defined with the `CRITICAL CRACK OPENING STRAIN` command line. This component of strain is aligned with the maximum-principal-stress direction at failure.

Output variables available for this model are listed in Table 8.23. For information about the ductile fracture material model, consult Reference 1.

4.2.8 Multilinear Elastic-Plastic Hardening Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL MULTILINEAR_EP
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    YIELD STRESS = <real>yield_stress
    BETA = <real>beta_parameter(1.0)
    HARDENING FUNCTION = <string>hardening_function_name
    YOUNGS MODULUS FUNCTION = <string>ym_function_name
    POISSONS RATIO FUNCTION = <string>pr_function_name
    YIELD STRESS FUNCTION = <string>yield_stress_function_name
  END [PARAMETERS FOR MODEL MULTILINEAR_EP]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

This model is similar to the power-law hardening model except that the hardening behavior is described with a piecewise-linear curve as opposed to a power law.

The command block for a multi-linear elastic-plastic hardening material starts with the line:

```
BEGIN PARAMETERS FOR MODEL MULTILINEAR_EP
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL MULTILINEAR_EP]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.

- The Biot's coefficient of the material is defined with the `BIOTS COEFFICIENT` command line.

- The `thermal strain option` is used to define thermal strains. See Section 4.1.3.1 and Section 4.1.3.2 for further information on defining and activating thermal strains.

- Any two of the following elastic constants are required:

  - Young's modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson's ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.

- The yield stress is defined with the `YIELD STRESS` command line.

- The beta parameter is defined with the `BETA` command line.

- The `HARDENING FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope that describes the hardening behavior of the material as a stress versus equivalent plastic strain. This curve is expressed as the additional increment of stress over the yield stress versus equivalent plastic strain, thus the first point on the curve should be (0.0, 0.0).

- The `YOUNGS MODULUS FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope that describes a scale factor on Young's modulus as a function of temperature.

- The `POISSONS RATIO FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope that describes a scale factor on Poisson's ratio as a function of temperature.

- The `YIELD STRESS FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope that describes a scale factor on the yield stress as a function of temperature.

Output variables available for this model are listed in Table 8.24.

4.2.9 Multilinear Elastic-Plastic Hardening Model with Failure

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL ML_EP_FAIL
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    YIELD STRESS = <real>yield_stress
    BETA = <real>beta_parameter(1.0)
    HARDENING FUNCTION = <string>hardening_function_name
    YOUNGS MODULUS FUNCTION = <string>ym_function_name
    POISSONS RATIO FUNCTION = <string>pr_function_name
    YIELD STRESS FUNCTION = <string>yield_stress_function_name
    CRITICAL TEARING PARAMETER = <real>crit_tearing
    CRITICAL CRACK OPENING STRAIN = <real>critical_strain
  END [PARAMETERS FOR MODEL ML_EP_FAIL]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

This model is similar to the power-law hardening model except that the hardening behavior is described with a piecewise-linear curve as opposed to a power law. This model incorporates a failure criterion and a post-failure isotropic decay of the stress to zero within the constitutive model. The point at which failure occurs is defined by a critical tearing parameter. The critical tearing parameter t_p is related to the plastic strain at failure ε_f by the evolution integral:

$$t_p = \int_0^{\varepsilon_f} \langle \frac{2\sigma_{\max}}{3\,(\sigma_{\max} - \sigma_m)} \rangle^4 \, d\varepsilon_p \,. \tag{4.3}$$

In Equation (4.3), $\sigma_{\max}$ is the maximum principal stress, and σ_m is the mean stress. The quantity in the angle brackets, the expression

$$\frac{2\sigma_{\max}}{3\,(\sigma_{\max} - \sigma_m)} \,, \tag{4.4}$$

is nonzero only if it evaluates to a positive value. This quantity is set to zero if it has a negative value.

The stress decays isotropically based on the component of strain parallel to the maximum principal stress. The value of the component of strain over which the stress is decayed to zero is a user-defined parameter for the model. This strain parameter can be adjusted so that failure is mesh independent.

The command block for a multi-linear elastic-plastic hardening material with failure starts with the line:

```
BEGIN PARAMETERS FOR MODEL ML_EP_FAIL
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL ML_EP_FAIL]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.
- The Biot's coefficient of the material is defined with the `BIOTS COEFFICIENT` command line.
- The `thermal strain option` is used to define thermal strains. See Section 4.1.3.1 and Section 4.1.3.2 for further information on defining and activating thermal strains.
- Any two of the following elastic constants are required:
  - Young's modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson's ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.
- The yield stress is defined with the `YIELD STRESS` command line.
- The beta parameter is defined with the `BETA` command line.
- The `HARDENING FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope that describes the hardening behavior of the material as a stress versus equivalent plastic strain. This curve is expressed as the additional increment of stress over the yield stress versus equivalent plastic strain, thus the first point on the curve should be (0.0, 0.0).

- The `YOUNGS MODULUS FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope that describes a scale factor on Young's modulus as a function of temperature.

- The `POISSONS RATIO FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope that describes a scale factor on Poisson's ratio as a function of temperature.

- The `YIELD STRESS FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope that describes a scale factor on the yield stress as a function of temperature.

- The critical tearing parameter is defined with the `CRITICAL TEARING PARAMETER` command line.

- The component of strain over which the stress decays to zero is defined with the `CRITICAL CRACK OPENING STRAIN` command line. This component of strain is aligned with the maximum-principal-stress direction at failure.

Output variables available for this model are listed in Table 8.25.

4.2.10 Johnson-Cook Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL JOHNSON_COOK
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    YIELD STRESS = <real>yield_stress
    HARDENING CONSTANT = <real>hardening_constant
    HARDENING EXPONENT = <real>hardening_exponent
    RHOCV = <real>rho_cv
    RATE CONSTANT = <real>rate_constant
    THERMAL EXPONENT = <real>thermal_exponent
    REFERENCE TEMPERATURE = <real>reference_temperature
    MELT TEMPERATURE = <real>melt_temperature
  END [PARAMETERS FOR MODEL JOHNSON_COOK]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The Johnson-Cook model is used to model materials, typically metals, undergoing plastic deformation at finite strains. The hardening function is defined by:

$$\sigma = (\sigma_y + B(\bar{\epsilon}_p)^N)(1 + C\ln(e^*))(1 - (T^*)^M)\,, \tag{4.5}$$

where σ_y is the yield stress, B is the hardening constant, $\bar{\epsilon}_p$ is the equivalent plastic strain, N is the hardening exponent, C is the rate constant, e^* is the non-dimensional effective total strain rate, and T^* is the homologous temperature. T^* is defined as:

$$T^* = (T - T_{ref})/(T_{melt} - T_{ref})\,, \tag{4.6}$$

where T is the current temperature, T_{ref} is the reference temperature, and T_{melt} is the melt temperature. In the case where $M <= 0$, $(1 - (T^*)^M) = 1$.

Plastic work results in adiabatic heating. The resulting change in temperature is computed according to the function:

$$\Delta T = \frac{0.95\sigma_y \Delta\bar{\epsilon}_p}{\rho c_v}, \tag{4.7}$$

where ρ is the material density and c_v is the specific heat.

For more information about the Johnson-Cook material model, consult Reference 22.

In the command blocks that define the Johnson-Cook model:

- The density of the material is defined with the `DENSITY` command line.
- The Biot's coefficient of the material is defined with the `BIOTS COEFFICIENT` command line.
- The `thermal strain option` is used to define thermal strains. See Section 4.1.3.1 and Section 4.1.3.2 for further information on defining and activating thermal strains.
- Any two of the following elastic constants are required:
  - Young's modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson's ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.
- The yield stress is defined with the `YIELD STRESS` command line.
- The hardening constant is defined with the `HARDENING CONSTANT` command line.
- The hardening exponent is defined with the `HARDENING EXPONENT` command line.
- The product ρc_v is defined with the `RHOCV` command line.
- The thermal exponent is defined with the `THERMAL EXPONENT` command line.
- The reference temperature is defined with the `REFERENCE TEMPERATURE` command line.
- The melt temperature is defined with the `MELT TEMPERATURE` command line.

4.2.11 BCJ Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL BCJ
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    C1 = <real>c1
    C2 = <real>c2
    C3 = <real>c3
    C4 = <real>c4
    C5 = <real>c5
    C6 = <real>c6
    C7 = <real>c7
    C8 = <real>c8
    C9 = <real>c9
    C10 = <real>c10
    C11 = <real>c11
    C12 = <real>c12
    C13 = <real>c13
    C14 = <real>c14
    C15 = <real>c15
    C16 = <real>c16
    C17 = <real>c17
    C18 = <real>c18
    C19 = <real>c19
    C20 = <real>c20
    DAMAGE EXPONENT = <real>damage_exponent
    INITIAL ALPHA_XX = <real>alpha_xx
    INITIAL ALPHA_YY = <real>alpha_yy
    INITIAL ALPHA_ZZ = <real>alpha_zz
    INITIAL ALPHA_XY = <real>alpha_xy
```

```
    INITIAL ALPHA_YZ = <real>alpha_yz
    INITIAL ALPHA_XZ = <real>alpha_xz
    INITIAL KAPPA = <real>initial_kappa
    INITIAL DAMAGE = <real>initial_damage
    YOUNGS MODULUS FUNCTION = <string>ym_function_name
    POISSONS RATIO FUNCTION = <string>pr_function_name
    SPECIFIC HEAT = <real>specific_heat
    THETA OPT = <integer>theta_opt
    FACTOR = <real>factor
    RHO = <real>rho
    TEMP0 = <real>temp0
  END [PARAMETERS FOR MODEL BCJ]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The BCJ plasticity model is a state-variable model for describing the finite deformation behavior of metals. It uses a multiplicative decomposition of the deformation gradient into elastic, volumetric plastic, and deviatoric parts. The model considers the natural configuration defined by this decomposition and its associated thermodynamics. The model incorporates strain rate and temperature sensitivity, as well as damage, through a yield-surface approach in which state variables follow a hardening-minus-recovery format.

Because the BCJ model has such an extensive list of parameters, we will not present the usual synopsis of parameter names with command lines. As with most other material models, the `thermal strain option` is used to define thermal strains. See Section 4.1.3.1 and Section 4.1.3.2 for further information on defining and activating thermal strains. In addition, only two of the five elastic constants are required. The user should consult References 2, 3, and 4 for a description of the various parameters. Note that the parameters for the `SPECIFIC HEAT`, `THETA OPT`, `FACTOR`, `RHO`, and `TEMP0` command lines are used to accommodate changes to the model for heat generation due to plastic dissipation. For coupled solid/thermal calculations, the plastic dissipation rate is stored as a state variable and passed to a thermal code as a heat source term. For uncoupled calculations, temperature is stored as a state variable, and temperature increases due to plastic dissipation are calculated within the material model.

If temperature is provided from an external source, `theta_opt` is set to 0. If the temperature is calculated by the BCJ model, `theta_opt` is set to 1.

4.2.12 Power Law Creep

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL POWER_LAW_CREEP
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    CREEP CONSTANT = <real>creep_constant
    CREEP EXPONENT = <real>creep_exponent
    THERMAL CONSTANT = <real>thermal_constant
  END [PARAMETERS FOR MODEL POWER_LAW_CREEP]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The power law creep model is a secondary creep model that can be used to model the time-dependent behavior of metals, brazes or solders at high homologous temperatures. It can also be used as a simple model for the time-dependent behavior of geologic materials such as salt.

In the power law creep model, the effective creep strain rate is related to the effective stress raised to a power

$$\dot{\bar{\varepsilon}}^c = A\bar{\sigma}^m \exp\left(\frac{-Q}{RT}\right), \tag{4.8}$$

where $\dot{\bar{\varepsilon}}^c$ is the effective creep strain rate, $\bar{\sigma}$ is the effective stress, A is the creep constant, m is the creep exponent, Q is the activation energy, R is the universal gas constant (1.987 cal/mole K), and T is the absolute temperature.

If an analysis is run isothermally, then the `THERMAL CONSTANT` is simply Q/RT for the given temperature. If the analysis is a thermal analysis, then the `THERMAL CONSTANT` is Q/R, and T is in general a function of space and time.

The command block for a power law creep material starts with the line:

```
BEGIN PARAMETERS FOR MODEL POWER_LAW_CREEP
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL POWER_LAW_CREEP]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.
- The Biot's coefficient of the material is defined with the `BIOTS COEFFICIENT` command line.
- The `thermal strain option` is used to define thermal strains. See Section 4.1.3.1 and Section 4.1.3.2 for further information on defining and activating thermal strains.
- Any two of the following elastic constants are required:
  - Young's modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson's ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.
- The creep constant, A, in Equation (4.8) is defined with the `CREEP CONSTANT` command line.
- The creep exponent, m, in Equation (4.8) is defined with the `CREEP EXPONENT` command line.
- The thermal constant, the particular form depending on if the analysis is isothermal or not, is defined with the `THERMAL CONSTANT` command line.

Output variables available for this model are listed in Table 8.37.

4.2.13 Soil and Crushable Foam Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL SOIL_FOAM
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    A0 = <real>const_coeff_yieldsurf
    A1 = <real>lin_coeff_yieldsurf
    A2 = <real>quad_coeff_yieldsurf
    PRESSURE CUTOFF = <real>pressure_cutoff
    PRESSURE FUNCTION = <string>function_press_volstrain
  END [PARAMETERS FOR MODEL SOIL_FOAM]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The soil and crushable foam model is a plasticity model that can be used for modeling soil or crushable foam. Given the right input, the model is a Drucker-Prager model.

For the soil and crushable foam model, the yield surface is a surface of revolution about the hydrostat in principal stress space. A planar end cap is assumed for the yield surface so that the yield surface is closed. The yield stress σ_{yd} is specified as a polynomial in pressure p. The yield stress is given as:

$$\sigma_{yd} = a_0 + a_1 p + a_2 p^2 \,, \tag{4.9}$$

where p is positive in compression. The determination of the yield stress from Equation (4.9) places severe restrictions on the admissible values of a_0, a_1, and a_2. There are three valid cases for the yield surface. In the first case, there is an elastic–perfectly plastic deviatoric response, and the yield surface is a cylinder oriented along the hydrostat in principal stress space. In this case, a_0 is positive, and a_1 and a_2 are zero. In the second case, the yield surface is conical. A conical yield surface is obtained by setting a_2 to zero and using appropriate values for a_0 and a_1. In the third case, the yield surface has a parabolic shape. For the parabolic yield surface, all three coefficients

in Equation (4.9) are nonzero. The coefficients are checked to determine that a valid negative tensile-failure pressure can be derived based on the specified coefficients.

For the case of the cylindrical yield surface (e.g., $a_0 > 0$ and $a_1 = a_2 = 0$), there is no tensile-failure pressure. For the other two cases, the computed tensile-failure pressure may be too low. To handle the situations where there is no tensile-failure pressure or the tensile-failure pressure is too low, a pressure cutoff can be defined. If a pressure cutoff is defined, the tensile-failure pressure is the larger of the computed tensile-failure pressure and the defined cutoff pressure.

The plasticity theories for the volumetric and deviatoric parts of the material response are completely uncoupled. The volumetric response is computed first. The mean pressure p is assumed to be positive in compression, and a yield function ϕ_p is written for the volumetric response as:

$$\phi_p = p - f_p(\varepsilon_V) \ , \tag{4.10}$$

where $f_p(\varepsilon_V)$ defines the volumetric stress-strain curve for the pressure. The yield function ϕ_p determines the motion of the end cap along the hydrostat.

The command block for a soil and crushable foam material starts with the line:

```
BEGIN PARAMETERS FOR MODEL SOIL_FOAM
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL SOIL_FOAM]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.
- The Biot's coefficient of the material is defined with the `BIOTS COEFFICIENT` command line.
- The `thermal strain option` is used to define thermal strains. See Section 4.1.3.1 and Section 4.1.3.2 for further information on defining and activating thermal strains.
- Any two of the following elastic constants are required:
  - Young's modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson's ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.
- The constant in the equation for the yield surface is defined with the `A0` command line.

- The coefficient for the linear term in the equation for the yield surface is defined with the `A1` command line.
- The coefficient for the quadratic term in the equation for the yield surface is defined with the `A2` command line.
- The user-defined tensile-failure pressure is defined with the `PRESSURE CUTOFF` command line.
- The pressure as a function of volumetric strain is defined with the function named on the `PRESSURE FUNCTION` command line.

For information about the soil and crushable foam model, see the PRONTO3D document listed as Reference 6. The soil and crushable foam model is the same as the soil and crushable foam model in PRONTO3D. The PRONTO3D model is based on a material model developed by Krieg [7]. The Krieg version of the soil and crushable foam model was later modified by Swenson and Taylor [8]. The soil and crushable foam model developed by Swenson and Taylor is the model in PRONTO3D and is also the shared model for Presto and Adagio.

Output variables available for this model are listed in Table 8.39.

4.2.14 Karagozian and Case Concrete Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
   DENSITY = <real>density_value
   BIOTS COEFFICIENT = <real>biots_value
   #
   # thermal strain option
   THERMAL STRAIN FUNCTION = <string>thermal_strain_function
   # or all three of the following
   THERMAL STRAIN X FUNCTION =
     <string>thermal_strain_x_function
   THERMAL STRAIN Y FUNCTION =
     <string>thermal_strain_y_function
   THERMAL STRAIN Z FUNCTION =
     <string>thermal_strain_z_function
   BEGIN PARAMETERS FOR MODEL KC_CONCRETE
      YOUNGS MODULUS = <real>youngs_modulus
      POISSONS RATIO = <real>poissons_ratio
      BULK MODULUS = <real>bulkmodulus
      SHEAR MODULUS = <real>shearmodulus
      COMPRESSIVE STRENGTH = <real>compressive_strength
      TENSILE STRENGTH = <real>tensile_strength
      LAMBDA = <real>lambda
      LAMBDAM = <real>lambda_m
      LAMBDAZ = <real>lambda_z
      SINGLE RATE ENHANCEMENT = <enum>TRUE|FALSE
      FRACTIONAL DILATANCY = <real>omega
      MAXIMUM AGGREGATE SIZE = <real>max_aggregate_size
      ONE INCH = <real>one_inch
      RATE SENSITIVITY FUNCTION = <string>rate_function_name
      PRESSURE FUNCTION = <string>pressure_function_name
      UNLOAD BULK MODULUS FUNCTION = <string>bulk_function_name
      HARDEN-SOFTEN FUNCTION = <string>harden_soften_function_name
   END PARAMETERS FOR MODEL KC_CONCRETE
END PROPERTY SPECIFICATION FOR MATERIAL name
```

The Karagozian & Case (or K&C) concrete model is an inelasticity model appropriate for approximating the constitutive behavior of concrete. Coupled with appropriate elements for capturing the embedded deformation of reinforcing steel, the K&C concrete model can be utilized effectively for simulating the mechanical response of reinforced concrete structures. The K&C model has several useful characteristics for estimating concrete response, including strain-softening capabilities, some degree of tensile response, and a nonlinear stress-strain characterization that robustly simulates the behavior of plain concrete. This model is described in detail in Reference 9.

The command block for the K&C concrete material model starts with the line:

```
BEGIN PARAMETERS FOR MODEL KC_CONCRETE
```

and terminates with the line:

```
END PARAMETERS FOR MODEL KC_CONCRETE
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.
- The Biot's coefficient of the material is defined with the `BIOTS COEFFICIENT` command line.
- The `thermal strain option` is used to define thermal strains. See Section 4.1.3.1 and Section 4.1.3.2 for further information on defining and activating thermal strains.
- Any two of the following elastic constants are required:
  - Young's modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson's ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.

In addition to these material moduli, the following constitutive parameters should be defined:

- The compressive strength for a uniaxial compression test is defined with the `COMPRESSIVE STRENGTH` command line.
- The tensile strength for the uniaxial tension test is defined with the `TENSILE STRENGTH` command line.
- The abscissa of the hardening/softening curve where this curve takes on the value of one is termed Lambda-M, and it is defined with the `LAMBDAM` command line (Reference 9, pg. B-3).
- The abscissa of the hardening/softening curve where this curve takes on the value of zero after its peak value has been attained is termed Lambda-Z, and it is defined with the `LAMBDAZ` command line. This parameter should satisfy LAMBDAZ > LAMBDAM (Reference 9, pg. B-3). This input is Sierra-specific, and differs from the previous PRONTO3D definitions.
- The `SINGLE RATE ENHANCEMENT` parameter indicates whether the rate enhancement of the model should be independent of the sign of the deformation. If this parameter is set to `TRUE`, the same enhancement function is used for both compression and tension. If it is set to `FALSE`, the enhancement function must assign values for both positive and negative values of strain rate (Reference 9, pg. B-5). This parameter is also Sierra-specific, and is different from the previous PRONTO3D definitions.

- The `FRACTIONAL DILATANCY` is an estimate of the size of the plastic volume strain increment relative to that corresponding to straining in the hydrostatic plane. This value normally ranges from 0.3 to 0.7, and a value of one-half is commonly utilized in practice.

- The `MAXIMUM AGGREGATE SIZE` parameter provides an estimate of the largest length dimension for the aggregate component of the concrete mix. The American Concrete Institute code [10] includes specifications for maximum aggregate size that are based on member depth and clear spacing between adjacent reinforcement elements.

- The parameter `ONE INCH` provides for conversion to units other than the pounds/inch system commonly used in U.S. concrete venues. This parameter should be set to the equivalent length in the system utilized for analysis, e.g., if centimeters are used, then this parameter is set to 2.54.

The following functions describe the evolution of material coefficients in this model:

- The function characterizing the enhancement of strength with strain rate is described via the `RATE SENSITIVITY FUNCTION` (Reference 9, pg. B-3).

Warning: The `RATE SENSITIVITY FUNCTION` command should be used with caution. The implementation appears to provide unconservative estimates of concrete strength in tension, and users are cautioned to provide rate sensitivity function values that have the value of 1.0 for positive (tensile) values of strain rate. These values correspond to no additional strength in tension due to strain rate, and are both physically realistic and properly conservative.

- The function describing the relationship between pressure and volumetric strain is described via the `PRESSURE FUNCTION`.

- The function characterizing the relationship between bulk modulus and volumetric strain during unloading is described via the `UNLOAD BULK MODULUS FUNCTION`.

- The function describing the hardening and softening functions function eta as a function of the material parameters lambda (see `LAMBDAM` and `LAMBDAZ`) is defined via the `HARDEN-SOFTEN FUNCTION` (Reference 9, pg. B-3).

4.2.15 Foam Plasticity Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL FOAM_PLASTICITY
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    PHI = <real>phi
    SHEAR STRENGTH  = <real>shear_strength
    SHEAR HARDENING = <real>shear_hardening
    SHEAR EXPONENT  = <real>shear_exponent
    HYDRO STRENGTH  = <real>hydro_strength
    HYDRO HARDENING = <real>hydro_hardening
    HYDRO EXPONENT  = <real>hydro_exponent
    BETA = <real>beta
  END [PARAMETERS FOR MODEL FOAM_PLASTICITY]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The foam plasticity model was developed to describe the response of porous elastic-plastic materials like closed-cell polyurethane foam to large deformation. Like solid metals, these foams can exhibit significant plastic deviatoric strains (permanent shape changes). Unlike metals, these foams can also exhibit significant plastic volume strains (permanent volume changes). The foam plasticity model is characterized by an initial yield surface that is an ellipsoid about the hydrostat.

When foams are compressed, they typically exhibit an initial elastic regime followed by a plateau regime in which the stress needed to compress the foam remains nearly constant. At some point in the compression process, the densification regime is reached, and the stress needed to compress the foam further begins to rapidly increase.

The foam plasticity model can be used to describe the response of metal foams and many closed-cell polymeric foams (including polyurethane, polystyrene bead, etc.) subjected to large deformation. This model is not appropriate for flexible foams that return to their undeformed shape after loads are removed.

The command block for a foam plasticity material starts with the line:

```
BEGIN PARAMETERS FOR MODEL FOAM_PLASTICITY
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL FOAM_PLASTICITY]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.
- The Biot's coefficient of the material is defined with the `BIOTS COEFFICIENT` command line.
- The `thermal strain option` is used to define thermal strains. See Section 4.1.3.1 and Section 4.1.3.2 for further information on defining and activating thermal strains.
- Any two of the following elastic constants are required:
  - Young's modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson's ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.
- The initial volume fraction of solid material in the foam, φ, is defined with the `PHI` command line. For example, solid polyurethane weighs 75 pounds per cubic foot (pcf); uncompressed 10 pcf polyurethane foam would have a φ of 0.133 = 10/75.
- The shear (deviatoric) strength of uncompressed foam is defined with the `SHEAR STRENGTH` command line.
- The shear hardening modulus for the foam is defined with the `SHEAR HARDENING` command line.
- The shear hardening exponent is defined with the `SHEAR EXPONENT` command line. The deviatoric strength is given by `(SHEAR STRENGTH) + (SHEAR HARDENING) * PHI**(SHEAR EXPONENT)`.
- The hydrostatic (volumetric) strength of the uncompressed foam is defined with the `HYDRO STRENGTH` command line.
- The hydrodynamic hardening modulus is defined with the `HYDRO HARDENING` command line.

- The hydrodynamic hardening exponent is defined with the `HYDRO EXPONENT` command line. The hydrostatic strength is given by `(HYDRO STRENGTH)` + `(HYDRO HARDENING) * PHI**(HYDRO EXPONENT)`.

- The prescription for nonassociated flow, β, is defined with the `BETA` command line. When $\beta = 0.0$, the flow direction is given by the normal to the yield surface (associated flow). When $\beta = 1.0$, the flow direction is given by the stress tensor. Values between 0.0 and 0.95 are recommended.

Output variables available for this model are listed in Table 8.26.

4.2.16 Low Density Foam Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL LOW_DENSITY_FOAM
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    A = <real>A
    B = <real>B
    C = <real>C
    NAIR  = <real>NAir
    P0  = <real>P0
    PHI = <real>Phi
  END [PARAMETERS FOR MODEL LOW_DENSITY_FOAM]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The `LOW_DENSITY_FOAM` material model is a phenomenological model for low density polyurethane foams, where `A`, `B`, and `C` are material constants, `NAIR` is the mole fraction of air, `P0` is the initial air pressure, and `PHI` is the volume fraction of solid material. The yield function for this model has the form

$$\bar{\sigma} = A \left\langle I_2' \right\rangle + B \left(1.0 + C I_1\right), \tag{4.11}$$

where $\langle\rangle$ denotes the Heaviside step function, I_1 is the first invariant of the deviatoric strain, and I_2' is the second invariant of the strain.

For more information on the low density foam material model, see [11].

4.2.17 Elastic Three-Dimensional Orthotropic Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  BEGIN PARAMETERS FOR MODEL ELASTIC_3D_ORTHOTROPIC
    # general parameters (any two are required)
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    # required parameters
    YOUNGS MODULUS AA = <real>Eaa_value
    YOUNGS MODULUS BB = <real>Ebb_value
    YOUNGS MODULUS CC = <real>Ecc_value
    POISSONS RATIO AB = <real>NUab_value
    POISSONS RATIO BC = <real>NUbc_value
    POISSONS RATIO CA = <real>NUca_value
    SHEAR MODULUS AB = <real>Gab_value
    SHEAR MODULUS BC = <real>Gbc_value
    SHEAR MODULUS CA = <real>Gca_value
    COORDINATE SYSTEM = <string>coordinate_system_name
    DIRECTION FOR ROTATION = <real>1|2|3
    ALPHA = <real>alpha_in_degrees
    SECOND DIRECTION FOR ROTATION = <real>1|2|3
    SECOND ALPHA = <real>second_alpha_in_degrees
    THERMAL STRAIN AA FUNCTION = <string>ethaa_function_name
    THERMAL STRAIN BB FUNCTION = <string>ethbb_function_name
    THERMAL STRAIN CC FUNCTION = <string>ethcc_function_name
  END [PARAMETERS FOR MODEL ELASTIC_3D_ORTHOTROPIC]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The elastic three-dimensional orthotropic model describes the linear elastic response of an orthotropic material where the orientation of the principal material directions can be arbitrary. These principal axes are here denoted as A, B, and C. Thermal strains are also given along the principal material axes. The specification of these material axes is accomplished by selecting a user-defined coordinate system that can then be rotated twice about one of its current axes to give the final desired directions.

The command block for an elastic three-dimensional orthotropic material starts with the line:

```
  BEGIN PARAMETERS FOR MODEL ELASTIC_3D_ORTHOTROPIC
```

and terminates with the line:

```
  END [PARAMETERS FOR MODEL ELASTIC_3D_ORTHOTROPIC]
```

In the above command blocks all of the following are required inputs, including two of the five general elastic material constants:

- The density of the material is defined with the `DENSITY` command line.
- The Biot's coefficient of the material is defined with the `BIOTS COEFFICIENT` command line.
- Any two of the following elastic constants are required:
  - Young's modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson's ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.
- The Youngs moduli corresponding to the principal material axes A, B, and C are given by the `YOUNGS MODULUS AA`, `YOUNGS MODULUS BB`, and `YOUNGS MODULUS CC` command lines.
- The Poisson's ratio defining the BB normal strain when the material is subjected only to AA normal stress is given by the `POISSONS RATIO AB` command line.
- The Poisson's ratio defining the CC normal strain when the material is subjected only to BB normal stress is given by the `POISSONS RATIO BC` command line.
- The Poisson's ratio defining the AA normal strain when the material is subjected only to CC normal stress is given by the `POISSONS RATIO CA` command line.
- The shear moduli for shear in the AB, BC, and CA planes are given by the `SHEAR MODULUS AB`, `SHEAR MODULUS BC`, and `SHEAR MODULUS CA` command lines, respectively.
- The specification of the principal material directions begins with the selection of a user-specified coordinate system given by the `COORDINATE SYSTEM` command line. This initial coordinate system can then be rotated twice to give the final material directions.
- The rotation of the initial coordinate system is defined using the `DIRECTION FOR ROTATION` and `ALPHA` command lines. The axis for rotation of the initial coordinate system is specified by the `DIRECTION FOR ROTATION` command line, while the angle of rotation is given by the `ALPHA` command line. This gives an intermediate specification of the material directions.
- The rotation of the intermediate coordinate system is defined using the `SECOND DIRECTION FOR ROTATION` and `SECOND ALPHA` command lines. The axis for rotation of the intermediate coordinate system is specified by the `SECOND DIRECTION FOR ROTATION` command line, while the angle of rotation is given by the `SECOND ALPHA` command line. The resulting coordinate system gives the final specification of the material directions.

- The thermal strain functions for normal thermal strains along the principal material directions are given by the `THERMAL STRAIN AA FUNCTION`, `THERMAL STRAIN BB FUNCTION`, and `THERMAL STRAIN CC FUNCTION` command lines.

See Reference 13 for more information about the elastic three-dimensional orthotropic model.

4.2.18 Wire Mesh Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL WIRE_MESH
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    YIELD FUNCTION = <string>yield_function
    TENSION = <real>tensile_strength
  END [PARAMETERS FOR MODEL WIRE_MESH]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The wire mesh constitutive model was developed at Sandia National Laboratories to model layers of mesh for analyses of packaging for transportation of hazardous materials.

The wire mesh model decomposes the Cauchy stress tensor into its principal components. It then checks each of the principal stress to see whether they exceed the yield criterion. If a principal stress is negative, i.e. in compression, the yield condition is

$$\psi = \sigma - f(e_v) \tag{4.12}$$

The yield function for this model can be input by the user, and defines the yield strength as a function of the volumetric engineering strain, e_v.

If the principal stress is tensile, a cutoff value of the principal tensile stress is used, and the yield condition is

$$\psi = \sigma - \tau \tag{4.13}$$

The value for τ is given by the value of `TENSION`.

The command block for a wire mesh material starts with the line:

```
BEGIN PARAMETERS FOR MODEL WIRE_MESH
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL WIRE_MESH]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.
- The Biot's coefficient of the material is defined with the `BIOTS COEFFICIENT` command line.
- The `thermal strain option` is used to define thermal strains. See Section 4.1.3.1 and Section 4.1.3.2 for further information on defining and activating thermal strains.
- Any two of the following elastic constants are required:
  - Young's modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson's ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.
- The yield function in compression is defined with the `YIELD FUNCTION` command line.
- The tensile strength is give by the `TENSION` command line.

Output variables available for this model are listed in Table 8.27.

More information on the model can be found in the report by Neilsen, et. al. [12]

4.2.19 Orthotropic Crush Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL ORTHOTROPIC_CRUSH
    EX  = <real>modulus_x_pre_lockup
    EY  = <real>modulus_y_pre_lockup
    EZ  = <real>modulus_z_pre_lockup
    GXY = <real>shear_modulus_xy_pre_lockup
    GYZ = <real>shear_modulus_yz_pre_lockup
    GZX = <real>shear_modulus_zx_pre_lockup
    CRUSH XX = <string>stress_volume_xx_function_name
    CRUSH YY = <string>stress_volume_yy_function_name
    CRUSH ZZ = <string>stress_volume_zz_function_name
    CRUSH XY = <string>shear_stress_volume_xy_function_name
    CRUSH YZ = <string>shear_stress_volume_yz_function_name
    CRUSH ZX = <string>shear_stress_volume_zx_function_name
    VMIN = <real>lockup_volumetric_strain
    YOUNGS MODULUS = <real>youngs_modulus_post_lockup
    POISSONS RATIO = <real>poissons_ratio_post_lockup
    SHEAR MODULUS = <real>shear_modulus_post_lockup
    BULK MODULUS = <real>bulk_modulus_post_lockup
    LAMBDA = <real>lambda_post_lockup
    YIELD STRESS = <real>yield_stress_post_lockup
  END [PARAMETERS FOR MODEL ORTHOTROPIC_CRUSH]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The orthotropic crush model is an empirically based constitutive relation that is useful for modeling materials like metallic honeycomb and wood. This particular implementation follows the formulation of the metallic honeycomb model in DYNA3D [14]. The orthotropic crush model divides material behavior into three phases:

- orthotropic elastic,
- volumetric crush (partially compacted), and

- elastic–perfectly plastic (fully compacted).

The command block for an orthotropic crush material starts with the line:

```
BEGIN PARAMETERS FOR MODEL ORTHOTROPIC_CRUSH
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL ORTHOTROPIC_CRUSH]
```

In the above command blocks:

- The uncompacted density of the material is defined with the `DENSITY` command line.
- The `thermal strain option` is used to define thermal strains. See Section 4.1.3.1 and Section 4.1.3.2 for further information on defining and activating thermal strains.
- The initial directional modulus E_{xx} is defined with the `EX` command line.
- The initial directional modulus E_{yy} is defined with the `EY` command line.
- The initial directional modulus E_{zz} is defined with the `EZ` command line.
- The initial directional shear modulus G_{xy} is defined with the `GXY` command line.
- The initial directional shear modulus G_{yz} is defined with the `GYZ` command line.
- The initial directional shear modulus G_{zx} is defined with the `GZX` command line.
- The compressive volumetric strain at lockup or full compaction is defined with the `VMIN` command line.
- The directional stress σ_{xx} as a function of the compressive volumetric strain is defined by the function referenced in the `CRUSH XX` command line.
- The directional stress σ_{yy} as a function of the compressive volumetric strain is defined by the function referenced in the `CRUSH YY` command line.
- The directional stress σ_{zz} as a function of the compressive volumetric strain is defined by the function referenced in the `CRUSH ZZ` command line.
- The directional stress σ_{xy} as a function of the compressive volumetric strain is defined by the function referenced in the `CRUSH XY` command line.
- The directional stress σ_{yz} as a function of the compressive volumetric strain is defined by the function referenced in the `CRUSH YZ` command line.
- The directional stress σ_{zx} as a function of the compressive volumetric strain is defined by the function referenced in the `CRUSH ZX` command line.

- Any two of the following elastic constants are required:
  - Young's modulus for the fully compacted state is defined with the `YOUNGS MODULUS` command line. This is the elastic–perfectly plastic value of Young's modulus.
  - Poisson's ratio for the fully compacted state is defined with the `POISSONS RATIO` command line. This is the elastic–perfectly plastic value of Poisson's ratio.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.
- The yield stress for the fully compacted state is defined with the `YIELD STRESS` command line. This is the elastic–perfectly plastic value of the yield stress.

Note that several of the command lines in this command block (those beginning with `CRUSH`) reference functions. These functions must be defined in the SIERRA scope. Output variables available for this model are listed in Table 8.34. For information about the orthotropic crush model, consult Reference 14.

4.2.20 Orthotropic Rate Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL ORTHOTROPIC_RATE
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    YIELD STRESS = <real>yield_stress
    MODULUS TTTT = <real>modulus_tttt
    MODULUS TTLL = <real>modulus_ttll
    MODULUS TTWW = <real>modulus_ttww
    MODULUS LLLL = <real>modulus_llll
    MODULUS LLWW = <real>modulus_llww
    MODULUS WWWW = <real>modulus_wwww
    MODULUS TLTL = <real>modulus_tltl
    MODULUS LWLW = <real>modulus_lwlw
    MODULUS WTWT = <real>modulus_wtwt
    TX = <real>tx
    TY = <real>ty
    TZ = <real>tz
    LX = <real>lx
    LY = <real>ly
    LZ = <real>lz
    MODULUS FUNCTION = <string>modulus_function_name
    RATE FUNCTION = <string>rate_function_name
    T FUNCTION = <string>t_function_name
    L FUNCTION = <string>l_function_name
    W FUNCTION = <string>w_function_name
    TL FUNCTION = <string>tl_function_name
    LW FUNCTION = <string>lw_function_name
    WT FUNCTION = <string>wt_function_name
  END [PARAMETERS FOR MODEL ORTHOTROPIC_RATE]
```

```
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The orthotropic rate model extends the functionality of the orthotropic crush constitutive model described in Section 4.2.19. The orthotropic rate model has been developed to describe the behavior of an aluminum honeycomb subjected to large deformation. The orthotropic rate model, like the original orthotropic crush model, has six independent yield functions that evolve with volume strain. Unlike the orthotropic crush model, the orthotropic rate model has yield functions that also depend on strain rate. The orthotropic rate model also uses an orthotropic elasticity tensor with nine elastic moduli in place of the orthotropic elasticity tensor with six elastic moduli used in the orthotropic crush model. A honeycomb orientation capability is included with the orthotropic rate model that allows users to prescribe initial honeycomb orientations that are not aligned with the original global coordinate system.

The command block for an orthotropic rate material starts with the line:

```
BEGIN PARAMETERS FOR MODEL ORTHOTROPIC_RATE
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL ORTHOTROPIC_RATE]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.
- The Biot's coefficient of the material is defined with the `BIOTS COEFFICIENT` command line.
- The `thermal strain option` is used to define thermal strains. See Section 4.1.3.1 and Section 4.1.3.2 for further information on defining and activating thermal strains.
- In the following list of elastic constants, only the elastic modulus (Young's modulus) is required for this model. If two elastic constants are supplied, the elastic constants will be completed. However, only the elastic modulus is used in this model.
    - Young's modulus for the fully compacted honeycomb is defined with the `YOUNGS MODULUS` command line.
    - Poisson's ratio for the fully compacted state is defined with the `POISSONS RATIO` command line.
    - The bulk modulus for the fully compacted state is defined with the `BULK MODULUS` command line.
    - The shear modulus for the fully compacted state is defined with the `SHEAR MODULUS` command line.
    - Lambda for the fully compacted state is defined with the `LAMBDA` command line.

- The yield stress for the fully compacted honeycomb is defined with the `YIELD STRESS` command line.

- The nine elastic moduli for the orthotropic uncompacted honeycomb are defined with the `MODULUS TTT`, `MODULUS TTLL`, `MODULUS TTWW`, `MODULUS LLLL`, `MODULUS LLWW`, `MODULUS WWWW`, `MODULUS TLTL`, `MODULUS LWLW`, and `MODULUS WTWT` command lines. The T-direction is usually associated with the generator axis for the honeycomb. The L-direction is in the ribbon plane (plane defined by flat sheets used in reinforced honeycomb) and orthogonal to the generator axis. The W-direction is perpendicular to the ribbon plane.

- The components of a vector defining the T-direction of the honeycomb are defined by the `TX`, `TY`, and `TZ` command lines. The values of `tx`, `ty`, and `tz` are components of a vector in the global coordinate system that define the orientation of the honeycomb's T-direction (generator axis).

- The components of a vector defining the L-direction of the honeycomb are defined by the `LX`, `LY`, and `LZ` command lines. The values of `lx`, `ly`, and `lz` are components of a vector in the global coordinate system that define the orientation of the honeycomb's L-direction. *Caution*: The vectors T and L must be orthogonal.

- The function describing the variation in moduli with compaction is given by the `MODULUS FUNCTION` command line. The moduli vary continuously from their initial orthotropic values to isotropic values when full compaction is obtained.

- The function describing the change in strength with strain rate is given by the `RATE FUNCTION` command line. Note that all strengths are scaled with the multiplier obtained from this function.

- The function describing the T-normal strength of the honeycomb as a function of compressive volumetric strain is given by the `T FUNCTION` command line.

- The function describing the L-normal strength of the honeycomb as a function of compressive volumetric strain is given by the `L FUNCTION` command line.

- The function describing the W-normal strength of the honeycomb as a function of compressive volumetric strain is given by the `W FUNCTION` command line.

- The function describing the TL-normal strength of the honeycomb as a function of compressive volumetric strain is given by the `TL FUNCTION` command line.

- The function describing the LW-normal strength of the honeycomb as a function of compressive volumetric strain is given by the `LW FUNCTION` command line.

- The function describing the WT-normal strength of the honeycomb as a function of compressive volumetric strain is given by the `WT FUNCTION` command line.

Note that several of the command lines in this command block reference functions. These functions must be defined in the SIERRA scope. Output variables available for this model are listed in Table 8.35.

4.2.21 Elastic Laminate Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  #
  BEGIN PARAMETERS FOR MODEL ELASTIC_LAMINATE
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    A11 = <real>a11_value
    A12 = <real>a12_value
    A16 = <real>a16_value
    A22 = <real>a22_value
    A26 = <real>a26_value
    A66 = <real>a66_value
    A44 = <real>a44_value
    A45 = <real>a45_value
    A55 = <real>a55_value
    B11 = <real>b11_value
    B12 = <real>b12_value
    B16 = <real>b16_value
    B22 = <real>b22_value
    B26 = <real>b26_value
    B66 = <real>b66_value
    D11 = <real>d11_value
    D12 = <real>d12_value
    D16 = <real>d16_value
    D22 = <real>d22_value
    D26 = <real>d26_value
    D66 = <real>d66_value
    COORDINATE SYSTEM = <string>coord_sys_name
    DIRECTION FOR ROTATION = 1|2|3
    ALPHA = <real>alpha_value_in_degrees
    THETA = <real>theta_value_in_degrees
    NTH11 FUNCTION = <string>nth11_function_name
    NTH22 FUNCTION = <string>nth22_function_name
    NTH12 FUNCTION = <string>nth12_function_name
    MTH11 FUNCTION = <string>mth11_function_name
    MTH22 FUNCTION = <string>mth22_function_name
    MTH12 FUNCTION = <string>mth12_function_name
  END [PARAMETERS FOR MODEL ELASTIC_LAMINATE]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The elastic laminate model can be used to describe the overall linear elastic response of layered shells. The response of each layer is pre-integrated through the thickness under an assumed vari-

ation of strain through the thickness. That is, the user inputs laminate stiffness matrices directly, and the overall response is calculated appropriately. This model allows the user to input laminate stiffness matrices that are consistent with a state of generalized plane stress for each layer. Each layer can be orthotropic with a unique orientation. This model is primarily intended for capturing the response of fiber-reinforced laminated composites. The user inputs the laminate stiffness matrices calculated with respect to a chosen coordinate system and then specifies this coordinate system's definition relative to the global coordinate system. Thermal stresses are handled via the input of thermal-force and thermal-force-couple resultants for the laminate as a whole. At present, the user cannot get layer stresses out from this material model. However, the overall section-force and force-couple resultants can be computed from available output. The details of this model are described in References 15 and 16.

The command block for an elastic laminate material starts with the line:

```
BEGIN PARAMETERS FOR MODEL ELASTIC_LAMINATE
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL ELASTIC_LAMINATE]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.
- Two of the five elastic constants must be defined with the `YOUNGS MODULUS`, `POISSONS RATIO`, `SHEAR MODULUS`, `BULK MODULUS`, or `LAMBDA` commands
- The elastic constants are unrelated to the laminate stiffness matrix. They are used along with the shell section thickness (defined in the shell section command block, see section 5.2.4) to calculate drilling and hourglass stiffnesses. Otherwise these values have no physical significance in the elastic laminate material model.
- The extensional stiffnesses are defined with the $\mathtt{A}_{ij}$ command lines, where the values of ij are 11, 12, 16, 22, 26, 66, 44, 45, and 55.
- The coupling stiffnesses are defined with the $\mathtt{B}_{ij}$ command lines, where the values of ij are 11, 12, 16, 22, 26, and 66.
- The bending stiffnesses are defined with the $\mathtt{D}_{ij}$ command lines, where the values of ij are 11, 12, 16, 22, 26, and 66.
- The initial laminate coordinate system is defined with the `COORDINATE SYSTEM` command line.
- The rotation of the initial laminate coordinate system is defined with the `DIRECTION FOR ROTATION` and `ALPHA` command lines. The axis of initial laminate coordinate system is specified by the `DIRECTION FOR ROTATION` command line, while the angle of rotation is given by the `ALPHA` command line. This produces an intermediate laminate coordinate system that is then projected onto the surface of each shell element.

- The projected intermediate laminate coordinate system is rotated about the element normal by angle theta, which is specified by the `THETA` command line.
- The thermal-force resultants are defined by functions that are referenced on the `NTH11 FUNCTION`, `NTH22 FUNCTION`, and `NTH12 FUNCTION` command lines.
- The thermal-force-couple resultants are defined by functions that are referenced on the `MTH11 FUNCTION`, `MTH22 FUNCTION`, and `MTH12 FUNCTION` command lines.

4.2.22 Fiber Membrane Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL FIBER_MEMBRANE
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    CORD DENSITY = <real>cord_density
    CORD DIAMETER = <real>cord_diameter
    MATRIX DENSITY = <real>matrix_density
    TENSILE TEST FUNCTION = <string>test_function_name
    PERCENT CONTINUUM = <real>percent_continuum
    EPL = <real>epl
    AXIS X = <real>axis_x
    AXIS Y = <real>axis_y
    AXIS Z = <real>axis_z
    MODEL = <string>RECTANGULAR
    STIFFNESS SCALE = <real>stiffness_scale
    REFERENCE STRAIN = <real>reference_strain
  END [PARAMETERS FOR MODEL FIBER_MEMBRANE]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The fiber membrane model is used for modeling membranes that are reinforced with unidirectional fibers. Through the use of a non-zero `PERCENT CONTINUUM`, a background isotropic material response can also be incorporated and is added in a manner such that the response in the fiber direction is unchanged. The fiber membrane model can be used in both Presto and Adagio. When the fiber membrane model is used in Adagio, the model can be used with or without the control-stiffness option in Adagio's multilevel solver. The control-stiffness option is implemented via the `CONTROL STIFFNESS` command block and is discussed in Chapter 3 of the Adagio user's guide. If the control-stiffness option is activated in Adagio, the response in the fiber direction is softened by lowering the fiber response. In all cases, the final material behavior that is used for equilibrium corresponds to the real material response. When the fiber membrane model is used in Presto, the fiber scaling, which is controlled by the `STIFFNESS SCALE` command line, is ignored.

The command block for a fiber membrane material starts with the line:

```
BEGIN PARAMETERS FOR MODEL FIBER_MEMBRANE
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL FIBER_MEMBRANE]
```

In the above command blocks, the following definitions are applicable. Usage requirements are identified both in this list of definitions and in the discussion that follows the list.

- The density of the material is defined with the `DENSITY` command line. This command line should be included, but its value will be recomputed (and hence replaced) if the `CORD DENSITY`, `CORD DIAMETER`, and `MATRIX DENSITY` command lines are specified.
- The `thermal strain option` is used to define thermal strains. See Section 4.1.3.1 and Section 4.1.3.2 for further information on defining and activating thermal strains.
- Any two of the following elastic constants are required. These are used to compute values for the elastic preconditioner only.
  - Young's modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson's ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.
- The density of the fibers is defined by the `CORD DENSITY` command line. This command line is optional. See the usage discussion below.
- The diameter of the fibers is defined by the `CORD DIAMETER` command line. This command line is optional. See the usage discussion below.
- The density of the matrix is defined by the `MATRIX DENSITY` command line. This command line is optional. See the usage discussion below.
- The `TENSILE TEST FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope that describes the fiber force versus strain data. This command line must be included.
- The fractional fiber stiffness to use in defining the background isotropic response is given by the `PERCENT CONTINUUM` command line. This command line must be included.
- The number of fibers per unit length is defined by the `EPL` command line. This command line must be included.

- The components of the vector defining the initial fiber direction is given by the `AXIS X`, `AXIS Y`, and `AXIS Z` command lines. These command lines must be included. See the usage discussion below.

- The coordinate system for specifying the fiber orientation is given by the `MODEL` command line. Only the option `RECTANGULAR` is available in this release. This command line must be included. See the usage discussion below.

- The fiber scaling is specified by the `STIFFNESS SCALE` command line. If the control-stiffness option is used in Adagio, this command line must be included. When the fiber membrane model is used in Presto, this command line is ignored.

- The reference strain is defined with the `REFERENCE STRAIN` command line. This command line is optional for Adagio and is not used in Presto. If the control-stiffness option is used in Adagio, this command line may be included. See the usage discussion below.

Certain command lines in the `PARAMETERS FOR MODEL FIBER_MEMBRANE` command block also have interdependencies or other factors that may impact their usage in Presto and Adagio, as discussed below.

The `CORD DENSITY`, `CORD DIAMETER`, and `MATRIX DENSITY` command lines are optional. When included, these three command lines are used for computation of the correct density corresponding to the fibers, the number of fibers per unit length, and the chosen matrix. When these three command lines are not included, the density is taken as that specified by the `DENSITY` command line.

The `AXIS X`, `AXIS Y`, and `AXIS Z` command lines must be specified if the value for the `MODEL` command line is `RECTANGULAR`. Currently, these axis-related command lines must be specified.

Specifying a reference strain (via the `REFERENCE STRAIN` command line) implies the use of strains for measuring part of the control-stiffness material constraint violation in Adagio. If this command line is not present, the material constraint violation is determined by comparing the change in the scaled fiber force over the current model problem.

4.2.23 Incompressible Solid Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL INCOMPRESSIBLE_SOLID
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    BULK MODULUS = <real>bulk_modulus
    SHEAR MODULUS = <real>shear_modulus
    LAMBDA = <real>lambda
    K SCALING = <real>k_scaling
    2G SCALING = <real>2g_scaling
    TARGET E = <real>target_e
    MAX POISSONS RATIO = <real>max_poissons_ratio
    REFERENCE STRAIN = <real>reference_strain
    SCALING FUNCTION = <string>scaling_function_name
  END [PARAMETERS FOR MODEL INCOMPRESSIBLE_SOLID]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The incompressible solid model is a variation of the elastic model and can be used in both Presto and Adagio. In Adagio, the incompressible solid model is used with the control-stiffness option in the multilevel solver. The control-stiffness option is implemented via the `CONTROL STIFFNESS` command block and is discussed in Chapter 3 of the Adagio user's guide. The model is used to model nearly incompressible materials where Poisson's ratio, ν, ≈ 0.5. In the course of solving a series of model problems in Adagio, the material response from this model incorporates scaling the bulk and/or shear behaviors to yield a material response that is more amenable to solution using Adagio's conjugate gradient solver. The final material behavior that is calculated corresponds to the actual moduli that are specified. When this model is used in Presto, the material scalings are ignored, and the model behaves like a linear elastic model.

The command block for an incompressible solid material starts with the line:

```
BEGIN PARAMETERS FOR MODEL INCOMPRESSIBLE_SOLID
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL INCOMPRESSIBLE_SOLID]
```

In the above command blocks, the following definitions are applicable. Usage requirements are identified both in this list of definitions and in the discussion that follows the list.

- The density of the material is defined with the `DENSITY` command line.
- The Biot's coefficient of the material is defined with the `BIOTS COEFFICIENT` command line.
- The `thermal strain option` is used to define thermal strains. See Section 4.1.3.1 and Section 4.1.3.2 for further information on defining and activating thermal strains.
- Any two of the following elastic constants are required to define the unscaled material response:
  - Young's modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson's ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.
- The following material-scaling command lines are used only in Adagio:
  - The nominal bulk scaling is defined with the `K SCALING` command line. This command line is optional. See the usage discussion below.
  - The nominal shear scaling is defined with the `2G SCALING` command line. This command line is optional. See the usage discussion below.
  - The target Young's modulus is defined with the `TARGET E` command line. This command line is optional. See the usage discussion below.
  - The maximum Poisson's ratio is defined with the `MAX POISSONS RATIO` command line. This command line is optional. See the usage discussion below.
  - The reference strain is defined with the `REFERENCE STRAIN` command line. This command line is optional. See the usage discussion below.
  - The `SCALING FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope that describes the time dependent scaling to be applied. This command line is optional. See the usage discussion below.

As noted previously, only two of the elastic constants are required to define the unscaled material response. This requirement applies to use of the incompressible solid model in Presto and in Adagio. Further, all the material-scaling command lines are only used in Adagio.

Several options exist for defining the bulk and/or shear scalings that can be used with the multilevel solver in Adagio.

- Option 1: You can provide the scalings directly by including both of the `K SCALING` and `2G SCALING` command lines or either of them. When both command lines are input, the user-specified values for their parameters will be used. If only the `K SCALING` command line is input, the bulk scaling is as specified in the `k_scaling` parameter, and the value of the shear scaling parameter, `2g_scaling`, is set to 1.0. On the other hand, if only the `2G SCALING` command line is input, then the shear scaling is as specified in the `2g_scaling` parameter, but the value of the bulk-scaling parameter, `k_scaling`, is not set to 1.0. Instead, the bulk scaling is determined by computing a scaled bulk modulus from the scaled shear modulus and a (scaled) Poisson's ratio of 0.3. Then, the bulk scaling is determined simply as the ratio of the scaled bulk modulus to the actual bulk modulus.

- Option 2: You can specify either or both of the `TARGET E` and `MAX POISSONS RATIO` command lines to define the scalings. If only the `TARGET E` command line is included, the bulk and shear scalings are computed by first finding scaled moduli using the value of the `target_e` parameter along with a (scaled) Poisson's ratio of 0.3. The bulk and shear scalings are then determined as the ratio of the appropriate scaled to unscaled modulus. If only the `MAX POISSONS RATIO` command line is included, the shear scaling is set to 1.0, and the bulk scaling is computed by first calculating a scaled bulk modulus from the actual shear modulus and the value of the `max_poissons_ratio` parameter. The bulk scaling is then calculated simply as the ratio of the scaled bulk modulus to the actual bulk modulus. If both the `TARGET E` and `MAX POISSONS RATIO` command lines are included, the bulk scaling (and shear scaling) is determined from the ratio of the bulk scaled modulus (and shear scaled modulus) computed using the values of the `target_e` and `max_poissons_ratio` parameters to the unscaled bulk (and shear) modulus.

- Option 3: You can choose not to include any of the `K SCALING`, `2G SCALING`, `TARGET E`, and `MAX POISSONS RATIO` command lines. In such case, the shear scaling is set to 1.0, and the bulk scaling is computed as the ratio of the scaled bulk modulus coming from the real shear modulus and a (scaled) Poisson's ratio of 0.3 to the actual bulk modulus.

The function referenced by the value of the parameter `scaling_function_name` in the `SCALING FUNCTION` command line can be used to modify the bulk and shear scalings in solution time. The actual scalings used are computed by taking the scalings specified by the parameter values in the `K SCALING`, `2G SCALING`, `TARGET E`, and `MAX POISSONS RATIO` command lines and simply multiplying them by the function value at the specified solution time. If the `SCALING FUNCTION` command line is not included, the bulk and shear scalings are fixed in time.

The `REFERENCE STRAIN` command line supplies a value for the reference strain that is used to create a normalized material constraint violation based on strains. Specifying a reference strain implies the use of strains for measuring the material constraint violation (or part of the control-stiffness error in Adagio). Otherwise, the material constraint violation is determined by using the change in the scaled stress response over the current model problem.

4.2.24 Mooney-Rivlin Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  BEGIN PARAMETERS FOR MODEL MOONEY_RIVLIN
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    BULK MODULUS = <real>bulk_modulus
    SHEAR MODULUS = <real>shear_modulus
    LAMBDA = <real>lambda
    C10 = <real>c10
    C01 = <real>c01
    C10 FUNCTION = <string>c10_function_name
    C01 FUNCTION = <string>c01_function_name
    BULK FUNCTION = <string>bulk_function_name
    THERMAL EXPANSION FUNCTION = <string>eth_function_name
    TARGET E = <real>target_e
    TARGET E FUNCTION = <string>etar_function_name
    MAX POISSONS RATIO = <real>max_poissons_ratio(0.5)
    REFERENCE STRAIN = <real>reference_strain
  END [PARAMETERS FOR MODEL MOONEY_RIVLIN]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

Mooney-Rivlin is a hyperelastic model that is used to model rubber. The Mooney-Rivlin model incorporates temperature-dependent material moduli and can be used in both Presto and Adagio. When the model is used in Adagio, it can be used with or without the control-stiffness option in Adagio's multilevel solver. The control-stiffness option is implemented via the `CONTROL STIFFNESS` command block and is discussed in Chapter 3 of the Adagio user's guide. The model is used to model nearly incompressible materials where Poisson's ratio, ν, $\approx$ 0.5. In the course of solving a series of model problems in Adagio, the material response from this model incorporates scaling the bulk and/or shear behaviors to yield a material response that is more amenable to solution using Adagio's conjugate gradient solver. The final material behavior that is calculated corresponds to the actual moduli that are specified. When this model is used in Presto, the material scalings are ignored.

The command block for a Mooney-Rivlin material starts with the line:

```
BEGIN PARAMETERS FOR MODEL MOONEY_RIVLIN
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL MOONEY_RIVLIN]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.

- The Biot's coefficient of the material is defined with the `BIOTS COEFFICIENT` command line.

- Any two of the following elastic constants are required to define the unscaled bulk behavior:

  - Young's modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson's ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.

- The nominal value for C10 is defined with the `C10` command line. This command line is required. See the usage discussion below.

- The nominal value for C01 is defined with the `C01` command line. This command line is required. See the usage discussion below.

- The `C10 FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope that describes the temperature dependence of the C10 material parameter. This command line is optional. If it is not present, there is no temperature dependence in the C10 parameter. See the usage discussion below.

- The `C01 FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope that describes the temperature dependence of the C01 material parameter. This command line is optional. If it is not present, there is no temperature dependence in the C01 parameter. See the usage discussion below.

- The `BULK FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope that describes the temperature dependence of the bulk modulus. This command line is optional. If it is not present, there is no temperature dependence in the bulk modulus. See the usage discussion below.

- The `THERMAL EXPANSION FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope that describes the linear thermal expansion as function of temperature. This command line is optional. If it is not present, there is no thermal expansion. See the usage discussion below.

- The following material-scaling command lines are used only in Adagio:

  - The target Young's modulus is defined with the `TARGET E` command line. This command line is optional. See the usage discussion below.

- The `TARGET E FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope that describes the time variation of the target Young's modulus. This command line is optional. If it is not present, there is no time dependence in the Target E parameter. See the usage discussion below.
- The maximum Poisson's ratio is defined with the `MAX POISSONS RATIO` command line. This command line is optional and will default to 0.5 if not specified. See the usage discussion below.
- The reference strain is defined with the `REFERENCE STRAIN` command line. This command line is optional. See the usage discussion below.

As noted previously, only two of the elastic constants are required to define the unscaled bulk behavior. Together, the values for C10 and C01 determine the shear behavior, and thus the `C10` and `C01` command lines must be included in this model.

The command lines for functions that specify the temperature dependence of C10, C01, and bulk modulus are optional, e.g., the `C10 FUNCTION`, `C01 FUNCTION` and `BULK FUNCTION` command lines. If these command lines are not included, their corresponding material parameters are taken to be independent of temperature. Mooney-Rivlin, like other material models, allows for the specification of thermal strain behavior within the material model itself, via the `THERMAL EXPANSION FUNCTION` command line. This command line, like the other "function-type" command lines in this model requires that a function associated with the name be defined in the SIERRA scope.

The bulk and shear scalings that can be used with the multilevel solver in Adagio are specified via a combination of the `TARGET E`, `TARGET E FUNCTION`, and `MAX POISSONS RATIO` command lines. If the `TARGET E` command line is not included (and the `MAX POISSONS RATIO` command line is included), the shear scaling is set to 1.0, and the bulk scaling is determined from the ratio of the scaled bulk modulus to its unscaled value, where the scaled bulk modulus is computed using the value of the `max_poissons_ratio` parameter along with the unscaled initial shear modulus that is determined from the value of the parameters specified in the `C10` and `C01` command lines. On the other hand, if both the `TARGET E` command line and the `MAX POISSONS RATIO` command line are included, bulk and shear scaling values are computed using scaled moduli that are calculated from the `target_e` and `max_poissons_ratio` parameter values.

Including the `TARGET E FUNCTION` command line allows time-dependent bulk and shear scaling to be used. If this command line is not specified, the bulk and shear scalings remain constant in solution time. If the command line is specified, the target Young's modulus that is used for computing the scaled moduli is multiplied by the function value.

The `REFERENCE STRAIN` command line supplies a value for the reference strain used to create a normalized material constraint violation that is based on strains. Specifying a reference strain implies the use of strains for measuring the material constraint violation (or part of the control-stiffness error in Adagio). Otherwise, the material constraint violation is determined using the change in the scaled stress response over the current model problem.

Brief documentation on the theoretical basis for the Mooney-Rivlin model is given in Reference 17.

4.2.25 NLVE 3D Orthotropic Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  BEGIN PARAMETERS FOR MODEL NLVE_3D_ORTHOTROPIC
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    COORDINATE SYSTEM = <string>coordinate_system_name
    DIRECTION FOR ROTATION = <real>1|2|3
    ALPHA = <real>alpha_in_degrees
    SECOND DIRECTION FOR ROTATION = <real>1|2|3
    SECOND ALPHA = <real>second_alpha_in_degrees
    FICTITIOUS LOGA FUNCTION = <string>fict_loga_function_name
    FICTITIOUS LOGA SCALE FACTOR = <real>fict_loga_scale_factor
    # In each of the five ``PRONY'' command lines and in
    # the RELAX TIME command line, the value of i can be from
    # 1 through 30
    1PSI PRONY <integer>i = <real>psi1_i
    2PSI PRONY <integer>i = <real>psi2_i
    3PSI PRONY <integer>i = <real>psi3_i
    4PSI PRONY <integer>i = <real>psi4_i
    5PSI PRONY <integer>i = <real>psi5_i
    RELAX TIME <integer>i = <real>tau_i
    REFERENCE TEMP = <real>tref
    REFERENCE DENSITY = <real>rhoref
    WLF C1 = <real>wlf_c1
    WLF C2 = <real>wlf_c2
    B SHIFT CONSTANT = <real>b_shift
    SHIFT REF VALUE = <real>shift_ref
    WWBETA 1PSI = <real>wwb_1psi
    WWTAU 1PSI = <real>wwt_1psi
    WWBETA 2PSI = <real>wwb_2psi
    WWTAU 2PSI = <real>wwt_2psi
    WWBETA 3PSI = <real>wwb_3psi
    WWTAU 3PSI = <real>wwt_3psi
    WWBETA 4PSI = <real>wwb_4psi
    WWTAU 4PSI = <real>wwt_4psi
    WWBETA 5PSI = <real>wwb_5psi
    WWTAU 5PSI = <real>wwt_5psi
    DOUBLE INTEG FACTOR = <real>dble_int_fac
    REF RUBBERY HCAPACITY = <real>hcapr
    REF GLASSY HCAPACITY = <real>hcapg
```

```
GLASS TRANSITION TEM = <real>tg
REF GLASSY C11 = <real>c11g
REF RUBBERY C11 = <real>c11r
REF GLASSY C22 = <real>c22g
REF RUBBERY C22 = <real>c22r
REF GLASSY C33 = <real>c33g
REF RUBBERY C33 = <real>c33r
REF GLASSY C12 = <real>c12g
REF RUBBERY C12 = <real>c12r
REF GLASSY C13 = <real>c13g
REF RUBBERY C13 = <real>c13r
REF GLASSY C23 = <real>c23g
REF RUBBERY C23 = <real>c23r
REF GLASSY C44 = <real>c44g
REF RUBBERY C44 = <real>c44r
REF GLASSY C55 = <real>c55g
REF RUBBERY C55 = <real>c55r
REF GLASSY C66 = <real>c66g
REF RUBBERY C66 = <real>c66r
REF GLASSY CTE1 = <real>cte1g
REF RUBBERY CTE1 = <real>cte1r
REF GLASSY CTE2 = <real>cte2g
REF RUBBERY CTE2 = <real>cte2r
REF GLASSY CTE3 = <real>cte3g
REF RUBBERY CTE3 = <real>cte3r
LINEAR VISCO TEST = <real>lvt
T DERIV GLASSY C11 = <real>dc11gdT
T DERIV RUBBERY C11 = <real>dc11rdT
T DERIV GLASSY C22 = <real>dc22gdT
T DERIV RUBBERY C22 = <real>dc22rdT
T DERIV GLASSY C33 = <real>dc33gdT
T DERIV RUBBERY C33 = <real>dc33rdT
T DERIV GLASSY C12 = <real>dc12gdT
T DERIV RUBBERY C12 = <real>dc12rdT
T DERIV GLASSY C13 = <real>dc13gdT
T DERIV RUBBERY C13 = <real>dc13rdT
T DERIV GLASSY C23 = <real>dc23gdT
T DERIV RUBBERY C23 = <real>dc23rdT
T DERIV GLASSY C44 = <real>dc44gdT
T DERIV RUBBERY C44 = <real>dc44rdT
T DERIV GLASSY C55 = <real>dc55gdT
T DERIV RUBBERY C55 = <real>dc55rdT
T DERIV GLASSY C66 = <real>dc66gdT
T DERIV RUBBERY C66 = <real>dc66rdT
T DERIV GLASSY CTE1 = <real>dcte1gdT
T DERIV RUBBERY CTE1 = <real>dcte1rdT
T DERIV GLASSY CTE2 = <real>dcte2gdT
```

```
T DERIV RUBBERY CTE2 = <real>dcte2rdT
T DERIV GLASSY CTE3 = <real>dcte3gdT
T DERIV RUBBERY CTE3 = <real>dcte3rdT
T DERIV GLASSY HCAPACITY = <real>dhcapgdT
T DERIV RUBBERY HCAPACITY = <real>dhcaprdT
REF PSIC = <real>psic_ref
T DERIV PSIC = <real>dpsicdT
T 2DERIV PSIC = <real>d2psicdT2
PSI EQ 2T = <real>psitt
PSI EQ 3T = <real>psittt
PSI EQ 4T = <real>psitttt
PSI EQ XX 11 = <real>psiXX11
PSI EQ XX 22 = <real>psiXX22
PSI EQ XX 33 = <real>psiXX33
PSI EQ XX 12 = <real>psiXX12
PSI EQ XX 13 = <real>psiXX13
PSI EQ XX 23 = <real>psiXX23
PSI EQ XX 44 = <real>psiXX44
PSI EQ XX 55 = <real>psiXX55
PSI EQ XX 66 = <real>psiXX66
PSI EQ XXT 11 = <real>psiXXT11
PSI EQ XXT 22 = <real>psiXXT22
PSI EQ XXT 33 = <real>psiXXT33
PSI EQ XXT 12 = <real>psiXXT12
PSI EQ XXT 13 = <real>psiXXT13
PSI EQ XXT 23 = <real>psiXXT23
PSI EQ XXT 44 = <real>psiXXT44
PSI EQ XXT 55 = <real>psiXXT55
PSI EQ XXT 66 = <real>psiXXT66
PSI EQ XT 1 = <real>psiXT1
PSI EQ XT 2 = <real>psiXT2
PSI EQ XT 3 = <real>psiXT3
PSI EQ XTT 1 = <real>psiXTT1
PSI EQ XTT 2 = <real>psiXTT2
PSI EQ XTT 3 = <real>psiXTT3
REF PSIA 11 = <real>psiA11
REF PSIA 22 = <real>psiA22
REF PSIA 33 = <real>psiA33
REF PSIA 12 = <real>psiA12
REF PSIA 13 = <real>psiA13
REF PSIA 23 = <real>psiA23
REF PSIA 44 = <real>psiA44
REF PSIA 55 = <real>psiA55
REF PSIA 66 = <real>psiA66
T DERIV PSIA 11 = <real>dpsiA11dT
T DERIV PSIA 22 = <real>dpsiA22dT
T DERIV PSIA 33 = <real>dpsiA33dT
```

```
    T DERIV PSIA 12 = <real>dpsiA12dT
    T DERIV PSIA 13 = <real>dpsiA13dT
    T DERIV PSIA 23 = <real>dpsiA23dT
    T DERIV PSIA 44 = <real>dpsiA44dT
    T DERIV PSIA 55 = <real>dpsiA55dT
    T DERIV PSIA 66 = <real>dpsiA66dT
    REF PSIB 1 = <real>psiB1
    REF PSIB 2 = <real>psiB2
    REF PSIB 3 = <real>psiB3
    T DERIV PSIB 1 = <real>dpsiB1dT
    T DERIV PSIB 2 = <real>dpsiB2dT
    T DERIV PSIB 3 = <real>dpsiB3dT
    PSI POT TT = <real>psipotTT
    PSI POT TTT = <real>psipotTTT
    PSI POT TTTT = <real>psipotTTTT
    PSI POT XT 1 = <real>psipotXT1
    PSI POT XT 2 = <real>psipotXT2
    PSI POT XT 3 = <real>psipotXT3
    PSI POT XTT 1 = <real>psipotXTT1
    PSI POT XTT 2 = <real>psipotXTT2
    PSI POT XTT 3 = <real>psipotXTT3
    PSI POT XXT 11 = <real>psipotXXT11
    PSI POT XXT 22 = <real>psipotXXT22
    PSI POT XXT 33 = <real>psipotXXT33
    PSI POT XXT 12 = <real>psipotXXT12
    PSI POT XXT 13 = <real>psipotXXT13
    PSI POT XXT 23 = <real>psipotXXT23
    PSI POT XXT 44 = <real>psipotXXT44
    PSI POT XXT 55 = <real>psipotXXT55
    PSI POT XXT 66 = <real>psipotXXT66
  END [PARAMETERS FOR MODEL NLVE_3D_ORTHOTROPIC]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The NLVE three-dimensional orthotropic model is a nonlinear viscoelastic orthotropic continuum model that describes the behavior of fiber-reinforced polymer-matrix composites. In addition to being able to model the linear elastic and linear viscoelastic behaviors of such composites, it also can capture both “weak” and “strong” nonlinear viscoelastic effects such as stress dependence of the creep compliance and viscoelastic yielding. This model can be used in both Presto and Adagio.

Because the NLVE model is still under active development and also because it has an extensive list of command lines, we have not followed the typical approach in documenting this model.

4.2.26 Stiff Elastic

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL STIFF_ELASTIC
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    BULK MODULUS = <real>bulk_modulus
    SHEAR MODULUS = <real>shear_modulus
    LAMBDA = <real>lambda
    SCALE FACTOR = <real>scale_factor
    REFERENCE STRAIN = <real>reference_strain
  END [PARAMETERS FOR MODEL STIFF_ELASTIC]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The stiff elastic model is a variation of the isotropic elastic model. The stiff elastic model can be used in both Presto and Adagio. When the model is used in Adagio, it is typically used with the control-stiffness option in Adagio's multilevel solver. The control-stiffness option is implemented via the `CONTROL STIFFNESS` command block and is discussed in Chapter 3 of the Adagio user's guide. The stiff elastic model is used to lower the stiffness of the bulk and shear behaviors of relatively stiff materials to yield a material response more amenable to solution using Adagio's conjugate gradient solver. The final material behavior that is calculated corresponds to the actual moduli that are specified. When this model is used in Presto, the material scalings are ignored.

The command block for a stiff elastic material starts with the line:

```
BEGIN PARAMETERS FOR MODEL STIFF_ELASTIC
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL STIFF_ELASTIC]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.
- The Biot's coefficient of the material is defined with the `BIOTS COEFFICIENT` command line.
- The `thermal strain option` is used to define thermal strains. See Section 4.1.3.1 and Section 4.1.3.2 for further information on defining and activating thermal strains.
- Any two of the following elastic constants are required to define the unscaled material response:
    - Young's modulus is defined with the `YOUNGS MODULUS` command line.
    - Poisson's ratio is defined with the `POISSONS RATIO` command line.
    - The bulk modulus is defined with the `BULK MODULUS` command line.
    - The shear modulus is defined with the `SHEAR MODULUS` command line.
    - Lambda is defined with the `LAMBDA` command line.
- The following command lines are used only in Adagio:
    - The material scaling is defined with the `SCALE FACTOR` command line.
    - The reference strain is defined with the `REFERENCE STRAIN` command line.

As noted previously, only two of the elastic constants are required to define the unscaled material response.

The scaled bulk and shear moduli are computed using a Young's modulus scaled by the value given by the `SCALE FACTOR` line command.

The `REFERENCE STRAIN` command line supplies a value for the reference strain used to create a normalized material constraint violation that is based on strains. Specifying a reference strain implies the use of strains for measuring the material constraint violation (or part of the control-stiffness error in Adagio). Otherwise, the material constraint violation is determined using the change in the scaled stress response over the current model problem.

4.2.27 Swanson Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  BEGIN PARAMETERS FOR MODEL SWANSON
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    BULK MODULUS = <real>bulk_modulus
    SHEAR MODULUS = <real>shear_modulus
    LAMBDA = <real>lambda
    A1 = <real>a1
    P1 = <real>p1
    B1 = <real>b1
    Q1 = <real>q1
    C1 = <real>c1
    R1 = <real>r1
    CUT OFF STRAIN = <real>ecut
    THERMAL EXPANSION FUNCTION = <string>eth_function_name
    TARGET E = <real>target_e
    TARGET E FUNCTION = <string>etar_function_name
    MAX POISSONS RATIO = <real>max_poissons_ratio(0.5)
    REFERENCE STRAIN = <real>reference_strain
  END [PARAMETERS FOR MODEL SWANSON]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The Swanson model is a hyperelastic model that is used to model rubber. The Swanson model can be used in both Presto and Adagio. When the model is used in Adagio, it can be used with or without the control-stiffness option in Adagio's multilevel solver for nearly incompressible materials where Poisson's ratio, ν, $\approx$ 0.5. The control-stiffness option is implemented via the `CONTROL STIFFNESS` command block and is discussed in Chapter 3 of the Adagio user's guide. In the course of solving a series of model problems in Adagio, the material response from this model incorporates scaling the bulk and/or shear behaviors to yield a material response that is more amenable to solution using Adagio's conjugate gradient solver. The final material behavior that is calculated corresponds to the actual moduli that are specified. When this model is used in Presto, the material scalings are ignored.

The command block for a Swanson material starts with the line:

```
BEGIN PARAMETERS FOR MODEL SWANSON
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL SWANSON]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.
- The Biot's coefficient of the material is defined with the `BIOTS COEFFICIENT` command line.
- Any two of the following elastic constants are required to define the unscaled bulk behavior:
  - Young's modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson's ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.
- The following command lines are required:
  - The material constant A1 is defined with the `A1` command line.
  - The material constant P1 is defined with the `P1` command line.
  - The material constant B1 is defined with the `B1` command line.
  - The material constant Q1 is defined with the `Q1` command line.
  - The material constant C1 is defined with the `C1` command line.
  - The material constant R1 is defined with the `R1` command line.
  - The small-strain value used for computing the initial shear modulus is defined with the `CUT OFF STRAIN` command line.
- The `THERMAL EXPANSION FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope that describes the linear thermal expansion as function of temperature. This command line is optional. If it is not present, there is no thermal expansion. See the usage discussion below.
- The following material-scaling command lines are used only in Adagio:
  - The target Young's modulus is defined with the `TARGET E` command line. This command line is optional. See the usage discussion below.
  - The `TARGET E FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope that describes the time variation of the target Young's modulus. This command line is optional. If it is not present, there is no time dependence in the Target E parameter. See the usage discussion below.
  - The maximum Poisson's ratio is defined with the `MAX POISSONS RATIO` command line. This command line is optional and will default to 0.5 if not specified. See the usage discussion below.
  - The reference strain is defined with the `REFERENCE STRAIN` command line. This command line is optional. See the usage discussion below.

As noted previously, only two of the elastic constants are required to define the unscaled bulk behavior. Together, the values for parameters in the `A1`, `P1`, `B1`, `Q1`, `C1`, and `R1` command lines define the unscaled shear behavior, so these command lines must be present. The initial unscaled shear modulus is determined from those parameter values along with the value of the parameter in the `CUT OFF STRAIN` command line, so this command line must also be present.

The Swanson model, like a few of the material models, allows for the specification of thermal strain behavior within the material model itself, via the `THERMAL EXPANSION FUNCTION` command line. This command line, like the other "function-type" command lines in this model, requires that a function associated with the name be defined in the SIERRA scope.

The bulk and shear scalings that can be used with the multilevel solver in Adagio are specified via a combination of the `TARGET E`, `TARGET E FUNCTION`, and `MAX POISSONS RATIO` command lines. If the `TARGET E` command line is not included (and the `MAX POISSONS RATIO` command line is included), the shear scaling is set to 1.0, and the bulk scaling is determined from the ratio of the scaled bulk modulus to its unscaled value, where the scaled bulk modulus is computed using the value of the `max_poissons_ratio` parameter along with the unscaled shear modulus. On the other hand, if both the `TARGET E` command line and the `MAX POISSONS RATIO` are included, bulk and shear scaling values are computed using scaled moduli that are calculated from the `target_e` and `max_poissons_ratio` parameter values.

Including the `TARGET E FUNCTION` command line allows time-dependent bulk and shear scaling to be used. If this command line is not specified, the bulk and shear scalings remain constant in solution time. If the command line is specified, the target Young's modulus that is used for computing the scaled moduli is multiplied by the function value.

The `REFERENCE STRAIN` command line supplies a value for the reference strain used to create a normalized material constraint violation that is based on strains. Specifying a reference strain implies the use of strains for measuring the material constraint violation (or part of the control-stiffness error in Adagio). Otherwise, the material constraint violation is determined using the change in the scaled stress response over the current model problem.

Output variables available for this model are listed in Table 8.40. Brief documentation on the theoretical basis for the Swanson model is given in Reference 17.

4.2.28 Viscoelastic Swanson Model

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  BEGIN PARAMETERS FOR MODEL VISCOELASTIC_SWANSON
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    BULK MODULUS = <real>bulk_modulus
    SHEAR MODULUS = <real>shear_modulus
    LAMBDA = <real>lambda
    A1 = <real>a1
    P1 = <real>p1
    B1 = <real>b1
    Q1 = <real>q1
    C1 = <real>c1
    R1 = <real>r1
    CUT OFF STRAIN = <real>ecut
    THERMAL EXPANSION FUNCTION = <string>eth_function_name
    PRONY SHEAR INFINITY = <real>ginf
    PRONY SHEAR 1 = <real>g1
    PRONY SHEAR 2 = <real>g2
    PRONY SHEAR 3 = <real>g3
    PRONY SHEAR 4 = <real>g4
    PRONY SHEAR 5 = <real>g5
    PRONY SHEAR 6 = <real>g6
    PRONY SHEAR 7 = <real>g7
    PRONY SHEAR 8 = <real>g8
    PRONY SHEAR 9 = <real>g9
    PRONY SHEAR 10 = <real>g10
    SHEAR RELAX TIME 1 = <real>tau1
    SHEAR RELAX TIME 2 = <real>tau2
    SHEAR RELAX TIME 3 = <real>tau3
    SHEAR RELAX TIME 4 = <real>tau4
    SHEAR RELAX TIME 5 = <real>tau5
    SHEAR RELAX TIME 6 = <real>tau6
    SHEAR RELAX TIME 7 = <real>tau7
    SHEAR RELAX TIME 8 = <real>tau8
    SHEAR RELAX TIME 9 = <real>tau9
    SHEAR RELAX TIME 10 = <real>tau10
    WLF COEF C1 = <real>wlf_c1
    WLF COEF C2 = <real>wlf_c2
    WLF TREF = <real>wlf_tref
    NUMERICAL SHIFT FUNCTION = <string>ns_function_name
    TARGET E = <real>target_e
    TARGET E FUNCTION = <string>etar_function_name
```

```
    MAX POISSONS RATIO = <real>max_poissons_ratio(0.5)
    REFERENCE STRAIN = <real>reference_strain
  END [PARAMETERS FOR MODEL VISCOELASTIC_SWANSON]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The viscoelastic Swanson model is a finite strain viscoelastic model that has an initial elastic response that matches the Swanson material model. The bulk response is elastic, while the shear response is viscoelastic. This model is commonly employed in simulating the response of rubber materials. The viscoelastic Swanson model can be used in both Presto and Adagio. When the model is used in Adagio, it can be used with or without the control-stiffness option in Adagio's multilevel solver for nearly incompressible materials where Poisson's ratio, ν, ≈ 0.5. The control-stiffness option is implemented via the `CONTROL STIFFNESS` command block and is discussed in Chapter 3 of the Adagio user's guide. In the course of solving a series of model problems in Adagio, the material response from this model incorporates scaling the bulk and/or shear behaviors to yield a material response that is more amenable to solution using Adagio's conjugate gradient solver. The final material behavior that is calculated corresponds to the actual moduli that are specified. When this model is used in Presto, the material scalings are ignored.

The command block for a viscoelastic Swanson material starts with the line:

```
BEGIN PARAMETERS FOR MODEL VISCOELASTIC_SWANSON
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL VISCOELASTIC_SWANSON]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.
- The Biot's coefficient of the material is defined with the `BIOTS COEFFICIENT` command line.
- Any two of the following elastic constants are required to define the unscaled bulk behavior:
  - Young's modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson's ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.
- The following command lines are required:
  - The material constant A1 is defined with the `A1` command line.

- The material constant P1 is defined with the `P1` command line.
- The material constant B1 is defined with the `B1` command line.
- The material constant Q1 is defined with the `Q1` command line.
- The material constant C1 is defined with the `C1` command line.
- The material constant R1 is defined with the `R1` command line.
- The small-strain value used for computing the glassy shear modulus is defined with the `CUT OFF STRAIN` command line.

- The `THERMAL EXPANSION FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope that describes the linear thermal expansion as function of temperature. This command line is optional. If it is not present, there is no thermal expansion. See the usage discussion below.

- `PRONY SHEAR INFINITY` command line. This command line is required.

- The normalized relaxation spectra coefficients are specified with the `PRONY SHEAR I` command lines, where the value of `I` varies sequentially from 1 to 10. These command lines are optional.

- The normalized relaxation spectra time constants are specified with the `SHEAR RELAX TIME I` command lines, where the value of `I` varies sequentially from 1 to 10. These command lines are optional.

- `WLF COEF C1` command line. This command line is required.

- `WLF COEF C2` command line. This command line is required.

- `WLF TREF` command line. This command line is required.

- `NUMERICAL SHIFT FUNCTION` command line. This command line is optional.

- The following material-scaling command lines are used only in Adagio:

  - The target Young's modulus is defined with the `TARGET E` command line. This command line is required. See the usage discussion below.
  - The `TARGET E FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope that describes the time variation of the target Young's modulus. This command line is optional. If it is not present, there is no time dependence in the Target E parameter. See the usage discussion below.
  - The maximum Poisson's ratio is defined with the `MAX POISSONS RATIO` command line. This command line is optional and will default to 0.5 if not specified. See the usage discussion below.
  - The reference strain is defined with the `REFERENCE STRAIN` command line. This command line is required. See the usage discussion below.

As noted previously, only two of the elastic constants are required to define the unscaled bulk behavior. Together, the values for parameters in the `A1`, `P1`, `B1`, `Q1`, `C1`, and `R1` command lines define the unscaled glassy shear behavior, so these command lines must be present. The unscaled glassy shear modulus is determined from those parameter values along with the value of the parameter in the `CUT OFF STRAIN` command line, so this command line must also be present.

The viscoelastic Swanson model, like a few of the material models, allows for the specification of thermal strain behavior within the material model itself, via the `THERMAL EXPANSION FUNCTION` command line. This command line, like the other "function-type" command lines in this model requires that a function associated with the name be defined in the SIERRA scope.

The bulk and shear scalings that can be used with the multilevel solver in Adagio are specified via a combination of the `TARGET E`, `TARGET E FUNCTION`, and `MAX POISSONS RATIO` command lines. If the `TARGET E` command line is not included (and the `MAX POISSONS RATIO` command line is included), the shear scaling is set to 1.0, and the bulk scaling is determined from the ratio of the scaled bulk modulus to its unscaled value, where the scaled bulk modulus is computed using the value of the `max_poissons_ratio` parameter along with the unscaled shear modulus. On the other hand, if both the `TARGET E` command line and the `MAX POISSONS RATIO` command line are included, bulk and shear scaling values are computed using scaled moduli that are calculated from the `target_e` and `max_poissons_ratio` parameter values.

Including the `TARGET E FUNCTION` command line allows time-dependent bulk and shear scaling to be used. If this command line is not specified, the bulk and shear scalings remain constant in solution time. If the command line is specified, the target Young's modulus that is used for computing the scaled moduli is multiplied by the function value.

The `REFERENCE STRAIN` command line supplies a value for the reference strain used to create a normalized material constraint violation that is based on strains. Specifying a reference strain implies the use of strains for measuring the material constraint violation (or part of the control-stiffness error in Adagio). Otherwise, the material constraint violation is determined using the change in the scaled stress response over the current model problem.

Output variables available for this model are listed in Table 8.41. Brief documentation on the theoretical basis for the viscoelastic Swanson model is given in References 17, 18, 19, and 20.

4.3 Cohesive Zone Material Models

Several material models are available for use with cohesive zone elements, and are described in this section.

Traction separation models used for cohesive surface elements are input within `BEGIN PROPERTY SPECIFICATION FOR MATERIAL` blocks in the same manner as continuum models. Although density is not a property used by cohesive zone elements, because of their specification within this block, all of these models currently require a density to be provided as part of their input.

4.3.1 Traction Decay

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  #
  DENSITY = <real>density_value
  #
  BEGIN PARAMETERS FOR MODEL TRACTION_DECAY
    NORMAL DECAY LENGTH = <real>
    TANGENTIAL DECAY LENGTH = <real>
  END [PARAMETERS FOR MODEL TRACTION_DECAY]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The Traction Decay cohesive model is a simple model that get initialized with a traction upon activation or insertion of the cohesive element, and decays that traction to zero over specified values of normal and tangential separation. This model is only valid to use in conjunction with dynamic cohesive zone activation through MPC deactivation or dynamic insertion of cohesive surface elements.

The command block for a traction decay material starts with the line:

```
BEGIN PARAMETERS FOR MODEL TRACTION_DECAY
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL TRACTION_DECAY]
```

In the above command block:

- The density of the material is defined with the `DENSITY` command line. Although this is not used in the model, it is currently a required input parameter.
- The separation length over which the normal traction decays to zero is set by the `NORMAL DECAY LENGTH` command line.
- The separation length over which the tangential traction decays to zero is set by the `TANGENTIAL DECAY LENGTH` command line.

4.3.2 Tvergaard Hutchinson

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  #
  DENSITY = <real>density_value
  #
  BEGIN PARAMETERS FOR MODEL TVERGAARD_HUTCHINSON
    INIT TRACTION METHOD = IGNORE|ADD (IGNORE)
    LAMBDA_1 = <real>
    LAMBDA_2 = <real>
    NORMAL LENGTH SCALE = <real>
    TANGENTIAL LENGTH SCALE = <real>
    PEAK TRACTION = <real>
    PENETRATION STIFFNESS MULTIPLIER = <real>
    NORMAL INITIAL TRACTION DECAY LENGTH = <real>
    TANGENTIAL INITIAL TRACTION DECAY LENGTH = <real>
    USE ELASTIC UNLOADING = NO|YES (YES)
  END [PARAMETERS FOR MODEL TVERGAARD_HUTCHINSON]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The Tvergaard Hutchinson cohesive model combines the normal and tangential separation into a single normalized separation and calculates a traction per unit length based on this value. This model then calculates normal and tangential traction based on the ratio of the normal and tangential length scales.

For a Tvergaard Hutchinson surface model, a Tvergaard Hutchinson command block starts with the input line: The command block for a traction decay material starts with the line:

```
BEGIN PARAMETERS FOR MODEL TVERGAARD_HUTCHINSON
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL TVERGAARD_HUTCHINSON]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line. Although this is not used in the model, it is currently a required input parameter.
- For dynamically activated or dynamically inserted cohesive surface elements, an initial traction can be added to the calculated traction based on element properties specified in the `ELEMENT DEATH` block and is set via the `INIT TRACTION METHOD`. The default behavior is to ignore any initial tractions and let the traction-separation law dictate the behavior.
- `LAMBDA_1` indicates the normalized separation at which the traction response flattens with an additional increase in separation.
- `LAMBDA_2` indicates the normalized separation at which the traction begins to degrade with an additional increase in separation.

- The separation at which failure occurs in the normal direction is prescribed using the `NORMAL LENGTH SCALE` command.
- The maximum traction is specified through the `PEAK TRACTION` command.
- `NORMAL INITIAL TRACTION DECAY LENGTH` and `TANGENTIAL INITIAL TRACTION DECAY LENGTH` specify the length over which the initial traction will decay to zero in the normal and tangential direction respectively if the cohesive elements are initialized during element death. This decay length is independent of the `NORMAL LENGTH SCALE` and `TANGENTIAL LENGTH SCALE` specified for the calculated traction.
- The separation at which failure occurs in the tangential direction is prescribed using the `TANGENTIAL LENGTH SCALE` command.
- To help prevent interpenetration of the cohesive faces, use the `PENETRATION STIFFNESS MULTIPLIER` command to artificially increase the normal traction when penetration occurs. WARNING: cohesive elements are not well equipped to handle compression. This is an ad-hoc method to handle contact.
- Set the `USE ELASTIC UNLOADING` command to `YES` to force this model to unload elastically.

4.3.3 Thouless Parmigiani

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value

  BEGIN PARAMETERS FOR MODEL THOULESS_PARMIGIANI
    INIT TRACTION METHOD = IGNORE|ADD (IGNORE)
    LAMBDA_1_N = <real>
    LAMBDA_1_T = <real>
    LAMBDA_2_N = <real>
    LAMBDA_2_T = <real>
    NORMAL LENGTH SCALE = <real>
    PEAK NORMAL TRACTION = <real>
    TANGENTIAL LENGTH SCALE = <real>
    PEAK Tangential TRACTION = <real>
    PENETRATION STIFFNESS MULTIPLIER = <real>
    USE ELASTIC UNLOADING = NO|YES (YES)
  END [PARAMETERS FOR MODEL THOULESS_PARMIGIANI]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The Thouless Parmigiani model support mixed-mode fracture more accurately than the Tvergaard Hutchinson model by separating the normal and tangential components, allowing one to fail independently of the other. Failure of this model is dependent on the energy release of both normal and tangential components. The shape of the traction-separation curve for this model is hardening, followed by a plateau, followed by softening.

The command block for a Thouless Parmigiani material starts with the line:

```
BEGIN PARAMETERS FOR MODEL THOULESS_PARMIGIANI
```

and terminates with the line:

```
END [PARAMETERS FOR MODEL THOULESS_PARMIGIANI]
```

In the above command block:

- The density of the material is defined with the `DENSITY` command line. Although this is not used in the model, it is currently a required input parameter.
- For dynamically activated or dynamically inserted cohesive surface elements, an initial traction can be added to the calculated traction based on element properties specified in the `ELEMENT DEATH` block and is set via the `INIT TRACTION METHOD`. The default behavior is to ignore any initial tractions and let the traction-separation law dictate the behavior.
- `LAMBDA_1_N` indicates the normalized normal separation at which the traction response flattens with an additional increase in separation.
- `LAMBDA_1_T` indicates the normalized tangential separation at which the traction response flattens with an additional increase in separation.

- `LAMBDA_2_N` indicates the normalized normal separation at which the traction begins to decrease with an additional increase in separation.
- `LAMBDA_2_T` indicates the normalized tangential separation at which the traction begins to decrease with an additional increase in separation.
- The separation at which failure occurs in the normal direction is prescribed using the `NORMAL LENGTH SCALE` command.
- The maximum normal traction is specified through the `PEAK NORMAL TRACTION` command.
- The separation at which failure occurs in the tangential direction is prescribed using the `TANGENTIAL LENGTH SCALE` command.
- The maximum tangential traction is specified through the `PEAK TANGENTIAL TRACTION` command.
- To help prevent interpenetration of the cohesive faces, use the `PENETRATION STIFFNESS MULTIPLIER` command to artificially increase the normal traction when penetration occurs. WARNING: cohesive elements are not well equipped to handle compression. This is an ad-hoc method to handle contact.
- Set the `USE ELASTIC UNLOADING` command to `YES` to force this model to unload elastically.

4.4 References

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Chapter 5

Elements

This chapter explains how material, geometric, and other properties are associated with the various element blocks in a mesh file. A mesh file contains, for the most part, only topological information about elements. For example, there may be a group of elements in the mesh file that consists of four nodes defining a planar facet in three-dimensional space. Whether or not these elements are used as shells or membranes in our actual model of an object is determined by command lines in the input file. The specifics of a material type associated with these four node facets are also set in the input file.

Most elements can be used in either Presto or Adagio. If an element is available in one code but not the other, this information will be noted for the element. There are special element implementations in Presto for peridynamics and for smoothed particle hydrodynamics (SPH). These sections are included in the Presto manual but not the Adagio manual. This chapter also includes descriptions of the commands for mass property calculations, element death, and mesh rebalancing. Two “element-like" capabilities are discussed in Chapter 5—torsional springs and rigid bodies.

Highlights of chapter contents follow. Section 5.1 discusses the `FINITE ELEMENT MODEL` command block, which provides the description of a mesh that will be associated with the elements. Section 5.2 presents the section command blocks that are used to define the different element sections.

Next are descriptions of command blocks that exhibit element-like functionality. Section 5.3.1 explains the use of rigid bodies. Section 5.3.2 describes how to implement a torsional spring mechanism in Presto. Section 5.4 describes the `MASS PROPERTIES` command block, which lets the user compute the total mass of the model or the mass of sub-parts of the model once the element blocks are completely defined in terms of geometry and material. Section 5.5 details the `ELEMENT DEATH` command block, which lets the user delete (kill) elements based on various criteria during an analysis. A command block for derived quantities that are to be used with transfers or error estimation is discussed in Section 5.7. Finally, Section 5.8 presents various options for partitioning a mesh for parallel runs with Presto. The partitioning scheme can greatly influence the run time for a particular analysis. The command block for selecting a partitioning scheme is `REBALANCE`. The `REBALANCE` references a `ZOLTAN PARAMETERS` command block. The `ZOLTAN PARAMETERS` command block sets various parameters that control the partitioning.

Most of the command blocks and command lines described next appear within the SIERRA scope. There are some exceptions, and these exceptions are noted.

5.1 Finite Element Model

```
BEGIN FINITE ELEMENT MODEL <string>mesh_descriptor
  DATABASE NAME = <string>mesh_file_name
  DATABASE TYPE = <string>database_type(exodusII)
  ALIAS <string>mesh_identifier AS <string>user_name
  OMIT BLOCK <string>block_list
  COMPONENT SEPARATOR CHARACTER = <string>separator
  BEGIN PARAMETERS FOR BLOCK [<string list>block_names]
    #
    # Command lines that define attributes for
    # a particular element block appear in this
    # command block.
    #
  END [PARAMETERS FOR BLOCK <string list>block_names]
END [FINITE ELEMENT MODEL <string>mesh_descriptor]
```

The input file must point to a mesh file that is to be used for an analysis. The name of the mesh file appears within a `FINITE ELEMENT MODEL` command block, which appears in the SIERRA scope. In this command block, you will identify the particular mesh file that describes your model. Also within this command block, there will be one or more `PARAMETERS FOR BLOCK` command blocks. (All the `PARAMETERS FOR BLOCK` command blocks are embedded in the `FINITE ELEMENT MODEL` command block.) Within the `PARAMETERS FOR BLOCK` command block, you will set a material type and model, a section, and various other parameters for the element block. The concept of "section" is explained in Section 5.1.5.

The current element library is as follows:

- Eight-node, uniform-gradient hexahedron: Both a midpoint-increment formulation [1] and a strongly objective formulation are implemented [2]. These elements can be used with any of the material models described in Chapter 4.

- Eight-node, selective-deviatoric hexahedron: Only a strongly objective formulation is provided. This element can be used with any of the material models described in Chapter 4.

- Four-node tetrahedron: There is now the regular element formulation for the four-node tetrahedron and a node-based formulation for the four-node tetrahedron. For the regular element formulation, only a strongly objective formulation is implemented. The concept of a node-based four-node tetrahedron is described in Reference 3. The regular four-node tetrahedron can be used with any of the material models described in Chapter 4. The node-based tetrahedron can be used with any of the material models described in Chapter 4. When

using node-based tetrahedron it is important that nodal quantities are used where other element types use element quantities. For example, you evaluate element variable stress with a regular four-node tetrahedron but in node-based tetrahedron one should use nodal variable element_stress_## where ## is a number that increments from 1. Nodal variables for node-based tets will live on all nodes but are zero where they are not used. Element variables for node-based elements serve as intermediate variables and should not be used in post processing in the same way as other regular element variables.

- Eight-node tetrahedron: This tetrahedral element has nodes at the four vertices and nodes on the four faces. The eight-node tetrahedron has only a strongly objective formulation [4]. The eight-node tetrahedron uses a mean quadrature formulation even though it has the additional nodes. This element can be used with any of the material models described in Chapter 4.

- Ten-node tetrahedron: Only a strongly objective formulation is implemented. This element can be used with any of the material models described in Chapter 4.

- Four-node, quadrilateral, uniform-gradient membrane: Both a midpoint-increment formulation and a strongly objective formulation are implemented. This element is derived from the Key-Hoff shell formulation [5]. The strongly objective formulation has not been extensively tested, and it is recommended that the midpoint-increment formulation, which is the default, be used for this element type. These elements can be used with any of the following material models described in Chapter 4:

  – Elastic
  – Elastic-plastic
  – Elastic-plastic power-law hardening
  – Multilinear elastic-plastic hardening (no failure)

- Three-node, triangular shell: This shell uses the same formulation as the three-node triangular shell in Pronto [1]. A midpoint-increment formulation is implemented. This element can be used with any of the following material models described in Chapter 4:

  – Elastic
  – Elastic-plastic
  – Elastic-plastic power-law hardening
  – Multilinear elastic-plastic hardening without failure
  – Multilinear elastic-plastic hardening with failure

- Four-node, quadrilateral shell: This shell uses the Key-Hoff formulation [5]. Both a midpoint-increment formulation and a strongly objective formulation are implemented. The strongly objective formulation has not been extensively tested, and it is recommended that the midpoint-increment formulation, which is the default, be used for this element type. These elements can be used with any of the following material models described in Chapter 4:

  - Elastic
  - Elastic-plastic
  - Elastic-plastic power-law hardening
  - Multilinear elastic-plastic hardening without failure
  - Multilinear elastic-plastic hardening with failure

- Four-node, quadrilateral, selective-deviatoric membrane: Only a midpoint-increment formulation is implemented. These elements can be used with any of the following material models described in Chapter 4:

  - Elastic
  - Elastic-plastic
  - Elastic-plastic power-law hardening
  - Multilinear elastic-plastic hardening (no failure)

- Linear elastic shell element: The linear elastic shell element is linear in both a material and geometric sense. The linear elastic shell element can be used with any material, however it will use only the density and elastic material constants of that material. Use of the linear elastic shell element is specified with the `FORMULATION = NQUAD` command in the section command block.

- Two-node beam: The beam element is a uniform result model. Strains and stresses are computed only at the midpoint of the element. These midpoint values determine the forces and moments for the beam. The beam element is based on an incremental kinematic formulation that is accurate for large strains and rotations (e.g. this element exactly agrees with a logarithmic strain formulation under large strain axial loading). Thinning of the cross section is taken into account through a constant volume assumption. There are five different sections currently implemented for the beam: rod, tube, bar, box, and I. This element can be used with any of the following material models described in Chapter 4:

  - Elastic
  - Elastic-plastic

- Two-node truss: The two-node truss element carries only a uniform axial stress. Currently, there is a linear-elastic material model for the truss element.

- Two-node spring: The two-node spring element computes a uniaxial resistance force based on a non-linear force-engineering strain function. This element can handle preloads, mass per unit length, resetting of the initial length after preload and any arbitrary loading function.

- Two-node damper: (Code Usage: Presto only) The two-node damping element computes a damping force based on the relative velocity of the two nodes along the axis of the element. This element uses only a damping parameter for a material property.

- Point mass: The point mass element allows the user to put a specified mass and/or rotational inertia at a node. This element requires input for density, but does not make use of any other material properties.
- Particle elements: These are one-dimensional elements. These elements can be used with any of the material models described in Chapter 4.

The command block to describe a mesh file begins with

```
BEGIN FINITE ELEMENT MODEL <string>mesh_descriptor
```

and is terminated with:

```
END [FINITE ELEMENT MODEL <string>mesh_descriptor]
```

where `mesh_descriptor` is a user-selected name for the mesh. In this section, we will first discuss the command lines within the scope of the `FINITE ELEMENT MODEL` command block but outside the scope of the `PARAMETERS FOR BLOCK` command block. We will then discuss the `PARAMETERS FOR BLOCK` command block and the associated command lines for this particular block.

5.1.1 Identification of Mesh File

Nested within the `FINITE ELEMENT MODEL` command block are two command lines (`DATABASE NAME` and `DATABASE TYPE`) that give the mesh name and define the type for the mesh file, respectively. The command line

```
DATABASE NAME = <string>mesh_file_name
```

gives the name of the mesh file with the string `mesh_file_name`. If the current mesh file is in the default directory and is named `job.g`, then this command line would appear as:

```
DATABASE NAME = job.g
```

If the mesh file is in some other directory, the command line would have to show the path to that directory. For parallel runs, the string `mesh_file_name` is the base name for the spread of parallel mesh files. For example, for a four-processor run, the actual mesh files associated with a base name of `job.g` would be `job.g.4.0`, `job.g.4.1`, `job.g.4.2`, and `job.g.4.3`. The database name on the command line would be `job.g`.

Two metacharacters can appear in the name of the mesh file. If the `%P` character is found in the name, it will be replaced with the number processors being used for the run. For example, if you are running on 1024 processors and use the name `mesh-%P/job.g`, then the name would be expanded to `mesh-1024/job.g` and the actual mesh files would be `mesh-1024/job.g.1024.0000` to `mesh-1024/job.g.1024.1023`. The other recognized metacharacter is `%B` which is replaced with the base name of the input file containing the input commands. For example, if the commands are in the file `my_analysis_run.i` and the mesh database name is specified as `%B.g`, then the mesh would be read from the file `my_analysis_run.g`.

If the mesh file does not use the Exodus II format, you must specify the format for the mesh file using the command line:

```
DATABASE TYPE = <string>database_type(exodusII)
```

Currently, only the Exodus II database format is supported by Presto and Adagio for mesh input. Other options may be added in the future.

5.1.2 Alias

It is possible to associate a user-defined name with some mesh entity. The mesh entity names for Exodus II entities are typically the concatenation of the entity type (for example, "block", "nodelist", or "surface"), an underscore ("_"), and the entity id. This generated name can be aliased to a more descriptive name by using the `ALIAS command line`:

```
ALIAS <string>mesh_identifier AS <string>user_name
```

This alias can then be used in other locations in the input file in place of the Exodus II name.

Examples of this association are as follows:

```
Alias block_1   as Case
Alias block_10  as Fin
Alias block_12  as Nose
Alias surface_1 as Nose_Case_Interface
Alias surface_2 as OuterBoundary
```

The above examples use the Exodus II naming convention described in Section 1.5.

5.1.3 Omit Block

If the finite element mesh contains element blocks that should be omitted from the finite element analysis, the `OMIT BLOCK` line command is used.

```
OMIT BLOCK <string>block_list
```

The element blocks listed in the command are removed from the model. Any nodesets or surfaces only existing on nodes or elements in the omitted element blocks are also omitted. Note that if this command is used in a parallel analysis, it is possible for the resulting model to become unbalanced if, for example, the omitted element blocks make up a large portion of the elements on one or more processors. In this case, the mesh can be rebalanced using the `REBALANCE` command described in Section 5.8.1.

Examples of omitting element blocks are:

```
Omit Block block_1 block_2
Omit Block block_10
```

5.1.4 Component Separator Character

A variable defined on the mesh database can be used as an initial condition, or a prescribed temperature with the `READ VARIABLE` command. If the variable is a vector or a tensor, then the base name of the variable will be separated from the suffixes with a separator character. The default separator character is an underscore, but it can be changed with the `COMPONENT SEPARATOR CHARACTER` command.

```
COMPONENT SEPARATOR CHARACTER = <string>character|NONE
```

For example, the variable `displacement` can have the suffixes `x`, `y`, etc. By default, the base name is separated from the suffixes with an underscore character so that we have `displacement_x`, `displacement_y`, etc. in the mesh file. The underscore can be replaced as the default separator by using the above command line. If the data used the period as the separator, then the command would be

```
COMPONENT SEPARATOR CHARACTER = .
```

For the displacement example the components would then appear in the mesh file as `displacement.x`, `displacement.y`, etc.

The separator can be eliminated with an empty string or `NONE`.

5.1.5 Descriptors of Element Blocks

```
BEGIN PARAMETERS FOR BLOCK [<string list>block_names]
  MATERIAL <string>material_name
  SOLID MECHANICS USE MODEL <string>model_name
  INCLUDE ALL BLOCKS
  REMOVE BLOCK = <string list>block_names
  SECTION = <string>section_id
  LINEAR BULK VISCOSITY =
    <real>linear_bulk_viscosity_value(0.06)
  QUADRATIC BULK VISCOSITY =
    <real>quad_bulk_viscosity_value(1.20)
  HOURGLASS STIFFNESS =
    <real>hour_glass_stiff_value(solid = 0.05,
      shell/membrane = 0.0)
  HOURGLASS VISCOSITY =
    <real>hour_glass_visc_value(solid = 0.0,
      shell/membrane = 0.0)
  MEMBRANE HOURGLASS STIFFNESS =
    <real>memb_hour_glass_stiff_value(0.0)
  MEMBRANE HOURGLASS VISCOSITY =
    <real>memb_hour_glass_visc_value(0.0)
  BENDING HOURGLASS STIFFNESS =
    <real>bend_hour_glass_stiff_value(0.0)
  BENDING HOURGLASS VISCOSITY =
```

```
    <real>bend_hour_glass_visc_value(0.0)
  TRANSVERSE SHEAR HOURGLASS STIFFNESS =
    <real>tshr_hour_glass_stiff_value(0.0)
  TRANSVERSE SHEAR HOURGLASS VISCOSITY =
    <real>tshr_hour_glass_visc_value(0.0)
  EFFECTIVE MODULI MODEL = <string>PRESTO|PRONTO|CURRENT|
      ELASTIC(PRONTO)
  ELEMENT NUMERICAL FORMULATION = <string>OLD|NEW(OLD)
  ACTIVE FOR PROCEDURE <string>proc_name DURING PERIODS
    <string list>period_names
  INACTIVE FOR PROCEDURE <string>proc_name DURING PERIODS
    <string list>period_names
END [PARAMETERS FOR BLOCK <string list>block_names]
```

The finite element model consists of one or more element blocks. Associated with an element block or group of element blocks will be a `PARAMETERS FOR BLOCK` command block, which is also referred to in this document as an *element-block command block*. The basic information about the element blocks (number of elements, topology, connectivity, etc.) is contained in a mesh file. Specific attributes for an element block must be specified in the input file. If for example, a block of eight-node hexahedra is to use the selective-deviatoric versus mean-quadrature formulation, then the selective-deviatoric formulation must be specified in the input file. The element library is listed at the beginning of Section 5.1.

The element-block command block begins with the input line

```
BEGIN PARAMETERS FOR BLOCK [<string list>block_names]
```

and is terminated with the input line:

```
END [PARAMETERS FOR BLOCK <string list>block_names]
```

Here `block_names` is a list of element blocks assigned to the element-block command block. Such a list must be included on the `BEGIN PARAMETERS FOR BLOCK` input line if the `INCLUDE ALL BLOCKS` line command is not used. If the format for the mesh file is Exodus II, the typical form of a `block_name` is `block_integerID`, where `integerID` is the integer identifier for the block. If the element block is 280, the value of `block_name` would be `block_280`. It is also possible to generate an alias identifier for the element block and use this for the `block_name`. If `block_280` is aliased to `AL6061`, then `block_name` becomes `AL6061`.

All the element blocks listed on the `PARAMETERS FOR BLOCK` command line (or all the element blocks included using the line commands `INCLUDE ALL BLOCKS` and `REMOVE BLOCK`) will have the same mechanics properties. The mechanics properties are set by use of the various command lines. One of the key command lines, i.e., `MATERIAL`, will let you associate a material with the elements in the block. Another key command line is the `SECTION` command line. This command line lets you differentiate between elements with the same topology but different formulations. For example, assume that the topology of the elements in a block is a four-node quadrilateral. With the `SECTION` command line you can specify whether the element block will be used as a membrane or a shell. The `SECTION` command line also lets you assign a variety of parameters to an element, depending on the element formulation.

It is important to state here that the SECTION command line only specifies an identifier that maps to a section command block that is defined by the user. There are currently several kinds of section command blocks for the different elements: SOLID SECTION, COHESIVE SECTION, SHELL SECTION, MEMBRANE SECTION, BEAM SECTION, TRUSS SECTION, SPRING SECTION, DAMPER SECTION, POINT MASS SECTION, PARTICLE SECTION, PERIDYNAMICS SECTION, and SUPERELEMENT SECTION. It is within a section command block that the formulation-specific entities related to a particular element are specified. If no SECTION command line is present in an element-block command block, the code assumes the element block is a block of eight-node hexahedra using mean quadrature and the midpoint-increment formulation.

All the command lines that can be used for the element-block command block are described in Section 5.1.5.1 through Section 5.1.5.9.

5.1.5.1 Material Property

```
MATERIAL <string>material_name
SOLID MECHANICS USE MODEL <string>model_name
```

The material property specification for an element block is done by using the above two command lines. The property specification references both a PROPERTY SPECIFICATION FOR MATERIAL command block and a material-model command block, which has the general form PARAMETERS FOR MODEL model_name. These command blocks are described in Chapter 4. The PROPERTY SPECIFICATION FOR MATERIAL command block contains all the parameters needed to define a material, and is associated with an element block (PARAMETERS FOR BLOCK command block) by use of the MATERIAL command line. Some of the material parameters inside the property specification are grouped on the basis of material models. A material-model command block is associated with an element block by use of the SOLID MECHANICS USE MODEL command line.

Consider the following example. Suppose there is a PROPERTY SPECIFICATION FOR MATERIAL command block with a material_name of steel. Embedded within this command block for steel is a material-model command block for an elastic model of steel and an elastic-plastic model of steel. Suppose that for the current element block we would like to use the material steel with the elastic model. Then the element-block command block would contain the input lines:

```
MATERIAL steel
SOLID MECHANICS USE MODEL elastic
```

If, on the other hand, we would like to use the material steel with the elastic-plastic model, the element-block command block would contain the input lines:

```
MATERIAL steel
SOLID MECHANICS USE MODEL elastic_plastic
```

The user should remember that not all material types can be used with all element types.

5.1.5.2 Include All Blocks

The `INCLUDE ALL BLOCKS` line command is used to associate all element blocks with the same element parameters (which minimizes input).

```
INCLUDE ALL BLOCKS
```

5.1.5.3 Remove Block

The `REMOVE BLOCK` command line allows you to delete blocks from the set specified in the `PARAMETERS FOR BLOCK` command block or `INCLUDE ALL BLOCKS` command line(s) through the string list `block_names`.

```
REMOVE BLOCK <string>block_list
```

5.1.5.4 Section

```
SECTION = <string>section_id
```

The section specification for an element-block command block is done by using the above command line. The `section_id` is a string associated with a section command block. The various section command blocks are described in Section 5.2.

Suppose you wanted the current element-block command block to use the membrane formulation. You would define a `MEMBRANE SECTION` command block with some name, such as `membrane_rubber`. Inside the current element-block command block you would have the command line:

```
SECTION = membrane_rubber
```

The thickness of the membrane would be described in the `MEMBRANE SECTION` command block and then associated with the current element-block command block.

There can be only one `SECTION` command line in an element-block command block. Each element-block command block within the model description can reference a unique section command block, or several element-block command blocks can reference the same section command block. For example, in Figure 5.1, the section named `membrane_rubber` appears in two different `PARAMETERS FOR MODEL` command blocks, but there is only one specification for their associated `MEMBRANE SECTION` command block. When several element-block command blocks reference the same section, the input file is less verbose, and it is easier to maintain the input file.

5.1.5.5 Linear and Quadratic Bulk Viscosity

```
LINEAR BULK VISCOSITY =
  <real>linear_bulk_viscosity_value(0.06)
QUADRATIC BULK VISCOSITY =
  <real>quad_bulk_viscosity_value(1.20)
```

```
BEGIN FINITE ELEMENT MODEL mesh1
.
.
  BEGIN PARAMETERS FOR BLOCK block1
     .
    SECTION membrane_rubber
    .
  END PARAMETERS FOR BLOCK block1
  BEGIN PARAMETERS FOR BLOCK block2
    .
    SECTION membrane_rubber
    .
  END PARAMETERS FOR BLOCK block2
  .
  .
END FINITE ELEMENT MODEL mesh1

BEGIN MEMBRANE SECTION membrane_rubber
  .
  .
END MEMBRANE SECTION membrane_rubber
```

Figure 5.1: Association between `SECTION` command lines and a section command block.

The linear and quadratic bulk viscosity are set with these two command lines. Consult the documentation for the elements [6] for a description of the bulk viscosity parameters.

5.1.5.6 Hourglass Control

```
HOURGLASS STIFFNESS = <real>hour_glass_stiff_value(solid
  = 0.05, shell/membrane = 0.0)
HOURGLASS VISCOSITY = <real>hour_glass_visc_value(solid
  = 0.0, shell/membrane = 0.0)
MEMBRANE HOURGLASS STIFFNESS =
  <real>memb_hour_glass_stiff_value(0.0)
MEMBRANE HOURGLASS VISCOSITY =
  <real>memb_glass_visc_value(0.0)
BENDING HOURGLASS STIFFNESS =
  <real>bend_hour_glass_stiff_value(0.0)
BENDING HOURGLASS VISCOSITY =
  <real>bend_glass_visc_value(0.0)
TRANSVERSE SHEAR HOURGLASS STIFFNESS =
  <real>tshr_hour_glass_stiff_value(0.0)
TRANSVERSE SHEAR HOURGLASS VISCOSITY =
  <real>tshr_glass_visc_value(0.0)
```

These command lines set the hourglass control parameters for elements that use hourglass control. Currently, the included elements are the eight-node, uniform-gradient hexahedral elements; the

eight-node and ten-node tetrahedral elements; and the four-node membrane and shell elements. Consult the element documentation [6] for a description of the hourglass parameters.

Hourglass stiffness and viscosity parameters for hexahedral and tetrahedral elements are set using the `HOURGLASS STIFFNESS` and `HOURGLASS VISCOSITY` commands, respectively. If either of these commands are used for shell elements, they set the hourglass stiffness or viscosity for all three modes (membrane, bending, and transverse shear).

Hourglass parameters for the membrane, bending, and transverse shear modes can be set individually for shell elements. The membrane hourglass stiffness and viscosity can be set with the `MEMBRANE HOURGLASS STIFFNESS` and `MEMBRANE HOURGLASS VISCOSITY` commands. These membrane hourglass commands can also be used with membrane elements. The bending hourglass stiffness and viscosity are set with the `BENDING HOURGLASS STIFFNESS` and `BENDING HOURGLASS VISCOSITY` commands, and transverse shear hourglass stiffness and viscosity are set with the `TRANSVERSE SHEAR HOURGLASS STIFFNESS` and `TRANSVERSE SHEAR HOURGLASS VISCOSITY` commands. All of these commands will override either the default values and any value set in the generic `HOURGLASS STIFFNESS` and/or `HOURGLASS VISCOSITY` commands for the particular mode that is specified.

The hourglass stiffness parameter defaults to 0.05 for solids using hourglass control; it defaults to 0.0 for shell and membrane elements. A reasonable user defined hourglass stiffness (if needed) for shells and membranes is 0.005 (approximately an order of magnitude lower than for solid elements). The hourglass viscosity parameter defaults to 0.0 for all elements currently using hourglass control.

The hourglass stiffness is the same as the dilatational hourglass parameter, and the hourglass viscosity is the same as the deviatoric hourglass parameter.

The computation of the hourglass parameters can be strongly affected by the method that computes the effective moduli. The command line in Section 5.1.5.7 selects the method for computing the effective moduli.

5.1.5.7 Effective Moduli Model

```
EFFECTIVE MODULI MODEL =
  <string>PRESTO|PRONTO|CURRENT|ELASTIC(PRONTO)
```

The hourglass force computations require a measure of the material moduli to ensure appropriate scaling of the hourglass forces. For elastic, isotropic material models, the moduli are constant throughout the analysis. However, for nonlinear materials, the moduli are typically computed numerically from the stresses. For models with softening regimes or that approach perfect plasticity, the moduli may be difficult to define, and the way in which they are computed may adversely affect the analysis. Through the `EFFECTIVE MODULI MODEL` command line, Presto provides several methods for the computation of these effective moduli:

- `PRESTO`: This method includes a number of techniques for returning reasonable moduli for softening and perfectly plastic materials. The effective moduli that this approach produces are stiffer than those computed by the `PRONTO` approach.

- PRONTO: This method is the default and is identical to the method of computing effective moduli present in the Pronto3D code. It is similar to the PRESTO approach but generally produces moduli that are softer than the PRESTO approach.

- CURRENT: This method computes the effective moduli without any extra handling of negative or near-zero moduli cases. It generally provides the softest response but is also less stable.

- ELASTIC: This method simply uses the initial elastic moduli for the entire analysis. It is the most robust but also the most stiff, and may produce an overly stiff global response.

The EFFECTIVE MODULI MODEL command line should be used with caution because it can strongly affect the analysis results.

5.1.5.8 Element Numerical Formulation

```
ELEMENT NUMERICAL FORMULATION = <string>OLD|NEW(OLD)
```

For calculation of the critical time step, it is necessary to determine a characteristic length for each element. In one dimension, the correct characteristic element length is obviously the distance between the two nodes of the element. In higher dimensions, this length is usually taken to be the minimum distance between any of the nodes in the element. However, some finite element codes, primarily those based on Pronto3D [1], use as a characteristic length an eigenvalue estimate based on work by Flanagan and Belytschko [7]. That characteristic length provides a stable time step, but in many cases is far more conservative than the minimum distance between nodes. For a cubic element with side length equal to 1, and thus also surface area of each face and volume equal to 1, the minimum distance between nodes is 1. However, the eigenvalue estimate is $1\big/\sqrt{3}$, which is only 58% of the minimum distance. As the length of the element is increased in one direction while keeping surfaces in the lateral direction squares of area 1, the eigenvalue estimate asymptotes to $1\big/\sqrt{2}$ for very long elements. If the length is decreased, the eigenvalue estimate asymptotes to the minimum distance between nodes for very thin elements. In this case, the eigenvalue estimate is always more conservative than the minimum distance between nodes. However, consider an element whose cross section in one direction is not a square but a trapezoid with one side length much greater than the other. Assume the large side length is 1 and the other side length is arbitrarily small, ε. In this case, the minimum distance between nodes becomes ε, creating a very small and inefficient time step. However, the eigenvalue estimate is related to the length across the middle of the trapezoid, which for the conditions stated is $1/2$. Since both distances provide stable time steps, and one or the other can be much larger in various circumstances, the most efficient calculation is obtained by using the maximum of the two lengths, either the eigenvalue estimate or the minimum distance between nodes, to determine the time step.

By using the maximum of the lengths, the computed critical time step should be at the edge of instability, and the TIME STEP SCALE FACTOR command line should be used to provide a margin of safety. In this case the scale factor for the time step should not be greater than 0.9, and in some cases it may have to be reduced further. Thus, although the maximum of the lengths provides a

time step that is closer to the critical value and provides better accuracy and efficiency, you may need to specify a smaller-than-expected scale factor for stability. For this reason, the choice of which approach to use is left to the user and is determined by the command line:

```
ELEMENT NUMERICAL FORMULATION = <string>OLD|NEW(OLD)
```

If the input parameter is `OLD`, only the eigenvalue estimate is used; `NEW` means that the maximum of the two lengths is used. The default is `OLD` so that users will have to specifically choose the new approach and be aware of the scale factor for the time step.

The `ELEMENT NUMERICAL FORMULATION` command line is applicable to both the energy-dependent and purely mechanical material models. If this command line is applied to blocks using energy-dependent materials, only the determination of the characteristic length is affected. If this command line is applied to an element block with a purely mechanical model and the `OLD` option is used, the Pronto3D-based artificial viscosity, time step, and eigenvalue estimate will be used in the element calculations. If, however, the `NEW` option is used, the artificial viscosity and time step will be computed from equations associated with the energy-dependent models. You should consult Reference 8 for further details about the critical time-step calculations and the use of this command line.

5.1.5.9 Activation/Deactivation of Element Blocks by Time

```
ACTIVE FOR PROCEDURE <string>proc_name DURING PERIODS
  <string list>period_names
INACTIVE FOR PROCEDURE <string>proc_name DURING PERIODS
  <string list>period_names
```

This command line permits the activation and deactivation of element blocks by time period. The time periods are defined in the `TIME STEPPING BLOCK` command block (Section 3.1.1) within a specific procedure named in a `PRESTO PROCEDURE` command block (Section 2.2.1).

The `ACTIVE FOR PROCEDURE` or `INACTIVE FOR PROCEDURE` command lines can optionally be used to deactivate element blocks for a portion of the analysis. If the `ACTIVE FOR PROCEDURE` command is used, the element block is active for all periods listed for the named procedure, and is deactivated for all time periods that are absent from the list. If the `INACTIVE FOR PROCEDURE` command is used, the element block is deactivated for all periods listed for the named procedure. The element block is active for all time periods that are absent from the list. If neither command line is used, by default the block is active during all time periods. This command line controls the activation and deactivation of all elements in a block. Alternatively, individual elements can be deactivated with the `ELEMENT DEATH` command block (see Section 5.5).

5.2 Element Sections

Element sections are defined by section command blocks. There are currently nine different types of section command blocks. The section command blocks appear in the SIERRA scope, at the same level as the `FINITE ELEMENT MODEL` command block. In general, a section command block has the following form:

```
BEGIN section_type SECTION <string>section_name
  command lines dependent on section type
END [section_type SECTION <string>section_name]
```

Currently, `section_type` can be `SOLID`, `COHESIVE`, `SHELL`, `MEMBRANE`, `BEAM`, `TRUSS`, `SPRING`, `DAMPER`, `POINT MASS`, `PARTICLE`, `PERIDYNAMICS`,or `SUPERELEMENT`. These various section types are identified as individual section command blocks and are described below. The corresponding `section_name` parameter in each of these command blocks, e.g., `truss_section_name` in the `TRUSS SECTION` command block, is selected by the user. The method used to associate these names with individual `SECTION` command lines in `PARAMETERS FOR BLOCK` command blocks is discussed in Section 5.1.5.4.

5.2.1 Solid Section

```
BEGIN SOLID SECTION <string>solid_section_name
  COORDINATE SYSTEM = <string>Coordinate_system_name
  FORMULATION = <string>MEAN_QUADRATURE|
    SELECTIVE_DEVIATORIC|VOID(MEAN_QUADRATURE)
  DEVIATORIC PARAMETER = <real>deviatoric_param
  STRAIN INCREMENTATION = <string>MIDPOINT_INCREMENT|
    STRONGLY_OBJECTIVE|NODE_BASED(MIDPOINT_INCREMENT)
  NODE BASED ALPHA FACTOR = <real>bulk_stress_weight(0.01)
  NODE BASED BETA FACTOR = <real>shear stress_weight(0.35)
  HOURGLASS FORMULATION = <string>TOTAL|INCREMENTAL(INCREMENTAL)
  HOURGLASS INCREMENT = <string>ENDSTEP|MIDSTEP (ENDSTEP)
  HOURGLASS ROTATION = <string> APPROXIMATE|SCALED (APPROXIMATE)
  RIGID BODY = <string>rigid_body_name
  RIGID BODIES FROM ATTRIBUTES = <integer>first_id
    TO <integer>last_id
  USE LAME|STRUMENTO(LAME)
END [SOLID SECTION <string>solid_section_name]
```

The `SOLID SECTION` command block is used to specify the properties for solid elements (hexahedra and tetrahedra). This command block is to be referenced by an element block made up of solid elements. The two types of solid-element topologies currently supported are hexahedra and tetrahedra. The parameter `solid_section_name` is user-defined and is referenced by a `SECTION` command line in a `PARAMETERS FOR BLOCK` command block.

The COORDINATE SYSTEM command line specifies the name of a coordinate system definition block command that will be used to define a local coordinate system on each element of a block that uses this SOLID SECTION. The coordinate system can then be used to transform element stresses for solid elements from the global coordinate system to this local element coordinate system through the use of a BEGIN USER OUTPUT command block as described in Section out:user. It is also used for defining a local element coordinate system for representative volume analyses (see Section spec:rve).

The FORMULATION command line specifies whether the element will use a single-point integration rule (mean quadrature), use a selective-deviatoric rule, or act as a void element. The selective-deviatoric integration rule is a higher-order integration scheme, which is discussed below.

If the user wishes to use the selective-deviatoric rule, the DEVIATORIC PARAMETER command line must also appear in the SOLID SECTION command block. The selective-deviatoric parameter, deviatoric_param, which is valid from 0.0 to 1.0, indicates how much of the deviatoric response should be taken from a uniform-gradient integration and how much should be taken from a full integration of the element. A value of 0.0 will give a pure uniform-gradient response with no hourglass control. Thus, this value is of little practical use. A value of 1.0 will give a fully integrated deviatoric response. Although any value between 0.0 and 1.0 is perfectly valid, lower values are generally preferred.

The selective-deviatoric elements, when used with a value greater than 0.0, provide hourglass control without artificial hourglass parameters.

The VOID formulation is valid for 8-node hexahedral and 4-node tetrahedral element blocks. Void elements only compute volume. They do not contribute internal forces to the model. The material model and density associated with void elements are ignored. The volume and the first and second derivatives of the volume for each element are stored in the element variables volume, volume_first_derivative, and volume_second_derivative. The volume derivatives are computed using least squares fits of the volume history, which is stored for the previous five time steps.

In addition to the per-element volume and derivatives, the total volume and derivatives of that total volume for all elements in each void element block are written to the results file as global variables. The names for these variables are voidvol_blockID, voidvol_first_deriv_blockID, and voidvol_second_deriv_blockID. In these global variable names, blockID is the ID of the block. For example, the void volume for block 8 would be stored in voidvol_8.

Some of the solid elements support different strain-incrementation formulations. See the element summary at the beginning of Section 5.1 to determine which strain-incrementation formulations are available for which elements. The STRAIN INCREMENTATION command line lets you specify a midpoint-increment strain formulation (MIDPOINT_INCREMENT), a strongly objective strain formulation (STRONGLY_OBJECTIVE), or a node-based formulation (NODE_BASED) for some of the elements. Consult the element documentation [2,6] for a description of these strain formulations.

The node-based formulation can only be used with four-node tetrahedral elements. If your element-block command block (i.e., a PARAMETERS FOR BLOCK command block) has a SECTION command line that references a SOLID SECTION command block that uses:

```
STRAIN INCREMENTATION = NODE_BASED
```

then the element block must be a block of four-node tetrahedral elements.

The node-based formulation lets you calculate a solution that is some mixture of an element-based formulation (information from the center of an element) and a node-based formulation (information at a node that is based on all elements attached to the node). The node-based tetrahedron allows the user to model with four-node tetrahedral elements and avoid the main problems with regular tetrahedral elements. Regular tetrahedral elements are much too stiff and can produce very inaccurate results.

You can adjust the mixture of node-based versus element-based information incorporated into your solution with the `NODE BASED ALPHA FACTOR` and `NODE BASED BETA FACTOR` command lines. These two lines apply only if you have selected the `NODE BASED` option on the `STRAIN INCREMENTATION` command line. The value for `bulk_stress_weight` on the `NODE BASED ALPHA FACTOR` command line sets the element bulk stress weighting factor, while the value for `shear_stress_weight` on the `NODE BASED BETA FACTOR` command line sets the element shear stress weighting factor. You should consult Reference 3 to better understand the use of these weighting factors. If both of these factors are set to 0.0, you will be using a strictly node-based formulation. If both of these factors are set to 1.0, you will be using a strictly element-based formulation.

The `HOURGLASS FORMULATION` command is used to switch between total and incremental forms of hourglass control. This option can only be used with eight-noded uniform-gradient hexahedral elements using strongly objective strain incrementation (`STRAIN INCREMENTATION = STRONGLY_OBJECTIVE`). One of the following two arguments can be used with this command: `TOTAL` or `INCREMENTAL`. The total formulation performs stiffness hourglass force updates based on the rotation tensor from the polar decomposition of the total deformation gradient. The incremental formulation is the default and performs stiffness hourglass force updates based on the hourglass velocities and the incremental rotation tensor. The viscous hourglass forces and the hourglass parameters are unchanged by this command. Consult the element documentation [6] for a description of the hourglass forces and the incremental hourglass formulation.

The `HOURGLASS INCREMENT` and `HOURGLASS ROTATION` commands control the speed and accuracy of the hourglass control computation. These commands are only applicable to the uniform gradient hex with midpoint strain incrementation (`STRAIN INCREMENTATION = MIDPOINT_INCREMENT`). The `HOURGLASS INCREMENT` line command specifies whether the hourglass resistance increment is to be computed at the middle or end of the time step. The endstep calculation has a slightly reduced computational cost while the midstep computation is more accurate. The default is `ENDSTEP`. The `HOURGLASS ROTATION` command controls whether the hourglass resistance will be scaled after rotation to preserve the magnitude. Scaling requires additional computation time but will be more accurate, particularly when very large rotations are present in the analysis. The default is `APPROXIMATE`, meaning no scaling is done.

Rigid elements in a section are indicated by including the `RIGID BODY` command line. The `RIGID BODY` command line specifies an identifier that maps to a rigid body command block. See Section 5.3.1 for a full discussion of how to create rigid bodies and Section 5.3.1.1 for information on the use of the `RIGID BODIES FROM ATTRIBUTES` command.

You can request that the material model that will be used with this solid section come from the legacy Strumento material model library by using the `USE STRUMENTO` line command. LAME is the default material model library for all solid sections [9] but can be explicitly requested with the `USE LAME` line command. The versions of the material models in the Strumento library will be removed in a future release of Presto, so it is advised to switch to the LAME versions as soon as possible.

5.2.2 Cohesive Section

```
BEGIN COHESIVE SECTION <string>cohesive_section_name
  NUMBER OF INTEGRATION POINTS = <integer>num_int_points(1)
END [COHESIVE SECTION <string>cohesive_section_name]
```

Warning: In order for the cohesive elements to contribute to the global stable timestep, a node based timestep must be used. See Section 3.2.3 for details.

The `COHESIVE SECTION` command block is used to specify the properties for cohesive zone elements (quadrilateral and triangular). The name of this block (given by `cohesive_section_name`) is referenced by the element block for cohesive elements. If the option for adaptive insertion of cohesive zone elements is used, the name of this block is referenced by the `COHESIVE SECTION` command defined in Section 5.5.5.

`NUMBER OF INTEGRATION POINTS = <integer>num_int_points(1)`
The default number of integration points for a cohesive element is one. However, it should be noted that with a single integration point, spurious hour-glass like modes can be introduced to the deformation of the cohesive element. Currently, the quadrilateral cohesive element supports one and four integration points while the triangular cohesive element supports one and three integration points.

5.2.3 Localization Section

```
BEGIN LOCALIZATION SECTION <string>localization_section_name
  MEAN DILATATION FORMULATION
  NUMBER OF INTEGRATION POINTS = <integer>num_int_points
  THICKNESS = <real>thickness
END [LOCALIZATION SECTION <string>cohesive_section_name]
```

Warning: Currently the localization elements do not contribute to the global stable timestep. As such, the user must specify a timestep via the `INITIAL TIME STEP` and `TIME STEP INCREASE FACTOR` command lines. See Section 3.1 for details.

Localization elements are planar elements that lie between bulk (volumetric) elements and can employ the same underlying bulk material model. Topologically, localization elements are identical to cohesive surface elements. The reason this 2D element can access 3D material models is due to the multiplicative decomposition of the deformation gradient $\boldsymbol{F}$ such that $\boldsymbol{F} = \boldsymbol{F}^{\parallel}\boldsymbol{F}^{\perp}$ where $\boldsymbol{F}^{\parallel}$ encapsulates in-plane stretching and $\boldsymbol{F}^{\perp}$ is defined to be

$$\boldsymbol{F}^{\perp} = \boldsymbol{I} + \frac{\boldsymbol{\Delta}}{h} \otimes \boldsymbol{N} \tag{5.1}$$

where $\boldsymbol{N}$ is the normal to the mid-plane, $\boldsymbol{\Delta}$ is the gap vector, and h is the element "thickness" or the length scale governing the sub-grid separation progress. We note that because the length scale h is independent of the discretization, the methodology is regularized and ideal for employing local, softening material models to simulate the failure process. For full details on the theory, please see 15.

The `LOCALIZATION SECTION` command block is used to specify the properties for localization elements (quadrilateral and triangular). The name of this block (given by `localization_section_name`) is referenced by the element block for localization elements.

`MEAN DILATATION FORMULATION` This command line will yield a constant pressure formulation. The average pressure is obtained at all integration points through a modification of the kinematic quantities. For hypoelastic materials, we volume average the tr[$\boldsymbol{D}$]. For uncoupled hyperelastic models, we volume average det[$\boldsymbol{F}$]. After voluming averaging tr[$\boldsymbol{D}$] and det[$\boldsymbol{F}$], we remove local dilatational contributions and additively (hypoelastic) or multiplicatively (hyperelastic) include the average response. This results in an average pressure (by construction) and has been shown to be effective in avoiding element locking during isochoric deformations. Note that one can use a single integration point to achieve a constant pressure but we do not provide any hourglass control to suppress spurious modes. If isochoric deformations are of concern, we recommend using a fully-integrated element with `MEAN DILATATION FORMULATION`.

`NUMBER OF INTEGRATION POINTS = <integer>num_int_points` The default number of integration points for a localization element depends on the topology, but is always sufficient for full integration. For an 8 noded hex (planar 4 node quad) the default is 4 integration points while for a 6 noded wedge (planar 3 node tri) the default is 1 integration point. However, it should be noted that with a single integration point, spurious hourglass modes can be introduced into the deformation of the quadrilateral localization element. Currently, the quadrilateral localization element supports one and four integration points while the triangular localization element supports one integration point.

`THICKNESS = <real>thickness` The `THICKNESS` command line sets the localization element thickness h. In many respects, h should be considered a material parameter as it governs the evolution of surface separation. We note that the introduction of h generates the true length scale in the problem, the process zone size. Care must be taken to adequately resolve the process zone size or the methodology will not be regularized.

5.2.4 Shell Section

```
BEGIN SHELL SECTION <string>shell_section_name
```

```
    THICKNESS = <real>shell_thickness
    THICKNESS MESH VARIABLE =
      <string>THICKNESS|<string>var_name
    THICKNESS TIME STEP = <real>time_value
    THICKNESS SCALE FACTOR = <real>thick_scale_factor(1.0)
    INTEGRATION RULE = TRAPEZOID|GAUSS|LOBATTO|SIMPSONS|
      USER(TRAPEZOID)
    NUMBER OF INTEGRATION POINTS = <integer>num_int_points(5)
    FORMULATION = MEAN_QUADRATURE|NQUAD (MEAN_QUADRATURE)
    BEGIN USER INTEGRATION RULE
      <real>location_1 <real>weight_1
      <real>location_2 <real>weight_2
      .
      .
      <real>location_n <real>weight_n
    END [USER INTEGRATION RULE]
    LOFTING FACTOR = <real>lofting_factor(0.5)
    OFFSET MESH VARIABLE = <string>var_name
    ORIENTATION = <string>orientation_name
    DRILLING STIFFNESS FACTOR = <real>stiffness_factor(0.0)
    RIGID BODY = <string>rigid_body_name
    RIGID BODIES FROM ATTRIBUTES = <integer>first_id
      TO <integer>last_id
    USE LAME|STRUMENTO(LAME)
  END [SHELL SECTION <string>shell_section_name]
```

The `SHELL SECTION` command block is used to specify the properties for a shell element. If this command block is referenced in an element block of three-dimensional, four-node elements, the elements in the block will be treated as shell elements. The parameter, `shell_section_name`, is user-defined and is referenced by a `SECTION` command line in a `PARAMETERS FOR BLOCK` command block.

Either a `THICKNESS` command line or a `THICKNESS MESH VARIABLE` command line must appear in the `SHELL SECTION` command block.

If a shell element block references a `SHELL SECTION` command block with the command line:

```
THICKNESS = <real>shell_thickness
```

then all the shell elements in the block will have their thickness initialized to the value `shell_thickness`.

Presto can also initialize the thickness using an attribute defined on elements in the mesh file. Meshing programs such as PATRAN and CUBIT typically set the element thickness as an attribute on the elements. If the elements have one and only one attribute defined on the mesh, the `THICKNESS MESH VARIABLE` command line should be specified as:

```
THICKNESS MESH VARIABLE = THICKNESS
```

which causes the thickness of the element to be initialized to the value of the attribute for that element. If there are zero attributes or more than one attribute, the thickness variable will not be

automatically defined, and the command will fail.

The thickness may also be initialized by any other field present on the input mesh. To specify a field other than the single-element attribute, use this form of the THICKNESS MESH VARIABLE command line:

```
THICKNESS MESH VARIABLE = <string>var_name
```

Here, the string var_name is the name of the initializing field.

The input mesh may have values defined at more than one point in time. To choose the point in time in the mesh file that the variable should be read, use the command line:

```
THICKNESS TIME STEP = <real>time_value
```

The default time point in the mesh file at which the variable is read is 0.0.

Once the thickness of a shell element is initialized by using either the THICKNESS command line or the THICKNESS MESH VARIABLE command line, this initial thickness value can then be scaled using the scale-factor command line:

```
THICKNESS SCALE FACTOR = <real>thick_scale_factor
```

If the initial thickness of the shell is 0.15 inch, and the value for thick_scale_factor is 0.5, then the scaled thickness of the membrane will be 0.075.

The thickness mesh variable specification may be coupled with the THICKNESS SCALE FACTOR command line. In this case, the thickness mesh variable is scaled by the specified factor.

The shell formulation can be selected via the FORMULATION command line. The default formulation is MEAN_QUADRATURE. A fully elastic formulation may be selected with the NQUAD option.

For shell elements, the user can select from a number of integration rules, including a user-defined integration option. The integration rule is selected with the command line:

```
INTEGRATION RULE = <string>TRAPEZOID|GAUSS|LOBATTO|SIMPSONS|
     USER(TRAPEZOID)
```

Consult the element documentation [6] for a description of different integration schemes for shell elements.

The default integration scheme is TRAPEZOID with five integration points through the thickness. The number of integration points for TRAPEZOID can be set to any number greater than one by using the following command line:

```
NUMBER OF INTEGRATION POINTS = <integer>num_int_points(5)
```

The SIMPSONS, GAUSS, and LOBATTO integration schemes in the INTEGRATION RULE command line all default to five integration points. The number of integration points for these three schemes can be reset by using the NUMBER OF INTEGRATION POINTS command line. There are limitations on the number of integration points for some of these integration rules. The SIMPSONS rule can be set to any number greater than one, the GAUSS scheme can be set to one through seven integration points, and the LOBATTO integration scheme can be set to two through seven integration points.

In addition to these standard integration schemes, you may also define an integration scheme by using the USER INTEGRATION RULE command block.

```
BEGIN USER INTEGRATION RULE
  <real>location_1 <real>weight_1
  <real>location_2 <real>weight_2
  .
  .
  <real>location_n <real>weight_n
END [USER INTEGRATION RULE]
```

You may NOT specify both a standard integration scheme and a user scheme. If the USER option is specified in the INTEGRATION RULE command line, a set of integration locations with associated weight factors must be specified. This is done with tabular input command lines inside the USER INTEGRATION RULE command block. The number of command lines inside this command block should match the number of integration points specified in the NUMBER OF INTEGRATION POINTS command line. For example, suppose we wish to use a user-defined scheme with three integration points. The NUMBER OF INTEGRATION POINTS command line should specify three (3) integration points and the number of command lines inside the USER INTEGRATION RULE command block should be three (to give three locations and three weight factors).

For the user-defined rule, the integration point locations should fall between –1 and +1, and the weights should sum to 1.0.

The command line

```
LOFTING FACTOR = <real>lofting_factor(0.5)
```

allows the user to shift the location of the mid-surface of a shell element relative to the geometric location of the shell element. The lofting factor must be greater than or equal to 0.0 and less than or equal to 1.0. By default, the geometric location of a shell element in a mesh represents the mid-surface of the shell. If a shell has a thickness of 0.2 inch, the top surface of the shell is 0.1 inch above the geometric surface defined by the shell element, and the bottom surface of the shell is 0.1 inch below the geometric surface defined by the shell element. (The top surface of the shell is the surface with a positive element normal; the bottom surface of the shell is the surface with a negative element normal.)

Figure 5.2 shows an edge-on view of shell elements with a thickness of t and the location of the geometric plane in relation to the shell surfaces for three different values of the lofting factor—0.0, 0.5, and 1.0. For a lofting factor of 0.0, the geometric surface defined by the shell corresponds to the top surface of the shell element. A lofting factor of 1.0 puts the geometric surface at the bottom surface of the shell element. The geometric surface is midway between the top and bottom surfaces for a lofting factor of 0.5, which is the default. Lofting factors greater than 1.0 or less than 0.0 would put the geometric surface outside the shell element and are not allowed.

Consider the example of a lofting factor set to 1.0 for a shell with thickness of 0.2 inch. In this case, the top surface of the shell will be located at a distance of 0.2 inch from the geometric surface (measuring in the direction of the positive shell normal), and the bottom surface will be located at the geometric surface.

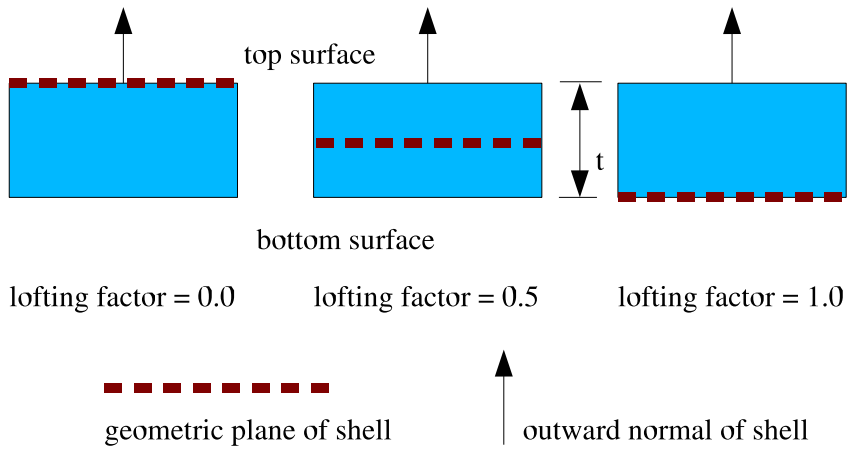

Figure 5.2: Location of geometric plane of shell for various lofting factors.

Both the shell mechanics and contact use shell lofting. See Section 7.2 for a discussion of lofting surfaces for shells and contact. It is recommended that shell lofting values other than 0.5 not be used if the shell is thick. If the shell is thicker than its in-plane width, the shell lofting algorithms may become unstable.

Lofting as described above may also be implemented through

```
OFFSET MESH VARIABLE = <string>var_name.
```

This command allows an offset value to be read from an attribute (or variable) on the mesh file. This attribute (or variable) must be named but may have any name, and this name is specified in place of `var_name` in the command. An offset is a dimensional value (i.e. not scaled by the shell thickness) that gives the shell mid-plane shift in the positive shell normal direction. Internal to Presto the offset value is converted to an equivalent lofting factor by dividing by the initial thickness and adding 0.5. Thus, an offset of zero gives a lofting factor of 0.5, an offset of one half of the thickness gives a lofting factor of one, and an offset of negative one half of the thickness gives a lofting factor of zero. There is no check that given offset values produce lofting values between zero and one, which allows any offset to be specified but requires that care be exercised to avoid unstable lofted shells.

Warning: An offset and a lofting factor may not be specified in the same shell section. Both determine the shell lofting and may conflict.

The `ORIENTATION` command line lets you select a coordinate system for output of in-plane stresses and strains. The `ORIENTATION` option makes use of an embedded coordinate system *rst* associated with each shell element. The *rst* coordinate system for a shell element is shown in Figure 5.3. The *r*-axis extends from the center of the shell to the midpoint of the side of the shell defined by nodes 1 and 2. The *t*-axis is located at the center of the shell and is normal to the surface of the shell at the center point. The *s*-axis is the cross-product of the *t*-axis and the *r*-axis. The *rst*-axes form a local coordinate system at the center of the shell; this local coordinate system

moves with the shell element as the element deforms.

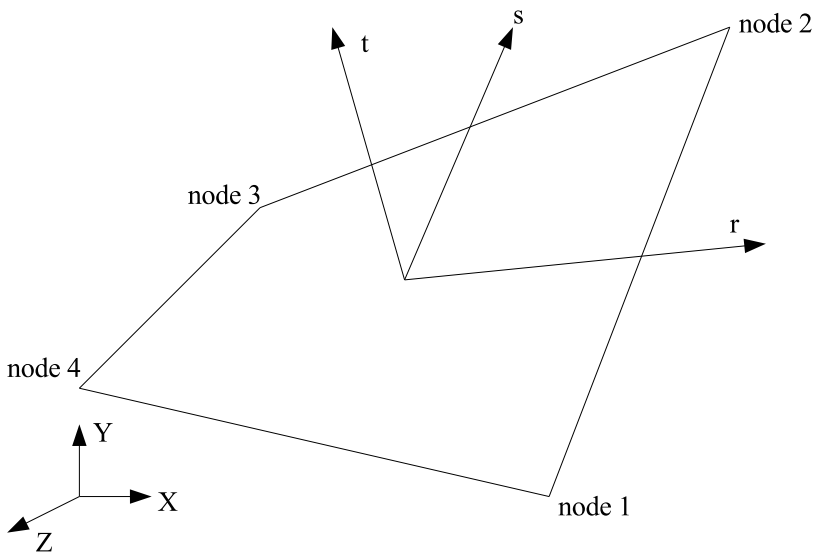

Figure 5.3: Local *rst* coordinate system for a shell element.

The `ORIENTATION` command line in the `SHELL SECTION` command block references an `ORIENTATION` command block that appears in the SIERRA scope. As described in Chapter 2 of this document, the `ORIENTATION` command block can be used to define a local co-rotational coordinate system $X''Y''Z''$ at the center of a shell element. In the original shell configuration (time 0), one of the axes—X'', Y'', or Z''—is projected onto the plane of the shell element. The angle between this projected axis of the $X''Y''Z''$ coordinate system and the r-axis is used to establish the transformation for in-plane stresses and strains. We will illustrate this with an example.

Suppose that in our `ORIENTATION` command block we have specified a rotation of 30 degrees about the 1-axis (X'-axis). The command line for this rotation in the `ORIENTATION` command block would be:

```
ROTATION ABOUT 1 = 30
```

For this case, we project the Y''-axis onto the plane of the shell (Figure 5.4). The angle between this projection and the r-axis establishes a transformation for the in-plane stresses of the shell (the stresses in the center of the shell lying in the plane of the shell). What will be output as the in-plane stress σ^{ip}_{xx} will be in the Y''-direction; what will be output as the in-plane stress σ^{ip}_{yy} will be in the Z''-direction. The in-plane stress σ^{ip}_{xy} is a shear stress in the $Y''Z''$-plane. The $X''Y''Z''$ coordinate system maintains the same relative position in regard to the *rst* coordinate system. This means that the $X''Y''Z''$ coordinate system is a local coordinate system that moves with the shell element as the element deforms.

The following permutations for output of the in-plane stresses occur depending on the axis (1, 2, or 3) specified in the `ROTATION ABOUT` command line:

- Rotation about the 1-axis (X'-axis): The in-plane stress σ^{ip}_{xx} will be in the Y''-direction; the in-plane stress σ^{ip}_{yy} will be in the Z''-direction. The in-plane stress σ^{ip}_{xy} is a shear stress in the

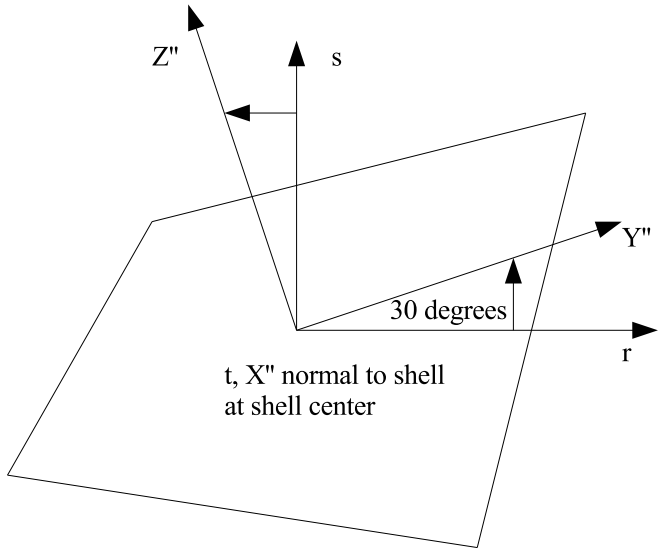

Figure 5.4: Rotation of 30 degrees about the 1-axis (X'-axis).

$Y''Z''$-plane.

- Rotation about the 2-axis (Y'-axis): The in-plane stress σ_{xx}^{ip} will be in the Z''-direction; the in-plane stress σ_{yy}^{ip} will be in the X''-direction. The in-plane stress σ_{xy}^{ip} is a shear stress in the $Z''X''$-plane.
- Rotation about the 3-axis (Z'-axis): The in-plane stress σ_{xx}^{ip} will be in the X''-direction; the in-plane stress σ_{yy}^{ip} will be in the Y''-direction. The in-plane stress σ_{xy}^{ip} is a shear stress in the $X''Y''$-plane.

If no orientation is specified, the in-plane stresses and strains are output in the consistent axes from a default orientation, which is a rectangular system with the X' and Y' axes taken as the global X and Y axes, respectively, and `ROTATION ABOUT 1 = 0.0`.

The command line

```
DRILLING STIFFNESS FACTOR = <real>stiffness_factor
```

adds stiffness in the drilling degrees of freedom to quadrilateral shells. Drilling degrees of freedom are rotational degrees of freedom in the direction orthogonal to the plane of the shell at each node. The formulation used for the quadrilateral shells has no rotational stiffness in this direction. This can lead to spurious zero-energy modes of deformation similar in nature to hourglass deformation. This makes obtaining a solution difficult in quasistatic problems and can result in singularities when using the full tangent preconditioner.

The `stiffness_factor` should be chosen as a quantity small enough to add enough stiffness to allow the solve to be successful without unduly affecting the solution. The default value for `stiffness_factor` is 0. If singularities are encountered in the solution or hourglass-like deformation is observed in the drilling degrees of freedom, it is recommend to try using a small amount of drilling stiffness. A suggested trial value for `stiffness_factor` is 1.0e-4.

Elements in a section can be made rigid by including the RIGID BODY command line. The RIGID BODY command line specifies an indenter that maps to a rigid body command block. See Section 5.3.1 for a full discussion of how to create rigid bodies and Section 5.3.1.1 for information on the use of the RIGID BODIES FROM ATTRIBUTES command.

You can request that the material model that will be used with this shell section come from the Strumento material model library by using the USE STRUMENTO line command. LAME is the default material model library for all shell sections [9], but can be explicitly requested with the USE LAME line command. The versions of the material models in the Strumento library will be removed in a future release of Presto, so it is advised to switch to the LAME versions as soon as possible.

5.2.5 Membrane Section

```
BEGIN MEMBRANE SECTION <string>membrane_section_name
  THICKNESS = <real>mem_thickness
  THICKNESS MESH VARIABLE =
    <string>THICKNESS|<string>var_name
  THICKNESS TIME STEP = <real>time_value
  THICKNESS SCALE FACTOR = <real>thick_scale_factor(1.0)
  FORMULATION = <string>MEAN_QUADRATURE|
    SELECTIVE_DEVIATORIC(MEAN_QUADRATURE)
  DEVIATORIC PARAMETER = <real>deviatoric_param
  LOFTING FACTOR = <real>lofting_factor(0.5)
  RIGID BODY = <string>rigid_body_name
  RIGID BODIES FROM ATTRIBUTES = <integer>first_id
    TO <integer>last_id
END [MEMBRANE SECTION <string>membrane_section_name]
```

The MEMBRANE SECTION command block is used to specify the properties for a membrane element. If a section defined by this command block is referenced in the parameters for a block of four-noded elements, the elements in that block will be treated as membranes. The parameter membrane_section_name is user-defined and is referenced by a SECTION command line in a PARAMETERS FOR BLOCK command block.

Either a THICKNESS command line or a THICKNESS MESH VARIABLE command line must appear in the MEMBRANE SECTION command block.

If a membrane element block references a MEMBRANE SECTION command block with the command line:

```
THICKNESS = <real>mem_thickness
```

then all the membrane elements in the block will have their thickness initialized to the value mem_thickness.

Presto can also initialize the thickness using an attribute defined on elements in the mesh file. Meshing programs such as PATRAN and CUBIT typically set the element thickness as an at-

tribute on the elements. If the elements have one and only one attribute defined on the mesh, the THICKNESS MESH VARIABLE command line should be specified as:

```
THICKNESS MESH VARIABLE = THICKNESS
```

which causes the thickness of the element to be initialized to the value of the attribute for that element. If there are zero attributes or more than one attribute, the thickness variable will not be automatically defined, and the command will fail.

The thickness may also be initialized by any other field present on the input mesh. To specify a field other than the single-element attribute, use this form of the THICKNESS MESH VARIABLE command line:

```
THICKNESS MESH VARIABLE = <string>var_name
```

where the string var_name is the name of the initializing field.

The input mesh may have values defined at more than one point in time. To choose the point in time in the mesh file that the variable should be read, use the command line:

```
THICKNESS TIME STEP = <real>time_value
```

The default time point in the mesh file at which the variable is read is 0.0.

Once the thickness of a membrane element is initialized by using either the THICKNESS command line or the THICKNESS MESH VARIABLE command line, this initial thickness value can then be scaled by using the scale-factor command line:

```
THICKNESS SCALE FACTOR = <real>thick_scale_factor
```

If the initial thickness of the membrane is 0.15 inch, and the value for thick_scale_factor is 0.5, then the scaled thickness of the membrane will be 0.075.

The FORMULATION command line specifies whether the element will use a single-point integration rule (mean quadrature) or a selective-deviatoric integration rule:

```
FORMULATION = <string>MEAN_QUADRATURE|SELECTIVE_DEVIATORIC
  (MEAN_QUADRATURE)
```

If the user wishes to use the selective-deviatoric rule, the DEVIATORIC PARAMETER command line must also appear in the MEMBRANE SECTION command block:

```
DEVIATORIC PARAMETER = <real>deviatoric_param
```

The selective-deviatoric elements, when used with a parameter greater than 0.0, provide hourglass control without artificial hourglass parameters. The selective-deviatoric parameter, deviatoric_param, which is valid from 0.0 to 1.0, indicates how much of the deviatoric response should be taken from a uniform-gradient integration and how much should be taken from a full integration of the element. A value of 0.0 will give a pure uniform-gradient response with no hourglass control. Thus, this value is of little practical use. A value of 1.0 will give a fully integrated deviatoric response. Although any value between 0.0 and 1.0 is perfectly valid, lower values are generally preferred.

The command line

```
LOFTING FACTOR = <real>lofting_factor(0.5)
```

allows the user to shift the location of the mid-surface of a membrane element relative to the geometric location of the membrane element. By default, the geometric location of a membrane element in a mesh represents the mid-surface of the membrane. If a membrane has a thickness of 0.2 inch, the top surface of the membrane is 0.1 inch above the geometric surface defined by the membrane element, and the bottom surface of the membrane is 0.1 inch below the geometric surface defined by the membrane element. (The top surface of the membrane is the surface with a positive element normal; the bottom surface of the membrane is the surface with a negative element normal.)

Figure 5.2, which shows lofting for shells, is also applicable to membranes. For membranes, Figure 5.2 represents an edge-on view of membrane elements with a thickness of t and the location of the geometric plane in relation to the membrane surfaces for three different values of the lofting factor—0.0, 0.5, and 1.0. For a lofting factor of 0.0, the geometric surface defined by the membrane corresponds to the top surface of the membrane element. A lofting factor of 1.0 puts the geometric surface at the bottom surface of the membrane element. The geometric surface is midway between the top and bottom surfaces for a lofting factor of 0.5, which is the default.

Consider the example of a lofting factor set to 1.0 for a membrane with thickness of 0.2 inch. In this case, the top surface of the membrane will be located at a distance of 0.2 inch from the geometric surface (measuring in the direction of the positive shell normal), and the bottom surface will be located at the geometric surface.

Both the membrane mechanics and contact use membrane lofting. See Section 7.2 for a discussion of lofting surfaces for membranes and contact.

Elements in a section can be made rigid by including the `RIGID BODY` command line. The `RIGID BODY` command line specifies an indenter that maps to a rigid body command block. Consult Section 5.3.1 for a full description of how to create rigid bodies and Section 5.3.1.1 for information on the use of the `RIGID BODIES FROM ATTRIBUTES` command.

5.2.6 Beam Section

```
BEGIN BEAM SECTION <string>beam_section_name
  SECTION = <string>ROD|TUBE|BAR|BOX|I
  WIDTH = <real>section_width
  WIDTH VARIABLE = <string>width_var
  HEIGHT = <real>section_width
  HEIGHT VARIABLE= <string>height_var
  WALL THICKNESS = <real>wall_thickness
  WALL THICKNESS VARIABLE = <string>wall_thickness_var
  FLANGE THICKNESS = <real>flange_thickness
  FLANGE THICKNESS VARIABLE = <string>flange_thickness_var
  T AXIS = <real>tx <real>ty <real>tz
  T AXIS VARIABLE = <string>t_axis_var
  REFERENCE AXIS = <string>CENTER|RIGHT|
    TOP|LEFT|BOTTOM(CENTER)
  AXIS OFFSET = <real>s_offset <real>t_offset
  AXIS OFFSET GLOBAL = <real>x_offset <real>y_offset <real>z_offset
  AXIS OFFSET VARIABLE = <string>axis_offset_var
  RIGID BODY = <string>rigid_body_name
  RIGID BODIES FROM ATTRIBUTES = <integer>first_id
    TO <integer>last_id
  USE LAME|STRUMENTO(LAME)
END [BEAM SECTION <string>beam_section_name]
```

The `BEAM SECTION` command block is used to specify the properties for a beam element. If this command block is referenced in an element block of three-dimensional, two-node elements, the elements in the block will be treated as beam elements. The parameter, `beam_section_name`, is user-defined and is referenced by a `SECTION` command line in a `PARAMETERS FOR BLOCK` command block.

Five different cross sections can be specified for the beam—`ROD`, `TUBE`, `BAR`, `BOX`, and `I`—via use of the `SECTION` command line. Each section requires a specific set of command lines for a complete geometric description. The command lines related to section geometry are `WIDTH`, `HEIGHT`, `WALL THICKNESS`, and `FLANGE THICKNESS`. We present a summary of the geometric parameter command lines required for each section as a quick reference.

- If the section is `ROD`, the following geometry command lines are required:

  ```
  WIDTH or WIDTH VARIABLE
  HEIGHT or HEIGHT VARIABLE
  ```

- If the section is `TUBE`, the following geometry command lines are required:

  ```
  WIDTH or WIDTH VARIABLE
  HEIGHT or HEIGHT VARIABLE
  WALL THICKNESS or WALL THICKNESS VARIABLE
  ```

- If the section is `BAR`, the following geometry command lines are required:

```
WIDTH or WIDTH VARIABLE
HEIGHT or HEIGHT VARIABLE
```

- If the section is `BOX`, the following geometry command lines are required:

```
WIDTH or WIDTH VARIABLE
HEIGHT or HEIGHT VARIABLE
WALL THICKNESS or WALL THICKNESS VARIABLE
```

- If the section is `I`, the following geometry command lines are required:

```
WIDTH or WIDTH VARIABLE
HEIGHT or HEIGHT VARIABLE
WALL THICKNESS or WALL THICKNESS VARIABLE
FLANGE THICKNESS or FLANGE THICKNESS VARIABLE
```

Most of the sections require the `T AXIS` or `T AXIS VARIABLE` command line. If the beam has a circular or tube cross section, and the width of the beam exactly equals the height, then the `T_AXIS` need not be specified. If the `T_AXIS` is not specified for one of these circularly symmetric cross sections the code will arbitrarily pick a t axis at each beam that is perpendicular to the the beam.

Beam section parameters can be specified as constant for all beams in the section with commands such as `WIDTH` or `T AXIS`. Alternatively a set of beam parameters that vary from element to element can be specified with variants of these commands with `VARIABLE` at the end, such as `WIDTH VARIABLE` or `T AXIS VARIABLE`. When the `VARIABLE` variants of commands are used, the command specifies the name of an attribute field on the input mesh that contains the parameter. For `WIDTH VARIABLE`, `HEIGHT VARIABLE`, `WALL THICKNESS VARIABLE`, and `FLANGE THICKNESS VARIABLE`, the field should contain one entry per element. For `AXIS OFFSET VARIABLE` the field should contain either two or three entries per element. If the field for the axis offset contains two entries, it specifies the offset in the local s, t coordinate system. If it contains three entries, it specifies the offset in the global x, y, z coordinate system. For `T AXIS VARIABLE` the field should contain three entries per element.

Before presenting details about the various sections, we will discuss the local coordinate system for the beam. (The geometric properties are related to this local coordinate system.) For the beam, it is necessary to specify a local Cartesian coordinate system, which will be designated as r, s, and t. The r-axis lies along the length of the beam and passes through the centroid of the beam. The t-axis is specified by the user as a vector in the global coordinate system. The s-axis is computed from the cross product of the t-axis and the r-axis. The t-axis is then recomputed as the cross product of the r-axis and the s-axis to ensure that the t-axis is orthogonal to the r-axis. These local direction vectors are all normalized, so the user-input vectors do not have to be unit vectors.

If we want the initial position of the t-axis to be parallel to the global Z-axis, then we would use the command line:

```
T AXIS = 0 0 1
```

If we wanted the initial position of the *t*-axis to be parallel to a vector (0.5, 0.8660, 0) in the global coordinate system, then we would use the command line:

```
T AXIS = 0.5 0.8660 0.0
```

The *t*-axis will change position as the beam deforms (rotates about the *r*-axis). This change in position is tracked internally by the computations for the beam element. The `HEIGHT` for the beam cross section is in the direction of the *t*-axis, and the `WIDTH` of the beam cross section is in the direction of the *s*-axis.

Now that the local coordinate system for the beam has been defined, we can describe the definition of each section.

- The `ROD` section is a solid elliptical section. The diameter along the height is specified by the `HEIGHT` command line, and the diameter along the width is specified by the `WIDTH` command line.
- The `TUBE` section is a hollow elliptical section. The diameter along the height is specified by the `HEIGHT` command line, and the diameter along the width is specified by the `WIDTH` command line. The wall thickness for the tube is specified by the `WALL THICKNESS` command line.
- The `BAR` section is a solid rectangular section. The height is specified by the `HEIGHT` command line, and the width is specified by the `WIDTH` command line.
- The `BOX` section is a hollow rectangular section. The height is specified by the `HEIGHT` command line, and the width is specified by the `WIDTH` command line. The wall thickness for the box is specified by the `WALL THICKNESS` command line.
- The `I` section is the standard I-section associated with a beam. The height of the I-section is given by the `HEIGHT` command line, and the width of the flanges is given by the `WIDTH` command line. The thickness of the vertical member is given by the `WALL THICKNESS` command line, and the thickness of the flanges is given by the `FLANGE THICKNESS` command line.

By default, the *r*-axis coincides with the geometric centerline of the beam. The geometric centerline of the beam is defined by the location of the two nodes defining the beam connectivity. It is possible to offset the local *r*-axis, *s*-axis, and *t*-axis from the geometric centerline of the beam. To do this, one can use either the `REFERENCE AXIS` command line or the `AXIS OFFSET` command line, but not both.

The `REFERENCE AXIS` command line has the options `CENTER`, `TOP`, `RIGHT`, `BOTTOM`, and `LEFT`. The `CENTER` option is the default, which means that the *r*-axis coincides with the geometric centerline of the beam. If the `TOP` option is used, the *r*-axis is moved in the direction of the original *t*-axis by a positive distance `HEIGHT/2` from the centroid so that it passes through the top of the beam section (top being defined in the direction of the positive *t*-axis). If the `RIGHT` option is used, the *r*-axis is moved in the direction of the original *s*-axis by a positive distance `WIDTH/2` so that it passes through the right side of the beam section (the section being viewed in the direction of the

negative r-axis). If the BOTTOM option is used, the r-axis is moved in the direction of the original t-axis by a distance HEIGHT/2 so that it passes through the bottom of the beam section (bottom being defined in the direction of the negative t-axis). If the LEFT option is used, the r-axis is moved in the direction of the original s-axis by a negative distance WIDTH/2 so that it passes through the left side of the beam section (the section being viewed in the direction of the negative r-axis). For all options, the s-axis and the t-axis remain parallel to their original positions before the translation of the r-axis.

The AXIS OFFSET command line allows the user to offset the local coordinate system from the geometric centerline by an arbitrary distance. The first parameter on the command line moves the r-axis a distance s_offset from the centroid of the section along the original s-axis. The second parameter on the command line moves the r-axis a distance t_offset from the centroid of the section along the original t-axis. The s-axis and t-axis remain parallel to their original positions before the translation of the r-axis.

Alternatively, the axis offset can be specified in global coordinates using the AXIS OFFSET GLOBAL command. This command takes three parameters, which are the x, y, and z components of the offset in the global coordinate system.

Strains and stresses are computed at the midpoint of the beam. The integration of the stresses over the cross section at the midpoint is used to compute the internal forces in the beam. Each beam section has its own integration scheme. The integration scheme for each of the sections is shown in Figure 5.5 through Figure 5.7. The numbers in these figures show the relative location of the integration points in regard to the centroid of the section and the s-axis and the t-axis.

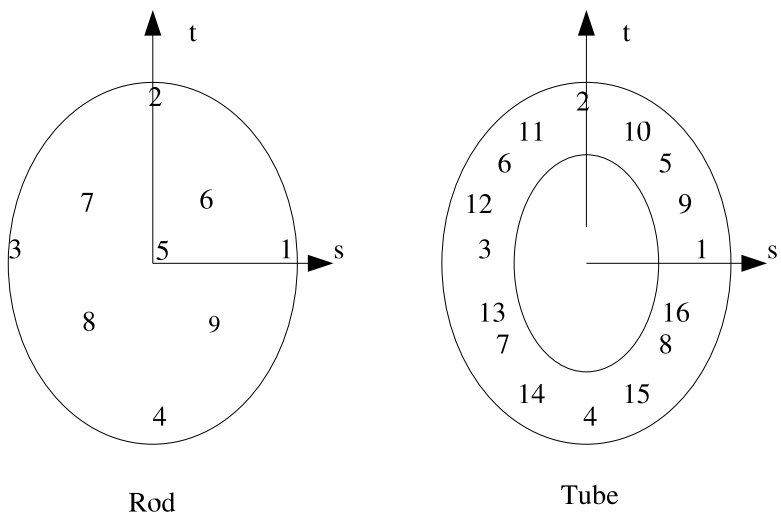

Figure 5.5: Integration points for rod and tube

At each integration point, there is an axial strain (with a corresponding axial stress) and an in-plane (in the plane of the cross section) shear strain (with a corresponding shear stress). The user can output this stress and strain information by using the RESULTS OUTPUT commands described in Chapter 8. The variable that will let users access the strain at the beam integration points is

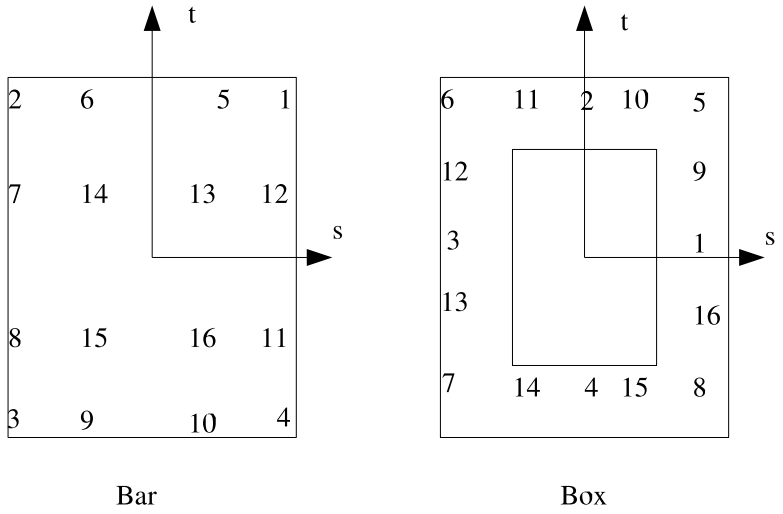

Figure 5.6: Integration points for bar and box.

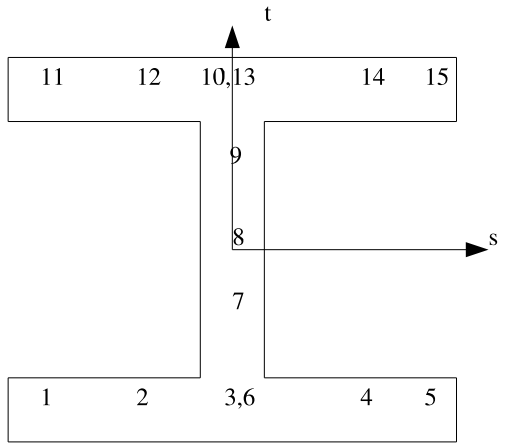

Figure 5.7: Integration points for I-section.

`beam_strain_inc`, and the variable that will let users access the stress at the beam integration points is `stress`. If the user requests output for the beam strain, 32 values are given for the strain. The first value (designated in the output as 01) is the axial strain at the first integration point, the second value (designated in the output as 02) is the shear strain at the first integration point, etc. The odd values for the strain output (01, 03, 05, etc.) are the axial strains at the integration points. The even values of the strain output (02, 04, 06, etc.) are the shear strains at the integration points. For the case where there are only nine integration points (the rod), only the first 18 values for strain have any meaning for the section (the values 19 through 32 are zero). For the I-section, only the first 30 of the strain values have meaning since this section only has 15 integration points. For all other sections, all 32 values have meaning. Output of stress is slightly different than the output

of strain because the stress is stored as a symmetric tensor that contains six components, although four of these components are never used. The axial stress at the first integration point is designated by `stress_xx_01` and the shear stress at the first integration point is `stress_xy_01`. The other four components, `stress_yy_01`, `stress_zz_01`, `stress_yz_01` and `stress_xz_01`, are unused and are set to zero. The stresses at other integration points are named `stress_xx_NN` and `stress_xy_NN`, where `NN` is a number from 01 to 16.

As an alternative for the stress output, you may use the variables `beam_stress_axial` and `beam_stress_shear`. The variable `beam_stress_axial` contains only the axial stresses. The first value associated with `beam_stress_axial` (designated as 01) corresponds to the axial stress at integration point 1, the second value associated with `beam_stress_axial` (designated as 02) corresponds to the axial stress at integration point 2, and so on. The variable `beam_stress_shear` contains only shear stresses. The correlation between numbering the values for `beam_stress_shear` (01, 02, ...) and the integration points is the same as for `beam_stress_axial`.

It is possible to access mean values for the internal forces at the midpoint of the beam. The axial force at the midpoint of the beam is obtained by referencing the variable `beam_axial_force`. The transverse forces at the midpoint of the beam in the *s*-direction and the *t*-direction are obtained by referencing `beam_transverse_force_s` and `beam_transverse_force_t`, respectively. The torsion at the midpoint of the beam (the moment about the *r*-axis), is obtained by referencing `beam_moment_r`. The moments about the *s*-axis and the *t*-axis are obtained by referencing `beam_moment_s` and `beam_moment_t`, respectively.

Elements in a section can be made rigid by including the `RIGID BODY` command line. The `RIGID BODY` command line specifies an identifier that maps to a rigid body command block. See Section 5.3.1 for a full discussion of how to create rigid bodies and Section 5.3.1.1 for information on the use of the `RIGID BODIES FROM ATTRIBUTES` command.

You can request that the material model that will be used with this beam section come from the Strumento material model library with the `USE STRUMENTO` line command. LAME is the default material model library for all beam sections [9] but can be explicitly requested by using the `USE LAME` line command. The versions of the material models in the Strumento library will be removed in a future release of Presto, so it is advised to switch to the LAME versions as soon as possible.

5.2.7 Truss Section

```
BEGIN TRUSS SECTION <string>truss_section_name
  AREA = <real>cross_sectional_area
  INITIAL LOAD = <real>initial_load
  PERIOD = <real>period
  RIGID BODY = <string>rigid_body_name
  RIGID BODIES FROM ATTRIBUTES = <integer>first_id
    TO <integer>last_id
  USE LAME|STRUMENTO(LAME)
END [TRUSS SECTION <string>truss_section_name]
```

The TRUSS SECTION command block is used to specify the properties for a truss element. If this command block is referenced in an element block of three-dimensional, two-node elements, the elements in the block will be treated as truss elements. The parameter, truss_section_name, is user-defined and is referenced by a SECTION command line in a PARAMETERS FOR BLOCK command block.

The cross-sectional area for truss elements is specified by the AREA command line. The value cross_sectional_area is the cross-sectional area of the truss members in the element block.

The truss can be given some initial load over some given time period. The magnitude of the load is specified by the INITIAL LOAD command line. If the load is compressive, the sign on the value initial_load should be negative; if the load is tensile, the sign on the value initial_value should be positive. The period is specified by the PERIOD command line.

The initial load is applied over some period by specifying the axial strain rate in the truss, $\dot{\varepsilon}$, over some period p. At some given time t, the strain rate is

$$\dot{\varepsilon} = \frac{ap}{2}\left[1 - \cos\left(\pi t/p\right)\right], \tag{5.2}$$

where

$$a = \frac{2F_i}{EAp}. \tag{5.3}$$

In Equation (5.3), F_i is the initial load, E is the modulus of elasticity for the truss, and A is the area of the truss. Over the period p, the total strain increment generates the desired initial load in the truss.

During the initial load period, the time increments should be reasonably small so that the integration of $\dot{\varepsilon}$ over the period is accurate. The period should be set long enough so that if the model was held in a steady state after time p, there would only be a small amount of oscillation in the load in the truss.

When doing an analysis, you may not want to activate certain boundary conditions until after the prestressing is done. During the prestressing, time-independent boundary conditions such as fixed displacement will most likely be turned on. Time-dependent boundary conditions such as prescribed acceleration or prescribed force will most likely be activated after the prestressing is complete.

Elements in a section can be made rigid by including the RIGID BODY command line. The RIGID BODY command line specifies an indenter that maps to a rigid body command block. See Section 5.3.1 for a full discussion of how to create rigid bodies and Section 5.3.1.1 for information on the use of the RIGID BODIES FROM ATTRIBUTES command.

It should be noted that the axial stress, which is the only stress component for a truss element, is output as a symmetric tensor with six components to be compatible with the notion of volumetric stress. Because of this, for every truss element, six values of stress are stored and output, but only the fist value is ever used. The axial stress is therefore output as stress_xx and the other five stress components, stress_yy, stress_zz, stress_xy, stress_yz, stress_zx are all

unused and set to zero.

You can request that the material model that will be used with this truss section come from the Strumento material model library with the `USE STRUMENTO` line command. LAME is the default material model library for all truss sections [9] but can be explicitly requested with the `USE LAME` line command. The versions of the material models in the Strumento library will be removed in a future release of Presto, so it is advised to switch to the LAME versions as soon as possible.

5.2.8 Spring Section

```
BEGIN SPRING SECTION <string>spring_section_name
  FORCE STRAIN FUNCTION = <string>force_strain_function
  DEFAULT STIFFNESS <real>default_stiffness
  PRELOAD = <real>preload_value
  PRELOAD DURATION = <real>preload_duration
  RESET INITIAL LENGTH AFTER PRELOAD = <string>NO|YES
  MASS PER UNIT LENGTH = <real>mass_per_unit_length
END [SPRING SECTION <string>spring_section_name]
```

The `SPRING SECTION` command block is used to specify the properties for a spring element. If this command block is referenced in an element block of three-dimensional, two node elements, the elements in the block will be treated as spring elements. The parameter, `spring_section_name`, is user-defined and is referenced by a `SECTION` command line in a `PARAMETERS FOR BLOCK` command block.

The spring behavior is governed by the force-engineering strain function which is specified by the `FORCE STRAIN FUNCTION` command line. The force generated by the spring element is based on the evaluation of the user specified `force_strain_function`, which has units of F vs dL/L_0 with the current engineering strain of the spring, dL/L_0. This allows the force-strain function to be length independent.

The `DEFAULT STIFFNESS` command block specifies the spring stiffness used during the first time step and during preload. In all other situations the spring stiffness is based on the slope of the force-strain function evaluated at the previous timestep and the current timestep. The unit of `default_stiffness` is force.

To specify a preload on the spring both the `PRELOAD` and `PRELOAD DURATION` command line must be specified. The `PRELOAD` command line specifies the magnitude of the preload force, while the `PRELOAD DURATION` command line specifies how long the preload application should take, in seconds.

An optional preload input, `RESET INITIAL LENGTH AFTER PRELOAD`, is used when the user would like the initial length of the spring to reset to the displaced length after the preload has occurred. If this command line is not specified, or is set to `NO`, the initial length of the spring is the undeformed length as calculated from the input mesh.

Springs can optionally have mass through the `MASS PER UNIT LENGTH` command line. However, this input parameter is required if the spring elements are not individual two-node elements, but

rather a string of spring elements, where the inter-spring nodes are only connected to the two adjacent springs. It should be noted, if the mass per unit length is not specified there is no critical timestep calculated for the spring elements.

5.2.9 Damper Section

```
BEGIN DAMPER SECTION <string>damper_section_name
  AREA = <real>damper_cross_sectional_area
END [DAMPER SECTION <string>damper_section_name]
```

The `DAMPER SECTION` command block is used to specify the properties for a damper element. If this command block is referenced in an element block of three-dimensional, two-node elements, the elements in the block will be treated as damper elements. The parameter, `damper_section_name`, is user-defined and is referenced by a `SECTION` command line in a `PARAMETERS FOR BLOCK` command block.

The cross-sectional area for damper elements is specified by the `DAMPER AREA` command line. The value `damper_cross_sectional_area` is the cross-sectional area of the dampers in the element block.

The damper area is used only to generate mass associated with the damper element. The mass is the density for the damper element multiplied by the original volume of the element (original length multiplied by the damper area).

The force generated by the damper element depends on the relative velocity along the current direction vector for the damper element. If $\boldsymbol{n}$ is a unit normal pointing in the direction from node 1 to node 2, if $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$ are the velocity vectors at nodes 1 and 2, respectively, then the force generated by the damper element is

$$F_d = \eta \mathbf{n} \cdot (\boldsymbol{v}_2 - \boldsymbol{v}_1)\,, \tag{5.4}$$

where η is the damping parameter. Currently, the damping parameter must be specified by using an elastic material model for the damper element. The value for Young's modulus in the elastic material model is used for the damping parameter η.

5.2.10 Point Mass Section

```
BEGIN POINT MASS SECTION <string>pointmass_section_name
  VOLUME = <real>volume
  MASS = <real>mass
  IXX = <real>Ixx
  IYY = <real>Iyy
  IZZ = <real>Izz
  IXY = <real>Ixy
  IXZ = <real>Ixz
  IYZ = <real>Iyz
```

```
  RIGID BODY = <string>rigid_body_name
  RIGID BODIES FROM ATTRIBUTES = <integer>first_id
    TO <integer>last_id
  MASS VARIABLE = <string>mass_variable_name
  INERTIA VARIABLE = <string>inertia_variable_name
  OFFSET VARIABLE = <string>offset_variable_name
  ATTRIBUTES VARIABLE NAME = <string>attrib_variable_name
END [POINT MASS SECTION <string>pointmass_section_name]
```

A point mass element is simply a mass at a node, which can be a convenient modeling tool in certain instances. The user can create an element block with one or more point masses. A point mass is a sphere element attached to a single node. A point mass will have its mass added to the mass at the connected node. (Other mass at the node will be derived from mass due to elements attached to the node.) The mass at a node due to a point mass is treated like any other mass at a node derived from an element. The mass due to point mass will be included in body force calculations and kinetic energy calculations, for example.

Point masses are a convenient modeling tool to be used in conjunction with rigid bodies. An element block including one or more point masses can be included in a collection of element blocks used to define a rigid body. The element block of point masses can be used to adjust the total mass and inertia properties for the rigid body. (The point mass element does not have to be used only in conjunction with rigid bodies. One can place a point mass at a node associated with solid or structural elements.)

An element block in which the connectivity for each element contains only one node can be used as a collection of point masses. This command block would have the following form:

```
BEGIN PARAMETERS FOR BLOCK <string>block_id
  MATERIAL = <string>material_name
  SOLID MECHANICS USE MODEL <string> material_model_name
  SECTION = <string>point_mass_section_name
END PARAMETERS FOR BLOCK <string>block_id
```

The element block associated with the point mass must reference a material command block just like any other element block. If the point mass section specifies a volume, then the product of the density specified in the material block and the volume specified in the section block is used to calculate the element mass.

The `VOLUME` command specifies the volume of a point mass element. The mass of the element is then found by multiplying that volume by the material model density.

The `MASS` command explicitly specifies the mass.

The `IXX`, `IYY`, `IZZ`, `IXY`, `IXZ`, `IYZ` commands are used to explicitly define the symmetric inertia tensor entries for the point mass. Note that currently, the trace of the inertial tensor is added to the nodal rotational mass and the rest of the inertia tensor entries are ignored.

The `OFFSET` is used to define the offset of the mass with respect to the connected node. Currently the offset effects only the rotational properties of the point mass. The rotational mass of the point mass is increased by mass times offset distance squared.

The `MASS VARIABLE` specifies that the mass of the point mass elements is to be read from the input mesh file from the variable with the specified name (use the name ”attribute” to read the mass from the mesh block attributes.)

The `INERTIA VARIABLE` specifies that the inertia tensor of the point mass elements is to be read from the input mesh file from the variable with the specified name (use the name ”attribute” to read the inertia tensor from the mesh block attributes.) When this command is used, the mesh file variable should contain six entries per element, ordered as follows: Ixx, Iyy, Izz, Ixy, Ixz, Iyz.

The `OFFSET VARIABLE` specifies that the offset vector of the point mass elements is to be read from the input mesh file from the variable with the specified name (use the name ”attribute” to read the offset vector from the mesh block attributes.) When this command is used, the mesh file variable should contain three entries per element, ordered as follows: Offset_x, Offset_y, Offset_z.

The `ATTRIBUTES VARIABLE NAME` specifies that all properties of the point mass element are to be read from the input mesh file of the variable with the specified name (use the name ”attribute” to read from the mesh block attributes.) When this command is used, the mesh file variable should contain ten entries per element, ordered as follows: Mass, Ixx, Iyy, Izz, Ixy, Ixz, Iyz, Offset_x, Offset_y, Offset_z.

Multiple ways are provided to specify the raw attributes of mass, inertia and offset for the point mass element. The user must be careful to only use one of these ways to define each property. Using multiple ways to define the mass will result in errors or warnings because of ambiguities.

If you have access to the SEACAS codes from Sandia National Laboratories, you may use the codes in this library to generate element blocks with point mass elements. See Reference 11 for an overview of the SEACAS codes. By using various SEACAS codes, you can easily generate an element block with one or more point masses. For each point mass in the element block, you should create an eight-node hexahedral element that is centered at the point where you want the point mass located. The hexahedron can have arbitrary dimensions, but it is best to work with a unit cube. Suppose you wanted a point mass at (13.5, 27.0, 3.1415). You could create a unit hexahedron (1 by 1 by 1) centered on (13.5, 27.0, 3.1415). The SEACAS program SPHGEN3D will convert the hexahedron to a zero-dimensional element in three-dimensional space located at the center of the hexahedron. For our specific example, the program SPHGEN3D would create a zero-dimensional element, basically an element consisting of a single node, at (13.5, 27.0, 3.1415).

Elements in a section can be made rigid by including the `RIGID BODY` command line. The `RIGID BODY` command line specifies an indenter that maps to a rigid body command block. See Section 5.3.1 for a full discussion of how to create rigid bodies and Section 5.3.1.1 for information on the use of the `RIGID BODIES FROM ATTRIBUTES` command.

5.2.11 Particle Section

```
BEGIN PARTICLE SECTION <string>sph_section_name
  RADIUS MESH VARIABLE = <string>var_name|<string>attribute|
    SPHERE INITIAL RADIUS = <real>rad
  RADIUS MESH VARIABLE TIME STEP = <string>time
  PROBLEM DIMENSION = <integer>1|2|3(3)
```

```
    CONSTANT SPHERE RADIUS
    FINAL RADIUS MULTIPLICATION FACTOR = <real>factor(1.0)
    FORMULATION = <string>GPA|MASS_PARTICLE|SPH(SPH)
    MONAGHAN EPSILON = <real>monaghan_epsilon(0.0)
    MONAGHAN N = <real>monaghan_n(0.0)
    SPH ALPHAQ PARAMETER = <real>alpha(1.0)
    SPH BETAQ PARAMETER = <real>beta(2.0)
    DENSITY FORMULATION = <string>MATERIAL|KERNEL(MATERIAL)
    USE LAME|STRUMENTO(LAME)
  END [PARTICLE SECTION <string>sph_section_name]
```

SPH (smoothed particle hydrodynamics) is useful for modeling fluids or for modeling materials that undergo extremely large distortions. One must be careful when using SPH for modeling. SPH tends to exhibit both accuracy and stability problems, particularly in tension. An SPH particle interacts with other nearest-neighbor SPH particles based on radius properties of all the elements involved; SPH particles react with other elements, such as tetrahedra, hexahedra, and shells, through contact. You should consult Reference 10 regarding the theoretical background for SPH.

You can define contact interaction between the particles in a particle element block and other element types. In order to do this, you must use the `CONTACT NODE SET` option described in Section 7.2.4. All of the particles in the particle element block must be included in a node set if you use the `CONTACT NODE SET` option.

The particle section should only be associated with elements with the `SPHERE` topology. Sphere elements are point elements that are connected to only a single node.

All of the particles contained in a particle element block must be given some initial radius. There are two options for setting the initial radius for each particle. First, each particle can be given the same radius. To set the radius for each particle in an element block to the same value, use the `SPHERE INITIAL RADIUS` command line. The parameter `rad` on this command line sets the radius for all the particles in the element block.

Alternatively, the radius for each particle can be read from a mesh file. The radii can be read from a variable on the mesh file from attributes associated with the element block. If you want to read some variable from the mesh file for the radii, then you would use:

```
RADIUS MESH VARIABLE = sph_radius
```

where `sph_radius` is the variable name on the mesh file. If you want to use the variable associated with a specific time on the mesh file, you should use the `RADIUS MESH VARIABLE TIME STEP` command line to select the specific time. If you want to read the attributes associated with the particles, then you should insert the command line

```
RADIUS MESH VARIABLE = attribute
```

(as shown) into the `PARTICLE SECTION` command block. Pronto3d [1] only offers the attribute option. To compare Presto and Pronto3d results, you should use the attribute option.

If the attribute option is used, each particle should have two attributes defined per element. The first attribute is the particle radius, and the second attribute is the particle volume. The most common way to generate a particle mesh is to first generate a solid element mesh and then use the utility

'sphgen3d' to convert the solid elements into sphere elements. Sphgen3d will convert each solid element into a sphere and place it at the source element centroid. In the output mesh file generated by sphgen3d The radius attribute of the element blocks will be proportional to the source element size and the volume attribute will be the volume of the source element.

The `FINAL RADIUS MULTIPLICATION FACTOR` command may be used to increase or decrease the initial particle radii. The factor specified will scale the particle radii input with either a constant or a mesh file attribute.

After the radii are initialized, you may determine whether the radii are to remain constant or are to change throughout the analysis. The `CONSTANT SPHERE RADIUS` command line is an optional command line that prevents the sphere radius from changing over the course of the calculation. By default, the sphere radii will expand or contract based on the changing density in the elements to satisfy the relation that element mass (a constant) equals element volume times element density. If the `CONSTANT SPHERE RADIUS` command line appears, then the radii for all particles will remain constant.

The `DENSITY FORMULATION` command controls the method used to update the density, and thus SPH radii, during the analysis. The default `MATERIAL` option uses the material density and nodal mass to compute a volume for each particle at a given time. The radius is then computed as the cube root of that volume. The alternative `KERNEL` option computes the current density for each particle using the mass of that particle and the SPH kernel density function. The `KERNEL` option may be necessary when large expansions of particles are expected (such as when modeling large density changes in gases). The `MATERIAL` option generally changes particle densities, and thus radii, less than the `KERNEL` option, so is appropriate for analyses that do not have large density fluctuations.

You can request that the material model that will be used with this particle section come from the Strumento material model library with the `USE STRUMENTO` line command. LAME is the default material model library for all particle sections [9] but can be explicitly requested by using the `USE LAME` line command. The versions of the material models in the Strumento library will be removed in a future release of Presto, so it is advised to switch to the LAME versions as soon as possible.

An analysis problem using SPH may be inherently one-, two-, or three-dimensional. You may indicate whether or not there is some inherent dimensionality in the problem by using the `PROBLEM DIMENSION` command line. The possible value for this command line is 1 (one-dimensional), 2 (two-dimensional), or 3 (three-dimensional). The default value is 3 for three-dimensional. The internal SPH kernel functions are modified depending on the value set on the `PROBLEM DIMENSION` command line. If, for example, your problem is inherently two-dimensional in nature, you may get more accurate results by specifying the dimension for your problem as 2 (as opposed to 1 or 3).

The `FORMULATION` command defines the SPH formulation to use, and has the following options:

- `SPH`, general smoothed particle hydrodynamics.

- `GPA`, Generalized particle algorithm (See separate GPA documentation.)

- MASS_PARTICLE, Particles only have mass, and no stiffness. Particles do not interact with each other in any way.

The MONAGHAN EPSILON and MONAGHAN N commands set the Monaghan viscosity coefficients. Monaghan viscosity may allow the SPH algorithm to behave better, particularly in tension. Standard values to use are 0.2 for epsilon and 4 for n. See (Reference 14) for more information on the usage of these parameters.

The SPH ALPHAQ PARAMETER and SPH BETAQ PARAMETER commands control the sph viscosity terms. Larger values lead to more viscosity. Alpha is associated with a viscosity parameter that is proportional to the dilatational modulus of the material. Betaq is associated with a viscosity parameter that is proportional to the change in material density over a time step.

Utility Commands. In addition to the SPH-related command lines just described (which appear in the PARTICLE SECTION command block) there is one other SPH-related command block:

```
BEGIN SPH OPTIONS
  SPH SYMMETRY PLANE <string>+X|+Y|+Z|-X|-Y|-Z
    <real>position_on_axis(0.0)
  SPH DECOUPLE STRAINS: <string>material1 <string>material2
END [SPH OPTIONS]
```

If used, this command block should be placed in the Presto region scope. (All other SPH-related command lines must be nested within the PARTICLE SECTION command block; the PARTICLE SECTION command block, like all other section command blocks, is in the SIERRA scope.) The symmetry conditions are applied to all SPH element blocks.

The SPH SYMMETRY PLANE command line may be used to reduce model sizes by specifying symmetry planes and modeling only a portion of the model. Due to the nonlocal nature of SPH element integration, symmetry planes cannot be defined with boundary conditions alone; these planes must be explicitly defined. A plane is defined by an outward normal vector aligned with one of the axes (+X, +Y, +Z, -X, -Y, -Z) and some point on the axis, which represents a point in the plane. Suppose for example, the outward normal to the plane of symmetry is in the negative Y-direction (-Y) and the plane of symmetry passes through the y-axis at $y = +2.56$. Then the definition for the symmetry plane would be:

```
SPH SYMMETRY PLANE -Y +2.56
```

The SPH DECOUPLE STRAINS command line prevents two dissimilar materials from directly interacting. Generally, the material properties at a particle are the average of the material properties from nearby particles. If particles with very dissimilar material properties are interacting, this interaction can create problems. The SPH DECOUPLE STRAINS command line ensures that particles with very dissimilar material properties do not directly interact by material-property averaging, but instead just interact with a contact-like interaction. The two material types that are not to interact are specified by the parameters material1 and material2. These parameters will appear as material names on a PROPERTY SPECIFICATION FOR MATERIAL command block.

Display. For purposes of visualizing the element stresses, it may be necessary to copy these element variables into nodal variables. This can easily be done by defining a `USER VARIABLE` command block (Section 10.2.4) in conjunction with a `USER OUTPUT` command block (Section 8.2.2). Once the nodal variable is defined, it can be output in a `RESULTS OUTPUT` command block (Section 8.2.1). An example is provided below. The `SPH` element blocks for the problem are element blocks 20, 21, and 22. All other element blocks are non-SPH elements.

- In the SIERRA scope:

```
BEGIN USER VARIABLE nodal_stress
  TYPE = NODE SYM_TENSOR LENGTH = 1
END
```

- In the region scope:

```
BEGIN USER OUTPUT
  BLOCK = block_20 block_21 block_22
  COPY ELEMENT VARIABLE stress TO NODAL VARIABLE
    nodal_stress
  END

  BEGIN RESULTS OUTPUT output_presto
    DATABASE NAME = sph.e
    DATABASE TYPE = exodusII
    AT TIME 0.0 INCREMENT = 1.0e-04
    NODAL nodal_stress
  END RESULTS OUTPUT output_presto
```

5.2.12 Superelement Section

```
BEGIN SUPERELEMENT SECTION <string>section_name
  BEGIN MAP
    <integer>node_index_1 <integer>component_index_1
    <integer>node_index_2 <integer>component_index_2
    ...
    <integer>node_index_n <integer>component_index_n
  END
  BEGIN STIFFNESS MATRIX
    <real>k_1_1 <real>k_1_2 ...  <real>k_1_n
    <real>k_2_1 <real>k_2_2 ...  <real>k_2_n
    ...         ...         ...  ...
    <real>k_n_1 <real>k_n_2 ...  <real>k_n_n
  END
  BEGIN DAMPING MATRIX
```

```
    <real>c_1_1 <real>c_1_2 ...  <real>c_1_n
    <real>c_2_1 <real>c_2_2 ...  <real>c_2_n
    ...         ...         ...  ...
    <real>c_n_1 <real>c_n_2 ...  <real>c_n_n
  END
  BEGIN MASS MATRIX
    <real>m_1_1 <real>m_1_2 ...  <real>m_1_n
    <real>m_2_1 <real>m_2_2 ...  <real>m_2_n
    ...          ...        ...  ...
    <real>m_n_1 <real>m_n_2 ...  <real>m_n_n
  END
  FILE = <string>netcdf_file_name
END [SUPERELEMENT SECTION <string>section_name]
```

A superelement allows definition of an element with a user defined stiffness, damping, and mass matrix. The superelement stiffness is linear and remains constant in time.

The superelement must be represented by an element in the mesh file. A block of elements used to define a superelement must contain exactly one finite element. The finite element that represents the superelement may have any topology. The topology may either be a valid geometric topology (hex, rod, tet, etc.) or may be be an arbitrary topology as defined in the input mesh file. The nodes of a superelement can be shared with other elements, or can be attached only to the superelement. In addition, the superelement can have additional internal degrees of freedom that are not present in the mesh file. If output values are desired on a node, that node must be present in the input mesh file.

Superelement nodes have all the same variables as regular nodes (mass, displacement, velocity, etc.) Only the element time step is defined as an output variable on the superelement itself.

5.2.12.1 Input Commands

```
BEGIN MAP
```

The `MAP` command block defines the mapping from nodal degrees of freedom to the local degrees of freedom in the stiffness and mass matrix for the superelement. The map should contain N pairs of integers, where N is the number of nodes in the superelement. The first integer of each pair is the index of the node in the superelement in the range $0 \ldots N$. The second integer is the component in the range $0 \ldots 6$.

A node index of 0 is a special value and marks the degree of freedom that is internal to the superelement. A superelement may have any number of internal degrees of freedom. Internal degrees of freedom are created internal to the code do not correspond to any nodes actually present in the mesh. A node index greater than zero represents that node index in the element. For example if the superelement was represented by an eight node hex element then node indexes could vary from one to eight and would match the first through eighth nodes in the hex element.

If an internal degree of freedom is used, the component index should be set to 0 along with the node index. If a regular node is used, components 1, 2, and 3 correspond to the X, Y, and Z translational

degrees of freedom. Components 4, 5, and 6 correspond to the X, Y, and Z rotational degrees of freedom.

The following is an example superelement definition for a three degree of freedom truss element lying along the x-axis. The superelement is defined in the mesh file using a two node rod element. Degrees of freedom 1 and 3 are mapped to x degrees of freedom of the end nodes of the rod element. Degree of freedom 2 is internal to the superelement.

```
BEGIN SUPERELEMENT SECTION truss_x3
  BEGIN MAP
    1 1
    0 0
    2 1
  END
  BEGIN STIFFNESS MATRIX
    100 -100    0
   -100  200 -100
      0 -100  100
  END
  BEGIN DAMPING MATRIX
    1 -1  0
   -1  2 -1
    0 -1  1
  END
  BEGIN MASS MATRIX
    0.25 0.00 0.00
    0.00 0.50 0.00
    0.00 0.00 0.025
  END
END [SUPERELEMENT SECTION <string>section_name]
```

`BEGIN STIFFNESS MATRIX`

The `STIFFNESS MATRIX` command block defines the NxN stiffness matrix for the superelement. The number of rows and columns in the stiffness matrix must be the same as the number of rows in the `MAP` command block. The stiffness matrix should be symmetric. If the input matrix is not symmetric, it will be made symmetric by $K_{sym} = 0.5 * (K_{input} + K_{input}^T)$. To guarantee stability for explicit dynamics and solution convergence for implicit statics/dynamics, the stiffness matrix should be positive definite.

`BEGIN DAMPING MATRIX`

The `DAMPING MATRIX` command block defines the NxN damping matrix for the superelement. The number of rows and columns in the damping matrix must be the same as the number of rows in the `MAP` command block. The damping matrix should generally be symmetric. This command block is optional. If a damping matrix is not defined, no damping will be used by default.

`BEGIN MASS MATRIX`

The `MASS MATRIX` command block defines the *NxN* mass matrix for the superelement. The mass matrix must have the same dimensions as the stiffness matrix. The mass matrix need not be symmetric, however to guarantee stability for explicit dynamics and solution convergence for implicit statics/dynamics the mass matrix should be positive definite.

```
FILE = <string>netcdf_file_name
```

As an alternative to defining stiffness and mass matrices in the input file, the stiffness and mass matrices may be imported from a NetCDF file. External codes (such as Salinas) are able to compress larger models into superelements and output the matrices in the NetCDF format. The `netcdf_file_name` defines the path to the file that contains the mass, damping, and stiffness matrix definitions. All superelement matrices should be defined either in the input deck or in the NetCDF file. The damping matrix is optional, so if it is not defined in the NetCDF file, no damping will be used by default. The connectivity map needs to be specified in the input file in either case.

In the netcdf file the stiffness matrix must be named `Kr`, the mass matrix `Mr`, and the damping matrix `Cr`.

Known Issue: Superelements are not compatible with several modeling capabilities. They cannot be used with element death. They cannot be used with node-based, power method, or Lanczos critical time step estimation methods. They are also not compatible with some preconditioners (such as FETI) for implicit solutions.

5.2.13 Peridynamics Section

```
BEGIN PERIDYNAMICS SECTION <string>section_name
  MATERIAL MODEL FORMULATION = <string>CLASSICAL|PERIDYNAMICS
  HORIZON = <real>horizon [SCALE BY ELEMENT RADIUS]
  BOND DAMAGE MODEL = <string>CRITICAL_STRETCH|NONE(NONE)
     [<real>critical_stretch]
  HOURGLASS STIFFNESS = <real>stiffness(0.0)
  BOND CUTTING BLOCK = <string list>block_names
  BOND VISUALIZATION = <string>OFF|ON(OFF)
END [PERIDYNAMICS SECTION <string>section_name]
```

Peridynamics is an extension of classical solid mechanics that allows for the modeling of bodies in which discontinuities occur spontaneously. For this reason, peridynamics is well suited for modeling phenomena such as cracking. This section describes the `PERIDYNAMICS SECTION` command block. Details regarding peridynamics methodology and suggested usage guidelines can be found in Section 9.3.

A `PERIDYNAMICS SECTION` should only be associated with elements with the `SPHERE` topology. Sphere elements are point elements that are connected to only a single node. Sphere elements may be created, for example, using the `sphgen3d` utility.

Warning: The default parallel decomposition for models containing sphere elements is typically very poor. It is recommended that an initial rebalance be carried out for parallel analyses with peridynamics. See Section 5.8 for details regarding the `INITIAL REBALANCE` command.

Within a `PERIDYNAMICS SECTION`, the `MATERIAL MODEL FORMULATION` command line specifies the application of either a peridynamics material model or a classical material model adapted for use with peridynamics as described in Section 9.3. Currently, only the `ELASTIC` material model is available with the `PERIDYNAMICS` material model formulation. Setting `MATERIAL MODEL FORMULATION = CLASSICAL` enables the interface between Presto peridynamics and the `LAME` material library. This interface allows the material models described in Section 4.2 to be used with peridynamics.

The peridynamic horizon is set with the `HORIZON` line command. As described in Section 9.3, the horizon determines the region of nonlocality for a given peridynamic element. A peridynamic element interacts directly with all peridynamic elements that are within a distance equal to the horizon in the reference configuration. The horizon may be specified as either a constant value or as a multiple of the element radius. By default, the command applies a constant horizon equal to the specified value of `horizon` to all elements associated with the given peridynamics section. If the optional `SCALE BY ELEMENT RADIUS` is included at the end of this command, the horizon for each peridynamic element is set to `horizon` times a given element's radius.

The bond damage model is specified by the `BOND DAMAGE MODEL` command. Bonds may be broken as dictated by a critical stretch bond breaking law, or bond breaking may be disabled. Two options are available: `CRITICAL_STRETCH` and `NONE`. The default option, `NONE`, causes bond breaking to be disabled. The critical stretch bond breaking law is activated by specifying `CRITICAL_STRETCH`. If this model is selected, the user must specify `critical_stretch`, the value of stretch at which bonds are broken, where stretch is computed as bond elongation divided by the initial bond length.

Hourglass stiffness for peridynamics is controlled with the `HOURGLASS STIFFNESS` command. Within the peridynamics hourglass stiffness routine, the parameter `stiffness` is multiplied by a material's bulk modulus to determine the resistance to deformation in potential zero-energy modes. By default, no hourglass stiffness is computed for peridynamics; hourglass stiffness must be activated by including a this command. Note that peridynamics hourglass control is completely independent from the hourglass control applied to underintegrated elements (Section 5.1.5.6).

By default, a peridynamic bond is formed between a given peridynamic element and all peridynamic elements within its horizon. In some cases, this results in the formation of bonds that are nonphysical. For example, bonds may be incorrectly formed between two components that are within a distance equal to the horizon in the reference configuration but that are not physically connected. The bond cutting feature provides a mechanism for controlling the formation of bonds. The `BOND CUTTING BLOCK` command designates blocks in the `block_names` list as bond cutting blocks. Any bond that would pass through a surface of a bond cutting block is omitted from the analysis. For example, to prevent the creation of bonds between two components that are in close proximity but are not physically connected, a user may include a block in the input mesh file that lies between these components and designate that block as a bond cutting block. The bond

cutting block may be any type of block (e.g., a shell, hex, or tet mesh), provided that Presto is capable of skinning it (see Section 7.2). If a sphere element mesh for use with peridynamics has been created from a hex-element mesh (for example, with `sphgen3d`), it may be convenient to simply include the original hex element mesh as a bond cutting block. Any block designated as a bond cutting block is automatically removed from the analysis following the initialization of bonds.

The `BOND VISUALIZATION` command provides a mechanism for visualizing bonds through the representation of bonds as bar elements in the output database. This feature is set to `OFF` by default and may be activated with the command `BOND VISUALIZATION = ON`. The bond visualization feature is intended as a verification tool for mesh creation and is not recommended for used for production runs.

Warning: Setting `BOND VISUALIZATION = ON` results in the creation of additional elements in the output file. Because each bond is represented by an additional element, the resulting output file may grow in size by several orders of magnitude relative to the standard output file. For this reason, `BOND VISUALIZATION` is recommended only as a mesh verification tool for small- to medium-sized problems and should not be used for production runs.

5.3 Element-like Functionality

This section describes functionality in Presto that behaves similarly to finite elements, although is not implemented as such. The functionality described in this section—rigid bodies and the torsional spring mechanism—is specified through command blocks that appear in the SIERRA scope and Presto region, respectively.

5.3.1 Rigid Body

```
BEGIN RIGID BODY <string>rb_name
  MASS = <real>mass
  POINT MASS = <real>mass [AT <real>X <real>Y <real>Z]
  REFERENCE LOCATION = <real>X <real>Y <real>Z
  INERTIA = <real>Ixx <real>Iyy <real>Izz <real>Ixy
    <real>Iyz <real>Izx
  POINT INERTIA = <real>Ixx <real>Iyy <real>Izz <real>Ixy
    <real>Iyz <real>Izx
  MAGNITUDE = <real>magnitude_of_velocity
  DIRECTION = <string>direction_definition
  ANGULAR VELOCITY = <real>omega
  CYLINDRICAL AXIS = <string>axis_definition
  INCLUDE NODES IN <string>surface_name
    [IF <string>field_name <|<=|=|>=|> <real>value]
END [RIGID BODY <string>rb_name]
```

A rigid body can consist of any combination of elements—solid elements, structural elements, and point masses—except SPH or peridynamics elements. All nodes associated with a rigid body maintain their relative position to each other as determined at time 0 when there is no deformation of the body. This means that the elements associated with the rigid body can translate and rotate through space, but they cannot deform. Element blocks defining the rigid body do not have to be contiguous. They can also adjoin deformable element blocks. Multiple rigid bodies are allowed in a model.

The non-deformable nature of the rigid body can put it in conflict with other constraints. Refer to Appendix D for information on how conflicting constraints are handled.

Warning: Kinematic boundary conditions prescribed on a rigid body must be applied to the rigid body reference node. Kinematic boundary conditions prescribed on a rigid body that are not prescribed on the rigid body reference node will be unenforced. To apply kinematic boundary conditions to a rigid body, use the `BLOCK =` or the `RIGID BODY =` line command with the rigid body's block id or name, respectively, in the appropriate boundary condition command block. Refer to Chapter 6.

Presto creates a new node for each rigid body in the analysis. The new nodes are true nodes in that they are associated with solution fields such as displacement, velocity, and rotational velocity. These nodes will appear in a results file along with other nodes. The global node number given to the new nodes is simply the total number of nodes in the mesh plus one, repeated for each new rigid body node.

If an element block is declared to be a part of a rigid body, the internal force calculations are not called for the elements in that block and element time steps are not computed. Hence, for a model where all the element blocks are included in rigid bodies, there is no estimate for a global time step. In this case an initial time must be specified in the `TIME CONTROL` command block (Section 3.1.1) with the command line

```
INITIAL TIME STEP = <real>time_step
```

Also, one should not override the default value of 1.0 for the time step scale factor (see Section 3.1.1). The time step for this particular case must remain constant. The value of 1.0×10^{-6} should work well for most problems, though any time step may be specified. However since a completely rigid problem does not impose a stability limit on the time step, specifying too large of a time step could cause loss of accuracy in the solution of the problem (due to numerical integration error, large rotations over a time step, etc.) even though the problem runs to completion.

Specification of a rigid body requires the above command block, which appears in the SIERRA scope, plus the `RIGID BODY` command line that appears in the various `SECTION` command blocks described in this chapter. Suppose, for example, `rigidbody_1` consists of element blocks 100, 110, and 280. The `PARAMETERS FOR BLOCK` command blocks for element blocks 100, 110, and 280 must all contain a `SECTION` command line. In each case, the Section must contain a line such as:

```
RIGID BODY = rigidbody_1
```

Once you have declared an element block or some collection of element blocks to be a rigid body and created a rigid body name (through the Section chosen), that rigid body name must appear as the name in a `RIGID BODY` command block. In our example, we must have a `RIGID BODY` command block with the value for `rb_name` set to `rigidbody_1`. Therefore, at a minimum, you must have a command block in the SIERRA scope with the form

```
BEGIN RIGID BODY rigidbody_1
END RIGID BODY rigidbody_1
```

for our example.

The `RIGID BODY` command block has several optional command lines, composing four groups of commands. One group consists of the `MASS`, `POINT MASS`, `REFERENCE LOCATION`, `POINT INERTIA`, and `INERTIA` command lines, a second group consists of the paired `MAGNITUDE` and `DIRECTION` command lines, a third group consists of the paired `ANGULAR VELOCITY` and `CYLINDRICAL AXIS` command lines, and a final group consists of the `INCLUDE NODES IN` command line. The command block can include none or any combination of these groups. If none of these commands is included, the command block simply supplies the value for `rb_name`.

Input to the `MASS` command line consists of a single real number that defines the total mass of the rigid body. If this line command is not present, the mass of the rigid body will be computed using

the elements in the rigid body and their densities. This is the translational mass at the reference location. This command does not change the inertia terms.

The `POINT MASS` command line requires a real number specifying the amount of mass added to the rigid body. Optionally, the location of that mass may be specified with three real numbers. If the location is not given, the additional mass will be placed at the reference location (and will not affect the moments and products of inertia).

The `REFERENCE LOCATION` command line requires three real numbers defining the reference location for the rigid body. If this line command is not present, the center of mass will be used. The center of mass is calculated from the mesh and the element densities.

Input to the `INERTIA` command line consists of six real numbers. If present, this command line will set the inertia for the rigid body. If it is not present, moments and products of inertia are computed for the rigid body based on the reference location of the rigid body and the element masses.

Input to the `POINT INERTIA` command line consists of six real numbers that define moments (`Ixx`, `Iyy`, `Izz`) and products (`Ixy`, `Iyx`, `Izx`) of inertia to be added to the inertia tensor of the rigid body. This modified inertia tensor (rather than the inertia tensor based solely on element mass) is then used to calculate the motion of the rigid body.

It should be noted, if a rigid body contains an element that has rotational resistance, i.e. shell, beam, etc, the nodal moment of inertia of that element is added to the diagonal components of the rigid body's inertia tensor.

An initial, translational-only velocity for the rigid body reference location should be specified with the `MAGNITUDE` and `DIRECTION` command lines. The `MAGNITUDE` command line gives the magnitude of the initial velocity applied to the reference location, and the `DIRECTION` command line gives a defined direction.

An initial rotational and translational velocity for a rigid body can be specified with the `ANGULAR VELOCITY` and `CYLINDRICAL AXIS` command lines. The `ANGULAR VELOCITY` command line gives the initial translational velocity of and rotational velocity about the reference location due to an angular velocity about some defined axis given on the `CYLINDRICAL AXIS` command line. If the defined cylindrical axis passes through the reference location, this command will impart only an initial rotational velocity to the rigid body reference node. If the axis does not pass through the reference location, this command will impart an initial translational velocity on the rigid body node as well as the initial rotational velocity.

The `INCLUDE NODES IN` command line allows a rigid body to include nodes of a surface or block of the mesh. Optionally, the nodes in the surface or block will be included in the rigid body only if the value of a field on the nodes meets a given criterion. For example, consider the rigid body block below.

```
begin rigid body rigid1
  include nodes in block_1
  include nodes in surface_3 if height = -1.0
end
```

Rigid body rigid1 will include all nodes in block_1 and those nodes on surface_3 whose value of the `height` field are equal to -1.0. The optional field (`height` in this case) must be a field known in the analysis. This field may be read in from restart, be a native field initialized upon startup, or be an initialized user-defined field. Since the entire set of nodes in block_1 will be in the rigid body, internal forces and critical time steps will not be computed for elements in block_1.

Presto automatically outputs quantities such as displacement for the reference location of the rigid body. The name assigned to a rigid body will be used to construct variable names that give the quantities. This lets you identify the output associated with a rigid body based on the name you assigned for the rigid body.

Immediately before the results file is written, the accelerations for nodes associated with a rigid body are updated to reflect the accelerations due to the rigid-body constraints. This ensures that the accelerations sent to the results output are correct for a given time.

In summary, if you use a rigid body in an analysis, you will do one or more of the following steps:

- Include a `RIGID BODY` command block in the SIERRA scope. If desired, set reference location, mass, point mass, etc.

- Create a rigid body using one or more element blocks (except `PARTICLE` or `PERIDYNAMICS` element blocks). A `RIGID BODY` command line must appear in the `SECTION` command block used in the `PARAMETERS FOR BLOCK` command block for any element block associated with a rigid body.

- Include point mass element blocks with the rigid body if appropriate. To include point mass element blocks in a rigid body, a `RIGID BODY` command line must appear in the `SECTION` command block used in the `PARAMETERS FOR BLOCK` command block for those point mass element blocks.

- Associate an initial velocity or initial rotation about an axis with the rigid body, if appropriate. If any of the blocks associated with a rigid body have been given an initial velocity or initial rotation, the rigid body must have the same specification for the initial velocity or initial rotation.

The above steps involve a number of different command blocks. To demonstrate how to fully implement a rigid body, we will provide a specific example that exercises the various options available to a user.

Let us assume that we want to create a rigid body named `part_a` consisting of three element blocks. Two of the element blocks, element block 100 and element block 535, are eight-node hexahedra; one of the element blocks, element block 600, consists of only point masses. The `RIGID BODY` command block, `SECTION` command block, and the element blocks we want to associate with the rigid body will be as follows:

```
begin solid section hex_section
  rigid body = part_a
end
```

```
begin point mass section pm_section
  rigid body = part_a
  volume = 0.1
end

begin parameters for block block_100
  material steel
  solid mechanics model use elastic
  section = hex_section
end
begin parameters for block block_535
  material = aluminum
  solid mechanics model use elastic
  section = hex_section
end
begin parameters for block block_600
  material = mass_for_pointmass
  solid mechanics model use elastic
  section = pm_section
end
```

Suppose we want to have the rigid body initially rotating at 600 radians/sec about an axis parallel to the x-axis and passing through a point at (0, 10, 20). We would define this axis using the following set of `DEFINE` command lines:

```
define direction parallel_to_x with vector 2.0 0.0 0.0
define point off_axis with coordinates 0.0 10.0 20.0
define axis body_axis with point off_axis direction parallel_to_x
```

The initial angular velocity specification in the `RIGID BODY` command block is as follows:

```
begin rigid body part_a
  cylindrical axis = body_axis
  angular velocity = 600
end rigid body part_a
```

Presto automatically generates and outputs global data associated with the rigid body (e.g. displacement and quaternion). See Section 8.8 for details on global variable output. Individual field components may be output as discussed in Section 8.1.4 and Table 8.2. In general the field component `fieldi` of the rigid body named `part_a` will be written to the output file(s) with the name `FIELDI_PART_A`.

5.3.1.1 Multiple Rigid Bodies from a Single Block

Typically, all of the elements in a block are assigned to a single rigid body. However, it is sometimes necessary to define a very large number of rigid bodies. It would be unwieldy to create a

separate block for each rigid body. To avoid this, it is possible to create an element attribute in the input mesh file that contains an integer ID used to denote the rigid body in which each element should belong. The `RIGID BODIES FROM ATTRIBUTES` command is used to associate the attribute with the rigid body IDs. This command must be used in conjunction with the `RIGID BODY` command. These commands are used in the context of the section block. They are shown here in the `SOLID SECTION` block, but they can be used with any section type that supports rigid bodies.

```
BEGIN SOLID SECTION <string>sec_name
  RIGID BODIES FROM ATTRIBUTES = <integer>first_id to
    <integer>last_id
  RIGID BODY = <string>rigid_body_name
END
```

If the `RIGID BODIES FROM ATTRIBUTES` command is used, a series of rigid bodies will be created. These rigid bodies are named using the specified `rigid_body_name`, followed by an underscore (_), and then by an integer ID, which ranges between the specified value of `first_id` and `last_id`. Elements having an attribute value equal to a given ID are added to the corresponding rigid body.

When referencing the rigid body name for to apply boundary conditions, it is important to specify the entire name of the rigid body, including the underscore and ID. For example, a name such as `part_a_1` would be used in a boundary condition.

5.3.2 Torsional Spring Mechanism

```
BEGIN TORSIONAL SPRING MECHANISM <string>spring_name
  NODE SETS = <string>nodelist_int1 <string>nodelist_int2
    <string>nodelist_int3 <string>nodelist_int4
  TORSIONAL STIFFNESS = <real>stiffness
  INITIAL TORQUE = <real>init_load
  PERIOD = <real>time_period
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [TORSIONAL SPRING MECHANISM <string>spring_name]
```

This feature was originally implemented to model a torsional spring wrapped around a fixed pin. One end of the pin is fixed to a base, and one end of the spring is attached to this base. There is an arm on the other end of the pin, and this arm can rotate around the pin. The second end of the spring is attached to this arm. The spring resists motion of the arm. Any similar mechanism can be modeled with the torsional spring. Although the torsional spring is element-like in its overall behavior, its implementation within the code structure is different from the other elements described in Chapter 5. The torsional spring does not make use of a section, and its command block (`TORSIONAL SPRING MECHANISM`) should appear in the region scope. A schematic for the torsional spring mechanism is shown in Figure 5.8.

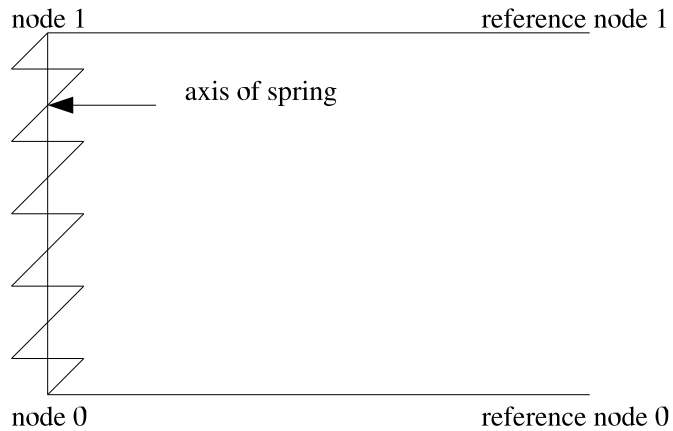

Figure 5.8: Schematic for torsional spring.

The mechanism consists of two nodes that represent the axis of a torsional spring. Node 0 is at the base of the torsional spring, and node 1 is at the top of the torsional spring. A third node, reference node 0, defines an arm extending from the axis of the torsional spring to some attachment point near the base of the spring. A fourth node, reference node 1, defines an arm extending from the axis of the torsional spring to some attachment point near the top of the spring. The rotation of the two arms relative to each other as measured along the axis of the torsional spring represents the angular deformation of the spring and determines the moment in the spring. The moment in the spring is translated into external forces at the two attachment points, reference node 0 and reference node 1.

In the `TORSIONAL SPRING MECHANISM` command block, the string `spring_name` is defined by the user. Via the `NODE SETS` command line, the mechanism is defined with four node sets, and each node set has a single node. The first set (`nodelist_int1`) defines node 0 in Figure 5.8; node 0 is the origin of a local coordinate system for the torsional spring mechanism. The second node set (`nodelist_int2`) defines node 1 in Figure 5.8; node 0 and node 1 define the axis of the torsional spring mechanism. The third node set (`nodelist_int3`) defines reference node 0; reference node 0 is an attachment point for the spring associated with node 0. The fourth node set (`node_int4`) defines reference node 1; reference node 1 is an attachment point for the spring associated with node 1.

The nodes defining the spring mechanism are used to set up a local coordinate system (x', y', z'). The (z'-axis runs along the axis of the spring from node 0 to node 1. The x'-axis extends from the axis of the spring and passes through reference node 0. If we are looking down the axis of the spring in the negative z'-direction, a positive rotation of the arm defined by node 1 and reference node 1 is in the counterclockwise direction. This is shown in Figure 5.9.

The torque, T, in the spring is simply

$$T = K\theta, \tag{5.5}$$

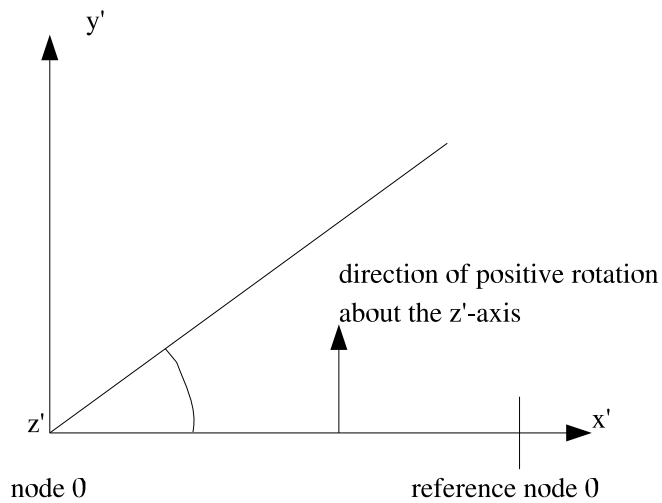

Figure 5.9: Positive direction of rotation for torsional spring.

where K is the torsional stiffness and θ is the rotation of the top arm relative to the bottom arm as measured along the axis of the spring. In the `TORSIONAL STIFFNESS` command line, K is specified by the real value `stiffness`.

The torque in the spring is converted to external forces with components in the global coordinate system XYZ. These external forces depend on the torque and the length of the spring arms. The length of the spring arms is automatically calculated.

You can apply an initial torque with the real value `init_load` in the `INITIAL TORQUE` command line. The maximum value of the torque is reached in the time specified by the real value `time_period` in the `PERIOD` command line.

The initial torque is applied over some period by specifying the angular rate of deformation in the torsional spring, $\dot{\theta}$, over some period p. At some given time t, the angular rate of deformation is

$$\dot{\theta} = \frac{ap}{2}\left[1 - \cos\left(\pi t/p\right)\right], \tag{5.6}$$

where

$$a = \frac{2T_i}{Kp}. \tag{5.7}$$

In Equation (5.7), T_i is the initial torque. Over the period p, the total strain increment generates the desired initial load in the truss.

During the initial load period, the time increments should be reasonably small so that the integration of $\dot{\theta}$ over the period is accurate. The period should be set long enough so that if the model was held in a steady state after time p, there would be only a small amount of oscillation in the load in the torsional spring.

When doing an analysis, you may not want to activate certain boundary conditions until after the prestressing is done. During the prestressing, time-independent boundary conditions such as fixed displacement will most likely be turned on. Time-dependent boundary conditions such as prescribed acceleration or prescribed force will most likely be activated after the prestressing is complete.

You can output the torque in the spring, the total rotation, and the last angle between the arms. The name specified on the command block is used to construct parameters for the mechanism. Suppose the input line is:

```
begin torsional spring mechanism lower_spring
```

where `lower_spring` is a user-specified name. The code will automatically generate the parameters `TS_lower_spring_MOMENT`, `TS_lower_spring_ROTATION`, and `TS_lower_spring_LAST_ANGLE`. These variables can then be output in a results file. For example, one could use

```
global TS_lower_spring_MOMENT as ts_lspring_m
global TS_lower_spring_ROTATION as ts_lspring_r
global TS_lower_spring_LAST_ANGLE as ts_lspring_la
```

in the `RESULTS OUTPUT` command block. If several torsional spring mechanisms appear in one model, you can generate unique names to keep track of the parameters associated with each spring. See Section 8.2 for further information about results output.

The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines determine when the torsional spring is active. See Section 2.5 for more information about these command lines. Although the active periods option is available in the `TORSIONAL SPRING` command block, use of this option to turn the torsional spring off and on repeatedly is not recommended. Turning the torsional spring off and on repeatedly may lead to erroneous behavior in the spring model.

5.4 Mass Property Calculations

```
BEGIN MASS PROPERTIES
  #
  # block set commands
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE BLOCK = <string list>block_names
  #
  # structure command
  STRUCTURE NAME = <string>structure_name
END [MASS PROPERTIES]
```

Presto automatically gives mass property information for the total model, which consists of all the element blocks. (The mass for the total model, for example, is the total mass of all the element blocks.) Presto also automatically gives mass property information for each element block.

In addition to the mass property information that is generated, Presto gives you the option of defining a structure that represents some combination of element blocks and then of calculating the mass properties for this particular structure. If you wish to define a structure that is a combination of some group of element blocks, you must use the `MASS PROPERTIES` command block. This command block appears in the region scope.

For the total model, each element block, and any user-defined structure, Presto reports the mass and the center of mass in the global coordinate system. It also reports the moments and products of inertia, as computed in the global coordinate system about the center of mass.

The `MASS PROPERTIES` command block contains two groups of commands—block set and structure. Each of these groups is basically independent of the other. Following are descriptions of the two command groups.

5.4.1 Block Set Commands

The `block set commands` portion of the `MASS PROPERTIES` command block defines a set of blocks for which mass properties are being requested, and can include some combination of the following command lines:

```
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of blocks. See Section 6.1.1 for more information about the use of these command lines for creating a set of blocks used by the command block. There must be at least one `BLOCK` or `INCLUDE ALL BLOCKS` command line in the command block.

The REMOVE BLOCK command line allows you to delete blocks from the set specified in the BLOCK and/or INCLUDE ALL BLOCKS command line(s) through the string list block_names. Typically, you would use the REMOVE BLOCK command line with the INCLUDE ALL BLOCKS command line. If you want to include all but a few of the element blocks, a combination of the REMOVE BLOCK command line and INCLUDE ALL BLOCKS should minimize input information.

Suppose that only one element block, block_300, is specified on the BLOCK command line. Then only the mass properties for that block will be calculated. If several element blocks are specified on the BLOCK command line, then that collection of blocks will be treated as one entity, and the mass properties for that single entity will be calculated. For example, if two element blocks, block_150 and block_210, are specified on the BLOCK command line, the total mass for the two element blocks will be reported as the total mass property.

5.4.2 Structure Command

The output for the mass properties will be identified by the command line:

```
STRUCTURE NAME = <string>structure_name
```

where the string structure_name is a user-defined name for the structure.

5.5 Element Death

```
BEGIN ELEMENT DEATH <string>death_name
  #
  # block set commands
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE BLOCK = <string list>block_names
  #
  # criterion commands
  CRITERION IS AVG|MAX|MIN NODAL VALUE OF
    <string>var_name <|<=|=|>=|> <real>tolerance
  CRITERION IS ELEMENT VALUE OF
    <string>var_name <|<=|=|>=|> <real>tolerance [KILL WHEN
    <integer>num_intg INTEGRATION POINTS REMAIN]
  CRITERION IS GLOBAL VALUE OF
    <string>var_name <|<=|=|>=|> <real>tolerance
  MATERIAL CRITERION
    = <string list>material_model_names [KILL WHEN
    <integer>num_intg INTEGRATION POINTS REMAIN]

  ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # evaluation commands
  CHECK STEP INTERVAL = <integer>num_steps
  CHECK TIME INTERVAL = <real>delta_t
  DEATH START TIME = <real>time
  #
  # miscellaneous option commands
  SUMMARY OUTPUT STEP INTERVAL = <integer>output_step_interval
  SUMMARY OUTPUT TIME INTERVAL = <real>output_time_interval

  DEATH ON INVERSION = OFF|ON(OFF)
  DEATH STEPS = <integer>death_steps(1)
  FORCE VALID ACME CONNECTIVITY
  AGGRESSIVE CONTACT CLEANUP = <string>OFF|ON(OFF)
  DEATH METHOD = <string>DEACTIVATE ELEMENT|DEACTIVATE NODAL MPCS|
  DISCONNECT ELEMENT|INSERT COHESIVE ZONES(DEACTIVATE ELEMENT)
  #
  # particle conversion commands
```

```
BEGIN PARTICLE CONVERSION
  PARTICLE SECTION = <string>section_name
  NEW MATERIAL = <string>material_name MODEL = <string>model_name
  TRANSFER = <string>NONE|ALL(ALL)
  MAX NUM PARTICLES = <integer>num(1)
  MIN PARTICLE CONVERSION VOLUME = <real>vol
END [PARTICLE CONVERSION]

ACTIVE PERIODS = <string list>period_names
INACTIVE PERIODS = <string list>period_names
#
# cohesive zone setup commands
COHESIVE SECTION = <string>sect_name
COHESIVE MATERIAL = <string>mat_name
COHESIVE MODEL = <string>model_name
COHESIVE ZONE INITIALIZATION METHOD = <string>NONE|
  ELEMENT STRESS AVG(NONE)

END [ELEMENT DEATH <string>death_name]
```

The `ELEMENT DEATH` command block is used to remove elements from an analysis. For example, the command block can be used to remove elements that have fractured, that are no longer important to the analysis results, or that are nearing inversion.This command block is located within the `PRESTO REGION` scope. The name of the command block, `death_name`, is user-defined and can be referenced in other commands to update boundary or contact conditions based on the death of elements creating new exposed surfaces.

Any element in an element block or element blocks selected in the `ELEMENT DEATH` command block is removed (killed) when one of the criteria specified in the `ELEMENT DEATH` command block is satisfied by that element. When an element dies, it is removed permanently. Any number of `ELEMENT DEATH` command blocks may exist within a region.

When an element is killed, the contribution of that element's mass to the attached nodal mass is removed from the attached nodes. If all of the elements attached to a node are killed, the mass for the node and all associated nodal quantities will be set to zero. If all of the elements in a region are killed, the analysis will terminate.

Elements may be killed based off of any internal variable, derived variable, material state variable, or user defined variable. Note that user-defined variables for triggering element death should be used with care. There are timing and parallel issues regarding the use of a user-defined variable with element death. User subroutines may work for element death in some situations where one might want to reference a user variable.

The quantity used in an element death criterion statement should have only a single value at each integration point. For example, the following command:

```
criterion is element value of stress(xx) > 10.0
```

is unambiguous and valid. However this command:

```
criterion is element value of stress > 10.0
```

is ambiguous, and will result in an error. Stress is a 3x3 tensor and there is no rational way to compare that tensor to the scalar value 10. If a variable is defined on multiple integration points, the criterion will be triggered if the value is exceeded at any of the integration points. If the command:

```
criterion is element value of stress(xx,:) > 10.0
```

were used with shells with five integration points, the shells would be killed if the value of `stress(xx)` at any of the five integration points exceeded 10.

The `ELEMENT DEATH` command block contains five groups of commands—block set, criteria, evaluation, miscellaneous, and cohesive zone setup. The command block must contain commands from the block set and criteria groups. Command lines from the evaluation and miscellaneous groups are optional, as are the cohesive zone commands.

Following are descriptions of the different command groups, an example of using the `ELEMENT DEATH` command block, and some concluding remarks related to element death visualization.

5.5.1 Block Set Commands

```
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE BLOCK = <string list>block_names
```

The `block set commands` portion of the `ELEMENT DEATH` command block defines a set of blocks for selecting the elements to be referenced. These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of blocks, as described in Section 6.1.1.

Element death must apply to a group of elements. There are two commands for selecting the elements to be referenced: `BLOCK` and `INCLUDE ALL BLOCKS`. In the `BLOCK` command line, you can list a series of blocks through the string list `block_names`. This command line may also be repeated multiple times. The `INCLUDE ALL BLOCKS` command line adds all the element blocks present in the region to the current element death definition. There must be at least one `BLOCK` or `INCLUDE ALL BLOCKS` command line in the `ELEMENT DEATH` command block.

The `REMOVE BLOCK` command line allows you to delete blocks from the set specified in the `BLOCK` and/or `INCLUDE ALL BLOCKS` command line(s) through the string list `block_names`. Typically, you will use the `REMOVE BLOCK` command line with the `INCLUDE ALL BLOCKS` command line. If you want to include all but a few of the element blocks, a combination of the `REMOVE BLOCK` command line and `INCLUDE ALL BLOCKS` command line should minimize input information.

5.5.2 Criterion Commands

Any combination of death criteria (`CRITERION IS NODAL`, `CRITERION IS ELEMENT`, `CRITERION IS GLOBAL`, `ELEMENT BLOCK SUBROUTINE`, `MATERIAL CRITERION`) can be

specified within a single `ELEMENT DEATH` command block. However, only one user subroutine criterion may appear in a set of criteria command lines. If multiple death criteria are specified for a given element, it will be killed when the first of those criteria are met. In other words, element death with multiple criteria is an `OR` condition rather than an `AND` condition.

A problem with a material that has both a tension cutoff and a compression cutoff would be an example for which you would want to use element death with multiple criteria. You would use one criterion to set failure in tension and another criterion to set failure in compression. If either the tension cutoff value, as set by the tension criterion, or the compression cutoff value, as set by the compression criterion, was exceeded for an element, the element would be killed.

As another example, you might have a problem that uses a nodal criterion and a user subroutine criterion. For this second example, you are precluded from using another subroutine criterion because you already have one. You could add some combination of nodal, element, global, or material criteria to the existing nodal and subroutine criteria, but you could not add another subroutine criterion.

5.5.2.1 Nodal Variable Death Criterion

```
CRITERION IS AVG|MAX|MIN NODAL VALUE OF
  <string>var_name <|<=|=|>=|> <real>tolerance
```

Any nodal variable may be used by an element death criterion. The input parameters are described as follows:

- Nodal variables are present on the nodes of an element, and these nodal values must be reduced to a single element value for use by the criterion. The available types of reduction are `AVG`, which takes the average of the nodal values; `MAX`, which takes the maximum of the nodal values; and `MIN`, which takes the minimum of the nodal values.

- The string `var_name` gives the name of the variable. See Section 8.9 for a listing of the variables. Parenthesis syntax may be used in the variable name for selection specific variable components or integration points, see Section 8.1.

- The specified variable, with an optional component specification if the variable has components, may be compared to a given tolerance with one of five operators. The operator is specified with the appropriate symbol for less than (<) less than or equal to (<=), equal to (=), greater than or equal to (>=), or greater than (>) The given tolerance is specified with the real value `tolerance`.

5.5.2.2 Element Variable Death Criterion

```
CRITERION IS ELEMENT VALUE OF
  <string>var_name[(<integer>component_num)]
  <|<=|=|>=|> <real>tolerance |
```

```
<string>derived_quantity[(<integer>int_num)]
<|<=|=|>=|> <real>tolerance [KILL WHEN <integer>num_intg
INTEGRATION POINTS REMAIN]
```

Any element variable may be used by an element death criterion. An element variable is present on the element itself, so no reduction is required, which is why the first line in the format of the above command line differs from that of the nodal criterion command line in Section 5.5.2.1.

For a criterion using an element variable, the variable name, component or integration point number, and tolerance can be specified in the same manner as defined for the nodal criterion command line.

Element state variables can also be used as criteria for element death. The syntax used to specify the variable name differs depending on the type of material model used.

- For Strumento solid material models, the variable name is called out as:

  `state_material_name(index)`

  where `material_name` is the name of the material model, e.g. `elastic_plastic`, and `index` is the index in the state variable array of the particular state variable to be used for the death criterion. For example, the command:

  `criterion = element value of state_elastic_plastic(1) > 0.9`

  uses the value of the first state variable for the elastic_plastic material, which is the equivalent plastic strain.

- For LAME solid material models, the variable name is called out directly by name.

- For shell material models, the variable name is called out directly by name. By default the element will be killed if the criteria is met at any integration point. Parenthesis syntax 8.1 may be used to kill based on the state of a specified integration point. For example:

  `criterion = element value of crack_opening_strain(2) > 0.01`

  would use the value of the state variable `crack_opening_strain` at the second shell integration point through the shell thickness as the criterion for element death.

Refer to Section 8.9.2 for tables with listings of state variables for the various material models.

Derived quantities can also be used for element death. For example the following command:

```
criterion = element value of von_mises > 1.0e+05
```

will cause elements to be killed any of the integration points reach a critical value of `von_mises`. Alternatively, the command:

```
criterion = element value of von_mises(3) > 1.0e+05
```

is used to kill an element if a specific integration point reaches the critical value of `von_mises`.

If the optional `KILL WHEN num_intg INTEGRATION POINTS REMAIN` portion of the command line is specified, the element will not die until there are `num_intg` integration points remaining. For example, for shells with five integration points, the following command:

```
criterion is element value of stress(xx,:) > 10.0 kill when 2 integration
points remain
```

will check the `xx` component of `stress` at each integration point, and when 3 of those 5 integration points exceed that criterion, leaving 2 integration points that have not reached the criterion, the element will die.

5.5.2.3 Global Death Criterion

```
CRITERION IS GLOBAL VALUE OF
<string>var_name[(<integer>component_num)]
<|<=|=|>=|> <real>tolerance
```

Any global variable may be used in an element death criterion. Once the global criterion is reached, all elements specified in the `ELEMENT DEATH` command block are killed. The variable name, component number, and tolerance can be specified in the same manner as defined for the nodal or element criterion command line.

The input parameters are described as follows:

- The string `var_name` gives the name of the global variable. See Section 8.9 for a listing of the global variables.
- Parenthesis syntax may be used in the variable name to specify specific components of the variable, see 8.1
- The specified variable, with an optional component specification if the variable has components, may be compared to a given tolerance with one of five operators. The operator is specified with the appropriate symbol for less than (<), less than or equal to (<=), equal to (=), greater than or equal to (>=), or greater than (>). The given tolerance is specified with the real value `tolerance`.

5.5.2.4 Material Death Criterion

```
MATERIAL CRITERION = <string list>material_model_names [KILL WHEN
  <integer>num_intg INTEGRATION POINTS REMAIN]
```

Some material models have a failure criterion. When this failure criterion is satisfied within an element, the element has fractured or disintegrated. The material models reduce the stress in these fractured or disintegrated elements to zero. The `MATERIAL CRITERION` command line can be used to remove these fractured or disintegrated elements from an analysis. Removal of the fractured elements can speed computations, enhance visualization, and prevent spurious inversion of these elements that may stop the analysis.

The material models currently supported for use with the `MATERIAL CRITERION` command line are:

- ELASTIC_FRACTURE (Solid only, see Section 4.2.4)

- DUCTILE_FRACTURE (Solid only, see Section 4.2.7)

- ML_EP_FAIL (Solid and Shell, see Section 4.2.9)

Element death will kill an element based on a material criterion when the material model indicates that the element is failed and can carry no more load. For a single integration point element, this occurs when the one integration point in the element fails. For elements with multiple integration points, the default behavior is for the element to be killed when all but one of the integration points has failed. This behavior is the default because for multi-integration point elements, particularly shells, if there is only a single integration point left, the element is severely under-integrated. The final integration point will generally not attract more load and will never fail. This default behavior can be changed by using the optional KILL WHEN num_intg INTEGRATION POINTS REMAIN command. In this command, num_intg specifies the number of remaining integration points when the element is to be killed.

Suppose you have an element block named part1_ss304 that references a material named SS304. This material, SS304, uses the DUCTILE_FRACTURE material model (see Section 4.2.7). You also have an element block named ring5_al6061 that references a material named al6061. This material, al6061, uses the ML_EP_FAIL material model (see Section 4.2.9). If you have an ELEMENT DEATH command block with the command line:

```
BLOCK = part1_ss304 ring5_al6061
```

and the command line:

```
MATERIAL CRITERION = DUCTILE_FRACTURE ML_EP_FAIL
```

then any element in part1_ss304 that fails according to the material model DUCTILE_FRACTURE (in material SS304) and any element in ring5_al6061 that fails according to the material model ML_EP_FAIL (in material al6061) will be killed by element death.

5.5.2.5 Subroutine Death Criterion

```
ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value
```

A death criterion can be specified via a user-defined subroutine (see Chapter 10), which is invoked by the ELEMENT BLOCK SUBROUTINE command line. The string subroutine_name is the name of a FORTRAN subroutine that is written by the user. The user-defined subroutine for

element death must be an element subroutine signature (see Section 10.2.2). The element subroutine will return an output values array and a flag array of one flag per element (see Table 10.2 in Chapter 10). The output values array is ignored. Death is determined by the flag return value. For user-defined subroutines, a flag return value of –1 indicates that the element should die. A flag return value greater than or equal to 0 indicates that the element should remain alive.

Following the `ELEMENT BLOCK SUBROUTINE` command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 10.2.2 and consist of `SUBROUTINE DEBUGGING OFF`, `SUBROUTINE DEBUGGING ON`, `SUBROUTINE REAL PARAMETER`, `SUBROUTINE INTEGER PARAMETER`, and `SUBROUTINE STRING PARAMETER`. Examples of using these command lines are provided throughout Section 10.

5.5.3 Evaluation Commands

```
CHECK STEP INTERVAL = <integer>num_steps
CHECK TIME INTERVAL = <real>delta_t
DEATH START TIME = <real>time
```

Evaluation of element death criteria may be time consuming. Additionally, reconstruction of contact or other boundary conditions after element death can be very time consuming. For these reasons, three command lines are available for determining the frequency at which element death is evaluated. The default is to evaluate element death at every time step. You can limit the number of times at which the element death evaluation is done by using the following commands.

- The `CHECK STEP INTERVAL` command line instructs element death to evaluate the element death criteria only every `num_steps` time steps.
- The `CHECK TIME INTERVAL` command line instructs element death to evaluate the element death criteria only every `delta_t` time units.
- The `DEATH START TIME` command line instructs element death not to evaluate death criteria before a user-specified time, as given by the real value `time`.

You may use both the `CHECK STEP INTERVAL` and `CHECK TIME INTERVAL` command lines in a command block. Evaluations for element death will be made at both the time and step intervals if both of these command lines are included.

All three of the above command lines—`CHECK STEP INTERVAL`, `CHECK TIME INTERVAL`, and `DEATH START TIME`—are optional command lines.

5.5.4 Miscellaneous Option Commands

The command lines listed below need not be present in the `ELEMENT DEATH` command block unless the conditions addressed by each call for their inclusion.

5.5.4.1 Summary Output Commands

At the end of a run, a summary of all element death blocks is output to the log file. The `SUMMARY OUTPUT STEP INTERVAL` or `SUMMARY OUTPUT STEP INTERVAL` commands can be used to request that the summary be output to the log file at regular intervals during the run. The `SUMMARY OUTPUT TIME INTERVAL` command results in the summary being printed every `output_step_interval` steps, while the `SUMMARY OUTPUT TIME INTERVAL` results in the summary being printed once every `output_time_interval` time units. These two commands can be supplied individually, together or not at all. If neither are used, the summary is printed only at the end of execution.

It should be noted that this command applies to all element death blocks. If these commands appear in multiple element death blocks, the values specified in the last instance of each of these commands prevails.

5.5.4.2 Death on Inversion

```
DEATH ON INVERSION = ON|OFF(OFF)
```

If the `DEATH ON INVERSION` command line is on, any element that inverts will be killed. This command currently only works for uniform gradient 8-noded hex elements 4, 8, and 10 noded tet elements, and 4 noded shells.

5.5.4.3 Death Steps

```
DEATH STEPS = <integer>death_steps(1)
```

If the `DEATH STEPS` command line is used and the value for `death_steps` is set to some value greater than 1, the stress in a killed element will not be set to 0 until the prescribed number of steps has occurred. The stress in the killed element will decrease (if it is positive) to 0 in a linear fashion over the prescribed number of steps; the stress in the killed element will increase (if it is negative) to 0 over the prescribed number of steps. If the stress in a killed element is set to 0 over a single time step, the resulting change in stress can sometimes cause instabilities due to the sudden release of energy. However, elimination of the stress over an excessive number of load steps can make it appear as if the element is present long after it has been killed. The default number of steps, as provided in the integer value `death_steps`, is 1.

The value you select for `death_steps` will depend on your analysis. A small number such as 3 or 5 may be sufficient to prevent instabilities for most cases. However, in some cases it may be necessary to use a value for `death_steps` of 10 or larger. The loads, material models, and model complexity in your analysis will impact the value of `death_steps`.

5.5.4.4 Degenerate Mesh Repair

```
FORCE VALID ACME CONNECTIVITY
```

If the FORCE VALID ACME CONNECTIVITY command line is present, degenerate mesh occurrences will be repaired. Element death has the possibility of creating degenerate mesh occurrences that will not be accepted by the ACME (see Reference 12) contact algorithms used by Presto. For example, if two continuum elements are connected only by an edge, ACME will not accept the mesh as a valid mesh. For this degenerate mesh occurrence (continuum elements connected only at an edge), the degeneracy is repaired by deleting all elements attached to the offending edge if we have turned on this repair option.

The option to repair degenerate mesh occurrences is on by default if there is a CONTACT DEFINITION command block that includes the command line:

```
UPDATE ALL SURFACES FOR ELEMENT DEATH = ON
```

See Section 7.4 for a full description of the UPDATE ALL SURFACES FOR ELEMENT DEATH command line.

If you do not have a CONTACT DEFINITION command block and want to repair degenerate mesh occurrences for whatever purposes, you should include the FORCE VALID ACME CONNECTIVITY command line.

5.5.4.5 Aggressive Contact Cleanup

```
AGGRESSIVE CONTACT CLEANUP = <string>OFF|ON(OFF)
```

The AGGRESSIVE CONTACT CLEANUP command line enables the use of element death in an attempt to guarantee a valid contact mesh. Certain complex meshes with extensive element death can be problematic for the contact algorithms on some mesh decompositions. This command allows element death to query the contact algorithm and then remove any elements that the contact algorithm flags as having the potential to cause contact to fail.

5.5.4.6 Death Method

```
DEATH METHOD = <string>DEACTIVATE ELEMENT|DEACTIVATE NODAL MPCS|
  DISCONNECT ELEMENT|INSERT COHESIVE ZONES(DEACTIVATE ELEMENT)
```

The DEATH METHOD command specifies what happens when an element meets the death criterion. The following strings can be used as arguments to this command: DEACTIVATE ELEMENT, DEACTIVATE NODAL MPCS, DISCONNECT ELEMENT, and INSERT COHESIVE ZONES. The behavior controlled by these options is described below.

- With the default option, DEACTIVATE ELEMENT, the element is deactivated, effectively removing it from the mesh.
- The DEACTIVATE NODAL MPCS option removes the nodes of a killed element from any multi-point constraints. This only has an effect if the element has nodes that are in multi-point constraints. The multi-point constraint deactivation option can be used to break an

element away from the mesh, allowing it to move independently. It can also be used to activate cohesive zones.

- The `DISCONNECT ELEMENT` option disconnects the element from the mesh, allowing the element to move independently. The disconnected element will no longer share any nodes with neighboring elements, and will only interact with the remainder of the mesh through contact.

- The `INSERT COHESIVE ZONE` option disconnects the element from the mesh and places a cohesive zone between the element and each face-adjacent neighbor. If this option is used, the commands `COHESIVE SECTION`, `COHESIVE MATERIAL`, and `COHESIVE MODEL` must be used to define the type of cohesive zone to be inserted, and are documented in Section 5.5.5.

When using element disconnection, it is necessary to use at least some hourglass stiffness and/or viscosity to prevent large deformations of the disconnected elements in zero energy modes. In addition, it is recommended that a secondary shape-based criterion be used in a separate element death command block to fully remove the disconnected elements if they begin to deform too much. The following example of an additional element death block to be used together with element disconnection shows recommended shape criteria:

```
begin element death
  include all blocks
  #Kill an element if it has negative volume
  death on inversion = on
  #Kill an element if it has become locally inverted (i.e., concave)
  criterion is element value of nodal_jacobian_ratio <= 0.0
  #Kill an element that is becoming very large (shells only)
  criterion is element value of perimeter_ratio > 10.0
end
```

5.5.4.7 Particle Conversion

```
BEGIN PARTICLE CONVERSION
  PARTICLE SECTION = <string>section_name
  NEW MATERIAL = <string>material_name MODEL = <string>model_name
  TRANSFER = <string>NONE|ALL(ALL)
  MAX NUM PARTICLES = <integer>num(1)
  MIN PARTICLE CONVERSION VOLUME = <real>vol
END [PARTICLE CONVERSION]
```

Presto provides the option to convert elements to particles when they are killed, rather than simply removing them from the mesh. This option is activated by using the `BEGIN PARTICLE CONVERSION` command block inside the `ELEMENT DEATH` command block. Particle conversion can be useful when elements become too highly deformed to be represented by solid elements.

This allows for the highly deformed solid elements to be removed from the mesh, while retaining the mass associated with those elements in the form of particles.

The name of a particle section block (defined with a `PARTICLE SECTION` command block, see Section 5.2.11) must be provided with the `PARTICLE SECTION` command line to define the properties of the created particles. Particles may be created that use the SPH or mass particle formulation, as defined by the section.

The material models for the created particles may be optionally prescribed by providing the name and model for a defined material in the `NEW MATERIAL` command. By default, the particle uses the material model of the solid element from which it has been converted, and all element data that can be retained, including material state variables, are transferred during conversion. This behavior may be modified by specifying the transfer type through the `TRANSFER` command. If all the applicable element data should be transferred, the `ALL` option should be specified (this is the default if no transfer type is specified). If the particles should be created with reinitialized state data, the `NONE` option should be specified. Moreover, if a new material type is specified for conversion, the `TRANSFER` option will apply, but likely much of the material state data will not be transferable and will be lost as the element is converted to a particle. The best option when using a new material is to also specify a transfer type of `NONE`.

Particle conversion works with most element types including hexahedra, tetrahedra, shells, beams, and other particles. The converted particle is placed at the centroid of the removed element. For shells, beams and particles the new particle is placed inside of the lofted volume that the structural element represents. The mass of the particle equals the mass of the converted element. The velocity and/or temperature of the converted particle is set to the average velocity/temperature of the source element's nodes. The radius of the converted particle is computed to allow the particle to fit inside the void space left by removal of the solid element. If no particle can fit in that space, no particle is created. This typically occurs when an element has inverted or the center of mass is not on the interior of the element, as seen in Figure 5.10.

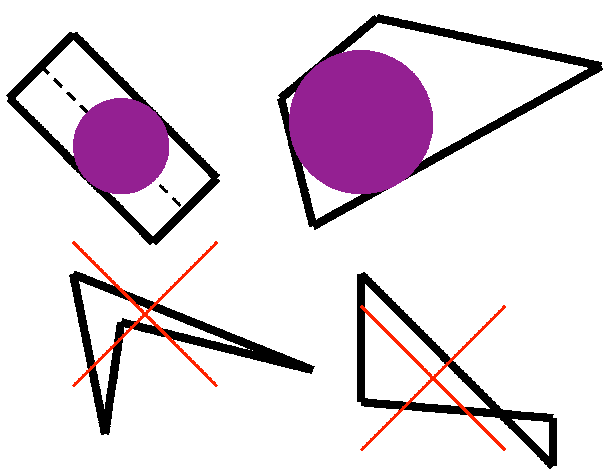

Figure 5.10: Examples of how an element is converted and when it is not converted.

A single element can optionally be converted into multiple particles. The number of particles to convert to is specified with the `MAX NUM PARTICLES` command and `MIN PARTICLE`

CONVERSION VOLUME command. The usage of these commands is as follows:

If neither of these command lines is present, one particle is placed at the centroid of the element.

If only the MAX NUM PARTICLES command line is present, the element will be cut into the specified number of roughly equal volume sections. A particle will then be placed at the centroid of each of these sections.

If only the MIN PARTICLE CONVERSION VOLUME command line is present, the element will be subdivided until a number of volumes each of roughly the specified volume is reached. A new particle will then be placed at the centroid of each of these sub-volumes.

If both the MAX NUM PARTICLES and MIN PARTICLE CONVERSION VOLUME commands are specified, the element will be subdivided until either the minimum volume of the sub-parts is reached, or the maximum number of sub-parts is reached. When one of these criteria is reached, a new particle is placed into each created sub-volume.

5.5.4.8 Active Periods

The following command lines can optionally be used in the ELEMENT DEATH command block:

```
ACTIVE PERIODS = <string list>period_names
INACTIVE PERIODS = <string list>period_names
```

These command lines determine when element death is active. See Section 2.5 for more information about these optional command lines.

5.5.5 Cohesive Zone Setup Commands

The commands listed here are all related to adaptive insertion or activation of cohesive zones by element death.

```
COHESIVE SECTION = <string>sect_name
COHESIVE MATERIAL = <string>mat_name
COHESIVE MODEL = <string>model_name
COHESIVE ZONE INITIALIZATION METHOD = <string>NONE|
  ELEMENT STRESS AVG(NONE)
```

The first three of these commands are only applicable to adaptive insertion of cohesive elements by element death. They are used together to fully define the properties of the elements that are adaptively inserted.

The COHESIVE SECTION command is used to specify the name of a section used to define the section properties of the cohesive zone elements to be adaptively inserted. See Section 5.2.2 for a description of cohesive sections.

The COHESIVE MATERIAL command is used to specify the name of the material model to be used for the newly-created cohesive elements. This material model name is the user-provide name for the cohesive zone material provided by the parameter mat_name in the BEGIN PROPERTY SPECIFICATION FOR MATERIAL mat_name command block. The material models available for cohesive zones are documented in Section 4.3.

The COHESIVE MODEL command is used to select the material model to be used for the newly-created cohesive elements. This references the name of the material model model_name defined in a BEGIN PARAMETERS FOR MODEL model_name block. The material models available for cohesive zones are documented in Section 4.3.

The COHESIVE ZONE INITIALIZATION METHOD command controls the initialization of cohesive zones that are dynamically inserted or activated through element death. This command should only be used if there are cohesive zones between elements and all nodes of those elements are initially attached together via multi-point constraints, or the INSERT COHESIVE ZONES death method is being used. When element death is used to deactivate the constraints or insert a cohesive element (with the DEATH METHOD = DEACTIVATE NODAL MPCS option or DEATH METHOD = INSERT COHESIVE ZONES option), the exposed cohesive zone can be given an initial state. The options are to either do nothing (NONE) or to initialize the tractions in the cohesive element based on the stresses in the two elements on either side of the cohesive zone (ELEMENT STRESS AVG). How the cohesive zone uses the initial traction will depend on the cohesive surface material model used.

5.5.6 Example

The following example provides instructions to kill elements in block_1 when they leave a bounding box. This type of element death can be useful in an analysis where some peripheral parts, because of fracture, separate and fly away from a central body, this central body being our part of interest. In this case, these peripheral parts no longer impact the solution. The instructions in this ELEMENT DEATH command block will cause the parts to be killed, thus speeding up the computation.

```
begin element death out_of_bounds
  block = block_1
  # check x coordinates
  criterion is avg nodal value of coordinates(1) >=  10
  criterion is avg nodal value of coordinates(1) <= -10
  # check y coordinates
  criterion is avg nodal value of coordinates(2) >=  10
  criterion is avg nodal value of coordinates(2) <= -10
  # check z coordinates
  criterion is avg nodal value of coordinates(3) >=  10
  criterion is avg nodal value of coordinates(3) <= -10
end element death out_of_bounds
```

5.5.7 Element Death Visualization

When an element dies, information about this element will still be sent, along with information for all other elements, to the Exodus II results file. (Chapter 8 describes the output of element variables to the results file.) The death status of the elements may be output to the results file by requesting element variable output for the element variable `DEATH_STATUS`. Including the command line

```
ELEMENT DEATH_STATUS as death_var
```

in a `RESULTS OUTPUT` command block (Chapter 8) will output this element variable with the name `death_var` in the results file.

The convention for `DEATH_STATUS` is as follows: An element with a value of 1.0 for `DEATH_STATUS` is a living element. An element with a value of 0.0 for `DEATH_STATUS` is a dead element. A value less than 0.0 indicates that the element was killed due to a code related issue (e.g. an unsupported geometry issue related to ACME). A value between 1.0 and 0.0 indicates an element in the process of dying. A dying element has its material stress scaled down over a number of time steps. The current scaling factor for an element is given by `DEATH_STATUS`. Whether or not an element can have a value for `DEATH_STATUS` other than 0.0 or 1.0 will depend on whether or not you have used the `DEATH STEPS` option in the `ELEMENT DEATH` command block. If the number of steps over which death occurs is greater than 1, then `DEATH_STATUS` can be some value between 0.0 and 1.0.

If `DEATH_STATUS` is written to a results file, and the results file is used in a visualization program to examine the mesh for the model, it is possible to use `DEATH_STATUS` to exclude killed elements from any view of the model. A subset of the mesh showing just the living elements can be created by visualizing only those elements for which `DEATH_STATUS` = 1.0. The procedure for visualizing results in this way varies for different postprocessing tools.

When an analysis is using element death the log file contains a table of marker values that will be applied to dead elements. The marker values allow determining which elements where killed and by which criterion. The marker variables are stored in the element variable `KILLED_BY_CRITERION` and are available for output on the mesh results file. Additionally, a global count of how many elements were killed by each criterion is printed at the end of the run log file.

5.6 Particle Embedding

```
BEGIN PARTICLE EMBEDDING <string>particle_embedding_name
  BLOCK = <string>block_name
  INCLUDE ALL BLOCKS
  REMOVE BLOCK = <string>block_name
  PARTICLE SECTION = <string>section_name
  NEW MATERIAL = <string>material_name MODEL = <string>model_name
  TRANSFER = <string>NONE|ALL(ALL)
  MAX NUM PARTICLES = <integer>num(1)
  MIN PARTICLE CONVERSION VOLUME = <real>vol
END [PARTICLE EMBEDDING]
```

Particle embedding allows the user to specify element blocks in which each element is embedded with particles during initialization (i.e. before the first time step is taken). This capability can remove the need to create particles during element death and may be used for particle-solid interactions.

The embedded particles are created in the same way as during particle conversion for element death, except that the original solid element remains alive after the particles are created. Particles that are created are constrained to move with a material point in their controlling element (i.e. the element in which they were created). This constraint is released only if the controlling element dies. In addition, these embedded particles may interact with non-embedded particles to produce internal forces on the embedded particles. These internal forces are transferred to the controlling element using the embedded particle's location in the element. Note that the mass of the particles embedded in an element is assigned as in particle conversion for element death but that the particles' mass does not affect the solution until the controlling element dies. Once a particle's controlling element dies it is freed and behaves as a particle element.

The commands for this block are discussed in Section 5.5.4.7 and work for particle embedding in the same way, save `TRANSFER`. Particle embedding has two opportunities for transferring element data: at initialization and at controlling element death. For particle embedding the `TRANSFER` command applies to both of these transfers. If the `ALL` option is used, an embedded particle will be initialized with the initial element data of its controlling element and will have its element data reset to the evolved element data of its controlling element when its controlling element dies. If the `NONE` option is used, the embedded particle's element data will be initialized as a non-embedded particle's would be, and the particle's element data will not be modified at controlling element death.

5.7 Explicitly Computing Derived Quantities

```
BEGIN DERIVED OUTPUT
  COMPUTE AND STORE VARIABLE =
    <string>derived_quantity_name
END DERIVED OUTPUT
```

The above command block is used to explicitly compute and store a derived quantity into an internal field. This is useful if the field is needed by an outside capability such as a transfer or error estimation.

For example, to use a derived quantity in a transfer, you must use a `DERIVED OUTPUT` command block. To transfer the von Mises stress norm, you would use the following command block:

```
BEGIN DERIVED OUTPUT
  COMPUTE AND STORE VARIABLE = von_mises
END DERIVED OUTPUT
```

Tables 8.10 through 8.13 in Section 8 list element variables available for different types of elements. Variables that are only computed at user request are designated with a `yes` in the `Derived` column of these tables. These are the quanities that must be listed in a `BEGIN DERIVED OUTPUT` command block if they are to be transferred during a coupled analysis.

5.8 Mesh Rebalancing

Mesh rebalancing is a feature in Presto that may improve the efficiency of an analysis. Two command blocks can be used to control mesh rebalancing: `REBALANCE` and `ZOLTAN PARAMETERS`. The `REBALANCE` command block is required; the `ZOLTAN PARAMETERS` command block is optional. Sections 5.8.1 and 5.8.2 describe these command blocks.

5.8.1 Rebalance

```
BEGIN REBALANCE
  ELEMENT GROUPING TYPE = SPLIT SPH AND STANDARD ELEMENTS|
    UNIFORM UNIFIED(SPLIT SPH AND STANDARD ELEMENTS)
  INITIAL REBALANCE = ON|OFF(OFF)
  PERIODIC REBALANCE = ON|OFF|AUTO(OFF)
  REBALANCE STEP INTERVAL = <integer>step_interval
  LOAD RATIO THRESHOLD = <real>load_ratio
  COMMUNICATION RATIO THRESHOLD = <real>communication_ratio
  ZOLTAN PARAMETERS = <string>parameter_name
END [REBALANCE]
```

Initial decomposition of a mesh for parallel runs with Presto is done by a utility called `loadbal`. The initial decomposition provided by `loadbal` may not provide a decomposition for good-to-optimal parallel performance of Presto under certain circumstances. Therefore, Presto supports a simple mesh-rebalancing capability that can be used to improve the parallel performance of some problems. When mesh rebalancing is invoked, the parallel decomposition is changed, and elements are moved among the processors to balance the computational load and minimize the processor-to-processor communication. Mesh rebalancing may be useful in the following circumstances:

- The mesh decomposition produced by `loadbal` for sphere elements (i.e. for SPH or peridynamics) is nearly always poor. It is recommended that an initial mesh rebalance be done for all problems involving sphere elements.

- If a problem experiences very large deformations, periodic rebalancing may be helpful. In contact or SPH problems, communication is performed between physically nearby contact surfaces or SPH particles. To maintain optimum performance, it is helpful to have neighboring particles located on the same processors. Periodic mesh rebalancing can ensure that neighboring entities tend to remain on the same processor during large mesh deformations.

The `REBALANCE` command block is placed in the Presto region scope. The mesh rebalancing in Presto uses a mesh balancing library called Zoltan (Reference 13). Zoltan performs the actual rebalancing. By default, Presto creates a Zoltan object with a default set of parameters. However, a Zoltan object with a customized set of parameters can be created and referenced from the `REBALANCE` command block.

5.8.1.1 Rebalance Command Lines

```
ELEMENT GROUPING TYPE = SPLIT SPH AND STANDARD ELEMENTS|
  UNIFORM UNIFIED(SPLIT SPH AND STANDARD ELEMENTS)
INITIAL REBALANCE = on|off (off)
PERIODIC REBALANCE = on|off|auto (off)
REBALANCE STEP INTERVAL = <integer>step_interval
LOAD RATIO THRESHOLD = <real>load_ratio
COMMUNICATION RATIO THRESHOLD = <real>ratio
```

The above command lines control how and when the rebalancing is done.

The `ELEMENT GROUPING TYPE` command line specifies how the elements are grouped for rebalancing. If set to `SPLIT SPH AND STANDARD ELEMENTS`, which is the default behavior, this command causes SPH and standard elements to be split into separate groups. If it is set to the `UNIFORM UNIFIED` option, all elements can be grouped together.

The `INITIAL REBALANCE` command line is used to rebalance the mesh at time zero before any calculations occur. This option should be used if the initial mesh decomposition passed to Presto is poor.

If the `PERIODIC REBALANCE COMMAND` option is set to `on`, the mesh will be rebalanced every `step_interval` steps, where `step_interval` is the parameter specified by the `REBALANCE STEP INTERVAL` command line. If the option is `auto`, the mesh will be rebalanced every `step_interval` steps, when the communication ratio reaches a critical value, or when the load ratio reaches a critical value.

The communication ratio, currently defined only for SPH problems, is a measure of how much communication is required in the current mesh decomposition versus an estimate of the amount of communication with an optimal decomposition. Mesh rebalancing is expensive, so rebalancing should be done rarely. The `COMMUNICATION RATIO THRESHOLD` command line is used to specify the value of the communication ratio that triggers a rebalance. Setting this to a value between 1.25 and 1.5 is usually optimal.

The load ratio is the ratio of the current load (maximum number of elements on a processor divided by the average number of elements per processor) to that immediately after the previous rebalance. The `LOAD RATIO THRESHOLD` command specifies that a rebalance should occur when the load ratio exceeds the specified threshold. A specified value of 1.5 would trigger a rebalance when the load ratio is 50% higher than the previous rebalance (or initial decomposition, if no rebalances have yet occurred).

5.8.1.2 Zoltan Command Line

The command line

```
ZOLTAN PARAMETERS = <string>parameter_name
```

references a `ZOLTAN PARAMETERS` command block named `parameter_name`. Various parameters for Zoltan can be set in the `ZOLTAN PARAMETERS` command block. If you do not use the

ZOLTAN PARAMETERS command line, a default set of parameters is used. The default parameter command block is shown as follows:

```
BEGIN ZOLTAN PARAMETERS
  LOAD BALANCING METHOD = recursive coordinate bisection
    # string parameter
  OVER ALLOCATE MEMORY  = 1.5 # real parameter
  REUSE CUTS = true # string parameter
  ALGORITHM DEBUG LEVEL = 0 # integer parameter
  CHECK GEOMETRY = true # string parameter
  ZOLTAN DEBUG LEVEL = 0 # integer parameter
END ZOLTAN PARAMETERS
```

See Section 5.8.2 for a discussion of the ZOLTAN PARAMETERS command block. Section 5.8.2 lists the command lines that can be used to set Zoltan parameters.

5.8.2 Zoltan Parameters

```
BEGIN ZOLTAN PARAMETERS
  LOAD BALANCING METHOD  = <string>recursive coordinate bisection|
    recursive inertial bisection|hilbert space filling curve|
    octree
  DETERMINISTIC DECOMPOSITION = <string>false|true
  IMBALANCE TOLERANCE = <real>imb_tol
  OVER ALLOCATE MEMORY = <real>over_all_mem
  REUSE CUTS = <string>false|true
  ALGORITHM DEBUG LEVEL = <integer>alg_level
    #  0<=(alg_level)<=3
  CHECK GEOMETRY = <string>false|true
  KEEP CUTS = <string>false|true
  LOCK RCB DIRECTIONS = <string>false|true
  SET RCB DIRECTIONS = <string>do not order cuts|xyz|xzy|
    yzx|yxz|zxy|zyx
  RECTILINEAR RCB BLOCKS = <string>false|true
  RENUMBER PARTITIONS = <string>false|true
  OCTREE DIMENSION = <integer>oct_dimension
  OCTREE METHOD = <string>morton indexing|grey code|hilbert
  OCTREE MIN OBJECTS = <integer>min_obj  #  1<=(min_obj)
  OCTREE MAX OBJECTS = <integer>max_obj  #  1<=(max_obj)
  ZOLTAN DEBUG LEVEL = <integer>zoltan_level
    #  0<=(zoltan_level)<=10
  DEBUG PROCESSOR NUMBER = <integer>proc  #  1<=proc
  TIMER = <string> wall|cpu
  DEBUG MEMORY = <integer>dbg_mem  #  0<=(dbg_mem)<=3
END [ZOLTAN PARAMETERS]
```

The `ZOLTAN PARAMETERS` command block is used to set parameters for Zoltan (see Reference 13), a program that can be used for mesh rebalancing in Presto. The `ZOLTAN PARAMETERS` command block is used in association with the `REBALANCE` command block. A `REBALANCE` command block may reference a `ZOLTAN PARAMETERS` command block via the name, `parameter_name`, for the parameter command block. Reference Section 5.8.1 regarding the use of the `ZOLTAN PARAMETERS` command block for mesh rebalancing in Presto.

Setting the parameters for Zoltan involves some understanding of how Zoltan works. Consult Reference 13 for a discussion of the parameters that can be set by the various command lines in the `ZOLTAN PARAMETERS` command block. Note that some of the command lines in this command block have comments that provide additional information about the parameters. The "`#`" symbol precedes a comment.

In the above command block, = and `IS` are the allowed delimiters, which is different from the usual Presto convention of =, `IS`, and `ARE`. Note that the `ZOLTAN PARAMETERS` command block should be specified in the SIERRA scope when it is referenced from the `ZOLTAN PARAMETERS` command line in the `REBALANCE` command block. When the default set of parameters is used for a Zoltan object, the `ZOLTAN PARAMETERS` command block need not be included in the input file.

5.9 Remeshing

```
BEGIN REMESH
  MAX REMESH STEP INTERVAL = <integer>stepInterval (Infinity)
  MAX REMESH TIME INTERVAL = <real>timeInterval (Infinity)
  NEW MESH MAX EDGE LENGTH RATIO = <real>newMaxRatio (1.25)
  NEW MESH MIN EDGE LENGTH RATIO = <real>newMinRatio (0.25)
  NEW MESH MIN SHAPE = <real>newShape (0.125)
  REMESH AT MAX EDGE LENGTH RATIO = <real>maxCutoffRatio
    (newMaxEdgeLengthRatio*1.75)
  REMESH AT MIN EDGE LENGTH RATIO = <real>minCutoffRatio
    (newMinEdgeLengthRatio*0.25)
  REMESH AT SHAPE = <real>cutoffShape (0.025)
  CONTACT CLEANUP = AUTO|OFF|ON (AUTO)
  DEBUG OUTPUT LEVEL = <integer>level (0)
  MAX REMESH REBALANCE METRIC = <integer>rebalanceMetric (1.25)
  MAX NUMBER ELEMENTS = <integer>maxNumElem (500000)
  MIN SHAPE IMPROVEMENT = <real>minShapeImprovement(0.001)
  MAX NUM PATCH RECREATIONS = <integer>maxNumPatchRecreations(5)
  POISON CRITICAL VALUE = <integer>poisonCriticalValue(4)
  POISON SUBTRACTION INTERVAL =
    <integer>poisonSubtractionInterval(10)
  MAX ITERATIONS = <integer>maxIterations(5)

  BEGIN REMESH BLOCK SET
    #
    # Parameters for remesh block set
    #
  END [REMESH BLOCK SET]

  BEGIN ADAPTIVE REFINEMENT
    #
    # Parameters for adaptive refinement
    #
  END [ADAPTIVE REFINEMENT]
END [REMESH]
```

The `REMESH` command block, which is used within the region scope, sets parameters for remeshing a portion of the mesh. Remeshing involves removing badly shaped elements and inserting new elements of better quality that occupy the same volume. Depending on the degree to which the original elements are deformed, the new elements may occupy slightly more or slightly less volume than the original mesh. If regions of the mesh cannot be meshed with well-shaped elements having reasonable time steps, they may be removed entirely, potentially changing the topology. Examples of such regions include exterior slivers or very thin parts.

Remeshing is used exclusively with node-based tetrahedrons. Whenever possible, remeshing avoids moving, deleting or adding nodes. The node-based tetrahedron stores both material and

kinematic state information at the nodes and thus avoids many of the state advection problems associated with remeshing. However, some amount of state advection or non-conservation of energy, momentum, and mass may occur during remeshing.

In addition to remeshing locations with badly shaped elements, remeshing can be used to adaptively refine a mesh. Adaptive refinement may applied to an initially uniform mesh to produce one with a large number of elements in a region of interest and a coarse mesh elsewhere. Mesh refinement is fully conforming and works by altering the nodal characteristic edge lengths in an adapted mesh. The remeshing algorithm attempts to make the new mesh density consistent with the adapted characteristic edge lengths. Mesh adaptation happens only during remesh steps. Specifying a remesh step or a remesh time interval may be used to trigger adaptive refinement even if no large element deformation is taking place.

5.9.1 Remeshing Commands

The following commands control how and when remeshing is performed:

```
MAX REMESH STEP INTERVAL = <integer>stepInterval (Infinity)
MAX REMESH TIME INTERVAL = <real>timeInterval (Infinity)
NEW MESH MAX EDGE LENGTH RATIO = <real>newMaxRatio (1.25)
NEW MESH MIN EDGE LENGTH RATIO = <real>newMinRatio (0.25)
NEW MESH MIN SHAPE = <real>newShape (0.125)
REMESH AT MAX EDGE LENGTH RATIO = <real>maxCutoffRatio
  (newMeshMaxEdgeLengthRatio*1.75)
REMESH AT MIN EDGE LENGTH RATIO = <real>minCutoffRatio
  (newMeshMinEhgeLengthRatio*0.25)
REMESH AT SHAPE = <real>cutoffShape (0.025)
CONTACT CLEANUP = AUTO|OFF|ON (AUTO)
DEBUG OUTPUT LEVEL = <integer>level (0)
MAX REMESH REBALANCE METRIC = <integer>rebalanceMetric (1.25)
MAX NUMBER ELEMENTS = <integer> maxNumElems (500000)
MIN SHAPE IMPROVEMENT = <real>minShapeImprovement(0.001)
MAX NUM PATCH RECREATIONS = <integer>maxNumPatchRecreations(5)
POISON CRITICAL VALUE = <integer>poisonCriticalValue(4)
POISON SUBTRACTION INTERVAL =
  <integer>poisonSubtractionInterval(10)
MAX ITERATIONS = <integer>maxIterations(5)
```

The `MAX REMESH STEP INTERVAL` command defines the maximum number of simulation time steps that can pass between remeshing steps. Note that if any value of `MAX REMESH STEP INTERVAL` is specified, the code will perform a remesh step during initialization. This is useful for doing an initial mesh adaptation.

The `MAX REMESH TIME INTERVAL` command defines the maximum simulation time that can pass between remeshing steps.

The NEW MESH MAX EDGE LENGTH RATIO, NEW MESH MIN EDGE LENGTH RATIO, and NEW MESH MIN SHAPE commands specify target values for maximum edge length ratio, minimum edge length ratio, and minimum mesh shape in the new mesh. These metrics are described below in the definitions of the REMESH AT MAX EDGE LENGTH RATIO, REMESH AT MIN EDGE LENGTH RATIO, and REMESH AT SHAPE commands, respectively. It is recommended that the thresholds for triggering remeshing be at least a factor of four smaller than the new mesh values to prevent excessive remeshing calls.

The REMESH AT MAX EDGE LENGTH RATIO command specifies a threshold edge length ratio at which remeshing is triggered. The ratio is determined as the ratio of the longest edge connected to a given node to the characteristic initial mesh edge length associated with that node. Edge lengths that become large may no longer be able to represent required geometric details or accurately compute contact. The remeshing algorithm attempts to maintain edge lengths at roughly their original lengths, which may vary significantly across the mesh.

The REMESH AT MIN EDGE LENGTH RATIO command is similar to the REMESH AT MAX EDGE LENGTH RATIO command. This command triggers remeshing when the ratio of the shortest edge connected to a given node to the characteristic initial mesh edge length associated with that node falls below the specified threshold value. If edge lengths become too small, the mesh may have an excessively small time step or too many elements.

The REMESH AT SHAPE command defines the critical shape at which refinement is triggered. The element shape metric is based on a minimum tetrahedron face angle. The optimum tetrahedron has four equilateral faces and angles between those faces of approximately 50 degrees. A degenerate or inverted tetrahedron has a minimum face angle less than or equal to zero degrees. The element shape provides a measure of how close an element is to becoming degenerate or inverted.

The CONTACT CLEANUP command determines whether contact-related algorithms are run following remeshing. Remeshing near areas of contact may result in violations of contact constraints due to changes in element topology. Reapplying contact algorithms following remeshing ensures that contact requirements are maintained.

The DEBUG OUTPUT LEVEL command controls the amount of remeshing-related output printed to the the log file and terminal output. If this is set to zero, no output occurs, while larger numbers result in larger amounts of output. Output many include:

- Step-by-step values of metrics that trigger remeshing.
- The number of elements changed in a remesh step.
- Mass, energy, and momentum conservation balances during remeshing.

The MAX REMESH REBALANCE METRIC command line is used to control when the load rebalancing algorithm is called. During remeshing, the number of elements per processor can become out of balance, causing the parallel analyses to slow down. The specified rebalance_metric is a threshold for the ratio of the maximum number of elements on any processor to the average number of elements per processor. After each remeshing is performed, if that ratio exceeds the specified rebalance_metric, the rebalancing algorithm is called. The default value for this parameter is 1.25.

The MAX NUMBER ELEMENTS command line is used to set the maximum number of elements per processor that may be created during a remeshing analysis. If this value is exceeded, a warning is issued and no further remeshing is done. The default value for this parameter is 500000.

The MAX ITERATIONS command line is used to set the maximum number of remesh iterations that will be taken in a single time step. Lower values cause remesh to possibly run faster at the expense of worse elements or deleting difficult regions of the mesh. Valid values are 1 to infinity. The default value is 5.

The MAX NUM PATCH RECREATIONS command line is used to set the maximum number of patch recreations. This is an advanced remeshing algorithm option that relates to the iteration loop around remesh/parallel consolidation/overlap removal. Lower values cause remeshing to possibly run faster at the expense of quality elements (similar to max iterations described above). Valid values are 1 to infinity. The default value is 5.

The MIN SHAPE IMPROVEMENT command line is used to set what is considered a valid remesh operation. Generally larger values will cause remesh to function faster at expense of less overall mesh quality or more element deletion. Valid values are from 0.0 to approximately 0.1

The commands POISON CRITICAL VALUE and POISON SUBTRACTION INTERVAL are used to mark bad mesh regions. Each time an element is marked as bad all its nodes get a poison counter. Every subtraction interval steps all nodes remove one poison counter (never going below zero). If a node ever has more than the critical value of poison counters the node and all elements attached to it are removed from the mesh. This control is used to remove parts of the mesh that are frequently remeshing, likely due to a material model going haywire. Decreasing the critical value or increasing the subtraction interval cause the algorithm to more aggressively delete parts of the mesh. Increasing the critical value or decreasing the subtraction interval cause the code to avoid element deletion. Valid critical value 2 to Infinity. Valid subtraction interval 1 to Infinity. Note, setting subtraction interval to 1 in effect turns off the poison node element deletion.

5.9.2 Remesh Block Set

```
BEGIN REMESH BLOCK SET
  BLOCK = <string list>block_names
  REMOVE BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
END [REMESH BLOCK SET]
```

The BEGIN REMESH BLOCK SET command block, used in the scope of the REMESH command block, defines the element block or set of blocks that the given remesh command block applies to. The elements in the element block will be checked against the shape criteria and may be affected by remeshing. Note that it is currently assumed that all elements to be remeshed are part of a single material. Remeshing of equivalenced mesh blocks is not well supported.

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of blocks. See Section 6.1.1 for more information about the use of these command lines for creating a set of blocks used by the command block. There must be at least one BLOCK or

INCLUDE ALL BLOCKS command line in the command block.

The REMOVE BLOCK command line allows you to delete blocks from the set specified in the BLOCK and/or INCLUDE ALL BLOCKS command line(s) through the string list block_names. Typically, you would use the REMOVE BLOCK command line with the INCLUDE ALL BLOCKS command line. If you want to include all but a few of the element blocks, a combination of the REMOVE BLOCK command line and INCLUDE ALL BLOCKS should minimize input information.

5.9.3 Adaptive Refinement

```
BEGIN ADAPTIVE REFINEMENT
  #
  # adaptive refinement control commands
  ADAPT TYPE = NODE_PROXIMITY|POINT_PROXIMITY|SHARP_EDGE_PROXIMITY
  RADIUS = <real>radius
  ADAPT SHARP ANGLE = <real>angle (45)
  ADAPT SMOOTH ANGLE = <real>angle (10)
  GEOMETRIC POINT COORDINATES = <real>x <real>y <real>z
  ADAPT SIZE RATIO = <real>ratio (2.0)
  #
  # tool mesh entity commands
  NODE SET = <string list>nodelist_names
  REMOVE NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  REMOVE SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  REMOVE BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  #
  # activation commands
  ACTIVE PERIODS = <string>period_names
  INACTIVE PERIODS = <string>period_names
END [ADAPTIVE REFINEMENT]
```

The ADAPTIVE REFINEMENT command block, used in the context of the REMESH command block, contains commands related to adaptive refinement. Adaptive refinement can be useful when the desired level of refinement in a region of the mesh is unknown when the mesh is created, or when a refinement region should move during the analysis. For example, complex physics may occur near moving contact boundaries. Adaptive refinement can be used to produce a fine mesh only near these boundaries and then have that refined region move with the contact boundaries as they move.

5.9.3.1 Adaptive Refinement Control Commands

The following commands used within the ADAPTIVE REFINEMENT command block control the adaptive refinement algorithm:

```
ADAPT TYPE = NODE_PROXIMITY|POINT_PROXIMITY|SHARP_EDGE_PROXIMITY
RADIUS = <real>radius
ADAPT SHARP ANGLE = <real>angle (45)
ADAPT SMOOTH ANGLE = <real>angle (10)
GEOMETRIC POINT COORDINATES = <real>x <real>y <real>z
ADAPT SIZE RATIO = <real>ratio (2.0)
```

The `ADAPT TYPE` command specifies the type of refinement. Currently three options exist:

- The `NODE_PROXIMITY` option refines areas of the remesh blocks that are near nodes of the tool blocks.
- The `SHARP_EDGE_PROXIMITY` option refines areas of the remesh blocks that are near exterior sharp edges of tool blocks. This command is specialized to refine regions for contact. To correctly represent contacting geometries, small elements are often required to allow material flow around sharp intruding edges.
- The `POINT_PROXIMITY` option refines all nodes near a defined point in space.

The `RADIUS` command defines the minimum distance from a node to a given tool object in the remesh block for that node to be considered for refinement. For example, if the refinement type is `POINT_PROXIMITY`, each node within a distance of `RADIUS` to the defined point will be refined. If refinement type is `NODE_PROXIMITY`, each node within a distance of `RADIUS` to any node in the tool block will be refined. Nodes that are closer to the refinement point have more refinement applied to them than nodes that are farther away. Thus, refinement grades the mesh smoothly from fine to coarse elements over the distance `RADIUS`.

The `ADAPT SHARP ANGLE` and `ADAPT SMOOTH ANGLE` commands are used only with the `SHARP_EDGE_PROXIMITY` refinement type and define edge sharpness thresholds for full, partial, and no mesh refinement. Edges with angles sharper (smaller) than `SHARP ANGLE` trigger full mesh refinement. Edges with angles smoother (larger) than `ADAPT SMOOTH ANGLE` do not trigger mesh refinement. Edges with angles that fall between these two angles trigger a reduced level of mesh refinement. These two commands define a transition zone over which the level of mesh refinement varies smoothly from full refinement to zero refinement.

The `GEOMETRIC POINT COORDINATES` command is used only with the `POINT_PROXIMITY` refinement type. This command defines the spatial location of the refinement tool point. This command may be used multiple times to define multiple refinement points.

The `ADAPT SIZE RATIO` command defines the degree of refinement applied. The default value of 2.0 specifies that the mesh density should be doubled. A value less than one specifies that the mesh should be coarsened.

5.9.3.2 Tool Mesh Entity Commands

The `NODE_PROXIMITY` and `SHARP_EDGE_PROXIMITY` types of adaptive refinement are based on proximity to tool mesh objects, which are collections of nodes or edges. For example, in a

simulation of a sheet metal forming process, the punch tool may be defined as a tool mesh object, thus triggering adaptive refinement in the sheet metal that is in proximity to the punch tool.

These tool objects do not refine the body to be refined, but define objects that will trigger refinement if they are in the proximity of the body to be refined. The following commands are used within the `ADAPTIVE REFINEMENT` command block to define tool entities:

```
NODE SET = <string list>nodelist_names
REMOVE NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
REMOVE SURFACE = <string list>surface_names
BLOCK = <string list>block_names
REMOVE BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
```

These commands are a set of Boolean operators for constructing a set of mesh entities. See Section 6.1.1 for more information about the use of these command lines. Multiple types of these commands can be used together to form a set of nodes or edges.

It is important to note that for the `NODE_PROXIMITY` adaptivity type, any type of mesh entity can be used. A set of nodes is formed from those contained in all node sets, surfaces, and blocks listed. For the `SHARP_EDGE_PROXIMITY` adaptivity type, however, only blocks and surfaces may be used. That adaptivity type requires information about element edges that is not available from node sets.

5.9.3.3 Activation Commands

Adaptive refinement, if used, is by default active throughout an analysis. If desired, it can optionally be activated or deactivated during select time periods using the following commands in the `ADAPTIVE REFINEMENT` command block:

```
ACTIVE PERIODS = <string>period_names
INACTIVE PERIODS = <string>period_names
```

See Section 2.5 for more information regarding these commands.

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Chapter 6

Boundary Conditions and Initial Conditions

Presto offers a variety of options for defining boundary and initial conditions. Typically, boundary and initial conditions are defined on some subset of mesh entities (node, element face, element) defining a model. Presto offers a flexible means to define subsets of mesh entities. Section 6.1.1 describes commands that will let you define some subset of a mesh entity using a collection of commands that constitute a set of Boolean operators.

The remaining parts of this chapter discuss the following functionality:

- Section 6.2 presents methods for setting the initial values of variables in Presto. Presto has the flexibility to set a complex initial state for some variable such as nodal velocity or element stress.

- Kinematic boundary conditions typical of those you would expect in a solid mechanics code (fixed displacement, prescribed acceleration, etc.) are options in Presto and described in Section 6.3. Most of these boundary conditions let you specify a time history using a function, a user subroutine, or by reading values from a mesh file.

- Section 6.4 documents a number of initial velocity options available in Presto.

- Force boundary conditions typical of those you would expect in a solid mechanics code (prescribed force, traction, etc.) are options in Presto and described in Section 6.5. Most of these force boundary conditions let you specify a time history using a function or a user subroutine.

- Section 6.6 discusses the gravity load option. A gravity load is a body force boundary condition.

- Section 6.7 details a number of options available for describing a temperature field in Presto.

- Section 6.8 details the options available for describing a pore pressure field.

- Section 6.10 describes a number of specialized boundary conditions.

6.1 General Boundary Condition Concepts

There are general principles that apply to all of the available types of boundary conditions. To apply a boundary condition, a set of mesh entities and the magnitude and/or direction in which it is to be applied must be specified. Presto provides several methods for both specifying the set of mesh entities and for prescribing how the boundary condition is to be applied. The general concepts on how this is done are applicable to all of the boundary condition types, and are described in the following sections.

6.1.1 Mesh-Entity Assignment Commands

A number of standard command lines exist to define a set of mesh entities (node, element face, element) associated with some type of boundary, initial, or load condition. All these command lines exist within the command blocks for the various prescribed conditions, which in turn exist within the region scope. These command lines, taken collectively, constitute a set of Boolean operators for constructing sets of mesh entities.

The first set of command lines we will consider is as follows:

```
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
```

In the above command lines, the string list `nodelist_names` is used to represent one or more node sets as discussed in Section 1.5. A node set is referenced as `nodelist_id`, where id is some integer. For example, suppose you have three node lists in your model: 10, 23, and 105. If you want to combine all these node lists so that they form one set of nodes for, say, your boundary condition or initial condition, then you would use the command line:

```
NODE SET = nodelist_10 nodelist_23 nodelist_105
```

This convention applies as well to any surface-related command line that uses the string list `surface_names` or any block-related command line that uses the string list `block_names`.

The `NODE SET` command line associates a set of nodes with an initial, boundary, or load condition. A condition may be applied to multiple node sets by putting multiple node set names on the command line or by repeating the command line multiple times.

The `SURFACE` command line associates a set of element faces or their attached nodes with a boundary, initial, or load condition. A condition may be applied to multiple surfaces by putting multiple surface names on the command line or by repeating the command line multiple times. For example, suppose we wish to use the fixed displacement kinematic boundary condition. Although this is a nodal boundary condition (the condition is applied to individual nodes), a `SURFACE` command line can be used to establish the set of nodes. If the command line

```
SURFACE = surface_101
```

appears in a fixed displacement boundary condition, then all the nodes associated with surface 101 will be associated with the boundary condition.

The `BLOCK` command line associates a set of elements and its nodes and faces with a boundary condition. A boundary condition may be applied to multiple blocks by putting multiple block names on the command line or by repeating the command line multiple times.

The `BLOCK` must be used for kinematic boundary conditions on rigid bodies. If a block has been defined as a rigid body, the specified kinematic condition will be applied to the rigid body reference node.

For example, suppose we wish to use the fixed displacement kinematic boundary condition as in the previous example. If the command line

```
BLOCK = block_50
```

appears in a fixed displacement kinematic boundary condition, then all the nodes associated with block 50 will be associated with the boundary condition.

The `INCLUDE ALL BLOCKS` command line associates all blocks and hence all elements and nodes in the model with a boundary, initial, or load condition. The block command lines associated with boundary conditions, initial conditions, and gravity will NOT generate surfaces.

Any combination of the above command lines can be used to create a union of mesh entities. Suppose, for example, that the command lines

```
NODE SET = nodelist_2
SURFACE = surface_3
```

appear in a `FIXED DISPLACEMENT` command block for a kinematic boundary condition. The set of nodes associated with the boundary condition will be the union of the set of nodes associated with surface 3 and the set of nodes associated with node set 2.

When a union of mesh entities is created by using two or more of the above command lines, a node or element face may appear in more than one node set, surface or block. However, the prescribed condition is applied to each node or face only once. For example, node 67 may be a part of nodelist 2 and surface 3 but the boundary condition will only be applied to node 67 once.

The set of mesh entities associated with a boundary, initial, or load condition can be edited (mesh entities can be deleted from the set) by using the following command lines:

```
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
```

The `REMOVE NODE SET` command line deletes the nodes in the specified node set from the set of nodes used by the condition.

The `REMOVE SURFACE` command line deletes a set of element faces and their associated nodes from the set of element faces used by the prescribed condition.

The `REMOVE BLOCK` command line deletes a set of elements and their associated nodes from the set of elements used by the prescribed condition.

6.1.2 Methods for Specifying Boundary Conditions

There are three main methods which can be used to prescribe most types of boundary conditions available in Presto.

- The boundary condition can be prescribed using commands in the input file. These commands are categorized as "specification commands" in this document. Depending on the type of the boundary condition, it is be necessary to prescribe its direction and/or magnitude. Boundary conditions can be specified this way when a set of mesh entities is to experience a similar condition with a time variation that can be expressed by a function. One of the following commands is used to specify the direction of the boundary condition: `COMPONENT`, `DIRECTION`, `CYLINDRICAL AXIS`, or `RADIAL AXIS`. The magnitude is defined using one of `MAGNITUDE`, `FUNCTION` or `ANGULAR VELOCITY`. These commands are used in various combinations depending on the type of the boundary condition. The details of how to use them are provided in the descriptions of the various boundary condition types.

- If the nature of the boundary condition is such its variation in time and space can not be described easily by the combination of a function and a direction, it may be necessary to use a user-defined subroutine. User subroutines provide a very general capability to define how kinematic or force boundary conditions are applied. The use of user-defined subroutines does increase the complexity of defining the model, however. The user must write and debug the subroutine and compile and link it in with Presto. Because of the added complexity, user subroutines should only be used if the needed capability is not provided by the other methods of prescribing boundary conditions.

- For some types of boundary conditions, the values of the field to be prescribed can be read in from an existing output database. This is often used as a method to transfer results from one analysis code to another. One of the common uses for this capability is to compute temperatures using a thermal code, and then transfer the temperature fields to Presto to study combined mechanical and thermal effects. This capability can be used either to read in initial values or to read in a series of values that vary over time.

In the following sections describing specific types of boundary conditions, the commands are grouped according to these three categories.

6.2 Initial Variable Assignment

```
BEGIN INITIAL CONDITION
  #
  # mesh-entity set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # variable identification commands
  INITIALIZE VARIABLE NAME = <string>var_name
  VARIABLE TYPE = NODE|EDGE|FACE|ELEMENT|GLOBAL
  #
  # specification command
  MAGNITUDE = <real list>initial_values
  #
  # probability distribution commands
  DISTRIBUTION = WEIBULL PARAMETERS = <real list>dist_values
    SEED = <integer>dist_seed
  DISTRIBUTION REFERENCE = NODE|EDGE|FACE|ELEMENT|GLOBAL
    <string>size_var_name VALUE = <real>size_ref_val
  #
  # external database commands
  READ VARIABLE = <string>var_name
  COPY VARIABLE = <string>var_name [FROM MODEL <string>model_name]
  TIME = <real>time
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name |
    SURFACE SUBROUTINE = <string>subroutine_name |
    ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # additional command
  SCALE FACTOR = <real>scale_factor(1.0)
END [INITIAL CONDITION]
```

Presto supports a general initialization procedure for setting the value of any variable. This procedure can be used to set material state variables, shell thickness, initial stress, etc. The initialization is performed both before and after the element and material model initialization. This allows the elements and material models to compute other initial variables based on variables specified by the user and also ensures that the variables specified by the user are not overwritten by the elements and material models. However, there is minimal checking in Prestoto ensure that the changes made yield a consistent system. There is also no guarantee that the changes will not be overwritten or misinterpreted by some other internal routine depending on what variable is being changed. Thus, caution is advised when using this capability.

The `INITIAL CONDITION` command block, which appears in the region scope, is used to select a method and set values for initializing a variable. The command block specifies the initial value of a global variable or a variable associated with a set of mesh entities, i.e., nodes, edges, faces, or elements. The user has three options for setting initial values: with a constant magnitude, with an input mesh variable, or by a user subroutine. Only one of these three options can be specified in the command block.

The command block contains five groups of commands—mesh-entity set, variable identification, magnitude, input mesh variable, and user subroutine. In addition to the command lines in the five groups, there is one additional command line: `SCALE FACTOR`. Following are descriptions of the different command groups and the `SCALE FACTOR` command line.

6.2.1 Mesh-Entity Set Commands

The `mesh-entity set commands` portion of the `INITIAL CONDITION` command block specifies the nodes, element faces, or elements associated with the variable to be initialized. This portion of the command block can include some combination of the following command lines:

```
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes, element faces, or elements. See Section 6.1.1 for more information about the use of these command lines for mesh entities. There must be at least one `NODE SET`, `SURFACE`, `BLOCK`, or `INCLUDE ALL BLOCKS` command line in the command block.

6.2.2 Variable Identification Commands

Any variable used in the `INITIAL CONDITION` command block must exist in Presto. The variable can be any currently defined variable in Presto or any user-defined variable created with the `USER`

VARIABLE command block (see Section 10.2.4).

There are two command lines that identify the variable:

```
INITIALIZE VARIABLE NAME = <string>var_name
VARIABLE TYPE = [NODE|EDGE|FACE|ELEMENT|GLOBAL]
```

The INITIALIZE VARIABLE NAME command line gives the name of the variable for which initial values are being assigned. As mentioned, the string var_name must be some variable known to Presto; it cannot be an arbitrary user-selected name.

The VARIABLE TYPE command line provides additional information about the variable being initialized. The options NODE, EDGE, FACE, ELEMENT, and GLOBAL on the command line indicate whether the variable is, respectively, a nodal, edge, face, element, or global quantity. One of these options must appear in the VARIABLE TYPE command line.

Both of these command lines are required regardless of the option selected to set values for the variable.

6.2.3 Specification Command

If the constant magnitude command is used, one or more initial values are specified directly in the command block. This is done using the following command line:

```
MAGNITUDE = <real list>initial_values
```

The initial_values specified on the MAGNITUDE command line will set the values for the variable given by var_name in the INITIALIZE VARIABLE NAME command line. The number of values is dependent on the type of the variable specified in the INITIALIZE VARIABLE NAME command line. For example, if the user wanted to initialize the velocity at a set of nodes, three quantities would have to be specified since the velocity at a node is a vector quantity. If the user wanted to initialize the stress tensor for a set of uniform-gradient, eight-node hexahedral elements, six quantities would have to be specified since the stress tensor for this element type is described with six values.

6.2.4 Probability Distribution Commands

The field to be initialized can optionally be populated with random numbers generated to conform to a specified probability distribution function. This is accomplished by including the following command:

```
DISTRIBUTION = WEIBULL PARAMETERS = <real list>dist_values
  SEED = <integer>dist_seed
```

Currently, the Weibull distribution is the only supported probability distribution, but this command is intended to eventually support other types of probability distributions. The parameters that describe the probability distribution, `dist_values`, are provided as a list of real numbers.

There are two parameters to the Weibull distribution: the shape parameter, k, and the scale parameter λ. In this implementation, only one parameter, k is input in `dist_values`. The scale parameter λ is hardcoded to be 1.0.

The `DISTRIBUTION` command must be used in conjunction with the `MAGNITUDE` command. The specified magnitude is applied as a scale factor to the randomly generated numbers. Thus, the scale parameter for the Weibull distribution is specified through the `MAGNITUDE` command.

If a field is populated with randomly generated values conforming to the Weibull distribution, the realizations of random values at each point can be scaled to account for the size of the mesh at that location. This is accomplished by including the following command:

```
DISTRIBUTION REFERENCE = NODE|EDGE|FACE|ELEMENT|GLOBAL
  <string>size_var_name VALUE = <real>size_ref_value
```

In this command, `size_var_name` is the name of a variable, which can be of either nodal, edge, face, or element, or global type, and which should represent the size of the mesh at each point. The element `volume` field is a good example of such a variable. The reference value: `size_ref_value`, is a reference size for which no scaling is performed.

The randomly generated value for the variable is multiplied by the factor α, which is computed as:

$$\alpha = \left(\frac{v_i}{v_{ref}}\right)^{-\frac{1}{k}} \tag{6.1}$$

where v_i is the value of a field variable specified in `size_var_name` at the current point i, v_{ref} is the reference size, `size_ref_value`, and k is the Weibull shape parameter (also referred to as the Weibull modulus). The result of this scaling is that realizations of the random variable on larger elements are scaled down and those on smaller elements are scaled up. This accounts for the fact that a defect is more likely to be found within the volume represented by an element as the size of that element increases.

6.2.5 External Mesh Database Commands

If the external database option is used, the initial values for a variable are read from an external mesh database. As an example, suppose the mesh file contains a set of element temperatures. These temperature values (which can vary for each element) can be used to initialize a temperature value associated with each element.

The values are read from a finite element model defined via the `FINITE ELEMENT MODEL` command block described in Section 5.1. The finite element model can either be the model used by the region for its mesh definition as specified with the `USE FINITE ELEMENT MODEL` command (see Section 2.3), or it can be a different (but compatible) model. The following command lines control the use of an external mesh database to prescribe initial conditions:

```
READ VARIABLE = <string>var_name
COPY VARIABLE = <string>var_name [FROM MODEL <string>model_name]
TIME = <real>time
```

The `READ VARIABLE = <string>var_name` command is used to read the variable from the region's finite element mesh database. The `var_name` string specifies the name of the variable as it appears on the mesh database. The number of values associated with the variable in the mesh file must be the same number associated with the variable name specified in the `INITIALIZE VARIABLE NAME` command line. For example, if the variable specified by the `INITIALIZE VARIABLE NAME` has a single value, then the variable specified in the mesh file must also have a single value.

If the analysis will cause topology modifications due to the use of load balancing, remeshing, or other techniques that can result in nodes and/or elements being moved among processors, then the `COPY VARIABLE` command should be used. This command specifies that the variable named `var_name` will be used to specify the initial conditions. The `FROM MODEL <string>model_name` portion of the command is optional. If it is specified, the results are read from the mesh database named `model_name`. Otherwise, the region's finite element mesh database will be used as the model.

The primary difference between the behavior of the `COPY VARIABLE` command and the `READ VARIABLE` command is that the copy command handles topology modifications caused by load balancing and remeshing, which can move nodes and elements to different processors. The `COPY VARIABLE` command will correctly match the nodes from the external database to the corresponding nodes in the analysis and communicate the data between processors if needed. Note that the nodes in the two finite element models must match spatially, but they can be distributed on different processors.

The variable name used on the mesh file can be arbitrary. The name can be identical to or different from the variable name specified on the `INITIALIZE VARIABLE NAME` command line.

The field to be read may be specified at an arbitrary number of different times on the mesh file. The default behavior is to use the value of the variable at the initial time in the analysis to prescribe the initial condition. The time history is interpolated as needed for an initial analysis time that does not correspond exactly to a time on the mesh file. The `TIME` command line can optionally be used to select a specific time to initialize a variable. If the specified time on the `TIME` command line does not correspond exactly to a time on the mesh file, the data on the mesh file will be interpolated as needed.

6.2.6 User Subroutine Commands

If the user subroutine option is used, the initial values will be calculated by a subroutine that is written by the user explicitly for this purpose. The subroutine will be called by Presto at the appropriate time to perform the calculations.

Following are the command lines related to the user subroutine option:

```
NODE SET SUBROUTINE = <string>subroutine_name |
```

```
  SURFACE SUBROUTINE = <string>subroutine_name |
  ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value
```

Only one of the first three command lines listed above can be specified in the command block. The particular command line selected depends on the mesh-entity type of the variable being initialized. For example, variables associated with nodes would be initialized if you are using the `NODE SET SUBROUTINE` command line, variables associated with faces if you are using the `SURFACE SUBROUTINE` command line, and variables associated with elements if you are using the `ELEMENT BLOCK SUBROUTINE` command line. The string `subroutine_name` is the name of a FORTRAN subroutine that is written by the user.

Following the selected subroutine command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 10.2.2 and consist of `SUBROUTINE DEBUGGING OFF`, `SUBROUTINE DEBUGGING ON`, `SUBROUTINE REAL PARAMETER`, `SUBROUTINE INTEGER PARAMETER`, and `SUBROUTINE STRING PARAMETER`. Examples of using these command lines are provided throughout Chapter 10.

The application of user subroutines for variable initialization is essentially the same as the application of user subroutines in general. See Section 6.3.8 and Chapter 10 for more details on implementing the user subroutine option.

When the user subroutine option is used for variable initialization, the user subroutine is called only once. Also, when a user subroutine is being used, the returned value is the new (initial) variable value at each mesh entity, and the flags array is ignored.

6.2.7 Additional Command

This command line provides an additional option for the `INITIAL CONDITION` command block:

```
SCALE FACTOR = <real>scale_factor(1.0)
```

Any initial value can be scaled by use of the `SCALE FACTOR` command line. An initial value generated by any one of the three initial-value-setting options in this command block (i.e., constant magnitude, input mesh, or user subroutine) will be scaled by the real value `scale_factor`.

6.3 Kinematic Boundary Conditions

The various kinematic boundary conditions available in Presto are described in this section. The kinematic boundary conditions are nested inside the region scope.

Kinematic constraints can potentially be in conflict with other constraints. Refer to Appendix D for information on how conflicting constraints are handled.

6.3.1 Fixed Displacement Components

```
BEGIN FIXED DISPLACEMENT
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # specification commands
  COMPONENT = <string>X/Y/Z | COMPONENTS = <string>X/Y/Z
  #
  # additional commands
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [FIXED DISPLACEMENT]
```

The `FIXED DISPLACEMENT` command block fixes displacement components (X, Y, Z, or some combination thereof) for a set of nodes. This command block contains two groups of commands—node set and component. Each of these command groups is basically independent of the other. In addition to the command lines in the two command groups, there are two additional command lines: `ACTIVE PERIODS` and `INACTIVE PERIODS`. These are used to activate or deactivate this kinematic boundary condition for certain time periods.

For rigid bodies, any kinematic boundary condition is applied directly to the rigid body reference node. The kinematics for the nodes attached to the rigid body are applied via the rigid body constraint conditions. Since rigid bodies are defined using element blocks, only the `BLOCK` command may be used to specify fixed displacement conditions on rigid bodies.

Following are descriptions of the different command groups.

6.3.1.1 Node Set Commands

The `node set commands` portion of the `FIXED DISPLACEMENT` command block specifies the nodes associated with the boundary condition. This portion of the command block can include some combination of the following command lines:

```
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes used by the boundary condition. There must be at least one `NODE SET`, `SURFACE`, `BLOCK`, or `INCLUDE ALL BLOCKS` command line in the command block.

6.3.1.2 Specification Commands

There are two component specification commands available in the `FIXED DISPLACEMENT` command block:

```
COMPONENT = X/Y/Z | COMPONENTS = X/Y/Z
```

The displacement components that are to be fixed can be specified with either the `COMPONENT` command line or the `COMPONENTS` command line. There can be only one `COMPONENT` command line or one `COMPONENTS` command line in the command block. The user can specify any combination of the components to be fixed, as in `X`, `Z`, `X Z`, `Y X`, etc.

6.3.1.3 Additional Commands

The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines can optionally appear in the `FIXED DISPLACEMENT` command block:

```
ACTIVE PERIODS = <string list>period_names
INACTIVE PERIODS = <string list>period_names
```

These command lines determine when the boundary condition is active. See Section 2.5 for more information about these optional command lines.

6.3.2 Prescribed Displacement

```
BEGIN PRESCRIBED DISPLACEMENT
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # specification commands
  DIRECTION = <string>defined_direction |
    COMPONENT = <string>X|Y|Z |
    CYLINDRICAL AXIS = <string>defined_axis |
    RADIAL AXIS = <string>defined_axis
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # external database commands
  READ VARIABLE = <string>var_name
  COPY VARIABLE = <string>var_name [FROM MODEL <string>model_name]
  TIME = <real>time
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [PRESCRIBED DISPLACEMENT]
```

The `PRESCRIBED DISPLACEMENT` command block prescribes a displacement field for a given set of nodes. The displacement field associates a vector giving the magnitude and direction of the displacement with each node in the set of nodes. The displacement field may vary over time and space. If the displacement field has only a time-varying magnitude and uses one of four methods for setting direction, the specification commands in the above command block can be used to specify the displacement field. If the displacement field is more complex, a user subroutine is

used to specify the displacement field. The displacement field can also be read from an external mesh database. In a given boundary condition command block, commands from only one of the command groups (specification commands, user subroutine commands, or external database commands) may be used.

For rigid bodies, any kinematic boundary condition is applied directly to the rigid body reference node. The kinematics for the mesh nodes attached to the rigid body are applied via the rigid body constraint conditions. Since rigid bodies are defined using element blocks, only the `BLOCK` command may be used to specify prescribed displacement conditions on rigid bodies.

The `PRESCRIBED DISPLACEMENT` command block contains four groups of commands—node set, function, user subroutine, and external database. Each of these command groups is basically independent of the others. In addition to the command lines in the four command groups, there are three additional command lines: `SCALE FACTOR`, `ACTIVE PERIODS`, and `INACTIVE PERIODS`. The `SCALE FACTOR` command line can be used in conjunction with the specification commands the user subroutine commands, or the external database command. The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines are used to activate or deactivate this kinematic boundary condition for certain time periods. Following are descriptions of the different command groups and the `SCALE FACTOR` and `ACTIVE PERIODS` command lines.

6.3.2.1 Node Set Commands

The `node set commands` portion of the `PRESCRIBED DISPLACEMENT` command block defines a set of nodes associated with the prescribed displacement field and can include some combination of the following command lines:

```
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes used by the boundary condition. There must be at least one `NODE SET`, `SURFACE`, `BLOCK`, or `INCLUDE ALL BLOCKS` command line in the command block.

6.3.2.2 Specification Commands

If the specification commands are used, the displacement vector at any given time is the same for all nodes in the node set associated with the particular `PRESCRIBED DISPLACEMENT` command block.

Following are the command lines used to specify the prescribed displacement with a direction and a function:

```
DIRECTION = <string>defined_direction |
  COMPONENT = <string>X|Y|Z |
  CYLINDRICAL AXIS = <string>defined_axis |
  RADIAL AXIS = <string>defined_axis
FUNCTION = <string>function_name
```

The displacement can be specified along an arbitrary user-defined direction, along a component direction (X, Y, or Z), along the azimuthal direction in a cylindrical coordinate system (defined in reference to an axis), or along a radial direction (defined in reference to an axis). Only one of these options (i.e., command lines) is allowed. The displacement is prescribed only in the specified direction. A prescribed displacement boundary condition does not influence the motion in directions orthogonal to the prescribed direction.

- The `DIRECTION` command line is used to prescribe displacement in an arbitrary user-defined direction. The name in the string `defined_direction` is a reference to a direction, which is defined using the `DEFINE DIRECTION` command block within the SIERRA scope.

- The `COMPONENT` command line is used to specify that the prescribed displacement vector lies along one of the component directions. The `COMPONENT` command line is a shortcut to an internally defined direction vector; for example, component `x` corresponds to using direction vector (1, 0, 0).

- The `CYLINDRICAL AXIS` command line is used to specify that the prescribed displacement is to be applied in the azimuthal direction of a cylindrical coordinate system. The string `defined_axis` refers to the name of the axis of the cylindrical coordinate system, and which is defined via a `DEFINE AXIS` command block in the SIERRA scope. The displacement is prescribed as a rotation in radians about the axis. Nodes with this type of boundary condition are free to move in the radial and height directions in the cylindrical coordinate system. Restraints can be placed on the node set in those directions if desired by applying separate kinematic boundary conditions that contain `RADIAL AXIS` or `DIRECTION` commands that refer to the same axis. Note that this type of boundary condition is not a rotational boundary condition; it only affects translational degrees of freedom.

  Known Issue: If a prescribed displacement with the `CYLINDRICAL AXIS` option is applied to nodes that fall on the axis, it will have no effect. Separate boundary conditions should be applied to those nodes to fix them in the plane normal to the axis.

- The `RADIAL AXIS` command line requires an axis definition that appears in the SIERRA scope. The string `defined_axis` uses an `axis_name` that is defined in the SIERRA scope (via a `DEFINE AXIS` command line). For this option, a radial line is drawn from a node to the radial axis. The prescribed displacement vector lies along this radial line from the node to the radial axis.

The magnitude of the displacement is specified by the FUNCTION command line. This references a function_name (defined in the SIERRA scope using a DEFINITION FOR FUNCTION command block) that specifies the magnitude of the displacement vector as a function of time. The magnitude can be scaled by use of the SCALE FACTOR command line described in Section 6.3.2.5.

6.3.2.3 User Subroutine Commands

If the user subroutine option is used, the displacement vector may vary spatially at any given time for each of the nodes in the node set associated with the particular PRESCRIBED DISPLACEMENT command block. The user subroutine option allows for a more complex description of the displacement field than do the specification commands, but the user subroutine option also requires that you write a user subroutine to implement this capability. The user subroutine will be used to define a displacement direction and a magnitude for every node to which the boundary condition will be applied. The subroutine will be called by Presto at the appropriate time to generate the displacement field.

Following are the command lines related to the user subroutine option:

```
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value
```

The user subroutine option is invoked by using the NODE SET SUBROUTINE command line. The string subroutine_name is the name of a FORTRAN subroutine that is written by the user.

Following the NODE SET SUBROUTINE command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 10.2.2 and consist of SUBROUTINE DEBUGGING OFF, SUBROUTINE DEBUGGING ON, SUBROUTINE REAL PARAMETER, SUBROUTINE INTEGER PARAMETER, and SUBROUTINE STRING PARAMETER. Examples of using these command lines are provided throughout Chapter 10.

The magnitude set in the user subroutine can be scaled by use of the SCALE FACTOR command line, as described in Section 6.3.2.5.

See Section 6.3.8 and Chapter 10 for more details on implementing the user subroutine option.

6.3.2.4 External Mesh Database Commands

If the external database option is used, the displacement vector (or specified components of the vector) is read from an external mesh database. The displacements are read from a finite element model defined via the FINITE ELEMENT MODEL command block described in Section 5.1. The

finite element model can either be the model used by the region for its mesh definition as specified with the `USE FINITE ELEMENT MODEL` command (see Section 2.3), or it can be a different (but compatible) model. The following command lines control the use of an external mesh database to prescribe the displacement:

```
READ VARIABLE = <string>var_name
COPY VARIABLE = <string>var_name [FROM MODEL <string>model_name]
TIME = <real>time
```

The `READ VARIABLE = <string>var_name` command is used to read the displacement vector from the region's finite element mesh database. The `var_name` string specifies the name of the variable as it appears on the mesh database.

If the analysis will cause topology modifications due to the use of load balancing, remeshing, or other techniques that can result in nodes and/or elements being moved among processors, then the `COPY VARIABLE` command should be used. This command specifies that the variable named `var_name` will be used to specify the displacement. The `FROM MODEL <string>model_name` portion of the command is optional. If it is specified, the results are read from the mesh database named `model_name`. Otherwise, the region's finite element mesh database will be used as the model.

The primary difference between the behavior of the `COPY VARIABLE` command and the `READ VARIABLE` command is that the copy command handles topology modifications caused by load balancing and remeshing, which can move nodes and elements to different processors. The `COPY VARIABLE` command will correctly match the nodes from the external database to the corresponding nodes in the analysis and communicate the data between processors if needed. Note that the nodes in the two finite element models must match spatially, but they can be distributed on different processors.

The field to be read may be specified at an arbitrary number of different times on the mesh file. The default behavior is for the time history of the variable read from the file to be used to prescribe the boundary condition. The time history is interpolated as needed for analysis times that do not correspond exactly to times on the mesh file. The `TIME` command line can optionally be used to specify that the boundary condition be constant over time, based on the value of the variable read from the file at the specified time. If the specified time on the `TIME` command line does not correspond exactly to a time on the mesh file, the data on the mesh file will be interpolated as needed.

6.3.2.5 Additional Commands

These command lines in the `PRESCRIBED DISPLACEMENT` command block provide additional options for the boundary condition:

```
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
INACTIVE PERIODS = <string list>period_names
```

The `SCALE FACTOR` command line is used to apply an additional scaling factor, which is constant in both time and space, to all vector magnitude values of the field defined by the specification commands or the user subroutine. For example, if the magnitude of the displacement in a time history function is given as 1.5 from time 1.0 to time 2.0 and the scale factor is 0.5, then the magnitude of the displacement from time 1.0 to 2.0 is 0.75. The default value for the scale factor is 1.0.

The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines determine when the boundary condition is active. See Section 2.5 for more information about these command lines.

6.3.3 Prescribed Velocity

```
BEGIN PRESCRIBED VELOCITY
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # specification commands
  DIRECTION = <string>defined_direction |
    COMPONENT = <string>X|Y|Z |
    CYLINDRICAL AXIS = <string>defined_axis |
    RADIAL AXIS = <string>defined_axis
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # external database commands
  READ VARIABLE = <string>var_name
  COPY VARIABLE = <string>var_name [FROM MODEL <string>model_name]
  TIME = <real>time
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [PRESCRIBED VELOCITY]
```

The `PRESCRIBED VELOCITY` command block prescribes a velocity field for a given set of nodes. The velocity field associates a vector giving the magnitude and direction of the velocity with each node in the node set. The velocity field may vary over time and space. If the velocity field has only a time-varying magnitude and uses one of four methods for setting direction, the specification commands in the above command block can be used to specify the velocity field. If the velocity field is more complex, a user subroutine is used to specify the velocity field. The velocity field can also be

read from an external mesh database. In a given boundary condition command block, commands from only one of the command groups (specification commands, user subroutine commands, or external database commands) may be used.

For rigid bodies, any kinematic boundary condition is applied directly to the rigid body reference node. The kinematics for the mesh nodes attached to the rigid body are applied via the rigid body constraint conditions. Since rigid bodies are defined using element blocks, only the `BLOCK` command may be used to specify prescribed velocity conditions on rigid bodies.

The `PRESCRIBED VELOCITY` command block contains four groups of commands—node set, function, user subroutine, and external database. Each of these command groups is basically independent of the others. In addition to the command lines in the four command groups, there are three additional command lines: `SCALE FACTOR`, `ACTIVE PERIODS`, and `INACTIVE PERIODS`. The `SCALE FACTOR` command line can be used in conjunction with either the specification commands or the user subroutine commands. The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines are used to activate or deactivate this kinematic boundary condition for certain time periods. Following are descriptions of the different command groups.

6.3.3.1 Node Set Commands

The `node set commands` portion of the `PRESCRIBED VELOCITY` command block defines a set of nodes associated with the prescribed velocity field and can include some combination of the following command lines:

```
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes used by the boundary condition. There must be at least one `NODE SET`, `SURFACE`, `BLOCK`, or `INCLUDE ALL BLOCKS` command line in the command block.

6.3.3.2 Specification Commands

If the specification commands are used, the velocity vector at any given time is the same for all nodes in the node set associated with the particular `PRESCRIBED VELOCITY` command block.

Following are the command lines used to specify the prescribed velocity with a direction and a function:

```
DIRECTION = <string>defined_direction |
```

```
    COMPONENT = <string>X|Y|Z |
    CYLINDRICAL AXIS = <string>defined_axis |
    RADIAL AXIS = <string>defined_axis
  FUNCTION = <string>function_name
```

The velocity can be specified along an arbitrary user-defined direction, along a component direction (X, Y, or Z), along the azimuthal direction in a cylindrical coordinate system (defined in reference to an axis), or along a radial direction (defined in reference to an axis). Only one of these options (i.e., command lines) is allowed. The velocity is prescribed only in the specified direction. A prescribed velocity boundary condition does not influence the motion in directions orthogonal to the prescribed direction.

- The `DIRECTION` command line is used to prescribe velocity in an arbitrary user-defined direction. The name in the string `defined_direction` is a reference to a direction, which is defined using the `DEFINE DIRECTION` command block within the SIERRA scope.

- The `COMPONENT` command line is used to specify that the prescribed velocity vector lies along one of the component directions. The `COMPONENT` command line is a shortcut to an internally defined direction vector; for example, component `x` corresponds to using direction vector (1, 0, 0).

- The `CYLINDRICAL AXIS` command line is used to specify that the prescribed velocity is to be applied in the azimuthal direction of a cylindrical coordinate system. The string `defined_axis` refers to the name of the axis of the cylindrical coordinate system, and which is defined via a `DEFINE AXIS` command block in the SIERRA scope. The velocity is prescribed as a rotation in radians about the axis. Nodes with this type of boundary condition are free to move in the radial and height directions in the cylindrical coordinate system. Restraints can be placed on the node set in those directions if desired by applying separate kinematic boundary conditions that contain `RADIAL AXIS` or `DIRECTION` commands that refer to the same axis. Note that this type of boundary condition is not a rotational boundary condition; it only affects translational degrees of freedom.

  Known Issue: If a prescribed velocity with the `CYLINDRICAL AXIS` option is applied to nodes that fall on the axis, it will have no effect. Separate boundary conditions should be applied to those nodes to fix them in the plane normal to the axis.

- The `RADIAL AXIS` command line requires an axis definition that appears in the SIERRA scope. The string `defined_axis` uses an `axis_name` that is defined in the SIERRA scope (via a `DEFINE AXIS` command line). For this option, a radial line is drawn from a node to the radial axis. The velocity vector lies along this radial line from the node to the radial axis.

The magnitude of the velocity is specified by the `FUNCTION` command line. This references a `function_name` (defined in the SIERRA scope using a `DEFINITION FOR FUNCTION` command block) that specifies the magnitude of the velocity vector as a function of time. The magnitude can be scaled by use of the `SCALE FACTOR` command line described in Section 6.3.3.5.

6.3.3.3 User Subroutine Commands

If the user subroutine option is used, the velocity vector may vary spatially at any given time for each of the nodes in the node set associated with the particular `PRESCRIBED VELOCITY` command block. The user subroutine option allows for a more complex description of the velocity field than do the specification commands, but the user subroutine option also requires that you write a user subroutine to implement this capability. The user subroutine will be used to define a velocity direction and a magnitude for every node to which the boundary condition will be applied. The subroutine will be called by Presto at the appropriate time to generate the velocity field.

Following are the command lines related to the user subroutine option:

```
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value
```

The user subroutine option is invoked by using the `NODE SET SUBROUTINE` command line. The string `subroutine_name` is the name of a FORTRAN subroutine that is written by the user.

Following the `NODE SET SUBROUTINE` command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 10.2.2 and consist of `SUBROUTINE DEBUGGING OFF`, `SUBROUTINE DEBUGGING ON`, `SUBROUTINE REAL PARAMETER`, `SUBROUTINE INTEGER PARAMETER`, and `SUBROUTINE STRING PARAMETER`. Examples of using these command lines are provided throughout Chapter 10.

The magnitude set in the user subroutine can be scaled by use of the `SCALE FACTOR` command line, as described in Section 6.3.3.5.

6.3.3.4 External Mesh Database Commands

If the external database option is used, the velocity vector (or specified components of the vector) is read from an external mesh database. The velocities are read from a finite element model defined via the `FINITE ELEMENT MODEL` command block described in Section 5.1. The finite element model can either be the model used by the region for its mesh definition as specified with the `USE FINITE ELEMENT MODEL` command (see Section 2.3), or it can be a different (but compatible) model. The following command lines control the use of an external mesh database to prescribe the velocity:

```
READ VARIABLE = <string>var_name
COPY VARIABLE = <string>var_name [FROM MODEL <string>model_name]
TIME = <real>time
```

The READ VARIABLE = <string>var_name command is used to read the velocity vector from the region's finite element mesh database. The var_name string specifies the name of the variable as it appears on the mesh database.

If the analysis will cause topology modifications due to the use of load balancing, remeshing, or other techniques that can result in nodes and/or elements being moved among processors, then the COPY VARIABLE command should be used. This command specifies that the variable named var_name will be used to specify the velocity. The FROM MODEL <string>model_name portion of the command is optional. If it is specified, the results are read from the mesh database named model_name. Otherwise, the region's finite element mesh database will be used as the model.

The primary difference between the behavior of the COPY VARIABLE command and the READ VARIABLE command is that the copy command handles topology modifications caused by load balancing and remeshing, which can move nodes and elements to different processors. The COPY VARIABLE command will correctly match the nodes from the external database to the corresponding nodes in the analysis and communicate the data between processors if needed. Note that the nodes in the two finite element models must match spatially, but they can be distributed on different processors.

The field to be read may be specified at an arbitrary number of different times on the mesh file. The default behavior is for the time history of the variable read from the file to be used to prescribe the boundary condition. The time history is interpolated as needed for analysis times that do not correspond exactly to times on the mesh file. The TIME command line can optionally be used to specify that the boundary condition be constant over time, based on the value of the variable read from the file at the specified time. If the specified time on the TIME command line does not correspond exactly to a time on the mesh file, the data on the mesh file will be interpolated as needed.

6.3.3.5 Additional Commands

These command lines in the PRESCRIBED VELOCITY command block provide additional options for the boundary condition:

```
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
INACTIVE PERIODS = <string list>period_names
```

The SCALE FACTOR command line is used to apply an additional scaling factor, which is constant in both time and space, to all vector magnitude values of the field defined by the specification commands or the user subroutine. For example, if the magnitude of the velocity in a time history function is given as 1.5 from time 1.0 to time 2.0 and the scale factor is 0.5, then the magnitude of the velocity from time 1.0 to 2.0 is 0.75. The default value for the scale factor is 1.0.

The ACTIVE PERIODS and INACTIVE PERIODS command lines determine when the boundary condition is active. See Section 2.5 for more information about these command lines.

6.3.4 Prescribed Acceleration

```
BEGIN PRESCRIBED ACCELERATION
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # specification commands
  DIRECTION = <string>defined_direction |
    COMPONENT = <string>X|Y|Z
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # external database commands
  READ VARIABLE = <string>var_name
  COPY VARIABLE = <string>var_name [FROM MODEL <string>model_name]
  TIME = <real>time
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [PRESCRIBED ACCELERATION]
```

The `PRESCRIBED ACCELERATION` command block prescribes an acceleration field for a given set of nodes. The acceleration field associates a vector giving the magnitude and direction of the acceleration with each node in the node set. The acceleration field may vary over time and space. If the acceleration field has only a time-varying component, the specification commands in the above command block can be used to specify the acceleration field. If the acceleration field has both time-varying and spatially varying components, a user subroutine is used to specify the acceleration field. The acceleration field can also be read from an external mesh database. In a given boundary condition command block, commands from only one of the command groups

(specification commands, user subroutine commands, or external database commands) may be used.

For rigid bodies, any kinematic boundary condition is applied directly to the rigid body reference node. The kinematics for the mesh nodes attached to the rigid body are applied via the rigid body constraint conditions. Since rigid bodies are defined using element blocks, only the `BLOCK` command may be used to specify prescribed acceleration conditions on rigid bodies.

The `PRESCRIBED ACCELERATION` command block contains four groups of commands—node set, function, user subroutine, and external database. Each of these command groups is basically independent of the others. In addition to the command lines in the four command groups, there are three additional command lines: `SCALE FACTOR`, `ACTIVE PERIODS`, and `INACTIVE PERIODS`. The `SCALE FACTOR` command line can be used in conjunction with either the specification commands or the user subroutine commands. The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines are used to activate or deactivate this kinematic boundary condition for certain time periods. Following are descriptions of the different command groups.

6.3.4.1 Node Set Commands

The `node set commands` portion of the `PRESCRIBED ACCELERATION` command block defines a set of nodes associated with the prescribed acceleration field and can include some combination of the following command lines:

```
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes used by the boundary condition. There must be at least one `NODE SET`, `SURFACE`, `BLOCK`, or `INCLUDE ALL BLOCKS` command line in the command block.

6.3.4.2 Specification Commands

If the specification commands are used, the acceleration vector at any given time is the same for all nodes in the node set associated with the particular `PRESCRIBED ACCELERATION` command block. The direction of the acceleration vector is constant for all time; the magnitude of the acceleration vector may vary with time, however.

Following are the command lines used to specify the prescribed acceleration with a direction and a function:

```
DIRECTION = <string>defined_direction |
  COMPONENT = <string>X|Y|Z
FUNCTION = <string>function_name
```

The acceleration can be specified either along an arbitrary user-defined direction or along a component direction (X, Y, or Z), but not both. The acceleration is prescribed only in the specified direction. A prescribed acceleration boundary condition does not influence the motion in directions orthogonal to the prescribed direction.

- The `DIRECTION` command line is used to prescribe acceleration in an arbitrary user-defined direction. The name in the string `defined_direction` is a reference to a direction, which is defined using the `DEFINE DIRECTION` command block within the SIERRA scope.

- The `COMPONENT` command line is used to specify that the prescribed acceleration vector lies along one of the component directions. The `COMPONENT` command line is a shortcut to an internally defined direction vector; for example, component `x` corresponds to using direction vector (1, 0, 0).

The magnitude of the acceleration is specified by the `FUNCTION` command line. This references a `function_name` (defined in the SIERRA scope using a `DEFINITION FOR FUNCTION` command block) that specifies the magnitude of the acceleration vector as a function of time. The magnitude can be scaled by use of the `SCALE FACTOR` command line described in Section 6.3.4.5.

6.3.4.3 User Subroutine Commands

If the user subroutine option is used, the acceleration vector may vary spatially at any given time for each of the nodes in the node set associated with the particular `PRESCRIBED ACCELERATION` command block. The user subroutine option allows for a more complex description of the acceleration field than do the specification commands, but the user subroutine option also requires that you write a user subroutine to implement this capability. The user subroutine will be used to define an acceleration direction and a magnitude for every node to which the boundary condition will be applied. The subroutine will be called by Presto at the appropriate time to generate the acceleration field.

Following are the command lines related to the user subroutine option:

```
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value
```

The user subroutine option is invoked by using the NODE SET SUBROUTINE command line. The string subroutine_name is the name of a FORTRAN subroutine that is written by the user.

Following the NODE SET SUBROUTINE command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 10.2.2 and consist of SUBROUTINE DEBUGGING OFF, SUBROUTINE DEBUGGING ON, SUBROUTINE REAL PARAMETER, SUBROUTINE INTEGER PARAMETER, and SUBROUTINE STRING PARAMETER. Examples of using these command lines are provided throughout Chapter 10.

The magnitude set in the user subroutine can be scaled by use of the SCALE FACTOR command line, as described in Section 6.3.4.5.

See Section 6.3.8 and Chapter 10 for more details on implementing the user subroutine option.

6.3.4.4 External Mesh Database Commands

If the external database option is used, the acceleration vector (or specified components of the vector) is read from an external mesh database. The accelerations are read from a finite element model defined via the FINITE ELEMENT MODEL command block described in Section 5.1. The finite element model can either be the model used by the region for its mesh definition as specified with the USE FINITE ELEMENT MODEL command (see Section 2.3), or it can be a different (but compatible) model. The following command lines control the use of an external mesh database to prescribe the acceleration:

```
READ VARIABLE = <string>var_name
COPY VARIABLE = <string>var_name [FROM MODEL <string>model_name]
TIME = <real>time
```

The READ VARIABLE = <string>var_name command is used to read the acceleration vector from the region's finite element mesh database. The var_name string specifies the name of the variable as it appears on the mesh database.

If the analysis will cause topology modifications due to the use of load balancing, remeshing, or other techniques that can result in nodes and/or elements being moved among processors, then the COPY VARIABLE command should be used. This command specifies that the variable named var_name will be used to specify the acceleration. The FROM MODEL <string>model_name portion of the command is optional. If it is specified, the results are read from the mesh database named model_name. Otherwise, the region's finite element mesh database will be used as the model.

The primary difference between the behavior of the COPY VARIABLE command and the READ VARIABLE command is that the copy command handles topology modifications caused by load balancing and remeshing, which can move nodes and elements to different processors. The COPY VARIABLE command will correctly match the nodes from the external database to the corresponding nodes in the analysis and communicate the data between processors if needed. Note that the nodes in the two finite element models must match spatially, but they can be distributed on different processors.

The field to be read may be specified at an arbitrary number of different times on the mesh file. The default behavior is for the time history of the variable read from the file to be used to prescribe the boundary condition. The time history is interpolated as needed for analysis times that do not correspond exactly to times on the mesh file. The `TIME` command line can optionally be used to specify that the boundary condition be constant over time, based on the value of the variable read from the file at the specified time. If the specified time on the `TIME` command line does not correspond exactly to a time on the mesh file, the data on the mesh file will be interpolated as needed.

6.3.4.5 Additional Commands

These command lines in the `PRESCRIBED ACCELERATION` command block provide additional options for the boundary condition:

```
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
INACTIVE PERIODS = <string list>period_names
```

The `SCALE FACTOR` command line is used to apply an additional scaling factor, which is constant in both time and space, to all vector magnitude values of the field defined by the specification commands or the user subroutine. For example, if the magnitude of the acceleration in a time history function is given as 1.5 from time 1.0 to time 2.0 and the scale factor is 0.5, then the magnitude of the acceleration from time 1.0 to 2.0 is 0.75. The default value for the scale factor is 1.0.

The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines determine when the boundary condition is active. See Section 2.5 for more information about these command lines.

6.3.5 Fixed Rotation

```
BEGIN FIXED ROTATION
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # specification commands
  COMPONENT = <string>X/Y/Z | COMPONENTS = <string>X/Y/Z
  #
  # additional commands
  ACTIVE PERIODS = <string list>periods_names
  INACTIVE PERIODS = <string list>periods_names
END [FIXED ROTATION]
```

The `FIXED ROTATION` command is only applied to nodes that have rotational degrees of freedom such as shell element nodes and rigid body reference nodes. In the case of rigid bodies, the boundary condition must be specified on the block that defines the rigid body using the `BLOCK` line command.

The `FIXED ROTATION` command block fixes rotation about direction components (X, Y, Z, or some combination thereof) for a set of nodes. This command block contains two groups of commands—node set and component. Each of these command groups is basically independent of the other. In addition to the command lines in the two command groups, there are additional command lines: `ACTIVE PERIODS` and `INACTIVE PERIODS`. These command lines are used to activate or deactivate this kinematic boundary condition for certain time periods. Following are descriptions of the different command groups.

6.3.5.1 Node Set Commands

The `node set commands` portion of the command block specifies the nodes associated with the boundary condition. This portion of the command block can include some combination of the following command lines:

```
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes used by the boundary condition. There must be at least one `NODE SET`, `SURFACE`, `BLOCK`, or `INCLUDE ALL BLOCKS` command line in the command block.

6.3.5.2 Specification Commands

There are two component specification commands available in the `FIXED ROTATION` command block:

```
COMPONENT = X/Y/Z | COMPONENTS = X/Y/Z
```

The rotation components that are to be fixed can be specified with either the `COMPONENT` command line or the `COMPONENTS` command line. There can be only one `COMPONENT` command line or one `COMPONENTS` command line in the command block. The user can specify any combination of the components to be fixed, as in `X`, `Z`, `X Z`, `Y X`, etc.

6.3.5.3 Additional Commands

The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines can optionally appear in the `FIXED ROTATION` command block:

```
ACTIVE PERIODS = <string list>period_names
INACTIVE PERIODS = <string list>period_names
```

This command line determines when the boundary condition is active. See Section 2.5 for more information about this optional command line.

6.3.6 Prescribed Rotation

```
BEGIN PRESCRIBED ROTATION
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # specification commands
  DIRECTION = <string>defined_direction
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # external database commands
  READ VARIABLE = <string>var_name
  COPY VARIABLE = <string>var_name [FROM MODEL
    <string>model_name]
  TIME = <real>time
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [PRESCRIBED ROTATION]
```

Warning: The `BEGIN PRESCRIBED ROTATION` command is only applied to nodes that have rotational degrees of freedom such as shell element nodes and rigid body reference nodes. Displacements consistent with rotation about a fixed axis for nodes that do not have rotational degrees of freedom, are imposed using the `CYLINDRICAL AXIS` command line in the `PRESCRIBED DISPLACEMENT` command block described in Section 6.3.2.

For nodal rotational degrees of freedom, the rotations applied using the BEGIN PRESCRIBED ROTATION command are the three components of the rotational degree of freedom itself. In the case of rigid bodies, the rotations must be the nonlinear components that result in the desired quaternion on the rigid body reference node. For rigid bodies, the boundary condition is applied to the reference node and therefore must be specified on the block that defines the rigid body using the BLOCK line command.

The PRESCRIBED ROTATION command block prescribes the rotation about an axis for a given set of nodes. The rotation field associates a vector giving the magnitude and direction of the rotation with each node in the node set. The rotation field may vary over time and space. If the rotation field has only a time-varying component, the specification commands in the above command block can be used to specify the rotation field. If the rotation field has both time-varying and spatially varying components, a user subroutine is used to specify the rotation field. The rotation field can also be read from an external mesh database. In a given boundary condition command block, commands from only one of the command groups (specification commands, user subroutine commands, or external database commands) may be used.

The PRESCRIBED ROTATION command block contains four groups of commands—node set, function, user subroutine, and external database. Each of these command groups is basically independent of the others. In addition to the command lines in the four command groups, there are three additional command lines: SCALE FACTOR, ACTIVE PERIODS, and INACTIVE PERIODS. The SCALE FACTOR command line can be used in conjunction with either the specification commands or the user subroutine commands. The ACTIVE PERIODS and INACTIVE PERIODS command lines are used to activate or deactivate this kinematic boundary condition for certain time periods. Following are descriptions of the different command groups.

6.3.6.1 Node Set Commands

The node set commands portion of the PRESCRIBED ROTATION command block defines a set of nodes associated with the prescribed rotation field and can include some combination of the following command lines:

```
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes used by the boundary condition. There must be at least one NODE SET, SURFACE, BLOCK, or INCLUDE ALL BLOCKS command line in the command block.

6.3.6.2 Specification Commands

If the specification commands are used, the rotation vector at any given time is the same for all nodes in the node set associated with the particular `PRESCRIBED ROTATION` command block. The direction of the rotation vector is constant for all time; the magnitude of the rotation vector may vary with time, however.

Following are the command lines used to specify the prescribed rotation with a direction and a function:

```
DIRECTION = <string>defined_direction
FUNCTION = <string>function_name
```

The `DIRECTION` command line is used to prescribe rotation in an arbitrary user-defined direction. The name in the string `defined_direction` is a reference to a direction, which is defined using the `DEFINE DIRECTION` command block within the SIERRA scope. The rotation is prescribed only in the specified direction. A prescribed rotation boundary condition does not influence the rotation in directions orthogonal to the prescribed direction.

The magnitude of the rotation is specified by the `FUNCTION` command line. This references a `function_name` (defined in the SIERRA scope in a `DEFINITION FOR FUNCTION` command block) that specifies the magnitude of the rotation vector as a function of time. The magnitude can be scaled by use of the `SCALE FACTOR` command line described in Section 6.3.6.5.

The magnitude of the rotation, as specified by the product of the function and the scale factor, has units of radians per second.

6.3.6.3 User Subroutine Commands

If the user subroutine option is used, the rotation vector may vary spatially at any given time for each of the nodes in the node set associated with the particular `PRESCRIBED ROTATION` command block. The user subroutine option allows for a more complex description of the rotation field than do the specification commands, but the user subroutine option also requires that you write a user subroutine to implement this capability. The user subroutine will be used to define a rotation direction and a magnitude for every node to which the boundary condition will be applied. The subroutine will be called by Presto at the appropriate time to generate the rotation field.

Following are the command lines related to the user subroutine option:

```
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value
```

The user subroutine option is invoked by using the NODE SET SUBROUTINE command line. The string subroutine_name is the name of a FORTRAN subroutine that is written by the user.

Following the NODE SET SUBROUTINE command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 10.2.2 and consist of SUBROUTINE DEBUGGING OFF, SUBROUTINE DEBUGGING ON, SUBROUTINE REAL PARAMETER, SUBROUTINE INTEGER PARAMETER, and SUBROUTINE STRING PARAMETER. Examples of using these command lines are provided throughout Chapter 10.

The magnitude set in the user subroutine can be scaled by use of the SCALE FACTOR command line, as described in Section 6.3.6.5.

See Section 6.3.8 and Chapter 10 for more details on implementing the user subroutine option.

6.3.6.4 External Mesh Database Commands

If the external database option is used, the rotation vector (or specified components of the vector) is read from an external mesh database. The rotations are read from a finite element model defined via the FINITE ELEMENT MODEL command block described in Section 5.1. The finite element model can either be the model used by the region for its mesh definition as specified with the USE FINITE ELEMENT MODEL command (see Section 2.3), or it can be a different (but compatible) model. The following command lines control the use of an external mesh database to prescribe the rotation:

```
READ VARIABLE = <string>mesh_var_name
COPY VARIABLE = <string>var_name [FROM MODEL <string>model_name]
TIME = <real>time
```

The READ VARIABLE = <string>var_name command is used to read the rotation vector from the region's finite element mesh database. The var_name string specifies the name of the variable as it appears on the mesh database.

If the analysis will cause topology modifications due to the use of load balancing, remeshing, or other techniques that can result in nodes and/or elements being moved among processors, then the COPY VARIABLE command should be used. This command specifies that the variable named var_name will be used to specify the rotation. The FROM MODEL <string>model_name portion of the command is optional. If it is specified, the results are read from the mesh database named model_name. Otherwise, the region's finite element mesh database will be used as the model.

The primary difference between the behavior of the COPY VARIABLE command and the READ VARIABLE command is that the copy command handles topology modifications caused by load balancing and remeshing, which can move nodes and elements to different processors. The COPY VARIABLE command will correctly match the nodes from the external database to the corresponding nodes in the analysis and communicate the data between processors if needed. Note that the nodes in the two finite element models must match spatially, but they can be distributed on different processors.

The field to be read may be specified at an arbitrary number of different times on the mesh file. The default behavior is for the time history of the variable read from the file to be used to prescribe the boundary condition. The time history is interpolated as needed for analysis times that do not correspond exactly to times on the mesh file. The `TIME` command line can optionally be used to specify that the boundary condition be constant over time, based on the value of the variable read from the file at the specified time. If the specified time on the `TIME` command line does not correspond exactly to a time on the mesh file, the data on the mesh file will be interpolated as needed.

6.3.6.5 Additional Commands

These command lines in the `PRESCRIBED ROTATION` command block provide additional options for the boundary condition:

```
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
INACTIVE PERIODS = <string list>period_names
```

The `SCALE FACTOR` command line is used to apply an additional scaling factor, which is constant in both time and space, to all vector magnitude values of the field defined by the specification commands or the user subroutine. For example, if the magnitude of the rotation in a time history function is given as 1.5 from time 1.0 to time 2.0 and the scale factor is 0.5, then the magnitude of the rotation from time 1.0 to 2.0 is 0.75. The default value for the scale factor is 1.0.

The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines determine when the boundary condition is active. See Section 2.5 for more information about these command lines.

6.3.7 Prescribed Rotational Velocity

```
BEGIN PRESCRIBED ROTATIONAL VELOCITY
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # specification commands
  DIRECTION = <string>defined_direction |
   COMPONENT = <string>X|Y|Z
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # external database commands
  READ VARIABLE = <string>variable_name
  COPY VARIABLE = <string>variable_name [FROM MODEL
    <string>model_name]
  TIME = <real>time
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [PRESCRIBED ROTATIONAL VELOCITY]
```

Warning: The `PRESCRIBED ROTATIONAL VELOCITY` command is only applied to nodes that have rotational degrees of freedom such as shell element nodes and rigid body reference nodes. Velocities consistent with rotation about a fixed axis for nodes that do not have rotational degrees of freedom, are imposed with the `CYLINDRICAL AXIS` command line in the `PRESCRIBED VELOCITY` command block described in Section 6.3.3.

For nodal rotational degrees of freedom, the rotations applied using the BEGIN PRESCRIBED ROTATIONAL VELOCITY command are the components of the rotational degree of freedom itself. For rigid bodies, the boundary condition is applied to the reference node and therefore must be specified on the block that defines the rigid body using the BLOCK line command.

The PRESCRIBED ROTATIONAL VELOCITY command block prescribes the rotational velocity about an axis for a given set of nodes. The rotational velocity field associates a vector giving the magnitude and direction of the rotational velocity with each node in the node set. The rotational velocity field may vary over time and space. If the rotational velocity field has only a time-varying component, the specification commands in the above command block can be used to specify the rotational velocity field. If the rotational velocity field has both time-varying and spatially varying components, a user subroutine is used to specify the rotational velocity field. The rotational velocity field can also be read from an external mesh database. In a given boundary condition command block, commands from only one of the command groups (specification commands, user subroutine commands, or external database commands) may be used.

The PRESCRIBED ROTATIONAL VELOCITY command block contains four groups of commands—node set, function, user subroutine, and external database. Each of these command groups is basically independent of the others. In addition to the command lines in the four command groups, there are three additional command lines: SCALE FACTOR, ACTIVE PERIODS, and INACTIVE PERIODS. The SCALE FACTOR command line can be used in conjunction with either the specification commands or the user subroutine commands. The ACTIVE PERIODS and INACTIVE PERIODS command lines are used to activate or deactivate this kinematic boundary condition for certain time periods. Following are descriptions of the different command groups.

6.3.7.1 Node Set Commands

The node set commands portion of the PRESCRIBED ROTATIONAL VELOCITY command block defines a set of nodes associated with the prescribed rotational velocity field and can include some combination of the following command lines:

```
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes used by the boundary condition. There must be at least one NODE SET, SURFACE, BLOCK, or INCLUDE ALL BLOCKS command line in the command block.

6.3.7.2 Specification Commands

If the specification commands are used, the rotational velocity vector at any given time is the same for all nodes in the node set associated with the particular `PRESCRIBED ROTATIONAL VELOCITY` command block. The direction of the rotational velocity vector is constant for all time; the magnitude of the rotational velocity vector may vary with time, however.

Following are the command lines used to specify the prescribed rotational velocity with a direction and a function:

```
DIRECTION = <string>defined_direction |
  COMPONENT = <string>X|Y|Z
FUNCTION = <string>function_name
```

The rotational velocity can be specified either along an arbitrary user-defined direction or along a component direction (X, Y, or Z), but not both. The rotational velocity is prescribed only in the specified direction. A prescribed rotational velocity boundary condition does not influence the rotational velocity in directions orthogonal to the prescribed direction.

- The `DIRECTION` command line is used to prescribe rotational velocity in an arbitrary user-defined direction. The name in the string `defined_direction` is a reference to a direction, which is defined using the `DEFINE DIRECTION` command block within the SIERRA scope.
- The `COMPONENT` command line is used to specify that the prescribed rotational velocity vector lies along one of the component directions. The `COMPONENT` command line is a shortcut to an internally defined direction vector; for example, component `x` corresponds to using direction vector (1, 0, 0).

The magnitude of the rotational velocity is specified by the `FUNCTION` command line. This references a `function_name` (defined in the SIERRA scope in a `DEFINITION FOR FUNCTION` command block) that specifies the magnitude of the rotational velocity vector as a function of time. The magnitude can be scaled by use of the `SCALE FACTOR` command line described in Section 6.3.7.5.

The magnitude of the rotational velocity, as specified by the product of the function and the scale factor, has units of radians per second.

6.3.7.3 User Subroutine Commands

If the user subroutine option is used, the rotational velocity vector may vary spatially at any given time for each of the nodes in the node set associated with the particular `PRESCRIBED ROTATIONAL VELOCITY` command block. The user subroutine option allows for a more complex description of the rotational velocity field than do the specification commands, but the user subroutine option also requires that you write a user subroutine to implement this capability. The user subroutine will be used to define a rotational velocity direction and a magnitude for every

node to which the boundary condition will be applied. The subroutine will be called by Presto at the appropriate time to generate the rotational velocity field.

Following are the command lines related to the user subroutine option:

```
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value
```

The user subroutine option is invoked by using the `NODE SET SUBROUTINE` command line. The string `subroutine_name` is the name of a FORTRAN subroutine that is written by the user.

Following the `NODE SET SUBROUTINE` command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 10.2.2 and consist of `SUBROUTINE DEBUGGING OFF`, `SUBROUTINE DEBUGGING ON`, `SUBROUTINE REAL PARAMETER`, `SUBROUTINE INTEGER PARAMETER`, and `SUBROUTINE STRING PARAMETER`. Examples of using these command lines are provided throughout Chapter 10.

The magnitude set in the user subroutine can be scaled by use of the `SCALE FACTOR` command line, as described in Section 6.3.7.5.

See Section 6.3.8 and Chapter 10 for more details on implementing the user subroutine option.

6.3.7.4 External Mesh Database Commands

If the external database option is used, the rotational velocity vector (or specified components of the vector) is read from an external mesh database. The rotational velocities are read from a finite element model defined via the `FINITE ELEMENT MODEL` command block described in Section 5.1. The finite element model can either be the model used by the region for its mesh definition as specified with the `USE FINITE ELEMENT MODEL` command (see Section 2.3), or it can be a different (but compatible) model. The following command lines control the use of an external mesh database to prescribe the rotational velocity:

```
READ VARIABLE = <string>mesh_var_name
COPY VARIABLE = <string>var_name [FROM MODEL <string>model_name]
TIME = <real>time
```

The `READ VARIABLE = <string>var_name` command is used to read the rotational velocity vector from the region's finite element mesh database. The `var_name` string specifies the name of the variable as it appears on the mesh database.

If the analysis will cause topology modifications due to the use of load balancing, remeshing, or other techniques that can result in nodes and/or elements being moved among processors, then

the COPY VARIABLE command should be used. This command specifies that the variable named var_name will be used to specify the rotational velocity. The FROM MODEL <string>model_name portion of the command is optional. If it is specified, the results are read from the mesh database named model_name. Otherwise, the region's finite element mesh database will be used as the model.

The primary difference between the behavior of the COPY VARIABLE command and the READ VARIABLE command is that the copy command handles topology modifications caused by load balancing and remeshing, which can move nodes and elements to different processors. The COPY VARIABLE command will correctly match the nodes from the external database to the corresponding nodes in the analysis and communicate the data between processors if needed. Note that the nodes in the two finite element models must match spatially, but they can be distributed on different processors.

The field to be read may be specified at an arbitrary number of different times on the mesh file. The default behavior is for the time history of the variable read from the file to be used to prescribe the boundary condition. The time history is interpolated as needed for analysis times that do not correspond exactly to times on the mesh file. The TIME command line can optionally be used to specify that the boundary condition be constant over time, based on the value of the variable read from the file at the specified time. If the specified time on the TIME command line does not correspond exactly to a time on the mesh file, the data on the mesh file will be interpolated as needed.

6.3.7.5 Additional Commands

These command lines in the PRESCRIBED ROTATIONAL VELOCITY command block provide additional options for the boundary condition:

```
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
INACTIVE PERIODS = <string list>period_names
```

The SCALE FACTOR command line is used to apply an additional scaling factor, which is constant in both time and space, to all vector magnitude values of the field defined by the specification commands or the user subroutine. For example, if the magnitude of the rotational velocity in a time history function is given as 1.5 from time 1.0 to time 2.0 and the scale factor is 0.5, then the magnitude of the rotational velocity from time 1.0 to 2.0 is 0.75. The default value for the scale factor is 1.0.

The ACTIVE PERIODS and INACTIVE PERIODS command lines determine when the boundary condition is active. See Section 2.5 for more information about these command lines.

6.3.8 Subroutine Usage for Kinematic Boundary Conditions

The prescribed kinematic boundary conditions may be defined by a user subroutine. All these conditions use a node set subroutine. See Chapter 10 for an in-depth discussion of user subroutines. The kinematic boundary conditions will be applied to nodes. The subroutine that you write will have to return six output values per node and one output flag per node. The usage of the output values depends on the returned flag value for a node, as follows:

- If the flag value is negative, no constraint will be applied to the node.
- If the flag value is equal to zero, the constraint will be absolute. All components of the boundary condition will be specified. For example, suppose you have written a user subroutine to be called from a prescribed displacement subroutine. The prescribed displacements are to be passed through an array `output_values`. For a given node `inode`, the `output_values` array would have the following values:

```
output_values(1,inode) = displacement in x at inode
output_values(2,inode) = displacement in y at inode
output_values(3,inode) = displacement in z at inode
output_values(4,inode) = not used
output_values(5,inode) = not used
output_values(6,inode) = not used
```

- If the flag value is equal to one, the constraint will be a specified amount in a given direction. For example, suppose you have written a user subroutine to be called from a prescribed displacement subroutine. The prescribed displacements are to be passed through an array `output_values`. For a given node `inode`, the `output_values` array would have the following values:

```
output_values(1,inode) = magnitude of displacement
output(values(2,inode) = not used
output_values(3,inode) = not used
output_values(4,inode) = x component of direction vector
output_values(5,inode) = y component of direction vector
output_values(6,inode) = z component of direction vector
```

The direction in which the constraint will act is given by `output_values` 4 through 6 for `inode`. The magnitude of the displacement in the specified direction is given by `output_values` 1 at `inode`. To compute the constraint, Presto first normalizes the direction vector. Next, Presto multiplies the normalized direction vector by the magnitude of the displacement and applies the resultant constraint vector.

Displacements or velocities orthogonal to the prescribed direction will not be constrained. (This is true regardless of whether or not one uses a user subroutine for the prescribed kinematic boundary conditions.) Take the case of a prescribed displacement condition. The displacement orthogonal to a prescribed direction of motion depends on the internal and external forces orthogonal to the prescribed direction. Displacement orthogonal to the prescribed direction may or may not be zero.

6.4 Initial Velocity Conditions

```
BEGIN INITIAL VELOCITY
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # direction specification commands
  COMPONENT = <string>X|Y|Z |
    DIRECTION = <string>defined_direction
  MAGNITUDE = <real>magnitude_of_velocity
  #
  # angular velocity specification commands
  CYLINDRICAL AXIS = <string>defined_axis
  ANGULAR VELOCITY = <real>angular_velocity
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
END [INITIAL VELOCITY]
```

The `INITIAL VELOCITY` command block specifies an initial velocity field for a set of nodes. There are two simple options for specifying the initial velocity field: by direction and by angular velocity. The user subroutine option available is also available to specify an initial velocity. You may use only one of the available options—direction specification, angular velocity specification, or user subroutine.

The `INITIAL VELOCITY` command block contains four groups of commands—node set, direction specification, angular velocity specification, and user subroutine. Command lines associated with the node set commands must appear. As mentioned, command lines associated with one of the options must also appear. Following are descriptions of the different command groups.

6.4.1 Node Set Commands

The `node set commands` portion of the `INITIAL VELOCITY` command block defines a set of nodes associated with the initial velocity field and can include some combination of the following command lines:

```
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes used by the boundary condition. There must be at least one `NODE SET`, `SURFACE`, `BLOCK`, or `INCLUDE ALL BLOCKS` command line in the command block.

6.4.2 Direction Specification Commands

If the direction specification commands are used, the initial velocity is applied along a defined direction with a specific magnitude. Following are the command lines for the direction option:

```
COMPONENT = <string>X|Y|Z |
  DIRECTION = <string>defined_direction
MAGNITUDE = <real>magnitude_of_velocity
```

The initial velocity can be specified either along an arbitrary user-defined direction or along a component direction (X, Y, or Z), but not both. The velocity is prescribed only in the specified direction. A prescribed velocity boundary condition does not influence the movement in directions orthogonal to the prescribed direction.

- The `DIRECTION` command line is used to prescribe initial velocity in an arbitrary user-defined direction. The name in the string `defined_direction` is a reference to a direction, which is defined using the `DEFINE DIRECTION` command block within the SIERRA scope.
- The `COMPONENT` command line is used to specify that the initial velocity vector lies along one of the component directions. The `COMPONENT` command line is a shortcut to an internally defined direction vector; for example, component `x` corresponds to using direction vector (1, 0, 0).

The magnitude of the initial velocity is given by the `MAGNITUDE` command line with the real value `magnitude_of_velocity`.

Either the `COMPONENT` command line or the `DIRECTION` command line must be specified with the `MAGNITUDE` command line if you use the direction specification commands.

6.4.3 Angular Velocity Specification Commands

If the angular velocity specification commands are used, the initial velocity is applied as an initial angular velocity about some axis. Following are the command lines for angular velocity specification:

```
CYLINDRICAL AXIS = <string>defined_axis
ANGULAR VELOCITY = <real>angular_velocity
```

The axis about which the body is initially rotating is given by the `CYLINDRICAL AXIS` command line. The string `defined_axis` uses an `axis_name` that is defined in the SIERRA scope (via a `DEFINE AXIS` command line).

The magnitude of the angular velocity about this axis is specified by the `ANGULAR VELOCITY` command line with the real value `angular_velocity`. This value is specified in units of radians per unit of time. Typically, the value for the angular velocity will be radians per second.

Both the `CYLINDRICAL AXIS` command line and the `ANGULAR VELOCITY` command line are required if you use the angular velocity specification commands.

6.4.4 User Subroutine Commands

If the user subroutine option is used, the initial velocity vector may vary spatially at any given time for each of the nodes in the node set associated with the particular `INITIAL CONDITION` command block. The user subroutine option allows for a more complex description of the initial velocity field than do the direction and angular-velocity options, but the user subroutine option also requires that you write a user subroutine to implement this capability. The user subroutine will be used to define a velocity direction and a magnitude for every node to which the initial velocity field will be applied. The subroutine will be called by Presto at the appropriate time to generate the initial velocity field.

Following are the command lines related to the user subroutine option:

```
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value
```

The user subroutine option is invoked by using the `NODE SET SUBROUTINE` command line. The string `subroutine_name` is the name of a FORTRAN subroutine that is written by the user.

Following the `NODE SET SUBROUTINE` command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 10.2.2 and

consist of `SUBROUTINE DEBUGGING OFF`, `SUBROUTINE DEBUGGING ON`, `SUBROUTINE REAL PARAMETER`, `SUBROUTINE INTEGER PARAMETER`, and `SUBROUTINE STRING PARAMETER`. Examples of using these command lines are provided throughout Chapter 10.

See Section 6.3.8 and Chapter 10 for more details on implementing the user subroutine option.

6.5 Force Boundary Conditions

A variety of force boundary conditions are available in Presto. This section describes these boundary conditions.

6.5.1 Pressure

```
BEGIN PRESSURE
  #
  # surface set commands
  SURFACE = <string list>surface_names
  REMOVE SURFACE = <string list>surface_names
  #
  # specification command
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  SURFACE SUBROUTINE = <string>subroutine_name |
    NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # external pressure sources
  READ VARIABLE = <string>variable_name
  OBJECT TYPE = <string>NODE|FACE(NODE)
  TIME = <real>time
  FIELD VARIABLE = <string>field_variable
  #
  # output external forces from pressure
  EXTERNAL FORCE CONTRIBUTION OUTPUT NAME =
    <string>variable_name
  #
  # additional commands
  USE DEATH = <string>death_name
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [PRESSURE]
```

The `PRESSURE` command block applies a pressure to each face in the associated surfaces. The pressure field can either be constant over the faces and vary in time, or it can be determined by

a user subroutine. If the pressure field is constant over the faces and has only a time-varying component, the function command in the above command block can be used to specify the pressure field. If the pressure field has both time-varying and spatially varying components, user subroutine commands are used to specify the pressure field. The pressure field may also be obtained from a mesh file or from another SIERRA code through a transfer operator. You can use only one of these four options—function, user subroutine, mesh file, transfer from another code—to specify the pressure field.

Currently, the `PRESSURE` command block can be used for surfaces that have faces derived from solid elements (eight-node hexahedra, four-node tetrahedra, eight-node tetrahedra, etc.), membranes, and shells.

A pressure boundary condition generates nodal forces that are summed into the external force vector that is used to calculate the motion of a body. The external force vector contains the contribution from all forces acting on the body. There is an option in the `PRESSURE` command block to save information about the contribution to the external force vector due only to pressure loads. This option does not change the magnitude or time history of the pressure load (regardless of how they are defined), but merely stores information in a user-accessible variable.

The `PRESSURE` command block contains five groups of commands—surface set, function, user subroutine, external pressure, and output external forces. Each of these command groups is basically independent of the others. In addition to the command lines in the five command groups, there are three additional command lines: `USE DEATH`, `SCALE FACTOR` and `ACTIVE PERIODS`. The `USE DEATH` command line links the pressure boundary condition to an element death definition so that the underlying surface geometry is updated as elements are killed. The `SCALE FACTOR` command line can be used in conjunction with either the function command or the user subroutine commands. The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines are used to activate or deactivate this force boundary condition for certain time periods. Following are descriptions of the different command groups.

6.5.1.1 Surface Set Commands

The `surface set commands` portion of the `PRESSURE` command block defines a set of surfaces associated with the pressure field and can include some combination of the following command lines:

```
SURFACE = <string list>surface_names
REMOVE SURFACE = <string list>surface_names
```

In the `SURFACE` command line, you can list a series of surfaces through the string list `surface_names`. There must be at least one `SURFACE` command line in the command block. The `REMOVE SURFACE` command line allows you to delete surfaces from the set specified in the `SURFACE` command line(s) through the string list `surface_names`. See Section 6.1.1 for more information about the use of these command lines for creating a set of surfaces used by the boundary condition.

6.5.1.2 Specification Commands

If the function command is used, the pressure vector at any given time is the same for all surfaces associated with the particular PRESSURE command block. The direction of the pressure vector is constant for all time; the magnitude of the pressure vector may vary with time, however.

Following is the command line used to specify the pressure with a function:

```
FUNCTION = <string>function_name
```

The pressure is applied in the opposite direction to the outward normals of the faces that define the surfaces. The magnitude of the pressure is specified by the FUNCTION command line. This references a function_name (defined in the SIERRA scope in a DEFINITION FOR FUNCTION command block) that specifies the magnitude of the pressure vector as a function of time. The magnitude can be scaled by use of the SCALE FACTOR command line described in Section 6.5.1.6.

6.5.1.3 User Subroutine Commands

If the user subroutine option is used, the pressure may vary spatially at any given time for each of the surfaces associated with the particular PRESSURE command block. The user subroutine option allows for a more complex description of the pressure field than does the function command, but the user subroutine option also requires that you write a user subroutine to implement this capability. The user subroutine will be used to define a pressure for every face to which the boundary condition will be applied. The subroutine will be called by Presto at the appropriate time to generate the pressure field.

Following are the command lines related to the user subroutine option:

```
SURFACE SUBROUTINE = <string>subroutine_name |
  NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value
```

The user subroutine option is invoked by using the SURFACE SUBROUTINE command line or the NODE SET subroutine command line. The string subroutine_name in both command lines is the name of a FORTRAN subroutine that is written by the user. The particular command line selected depends on the mesh-entity type for which the pressure field is being calculated. Associating pressure values with faces would require the use of a SURFACE SUBROUTINE command line. Associating pressure values with nodes would require the use of a NODE SET SUBROUTINE command line.

Following the selected subroutine command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 10.2.2 and consist of `SUBROUTINE DEBUGGING OFF`, `SUBROUTINE DEBUGGING ON`, `SUBROUTINE REAL PARAMETER`, `SUBROUTINE INTEGER PARAMETER`, and `SUBROUTINE STRING PARAMETER`. Examples of using these command lines are provided throughout Chapter 10.

The magnitude set in the user subroutine can be scaled by use of the `SCALE FACTOR` command line, as described in Section 6.5.1.6.

Usage requirements. Following are the usage requirements for the two types of subroutines:

- The surface subroutine operates on a group of faces. The subroutine that you write will return one output value per face. Suppose you write a user subroutine that returns the pressure information through an array `output_value`. The value `output_value(1,iface)` corresponds to the average pressure on face `iface`. The values of the flags array are not used.
- The node set subroutine that you write will return one value per node. Suppose you write a user subroutine that returns the pressure information through an array `output_value`. The return value `output_value(1,inode)` is the pressure at the node `inode`. The total pressure on the each face is found by integrating the pressures at the nodes. The values of the flags array are not used.

See Chapter 10 for more details on implementing the user subroutine option.

6.5.1.4 External Pressure Sources

Pressure may be obtained from two different external sources. The first option for obtaining pressure from an external source uses a mesh file. The commands for obtaining pressure information from a mesh file are as follows:

```
READ VARIABLE = <string>variable_name
OBJECT TYPE = <string>NODE|FACE(NODE)
TIME = <real>time
```

The `READ VARIABLE` command line specifies the name of the variable on the mesh file, `variable_name`, that is used to prescribe the pressure field. The `OBJECT TYPE` command line specifies whether the pressure field on the mesh file is specified for nodes (the mesh object type is `NODE`) or for faces (the mesh object type is `FACE`). If the `OBJECT TYPE` command line is not present, it is assumed that the variable is for nodes. If the `TIME` command line is present, only the pressure field information at a given time, as set by the `time` parameter, is read from the mesh file. If the `TIME` command line is not present, the pressure field information for all times is read. Pressure field information will then be interpolated as necessary during an analysis.

The second option for obtaining pressure from and external sources relies on the transfer of information from another SIERRA code. The command for obtaining pressure information by transfer from another code is:

```
FIELD VARIABLE = <string>variable_name
```

Here `variable_name` is the name of the variable where pressure information is to be stored. The pressure information will be transferred into this variable from another SIERRA code via a transfer operator.

6.5.1.5 Output Command

This command line lets the user create a variable that stores information about the contribution to the external force vector at a node arising solely from a pressure:

```
EXTERNAL FORCE CONTRIBUTION OUTPUT NAME =
  <string>variable_name
```

If the above command line appears in a `PRESSURE` command block, then there will be a variable created with whatever name the user specifies for `variable_name`. The variable defines a three-dimensional vector at each node associated with this particular command block. The three-dimensional vector at each node represents the external force due solely to the pressure on the elements attached to that node. For example, if one of the nodes associated with this particular command block has four elements attached to it and each element has a pressure load, then the external force contribution at the node would be summed from the pressure load for all four elements.

Once this variable for the external force contribution from a pressure load is specified, it may be used like any other nodal variable. The user can, for example, specify the variable as a nodal variable to be output in a `RESULTS OUTPUT` command block. Or the user can reference the variable in a user subroutine.

6.5.1.6 Additional Commands

These command lines in the `PRESSURE` command block provide additional options for the boundary condition:

```
USE DEATH = <string>death_name
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
INACTIVE PERIODS = <string list>period_names
```

The `USE DEATH` command line links the pressure boundary condition to an element death definition. The string `death_name` must match a name used in an `ELEMENT DEATH` command block. When elements are killed by the named element death definition, the pressure boundary condition will be applied to the newly exposed faces.

The `SCALE FACTOR` command line is used to apply an additional scaling factor, which is constant in both time and space, to all vector magnitude values of the field defined by the function command

or the user subroutine. For example, if the magnitude of the pressure in a time history function is given as 1.5 from time 1.0 to time 2.0 and the scale factor is 0.5, then the magnitude of the pressure from time 1.0 to 2.0 is 0.75. The default value for the scale factor is 1.0.

The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines determine when the boundary condition is active. See Section 2.5 for more information about these command lines.

6.5.2 Traction

```
BEGIN TRACTION
  #
  # surface set commands
  SURFACE = <string list>surface_names
  REMOVE SURFACE = <string list>surface_names
  #
  # specification commands
  DIRECTION = <string>direction_name
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [TRACTION]
```

The `TRACTION` command block applies a traction to each face in the associated surfaces. The traction has units of force per unit area. (A traction, unlike a pressure, may not necessarily be in the direction of the normal to the face to which it is applied.) The given traction is integrated over the surface area of a face.

The traction field can be determined by a SIERRA function or a user subroutine. If the traction field is constant over the faces and has only a time-varying component, the specification commands in the above command block can be used to specify the traction field. If the traction field has both time-varying and spatially varying components, a user subroutine is used to specify the traction field.

The traction field can only be controlled by one method. Accordingly, a `TRACTION` command block can only contain one of the options: function or user subroutine.

Currently, the `TRACTION` command block can be used for surfaces that have faces derived from solid elements (eight-node hexahedra, four-node tetrahedra, eight-node tetrahedra, etc.), membranes, and shells.

The `TRACTION` command block contains three groups of commands—surface set and user subroutine. Each of these command groups is basically independent of the others. In addition to the command lines in the four command groups, there are three additional command lines:

SCALE FACTOR, ACTIVE PERIODS, and INACTIVE PERIODS. The SCALE FACTOR command line can be used in conjunction with the specification commands or the user subroutine option. The ACTIVE PERIODS and INACTIVE PERIODS command lines are used to activate or deactivate this force boundary condition for certain time periods. Following are descriptions of the different command groups.

6.5.2.1 Surface Set Commands

The surface set commands portion of the TRACTION command block defines a set of surfaces associated with the traction field and can include some combination of the following command lines:

```
SURFACE = <string list>surface_names
REMOVE SURFACE = <string list>surface_names
```

In the SURFACE command line, you can list a series of surfaces through the string list surface_names. There must be at least one SURFACE command line in the command block. The REMOVE SURFACE command line allows you to delete surfaces from the set specified in the SURFACE command line(s) through the string list surface_names. See Section 6.1.1 for more information about the use of these command lines for creating a set of surfaces used by the boundary condition.

6.5.2.2 Specification Commands

If the specification commands are used, the traction vector at any given time is the same for all surfaces associated with the particular TRACTION command block. The direction of the traction vector is constant for all time; the magnitude of the traction vector may vary with time, however.

Following are the command lines used to specify the traction with a direction and a function:

```
DIRECTION = <string>defined_direction
FUNCTION = <string>function_name
```

The traction is specified in an arbitrary user-defined direction, and is defined using the DIRECTION command line. The name in the string defined_direction is a reference to a direction, which is defined using the DEFINE DIRECTION command block within the SIERRA scope.

The magnitude of the traction is specified by the FUNCTION command line. This references a function_name (defined in the SIERRA scope in a DEFINITION FOR FUNCTION command block) that specifies the magnitude of the traction vector as a function of time. The magnitude can be scaled by use of the SCALE FACTOR command line described in Section 6.5.2.4.

6.5.2.3 User Subroutine Commands

If the user subroutine option is used, the traction vector may vary spatially at any given time for each of the surfaces associated with the particular TRACTION command block. The user subroutine option allows for a more complex description of the traction field than does the function option, but the user subroutine option also requires that you write a user subroutine to implement this capability. The user subroutine will be used to define a traction for every face to which the boundary condition will be applied. The subroutine will be called by Presto at the appropriate time to generate the traction field.

Following is the command line related to the user subroutine option:

```
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value
```

The user subroutine option is invoked by using the NODE SET subroutine command line. The string subroutine_name is the name of a FORTRAN subroutine that is written by the user. Associating traction values with nodes requires the use of a NODE SET SUBROUTINE command line.

Following the NODE SET SUBROUTINE command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 10.2.2 and consist of SUBROUTINE DEBUGGING OFF, SUBROUTINE DEBUGGING ON, SUBROUTINE REAL PARAMETER, SUBROUTINE INTEGER PARAMETER, and SUBROUTINE STRING PARAMETER. Examples of using these command lines are provided throughout Chapter 10.

The magnitude set in the user subroutine can be scaled by use of the SCALE FACTOR command line, as described in Section 6.5.2.4.

Usage requirements for the node set subroutine. The node set subroutine that you write will return six values per node. Suppose you have written a user subroutine that passes the output values through an array output_values. For a given node inode, the output_values array would have the following values:

```
output_values(1,inode) = magnitude of traction
output(values(2,inode) = not used
output_values(3,inode) = not used
output_values(4,inode) = x component of direction vector
output_values(5,inode) = y component of direction vector
output_values(6,inode) = z component of direction vector
```

The direction in which the traction will act is given by components 4 through 6 of `output_values` for `inode`. The magnitude of the traction in the specified direction is given by component 1 of `output_values` at `inode`. The total force on each node is found by integrating the local nodal tractions using the associated directions, which are normalized by Prestoover the face areas. The values of the flags array are not used.

See Chapter 10 for more details on implementing the user subroutine option.

6.5.2.4 Additional Commands

These command lines in the `TRACTION` command block provide additional options for the boundary condition:

```
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
INACTIVE PERIODS = <string list>period_names
```

The `SCALE FACTOR` command line is used to apply an additional scaling factor, which is constant in both time and space, to all vector magnitude values of the field defined by the specification commands or the user subroutine. For example, if the magnitude of the traction in a time history function is given as 1.5 from time 1.0 to time 2.0 and the scale factor is 0.5, then the magnitude of the traction from time 1.0 to 2.0 is 0.75. The default value for the scale factor is 1.0.

The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines determine when the boundary condition is active. See Section 2.5 for more information about these command lines.

6.5.3 Prescribed Force

```
BEGIN PRESCRIBED FORCE
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # specification commands
  DIRECTION = <string>defined_direction |
    COMPONENT = <string>X|Y|Z
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [PRESCRIBED FORCE]
```

The `PRESCRIBED FORCE` command block prescribes a force field for a given set of nodes. The force field associates a vector giving the magnitude and direction of the force with each node in the node set. The force field may vary over time and space. If the force field has only a time-varying component, the specification commands in the above command block can be used to specify the force field. If the force field has both time-varying and spatially varying components, a user subroutine is used to specify the force field. In a given boundary condition command block, commands from only one of the command groups (specification commands or user subroutine commands) may be used.

The `PRESCRIBED FORCE` command block contains three groups of commands—node set, function, and user subroutine. Each of these command groups is basically independent of the others. In addition to the command lines in the three command groups, there are three additional command lines: `SCALE FACTOR`, `ACTIVE PERIODS`, and `INACTIVE PERIODS`. The `SCALE FACTOR` com-

mand line can be used in conjunction with either the specification commands or the user subroutine commands. The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines are used to activate or deactivate this force boundary condition for certain time periods. Following are descriptions of the different command groups.

6.5.3.1 Node Set Commands

The `node set commands` portion of the `PRESCRIBED FORCE` command block defines a set of nodes associated with the prescribed force field and can include some combination of the following command lines:

```
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes used by the boundary condition. There must be at least one `NODE SET`, `SURFACE`, `BLOCK`, or `INCLUDE ALL BLOCKS` command line in the command block.

6.5.3.2 Specification Commands

If the specification commands are used, the force vector at any given time is the same for all nodes in the node set associated with the particular `PRESCRIBED FORCE` command block. The direction of the force vector is constant for all time; the magnitude of the force vector may vary with time, however.

Following are the command lines used to specify the prescribe force with a direction and a function:

```
DIRECTION = <string>defined_direction |
  COMPONENT = <string>X|Y|Z
FUNCTION = <string>function_name
```

The force can be specified either along an arbitrary user-defined direction or along a component direction (X, Y, or Z), but not both.

- The `DIRECTION` command line is used to prescribe force in an arbitrary user-defined direction. The name in the string `defined_direction` is a reference to a direction, which is defined using the `DEFINE DIRECTION` command block within the SIERRA scope.

- The COMPONENT command line is used to specify that the force vector lies along one of the component directions. The COMPONENT command line is a shortcut to an internally defined direction vector; for example, component x corresponds to using direction vector (1, 0, 0).

The magnitude of the force is specified by the FUNCTION command line. This references a function_name (defined in the SIERRA scope in a DEFINITION FOR FUNCTION command block) that specifies the magnitude of the force vector as a function of time. The magnitude can be scaled by use of the SCALE FACTOR command line described in Section 6.5.3.4.

The force is applied only in the prescribed direction, and is not applied in any direction orthogonal to that direction.

6.5.3.3 User Subroutine Commands

If the user subroutine option is used, the force vector may vary spatially at any given time for each of the nodes in the node set associated with the particular PRESCRIBED FORCE command block. The user subroutine option allows for a more complex description of the force field than does the function option, but the user subroutine option also requires that you write a user subroutine to implement this capability. The user subroutine will be used to define a force direction and a magnitude for every node to which the boundary condition will be applied. The subroutine will be called by Presto at the appropriate time to generate the force field.

Following are the command lines related to the user subroutine option:

```
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value
```

The user subroutine option is invoked by using the NODE SET SUBROUTINE command line. The string subroutine_name is the name of a FORTRAN subroutine that is written by the user.

Following the NODE SET SUBROUTINE command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 10.2.2 and consist of SUBROUTINE DEBUGGING OFF, SUBROUTINE DEBUGGING ON, SUBROUTINE REAL PARAMETER, SUBROUTINE INTEGER PARAMETER, and SUBROUTINE STRING PARAMETER. Examples of using these command lines are provided throughout Chapter 10.

The magnitude set in the user subroutine can be scaled by use of the SCALE FACTOR command line, as described in Section 6.5.3.4.

Usage requirements for the node set subroutine. The subroutine that you write will return three output values per node. Suppose you write a user subroutine that passes the output values through

an array output_values. For a given node inode, the output_values array would have the following values:

```
output_values(1,inode) = x component of force at inode
output_values(2,inode) = y component of force at inode
output_values(3,inode) = z component of force at inode
```

The three components of the force vector are given in output_values 1 through 3. The values of the flags array are ignored.

See Chapter 10 for more details on implementing the user subroutine option.

6.5.3.4 Additional Commands

These command lines in the PRESCRIBED FORCE command block provide additional options for the boundary condition:

```
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
INACTIVE PERIODS = <string list>period_names
```

The SCALE FACTOR command line is used to apply an additional scaling factor, which is constant in both time and space, to all vector magnitude values of the field defined by the specification commands or the user subroutine. For example, if the magnitude of the force in a time history function is given as 1.5 from time 1.0 to time 2.0 and the scale factor is 0.5, then the magnitude of the force from time 1.0 to 2.0 is 0.75. The default value for the scale factor is 1.0.

The ACTIVE PERIODS and INACTIVE PERIODS command lines determine when the boundary condition is active. See Section 2.5 for more information about these command lines.

6.5.4 Prescribed Moment

```
BEGIN PRESCRIBED MOMENT
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # specification commands
  DIRECTION = <string>defined_direction |
    COMPONENT = <string>X|Y|Z
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [PRESCRIBED MOMENT]
```

The `PRESCRIBED MOMENT` command block prescribes a moment field for a given set of nodes. Moments can only be defined for nodes attached to beam or shell elements. The moment field associates a vector giving the magnitude and direction of the moment with each node in the node set. If the moment field has only a time-varying component, the specification commands in the above command block can be used to specify the moment field. If the moment field has both time-varying and spatially varying components, a user subroutine option is used to specify the moment field. In a given boundary condition command block, commands from only one of the command groups (specification commands or user subroutine commands) may be used.

The `PRESCRIBED MOMENT` command block contains three groups of commands—node set, function, and user subroutine. Each of these command groups is basically independent of the others. In addition to the command lines in the four command groups, there are three additional command lines: `SCALE FACTOR`, `ACTIVE PERIODS`, and `INACTIVE PERIODS`. The `SCALE FACTOR` com-

mand line can be used in conjunction with either the specification commands or the user subroutine commands. The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines are used to activate or deactivate this force boundary condition for certain time periods. Following are descriptions of the different command groups.

6.5.4.1 Node Set Commands

The `node set commands` portion of the `PRESCRIBED MOMENT` command block defines a set of nodes associated with the prescribed moment field and can include some combination of the following command lines:

```
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes used by the boundary condition. There must be at least one `NODE SET`, `SURFACE`, `BLOCK`, or `INCLUDE ALL BLOCKS` command line in the command block.

6.5.4.2 Specification Commands

If the specification commands are used, the moment vector at any given time is the same for all nodes in the node set associated with the particular `PRESCRIBED MOMENT` command block. The direction of the moment vector is constant for all time; the magnitude of the moment vector may vary with time, however.

Following are the command lines used to specify the prescribed moment with a function and a direction:

```
DIRECTION = <string>defined_direction |
  COMPONENT = <string>X|Y|Z
FUNCTION = <string>function_name
```

The moment can be specified either along an arbitrary user-defined direction or along a component direction (X, Y, or Z), but not both.

- The `DIRECTION` command line is used to prescribe the moment in an arbitrary user-defined direction. The name in the string `defined_direction` is a reference to a direction, which is defined using the `DEFINE DIRECTION` command block within the SIERRA scope.

- The COMPONENT command line is used to specify that the moment vector lies along one of the component directions. The COMPONENT command line is a shortcut to an internally defined direction vector; for example, component x corresponds to using direction vector (1, 0, 0).

The magnitude of the moment is specified by the FUNCTION command line. This references a function_name (defined in the SIERRA scope in a DEFINITION FOR FUNCTION command block) that specifies the magnitude of the moment vector as a function of time. The magnitude can be scaled by use of the SCALE FACTOR command line described in Section 6.5.4.4.

The moment is applied only in the prescribed direction, and is not applied in any direction orthogonal to that direction.

6.5.4.3 User Subroutine Commands

If the user subroutine option is used, the moment vector may vary spatially at any given time for each of the nodes in the node set associated with the particular PRESCRIBED MOMENT command block. The user subroutine option allows for a more complex description of the moment field than do specification commands, but the user subroutine option also requires that you write a user subroutine to implement this capability. The user subroutine will be used to define a moment direction and a magnitude for every node to which the boundary condition will be applied. The subroutine will be called by Presto at the appropriate time to generate the moment field.

Following are the command lines related to the user subroutine option:

```
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value
```

The user subroutine option is invoked by using the NODE SET SUBROUTINE command line. The string subroutine_name is the name of a FORTRAN subroutine that is written by the user.

Following the NODE SET SUBROUTINE command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 10.2.2 and consist of SUBROUTINE DEBUGGING OFF, SUBROUTINE DEBUGGING ON, SUBROUTINE REAL PARAMETER, SUBROUTINE INTEGER PARAMETER, and SUBROUTINE STRING PARAMETER. Examples of using these command lines are provided throughout Chapter 10.

The magnitude set in the user subroutine can be scaled by use of the SCALE FACTOR command line, as described in Section 6.5.4.4.

Usage requirements for the node set subroutine. The subroutine that you write will return three output values per node. Suppose you write a user subroutine that passes the output values through

an array output_values. For a given node inode, the output_values array would have the following values:

```
output_values(1,inode) = moment about x-direction at inode
output_values(2,inode) = moment about y-direction at inode
output_values(3,inode) = moment about z-direction at inode
```

The three components of the moment vector are given in output_values 1 through 3. The values of the flags array are ignored.

See Chapter 10 for more details on implementing the user subroutine option.

6.5.4.4 Additional Commands

These command lines in the PRESCRIBED MOMENT command block provide additional options for the boundary condition:

```
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
INACTIVE PERIODS = <string list>period_names
```

The SCALE FACTOR command line is used to apply an additional scaling factor, which is constant in both time and space, to all vector magnitude values of the field defined by the specification commands or the user subroutine. For example, if the magnitude of the moment in a time history function is given as 1.5 from time 1.0 to time 2.0 and the scale factor is 0.5, then the magnitude of the moment from time 1.0 to 2.0 is 0.75. The default value for the scale factor is 1.0.

The ACTIVE PERIODS and INACTIVE PERIODS command lines determine when the boundary condition is active. See Section 2.5 for more information about these command lines.

6.6 Gravity

```
BEGIN GRAVITY
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  DIRECTION = <string>defined_direction
  FUNCTION = <string>function_name
  GRAVITATIONAL CONSTANT = <real>g_constant
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [GRAVITY]
```

A gravity load is generally referred to as a body force boundary condition. A gravity load generates a force at a node that is proportional to the mass of the node. This section describes how to apply a gravity load to a body.

The `GRAVITY` command block is used to specify a gravity load that is applied to all nodes selected within a command block. The gravity load boundary condition uses the function and scale (gravitational constant and scale factor) information to generate a body force at a node based on the mass of the node. Multiple `GRAVITY` command blocks can be defined on different sets of nodes. If two different `GRAVITY` command blocks reference the same node, the node will have gravity loads applied by both of the command blocks. Care must be taken to make sure you do not apply multiple gravity loads to one block if you only want one gravity load condition applied.

The `node set commands` portion of the `GRAVITY` command block defines a set of nodes associated with the gravity load and can include some combination of the following command lines:

```
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for

creating a set of nodes used by the boundary condition. There must be at least one `NODE SET`, `SURFACE`, `BLOCK`, or `INCLUDE ALL BLOCKS` command line in the command block.

The gravity load is specified along an arbitrary user-defined direction, and is defined using the `DIRECTION` command line. The name in the string `defined_direction` is a reference to a direction, which is defined using the `DEFINE DIRECTION` command block within the SIERRA scope.

The strength of the gravitational field can be varied with time by using the `FUNCTION` command line. This command line references a `function_name` defined in the SIERRA scope in a `DEFINITION FOR FUNCTION` command block.

A gravitational constant is specified by the `GRAVITATIONAL CONSTANT` command line in the real value `g_constant`. For example, the gravitational constant in units of inches and seconds would be 386.4 inches per second squared. You must set this quantity based on the actual units for your model.

The dependent variables in the function can be scaled by the real value `scale_factor` in the `SCALE FACTOR` command line. At any given time, the strength of the gravitational field is a product of the gravitational constant, the value of the function at that time, and the scale factor.

The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines provides an additional option for the gravity load condition. These command lines can activate or deactivate the gravity load for certain time periods. See Section 2.5 for more information about these command lines.

6.7 Prescribed Temperature

```
BEGIN PRESCRIBED TEMPERATURE
  #
  # block set commands
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE BLOCK = <string list>block_names
  #
  # specification command
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
  # external database commands
  READ VARIABLE = <string>var_name
  COPY VARIABLE = <string>var_name [FROM MODEL <string>model_name]
  TIME = <real>time
  TEMPERATURE TYPE = SOLID_ELEMENT|SHELL_ELEMENT (SOLID_ELEMENT)
  #
  # coupled analysis commands
  RECEIVE FROM TRANSFER [FIELD TYPE = NODE|ELEMENT(NODE)]
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [PRESCRIBED TEMPERATURE]
```

The `PRESCRIBED TEMPERATURE` command block prescribes a temperature field for a given set of nodes. The prescribed temperature is for each node in the node set. The temperature field may vary over time and space. If the temperature field has only a time-varying component, the function command in the above command block can be used to specify the temperature field. If the temperature field has both time-varying and spatially varying components, a user subroutine option can be used to specify the temperature field. Finally, you may also read the temperature as a variable from the mesh file. You can select only one of these options—function, user subroutine, or read variable—in a command block.

Temperature is applied to nodes, but it is frequently used at the element level, such as in the case for thermal strains. If the temperatures are used at the element level, the nodal values are averaged (depending on element) connectivity to produce an element temperature. The temperatures must

be defined for all the nodes defining the connectivity for any given element. For this reason, we use block commands to derive a set of nodes at which to define temperatures. If the temperatures are used on an element basis, then the temperature at all the necessary nodes will be defined.

The `PRESCRIBED TEMPERATURE` command block contains four groups of commands—block set, function, user subroutine, and read variable. Each of these command groups is basically independent of the others. In addition to the command lines in the four command groups, there are three additional command lines: `SCALE FACTOR`, `ACTIVE PERIODS`, and `INACTIVE PERIODS`. The `SCALE FACTOR` command line can be used in conjunction with the function command, the user subroutine option, or the read variable option. The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines are used to activate or deactivate this kinematic boundary condition for certain time periods. Following are descriptions of the different command groups.

6.7.1 Block Set Commands

The `block set commands` portion of the `PRESCRIBED TEMPERATURE` command block defines a set of nodes associated with the prescribed temperature field and can include some combination of the following command lines:

```
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes derived from some combination of element blocks. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes used by the boundary condition. There must be at least one `BLOCK` or `INCLUDE ALL BLOCKS` command line in the command block.

6.7.2 Specification Command

If the function command is used, the temperature at any given time is the same for all nodes in the node set associated with the particular `PRESCRIBED TEMPERATURE` command block. The command line

```
FUNCTION = <string>function_name
```

references a `function_name` (defined in the SIERRA scope using a `DEFINITION FOR FUNCTION` command block) that specifies the temperature as a function of time. The temperature can be scaled by use of the `SCALE FACTOR` command line described in Section 6.7.6.

6.7.3 User Subroutine Commands

If the user subroutine option is used, the temperature field may vary spatially at any given time for each of the nodes in the node set associated with the particular `PRESCRIBED TEMPERATURE` command block. The user subroutine option allows for a more complex description of the temperature field than does the function command, but the user subroutine option also requires that you write a user subroutine to implement this capability. The user subroutine will be used to define a temperature for every node to which the boundary condition will be applied. The subroutine will be called by Presto at the appropriate time to generate the temperature field.

Following are the command lines related to the user subroutine option:

```
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value
```

The user subroutine option is invoked by using the `NODE SET SUBROUTINE` command line. The string `subroutine_name` is the name of a FORTRAN subroutine that is written by the user.

Several other commands control the behavior of user subroutines: `SUBROUTINE DEBUGGING OFF`, `SUBROUTINE DEBUGGING ON`, `SUBROUTINE REAL PARAMETER`, `SUBROUTINE INTEGER PARAMETER`, and `SUBROUTINE STRING PARAMETER`. These are described in Section 10.2.2. Examples of using these command lines are provided throughout Chapter 10.

The temperature set in the user subroutine can be scaled by use of the `SCALE FACTOR` command line, as described in Section 6.7.6.

See Chapter 10 for more details on implementing the user subroutine option.

6.7.4 External Mesh Database Commands

If the external database option is used, the temperature field is read from an external mesh database. The temperatures are read from a finite element model defined via the `FINITE ELEMENT MODEL` command block described in Section 5.1. The finite element model can either be the model used by the region for its mesh definition as specified with the `USE FINITE ELEMENT MODEL` command (see Section 2.3), or it can be a different (but compatible) model. The following command lines control the use of an external mesh database to prescribe the temperature:

```
READ VARIABLE = <string>mesh_var_name
COPY VARIABLE = <string>var_name [FROM MODEL <string>model_name]
TIME = <real>time
TEMPERATURE TYPE = SOLID_ELEMENT|SHELL_ELEMENT (SOLID_ELEMENT)
```

The READ VARIABLE command is used to read the temperature from the region's finite element mesh database. The var_name string specifies the name of the variable as it appears on the mesh database.

If the analysis will cause topology modifications due to the use of load balancing, remeshing, or other techniques that can result in nodes and/or elements being moved among processors, then the COPY VARIABLE command should be used. This command specifies that the variable named var_name will be used to specify the temperature. The FROM MODEL <string>model_name portion of the command is optional. If it is specified, the results are read from the mesh database named model_name. Otherwise, the region's finite element mesh database will be used as the model.

The primary difference between the behavior of the COPY VARIABLE command and the READ VARIABLE command is that the copy command handles topology modifications caused by load balancing and remeshing, which can move nodes and elements to different processors. The COPY VARIABLE command will correctly match the nodes from the external database to the corresponding nodes in the analysis and communicate the data between processors if needed. Note that the nodes in the two finite element models must match spatially, but they can be distributed on different processors.

The field to be read may be specified at an arbitrary number of different times on the mesh file. The default behavior is for the time history of the variable read from the file to be used to prescribe the boundary condition. The time history is interpolated as needed for analysis times that do not correspond exactly to times on the mesh file. The TIME command line can optionally be used to specify that the boundary condition be constant over time, based on the value of the variable read from the file at the specified time. If the specified time on the TIME command line does not correspond exactly to a time on the mesh file, the data on the mesh file will be interpolated as needed.

If temperature is to be prescribed for shell elements, a linear or quadratic thermal gradient can optionally be specified through the thickness of the shells using the TEMPERATURE TYPE command line. The SOLID_ELEMENT option to this command is the default behavior, and results in a single temperature being read for each node into the temperature variable. With the SHELL_ELEMENT option, temperatures are read into the shell_temperature variable. Shell elements may potentially define a temperature gradient though the thickness, in which case there will be multiple temperatures at a node to describe the temperature gradient through the shell. The TEMPERATURE_TYPE command is only valid in conjunction with the READ VARIABLE command.

Though-thickness shell temperatures follow the Aria/Calore convention. If there is a single shell temperature defined at a node, the temperature is constant through the thickness.

If there are two shell temperatures defined at a node, the first is the temperature on the bottom of the shell and the second the temperature at the top. The temperature varies linearly between the top and bottom.

If there are three shell temperatures defined at node, the first is the temperature at the bottom of the shell, the second the temperature at the middle of the shell, and the third the temperature at the top of the shell. The temperature varies quadratically through the thickness.

SOLID_ELEMENT and SHELL_ELEMENT temperatures may be defined simultaneously in the same analysis through two different temperature command blocks. If both are defined, the shell element temperature results override any solid element temperature results on the shell elements.

6.7.5 Coupled Analysis Commands

The RECEIVE FROM TRANSFER command provides the ability to set the temperature in a coupled analysis by transferring results from another SIERRA code, such as Aria.

```
RECEIVE FROM TRANSFER [FIELD TYPE = NODE|ELEMENT(NODE)]
```

If this command is used in its default form, it is expected that the temperature is transferred to a nodal field named temperature in the Presto region. Presto performs an interpolation from the nodal field to an element field named temperature. The temperature can also be transferred directly to the element temperature field by using the optional FIELD TYPE = ELEMENT argument to this command.

If the RECEIVE FROM TRANSFER command is used, but the appropriate commands to perform the transfer between the two regions are missing, the temperature will be zero during the entire simulation.

It is also possible to use this line command to cause the initial temperatures obtained from a restart file to remain constant in time.

6.7.6 Additional Commands

These command lines in the PRESCRIBED TEMPERATURE command block provide additional options for the boundary condition:

```
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
INACTIVE PERIODS = <string list>period_names
```

The SCALE FACTOR command line is used to apply an additional scaling factor, which is constant in both time and space, to all temperature values of the field defined by the function command, the user subroutine, or the read variable option. For example, if the temperature in a time history function is given as 100.5 from time 1.0 to time 2.0 and the scale factor is 0.5, then the temperature from time 1.0 to 2.0 is 50.25. The default value for the scale factor is 1.0.

The ACTIVE PERIODS and INACTIVE PERIODS command lines determine when the boundary condition is active. See Section 2.5 for more information about these command lines.

6.8 Pore Pressure

```
BEGIN PORE PRESSURE
  #
  # block set commands
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE BLOCK = <string list>block_names
  #
  # specification command
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
  # external database commands
  READ VARIABLE = <string>var_name
  COPY VARIABLE = <string>var_name [FROM MODEL <string>model_name]
  TIME = <real>time
  #
  # coupled analysis commands
  RECEIVE FROM TRANSFER [FIELD TYPE = NODE|ELEMENT(NODE)]
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [PORE PRESSURE]
```

The `PORE PRESSURE` command block prescribes a pore pressure field for a given set of elements. The pore pressure is prescribed for each element in the block. The pore pressure field may vary over time and space. If the pore pressure field has only a time-varying component, the function command in the above command block can be used to specify the pore pressure field. If the pore pressure field has both time-varying and spatially varying components, a user subroutine option can be used to specify the pore pressure field. Finally, the pore pressure can be read as a variable from the mesh file. You can select only one of these options—function, user subroutine, or read variable—in a command block.

The `PORE PRESSURE` command block contains four groups of commands—block set, function, user subroutine, and read variable. Each of these command groups is basically independent of the others. In addition to the command lines in the four command groups, there are three additional command lines: `SCALE FACTOR`, `ACTIVE PERIODS`, and `INACTIVE PERIODS`. The

SCALE FACTOR command line can be used in conjunction with the function command, the user subroutine option, or the read variable option. The ACTIVE PERIODS and INACTIVE PERIODS command lines are used to activate or deactivate this kinematic boundary condition for certain time periods. Following are descriptions of the different command groups.

Biot's coefficient can be defined when prescribing pore pressure. See Section 4.1.2 for more information on Biot's coefficient.

6.8.1 Block Set Commands

The block set commands portion of the PORE PRESSURE command block defines a set of elements associated with the pore pressure field and can include a combination of the following command lines:

```
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of elements derived from some combination of element blocks. See Section 6.1.1 for more information about the use of these command lines for creating a set of elements used by the boundary condition. There must be at least one BLOCK or INCLUDE ALL BLOCKS command line in the command block.

6.8.2 Specification Command

If the FUNCTION command is used, the pore pressure at any given time is the same for all elements in the element set associated with the particular PORE PRESSURE command block. The command line

```
FUNCTION = <string>function_name
```

references a function_name (defined in the SIERRA scope using a DEFINITION FOR FUNCTION command block) that specifies the pore pressure as a function of time. The pore pressure can be scaled using the SCALE FACTOR command line described in Section 6.8.6.

6.8.3 User Subroutine Commands

If the user subroutine option is used, the pore pressure field may vary spatially at any given time for each of the elements in the element set associated with the particular PORE PRESSURE command block. The user subroutine option allows for a more complex description of the pore pressure field than does the FUNCTION command, but the user subroutine option also requires that a user

subroutine be written to implement this capability. The user subroutine will be used to define a pore pressure for every element to which the boundary condition will be applied. The subroutine will be called by Presto at the appropriate time to generate the pore pressure field.

Following are the command lines related to the user subroutine option:

```
ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value
```

The user subroutine option is invoked by using the `ELEMENT BLOCK SUBROUTINE` command line. The string `subroutine_name` is the name of a FORTRAN subroutine that is written by the user.

Several other commands control the behavior of user subroutines: `SUBROUTINE DEBUGGING OFF`, `SUBROUTINE DEBUGGING ON`, `SUBROUTINE REAL PARAMETER`, `SUBROUTINE INTEGER PARAMETER`, and `SUBROUTINE STRING PARAMETER`. These are described in Section 10.2.2. Examples of using these command lines are provided throughout Chapter 10.

The pore pressure set in the user subroutine can be scaled by use of the `SCALE FACTOR` command line, as described in Section 6.8.6.

See Chapter 10 for more details on implementing the user subroutine option.

6.8.4 External Mesh Database Commands

The pore pressure field can be read from an external mesh database. The finite element model from which pore pressures are read is defined via the `FINITE ELEMENT MODEL` command block described in Section 5.1. The finite element model can either be the model used by the region for its mesh definition as specified with the `USE FINITE ELEMENT MODEL` command (see Section 2.3), or it can be a different (but compatible) model. The following command lines control the use of an external mesh database to prescribe the pore pressure:

```
READ VARIABLE = <string>mesh_var_name
COPY VARIABLE = <string>var_name [FROM MODEL <string>model_name]
TIME = <real>time
```

The `READ VARIABLE` command is used to read the pore pressure from the region's finite element mesh database. The `var_name` string specifies the name of the variable as it appears on the mesh database.

If the analysis will cause topology modifications due to the use of load balancing, remeshing, or other techniques that can result in nodes and/or elements being moved among processors, the

COPY VARIABLE command should be used. This command specifies that the variable named var_name will be used to specify the pore pressure. The FROM MODEL <string>model_name portion of the command is optional. If it is specified, the results are read from the mesh database named model_name. Otherwise, the region's finite element mesh database will be used as the model.

The primary difference between the behavior of the COPY VARIABLE command and the READ VARIABLE command is that the copy command handles topology modifications caused by load balancing and remeshing, which can move nodes and elements to different processors. The COPY VARIABLE command will correctly match the nodes from the external database to the corresponding nodes in the analysis and communicate the data between processors if needed. Note that the nodes in the two finite element models must match spatially, but they can be distributed on different processors.

The field to be read may be specified at an arbitrary number of different times on the mesh file. The default behavior is for the time history of the variable read from the file to be used to prescribe the boundary condition. The time history is interpolated as needed for analysis times that do not correspond exactly to times on the mesh file. The TIME command line can optionally be used to specify that the boundary condition be constant over time, based on the value of the variable read from the file at the specified time. If the specified time on the TIME command line does not correspond exactly to a time on the mesh file, the data on the mesh file will be interpolated as needed.

6.8.5 Coupled Analysis Commands

The RECEIVE FROM TRANSFER command provides the ability to set the pore pressure in a coupled analysis by transferring results from another SIERRA code, such as Aria.

```
RECEIVE FROM TRANSFER [FIELD TYPE = NODE|ELEMENT(NODE)]
```

If this command is used in its default form, it is expected that the pore pressure is transferred to a nodal field named pore_pressure in the Presto region. Presto performs an interpolation from the nodal field to an element field named pore_pressure. The pore pressure can also be transferred directly to the element pore_pressure field by using the optional FIELD TYPE = ELEMENT argument to this command.

If the RECEIVE FROM TRANSFER command is used, but the appropriate commands to perform the transfer between the two regions are missing, the pore pressure will be zero during the entire simulation.

6.8.6 Additional Commands

These command lines in the PORE PRESSURE command block provide additional options for the boundary condition:

```
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
INACTIVE PERIODS = <string list>period_names
```

The `SCALE FACTOR` command line is used to apply an additional scaling factor, which is constant in both time and space, to all pore pressure values of the field defined by the function command, the user subroutine, or the read variable option. For example, if the pore pressure in a time history function is given as 100.5 from time 1.0 to time 2.0 and the scale factor is 0.5, then the pore pressure from time 1.0 to 2.0 is 50.25. The default value for the scale factor is 1.0.

The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines determine when the boundary condition is active. See Section 2.5 for more information about these command lines.

6.9 Fluid Pressure

```
BEGIN FLUID PRESSURE
  #
  # surface set commands
  SURFACE = <string list>surface_names
  #
  # specification commands
  DENSITY = <real>fluid_density
  DENSITY FUNCTION = <string>density_function_name
  GRAVITATIONAL CONSTANT = <real>gravitational_acceleration
  FLUID SURFACE NORMAL = <string>global_component_names
  DEPTH = <real>fluid_depth
  DEPTH FUNCTION = <string>depth_function_name
  REFERENCE POINT = <string>reference_point_name
  #
  # additional commands
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [PRESSURE]
```

The `FLUID PRESSURE` command block applies a hydrostatic pressure to each node of each face in the associated surfaces. The pressure at any node is determined from

$$P = \rho g h \tag{6.2}$$

where P is the pressure, ρ is the fluid density at the current time, g is the gravitational constant, and h is the current depth of the fluid above the node. The depth of the fluid is computed as the distance from the current fluid surface to the node in the direction of the fluid surface normal. The normal must be specified as one of the three global coordinate directions, x, y, or z. The global location of the fluid surface is found by adding the current depth to the appropriate coordinate component (the direction defined in the `FLUID SURFACE NORMAL` command) of a datum point. The datum point is either the point specified in the `REFERENCE POINT` line command, or, in the absence of this command, the minimum coordinate on the applied pressure surface in the component direction defined in the `FLUID SURFACE NORMAL` command. Once the current location of the fluid surface is computed, the depth at each node on the pressure surface is computed as the distance from the node to the fluid surface in the direction of the fluid surface normal.

Currently, the `FLUID PRESSURE` command block can be used for surfaces that have faces derived from solid elements (eight-node hexahedra, four-node tetrahedra, eight-node tetrahedra, etc.), membranes, and shells.

The `FLUID PRESSURE` command block contains three groups of commands—surface set, specification, and additional optional commands.

6.9.1 Surface Set Commands

The `surface set commands` portion of the `FLUID PRESSURE` command block defines a set of surfaces associated with the pressure field and consists of the following line:

```
SURFACE = <string list>surface_names
```

In the `SURFACE` command line, a series of surfaces can be listed through the string list `surface_names`. There must be at least one `SURFACE` command line in the command block. See Section 6.1.1 for more information about the use of command lines for creating a set of surfaces used by the boundary condition. The force computed from the hydrostatic pressure will be in the opposite direction of the face normal. When using shells or membranes, the analyst must ensure that all face normals composing the pressure application surface are in the correct direction.

6.9.2 Specification Commands

The density and the gravitational acceleration must be input by the user in units consistent with other material properties and the lengths in the mesh. To facilitate convergence of the initial load step, the gradual application of a hydrostatic load may be specified through a time history function for the density. A combination of the `DENSITY` and the `DENSITY FUNCTION` sets the value for the fluid density at each time. Either the `DENSITY` or the `DENSITY FUNCTION` must be input and both can be used together. If the `DENSITY` command is input without the `DENSITY FUNCTION` command, the density will be constant in time at that value. If the `DENSITY FUNCTION` command is input without a `DENSITY` command, the function is used as a time history of the density. If both the `DENSITY` and the `DENSITY FUNCTION` commands are input, the density value is used as a scale factor on the time history function. Finally, the `GRAVITATIONAL CONSTANT` sets the value for the acceleration due to gravity, g.

```
DENSITY = <real>fluid_density
DENSITY FUNCTION = <string>fluid_density_function
GRAVITATIONAL CONSTANT = <real>G
```

The following command lines are used to define the location of the fluid surface at any time during the analysis:

```
FLUID SURFACE NORMAL = <string>normal_component
DEPTH = <real>initial_fluid_depth
DEPTH FUNCTION = <string>depth_function_name
REFERENCE POINT = <string>point_name
```

The `FLUID SURFACE NORMAL` command sets the outward normal of the fluid surface to be one of the global component directions, x, y, or z. The fluid depth is then assumed to be in the direction opposite this global direction. The `DEPTH` command is used with the `DEPTH FUNCTION` command

to determine the fluid depth at any time. At least one of these commands must be input. If the DEPTH command is input without the DEPTH FUNCTION command, the fluid depth will be constant in time with that value. If the DEPTH FUNCTION command is input without a DEPTH command, the function is used as a time history of the depth. If both the DEPTH and the DEPTH FUNCTION commands are input, the specified depth is used as a scale factor on the time history function.

The depth and/or depth function are used to determine the current depth, which is added to the appropriate position of a datum point to compute the current location of the fluid surface in the FLUID SURFACE NORMAL component direction. The datum point is assumed to be the minimum coordinate in the component direction on the pressure surface defined in the SURFACE command if the optional REFERENCE POINT command described below is not used.

The REFERENCE POINT command line is used to specify the fluid surface relative to an external datum. When applying an external fluid pressure in a quasistatic analysis, a corresponding stiffness due to the external fluid is added to the diagonal terms of the stiffness matrix for the full tangent preconditioner to enhance convergence of the solver.

6.9.3 Additional Commands

These command lines in the FLUID PRESSURE command block provide additional options for the boundary condition:

```
ACTIVE PERIODS = <string list>period_names
INACTIVE PERIODS = <string list>period_names
```

By default, the FLUID PRESSURE boundary condition will be active throughout an analysis. However, use of the ACTIVE PERIODS and INACTIVE PERIODS commands can be used to limit the action of the boundary condition to specific time periods. The ACTIVE PERIODS command line specifies when the boundary condition is active implying that it is inactive during any periods not included on the command line. Alternatively, the INACTIVE PERIODS determines when the boundary condition will not be active. See Section 2.5 for more information about these commands.

6.10 Specialized Boundary Conditions

Specialized boundary conditions that are provided to enforce kinematic conditions or apply loads are described in this section.

6.10.1 Cavity Expansion

```
BEGIN CAVITY EXPANSION
  EXPANSION RADIUS = <string>SPHERICAL|CYLINDRICAL
    (spherical)
  SURFACE = <string list>surface_ids
  REMOVE SURFACE = <string list>surface_ids
  FREE SURFACE = <real>top_surface_zcoord
    <real>bottom_surface_zcoord
  NODE SETS TO DEFINE BODY AXIS =
    <string>nodelist_1 <string>nodelist_id2
  TIP RADIUS = <real>tip_radius
  BEGIN LAYER <string>layer_name
    LAYER SURFACE = <real>top_layer_zcoord
      <real>bottom_layer_zcoord
    PRESSURE COEFFICIENTS = <real>c0 <real>c1 <real>c2
    SURFACE EFFECT = <string>NONE|SIMPLE_ON_OFF(NONE)
    FREE SURFACE EFFECT COEFFICIENTS = <real>coeff1
      <real>coeff2
  END [LAYER <string>layer_name]
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [CAVITY EXPANSION]
```

The `CAVITY EXPANSION` command block is used to apply a cavity expansion boundary condition to a surface on a body. This boundary condition is typically used for earth penetration studies where some type of projectile (penetrator) strikes a target. For a more detailed explanation of the numerical implementation of the cavity expansion boundary condition and the parameters for this boundary condition, consult Reference 1. The cavity expansion boundary condition is a complex boundary condition with several options, and the detailed explanation of the implementation of the boundary condition in the above reference is required reading to fully understand the input parameters for this boundary condition.

There are two types of cavity expansion—cylindrical expansion and spherical expansion. You can select either the spherical or cylindrical option by using the `EXPANSION RADIUS` command line; the default is `SPHERICAL`. Reference 1 describes these two types of cavity expansion.

The boundary condition is applied to the surfaces (`surface_ids`) in the finite element model specified by the `SURFACE` command line. (Any surface specified on the `SURFACE` command line can be removed from the list of surfaces by using a `REMOVE SURFACE` command line.) This boundary condition generates a pressure at a node based on the velocity and surface geometry at

the node. Since cavity expansion is essentially a pressure boundary condition, cavity expansion must be specified for a surface.

The target has a top free surface with a normal in the global positive z-direction; the target has a bottom free surface with a normal in the global negative z-direction. The point on the global z-axis intersected by the top free surface is given by the parameter `top_surface_zcoord` on the `FREE SURFACE` command line. The point on the global z-axis intersected by the bottom free surface is given by the parameter `bottom_surface_zcoord` on the `FREE SURFACE` command line.

It is necessary to define two points that lie on the axis (usually the axis of revolution) of the penetrator. These two nodes are specified with the `NODE SETS TO DEFINE BODY AXIS` command line. The first node should be a node toward the tip of the penetrator (`nodelist_1`), and the second node should be a node toward the back of the penetrator (`nodelist_2`). Only one node is allowed in each node set.

It is necessary to compute either a spherical or cylindrical radius for nodes on the surface where the cavity expansion boundary condition is applied. This is done automatically for most nodes. The calculations for these radii break down if the node is close to or at the tip of the axis of revolution of the penetrator. For nodes where the radii calculations break down, a user-defined radius can be specified with the `TIP RADIUS` command line. For more information, consult Reference 1.

Embedded within the target can be any number of layers. Each layer is defined with a `LAYER` command block. The command block begins with

```
BEGIN LAYER <string>layer_name
```

and is terminated with:

```
END [LAYER <string>layer_name]
```

Here the string `layer_name` is a user-selected name for the layer. This name must be unique to all other layer names defined in the `CAVITY EXPANSION` command blocks. The layer properties are defined by several different command lines—`LAYER SURFACE`, `PRESSURE COEFFICIENTS`, `SURFACE EFFECT`, and `FREE SURFACE EFFECT COEFFICIENTS`. These command lines are described next.

- `LAYER SURFACE = <real>top_layer_zcoord`
  `<real>bottom_layer_zcoord`

  The layer has a top surface with a normal in the global positive z-direction; the layer has a bottom surface with a normal in the global negative z-direction. In the `LAYER SURFACE` command line, the point on the global z-axis intersected by the top layer surface is given by the parameter `top_layer_zcoord`, and the point on the global z-axis intersected by the bottom layer surface is given by the parameter `bottom_layer_zcoord`.

- `PRESSURE COEFFICIENTS = <real>c0 <real>c1 <real>c2`

The value of the pressure at a node is derived from an equation that is quadratic based on some scalar value derived from the velocity vector at the node. The three coefficients for the quadratic equation (`c0`, `c1`, `c2`) in the `PRESSURE COEFFICIENTS` command line define the impact properties of a layer.

- `SURFACE EFFECT = <string>NONE|SIMPLE_ON\str (NONE)`

  There can be no surface effects associated with a layer, or there can be a simple on/off surface effect model associated with a layer. The type of surface effect is determined by the `SURFACE EFFECT` command line. The default is no surface effects. If the `SIMPLE_ON_OFF` model is chosen, it is necessary to specify free surface effect coefficients with the `FREE SURFACE EFFECT COEFFICIENTS` command line.

- `FREE SURFACE EFFECT COEFFICIENTS = <real>coeff1 <real>coeff2`

  All the parameters defined in a `LAYER` command block apply to that layer. If a simple on/off surface effect is applied to a layer, the surface effect coefficients are associated with the layer values. The surface effect parameter associated with the top of the layer is `coeff1`; the surface effect parameter associated with the bottom of the layer is `coeff2`.

The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines provide an additional option for cavity expansion. These command lines can activate or deactivate cavity expansion for certain time periods. See Section 2.5 for more information about these command lines.

6.10.2 Blast Pressure

```
BEGIN BLAST PRESSURE
  SURFACE = <string list>surface_ids
  REMOVE SURFACE = <string list>surface_ids
  BURST TYPE = <string>SURFACE|AIR
  TNT MASS IN LBS = <real>tnt_mass_lbs
  BLAST TIME = <real>blast_time
  BLAST LOCATION = <real>loc_x <real>loc_y <real>loc_z
  ATMOSPHERIC PRESSURE IN PSI = <real>atmospheric_press
  AMBIENT TEMPERATURE IN FAHRENHEIT = <real>temperature
  FEET PER MODEL UNITS = <real>feet
  MILLISECONDS PER MODEL UNITS = <real>milliseconds
  PSI PER MODEL UNITS = <real>psi
  PRESSURE SCALE FACTOR = <real>pressure_scale(1.0)
  IMPULSE SCALE FACTOR = <real>impulse_scale(1.0)
  POSITIVE DURATION SCALE FACTOR = <real>duration_scale(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [BLAST PRESSURE]
```

The `BLAST PRESSURE` command block is used to apply a pressure load resulting from a conventional explosive blast. This boundary condition is based on Reference 2 and Reference 3, and Sachs scaling is implemented to match the ConWep code (Reference 4). Angle of incidence is accounted for by transitioning from reflected pressure to incident pressure according to:

$$P_{total} = P_{ref} * \cos\theta + P_{inc} * (1 - \cos\theta) \tag{6.3}$$

where θ is the angle between the face normal vector and the direction to the blast from the face, P_{total} is the total pressure, P_{ref} is the reflected portion of the pressure, and P_{inc} is the incident portion of the pressure. P_{ref} and P_{inc} are based on Friedlander's equation, as described in Reference 3.

If θ is greater than 90 degrees (i.e. the face is pointing away from the blast), only P_{inc} is applied to the face. In this case, the face variable `cosa`, which contains $\cos\theta$, is set to zero.

This boundary condition is applied to the surfaces in the finite element model specified by the `SURFACE` command line. (Any surface specified on the `SURFACE` command line can be removed from the list of surfaces by using a `REMOVE SURFACE` command line.)

Warning: Multiple `BLAST PRESSURE` command blocks may be used in an analysis to apply blast loads at different locations. However, only one should be applied to a given element face. Each instance of this boundary condition should be applied to a different set of surfaces, and those surfaces should not overlap surfaces used by other instances of this boundary condition. This is because face variables are used to store information used by this boundary condition, and those variables would be over-written by another instance of the boundary condition.

Table 8.9 lists the face variables used by the `BLAST PRESSURE` boundary condition. These can be requested for output in the standard manner (see Chapter 8), and can be useful for verifying that this boundary condition is correctly applied.

The type of burst load is specified with the `BURST TYPE` command, which can be `SURFACE` or `AIR`. The `SURFACE` option is used to define a hemispherical burst, while the `AIR` option is used for a spherical burst.

The equivalent TNT mass (in pounds) is defined with the `TNT MASS IN LBS` command. The time of the explosion is defined using the `BLAST TIME` command. This can be negative, and can be used to start the analysis at the time when the blast reaches the structure, saving computational time. The location of the blast is defined with the `BLAST LOCATION` command.

The current ambient pressure and temperature are defined using the `ATMOSPHERIC PRESSURE IN PSI` and `AMBIENT TEMPERATURE IN FAHRENHEIT` commands, respectively. As implied by the command names, these must be supplied in units of pounds per square inch and degrees Fahrenheit.

Because of the empirical nature of this method for computing an explosive load, appropriate conversion factors for the unit system used in the model must be supplied. The commands `FEET PER MODEL UNITS`, `MILLISECONDS PER MODEL UNITS`, and `PSI PER MODEL UNITS` are used to specify the magnitude of one foot, one millisecond, and one pound per square inch in the unit system of the model.

All of the commands listed above are required. Scaling factors can optionally be applied to modify the peak pressure, the impulse, and the duration of the loading. The `PRESSURE SCALE FACTOR` command scales the the peak value of both the reflected and incident portions of the applied pressure. The `IMPULSE SCALE FACTOR` command scales the impulse of the reflected and incident portions of the applied pressure. The `POSITIVE DURATION SCALE FACTOR` command scales the duration of the reflected and incident portions of the applied pressure. Each of these scaling factors only affects the quantity that it modifies, for example, scaling the pressure does not affect the impulse or duration.

The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines can optionally be used to activate or deactivate this boundary condition for certain time periods. See Section 2.5 for more information about these command lines.

6.10.3 Silent Boundary

```
BEGIN SILENT BOUNDARY
  SURFACE = <string list>surface_names
  REMOVE SURFACE = <string list>surface_names
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [SILENT BOUNDARY]
```

The `SILENT BOUNDARY` command block is also referred to as a non-reflecting surface boundary condition. A wave striking this surface is not reflected. This boundary condition is implemented with the techniques described in Reference 5. The method described in this reference is excellent at transmitting the low- and medium-frequency content through the boundary. While the method does reflect some of the high-frequency content, the amount of energy reflected is usually minimal. On the whole, the silent boundary condition implemented in Presto is highly effective.

In the `SURFACE` command line, you can list a series of surfaces through the string list `surface_names`. There must be at least one `SURFACE` command line in the command block. The `REMOVE SURFACE` command line allows you to delete surfaces from the set specified in the `SURFACE` command line(s) through the string list `surface_names`. See Section 6.1.1 for more information about the use of these command lines for creating a set of surfaces used by the boundary condition.

The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines provide an additional option for the boundary condition. These command lines are used to activate or deactivate the boundary condition for certain time periods. See Section 2.5 for more information about these command lines.

6.10.4 Spot Weld

```
BEGIN SPOT WELD
  NODE SET = <string list>nodelist_ids
  REMOVE NODE SET = <string list>nodelist_ids
  SURFACE = <string list>surface_ids
  REMOVE SURFACE = <string list>surface_ids
  SECOND SURFACE = <string>surface_id
  NORMAL DISPLACEMENT FUNCTION =
    <string>function_nor_disp
  NORMAL DISPLACEMENT SCALE FACTOR =
    <real>scale_nor_disp(1.0)
  TANGENTIAL DISPLACEMENT FUNCTION =
    <string>function_tang_disp
  TANGENTIAL DISPLACEMENT SCALE FACTOR =
    <real>scale_tang_disp(1.0)
  FAILURE ENVELOPE EXPONENT = <real>exponent(2.0)
  FAILURE FUNCTION = <string>fail_func_name
  FAILURE DECAY CYCLES = <integer>number_decay_cycles(10)
  SEARCH TOLERANCE = <real>search_tolerance
  IGNORE INITIAL OFFSET = NO|YES(NO)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [SPOT WELD]
```

The spot weld option lets the user model an "attachment" between a node on one surface and a face on another surface. This option models a weld or a small screw or bolt with a normal force-displacement curve like that shown in Figure 6.1 and a tangential force-displacement curve like that shown in Figure 6.2. The displacement shown in the figures is the distance, either normal or tangential, that the node moves from the nearest point on the face as measured in the original configuration. The force shown in the figure is the force at the attachment as a function of the distance between the two attachment points. (The force-displacement curve assumes the two attachment points are originally at the same location and the initial distance is zero, thus zero force at time zero. However, in most situations there is an initial gap which leads to non-zero forces at time zero.) Two force-displacement curves are required for the spot weld model; one curve models normal behavior, and the other curve models tangential behavior. It is worth noting the difference in how the normal and tangential components behave, therefore explaining why two curves are required. It is possible for the node to interpenetrate the surface resulting in a negative normal displacement between the connection points. Therefore, the normal force displacement curve must have the ability to capture negative displacements and thus negative forces. Although this penalty stiffness approach will work to prevent interpenetration, it is better to model this behavior using contact. The tangential displacement, however, is always positive.

The sign of the normal displacement of the spot weld (generally tension at positive displacement or compression at negative displacement) is determined by the relative motion of the attached node and face as well as the normal direction of the face. See Figure 6.3. If the relative normal motion of the face is along the face normal the spot weld becomes more compressive. If the relative normal

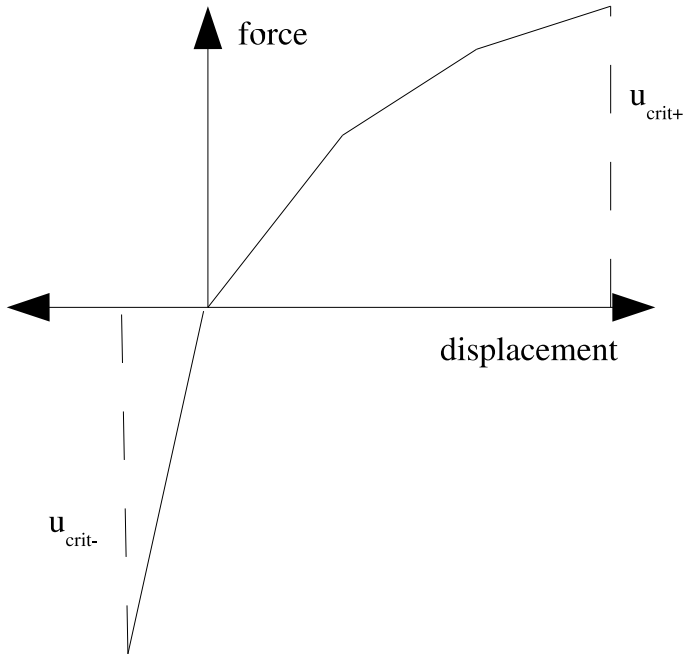

Figure 6.1: Force-displacement curve for spot weld normal force.

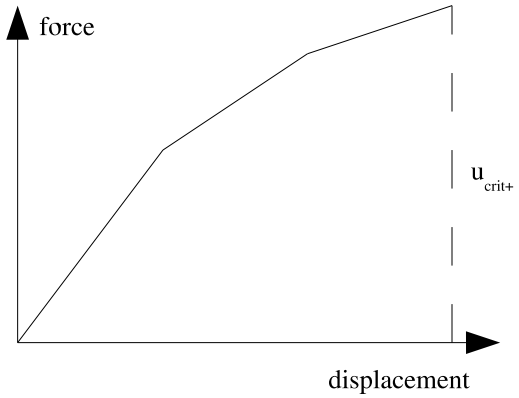

Figure 6.2: Force-displacement curve for spot weld tangential force.

motion of the face is opposite to the face normal the spot weld becomes more tensile.

The attachment in Presto is defined between a node on one surface and the closest point on an element face on the other surface. Since a face is used to define one of the attachment points, it is possible to compute a normal vector and a tangent vector associated with the face. This allows us to resolve the displacement (distance, both positive and negative) and force (both tensile

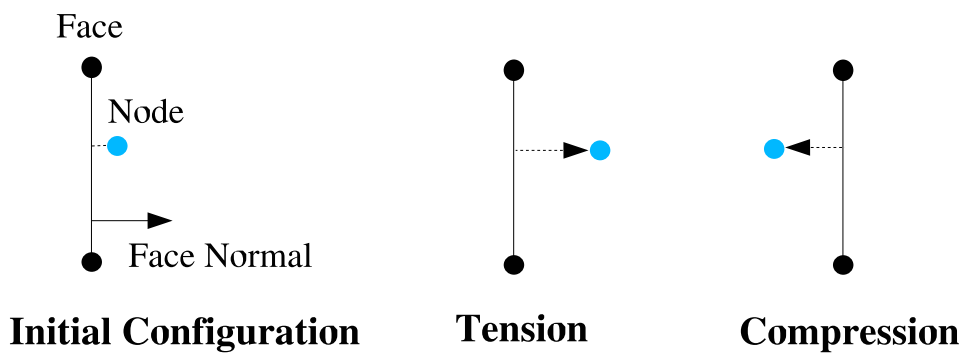

Figure 6.3: Sign convention for spot weld normal displacements.

and compressive) into normal and tangential components. With normal and tangential vectors associated with the attachment, the attachment can be characterized for the case of pure tension and pure shear.

Presto includes two mechanisms for determining failure for cases that fall between pure tension and pure shear. In the first case, failure is governed by the equation

$$(u_n/u_{n_{crit}})^p + (u_t/u_{t_{crit}})^p < 1.0\,. \tag{6.4}$$

In Equation 6.4, the distance from the node to the original attachment point on the face as measured normal to the face is u_n, which is defined as the normal distance. The maximum value given for u_n in the normal force-displacement curve is $u_{n_{crit}}$, but is different for positive and negative displacements. In Figure 6.1, the value used for $u_{n_{crit}}$ is u_{crit+} in the positive direction and u_{crit-} in the negative direction. The distance from the node to the original attachment point on the face as measured along a tangent to the face is u_t, which is defined as the tangential distance. The maximum value given for u_t in the tangential force-displacement curve is $u_{t_{crit}}$. The value p is a user-specified exponent that controls the shape of the failure surface.

Alternatively, Presto permits a user-specified function to determine the failure surface. The function defines the ratio of $u_t/u_{t_{crit}}$ at which failure will occur as a function of $u_n/u_{n_{crit}}$. The function must range from 0.0 to 1.0, and have a value of 1.0 at 0.0 and a value of 0.0 at 1.0. These restrictions preserve proper failure for the cases of pure tension and pure shear.

To use the spot weld option in Presto, a `SPOT WELD` command block begins with the input line:

```
BEGIN SPOT WELD
```

and is terminated with the input line :

```
END [SPOT WELD]
```

Within the command block, it is necessary to specify the set of nodes on one side of the spot weld with the `NODE SET` command line. The `NODE SET` command line can list one or more node sets. Any node set listed on the `NODE SET` command line can be deleted from the list of node sets by using a `REMOVE NODE SET` command line. A set of element faces on an opposing side of the spot weld (which we will refer to as the *first* surface) is specified with the `SURFACE` command line. The `SURFACE` command line can list one or more surfaces. Any surface listed on the `SURFACE` command line can be deleted from the list of surface by using a `REMOVE SURFACE` command line. For any node in the node set, the closest point to this node on the opposing surface should lie within the element faces specified by the `SURFACE` command line.

The normal force-displacement curve is specified by a function named by the value `function_nor_disp` in the `NORMAL DISPLACEMENT FUNCTION` command line. This function can be scaled by the real value `scale_nor_disp` in the `NORMAL DISPLACEMENT SCALE FACTOR` command line; the default for this factor is 1.0. The last points in the positive and negative directions are used as the displacements beyond which the spot weld fails. The tangential force-displacement curve is specified by a function named by the string `function_tang_disp` in the `TANGENTIAL DISPLACEMENT FUNCTION` command line. This function can be scaled by the real value `scale_tang_disp` given in the `TANGENTIAL DISPLACEMENT SCALE FACTOR` command line; the default for this factor is 1.0. The last point in the positive direction in the tangential curve is used as the displacement beyond which the spot weld fails.

The failure surface between pure tension and pure shear is controlled by specifying either the failure envelope exponent, p in Equation 6.4, or a failure function. The failure exponent is specified by the real value exponent in the `FAILURE ENVELOPE EXPONENT` command line. The failure function is specified by the `FAILURE FUNCTION` command line. If both a failure function and a failure exponent are given, then the failure function is used.

For an explicit, transient dynamics code like Presto, it is better to remove the force for the spot weld over several load steps rather than over a single load step once the failure criterion is exceeded. The `FAILURE DECAY CYCLES` command line controls the number of load steps over which the final force is removed (default value is 10). To remove the final force at a spot weld over five load increments, the integer specified by `number_decay_cycles` would be set to 5. Once the force at the spot weld is reduced to zero, it remains zero for all subsequent time (despite the function definition).

The spot weld can take on area-based behavior by specifying a surface in place of a set of nodes. The identifier of this surface is specified by the string `surface_id` in the `SECOND SURFACE` command line. The area-based spot weld creates a weld between all nodes on the second surface and the faces of the first surface. The load-resistance curve at each node is derived from the tributary area of the node times the given force-displacement curves. Thus, for the area-based spot welds, the force-displacement curves give the force per unit area resisted by the weld.

The user must set a tolerance for the node-to-face search with the

```
SEARCH TOLERANCE = <real>search_tolerance
```

command line. The value you select for `search_tolerance` will depend upon the distance between the nodes and surfaces used to define the spot weld.

If the user sets `IGNORE INITIAL OFFSET = YES`, the initial distance between the node and the face will be taken as the zero normal displacement distance for the spot weld. When using the `IGNORE INITIAL OFFSET = YES` command the initial normal force in the will be the value of the force-displacement curve at displacement=zero. The sign convention used to determine if a spot weld is in compression or tension is the same as without using `IGNORE INITIAL OFFSET = YES` as shown Figure 6.4.

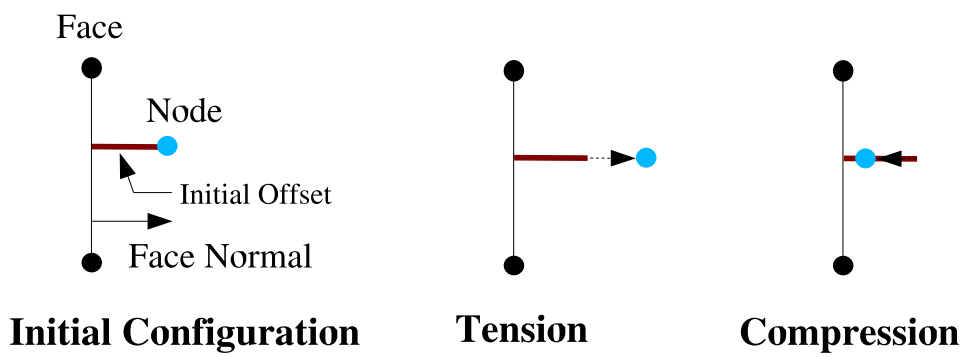

Figure 6.4: Sign convention for spot weld normal displacements with ignore initial offsets on.

The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines provide an additional option for the boundary condition. These command lines are used to activate or deactivate the boundary condition for certain time periods. See Section 2.5 for more information about these command lines.

In explicit dynamics, spot welds do not inherently have a critical time step due to the fact that they have zero mass. However, when a node-based time step estimate is used, spot welds contribute their stiffness to the nodes associated with the spot weld, thus influencing the time step calculated based on those nodes. The spot weld stiffness is calculated as the sum of the current derivative of the normal force function and the current derivative of the tangential force function, which is a conservative estimate. If the nodes attached to an element that governs the critical time step have spot weld stiffness contributions, a line is output to the log file stating the approximate percent reduction in critical time step due to the the spot weld stiffness contribution.

Output data can be obtained from spot welds. The list of available output variables is documented in Table 8.6.

6.10.5 Line Weld

```
BEGIN LINE WELD
  SURFACE = <string list> surface_names
  REMOVE SURFACE = <string list> surface_names
  BLOCK = <string list> block_names
  REMOVE BLOCK = <string list>block_names
  SEARCH TOLERANCE = <real>search_tolerance
  R DISPLACEMENT FUNCTION = <string>r_disp_function_name
  R DISPLACEMENT SCALE FACTOR = <real>r_disp_scale
  S DISPLACEMENT FUNCTION = <string>s_disp_function_name
  S DISPLACEMENT SCALE FACTOR = <real>s_disp_scale
  T DISPLACEMENT FUNCTION = <string>t_disp_function_name
  T DISPLACEMENT SCALE FACTOR = <real>t_disp_scale
  R ROTATION FUNCTION = <string>r_rotation_function_name
  R ROTATION SCALE FACTOR = <real>r_rotation_scale
  S ROTATION FUNCTION = <string>s_rotation_function_name
  S ROTATION SCALE FACTOR = <real>s_rotation_scale
  T ROTATION FUNCTION = <string>t_rotation_function_name
  T ROTATION SCALE FACTOR = <real>t_rotation_scale
  FAILURE ENVELOPE EXPONENT = <real>k
  FAILURE DECAY CYCLES = <integer>number_decay_cycles
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END LINE WELD
```

The line-weld capability is used to weld the edge of a shell to the face of another shell. The bond can transmit both translational and rotational forces. When failure of the line weld occurs, it breaks and no longer transmits any forces.

The edge of the shell that is tied to a surface is modeled with a block of one-dimensional elements (truss, beam, spring, etc.). The edge of the shell and the one-dimensional elements will share the same nodes. We will refer to the shell edge and the one-dimensional elements associated with it as the one-dimensional part of the line-weld model. The element blocks with the one-dimensional elements are specified by using the `BLOCK` command line. More than one element block can be listed on this command line. The element blocks referenced by the `BLOCK` command line must be one-dimensional elements—truss, beam, spring, etc.

The other part of the line weld is a set of faces defined by shell elements; this set of faces is the two-dimensional part of the line weld. The surface (the two-dimensional part of the model) to which the nodes (from the one-dimensional part of the model) are to be bonded is defined by any surface of element faces derived from shell elements. The line weld will bond each node in the element blocks listed in the `BLOCK` command line to the closest face (or faces) of element faces in the surfaces listed in the `SURFACE` command line. More than one surface can be listed on this command line.

The command line `SEARCH TOLERANCE` sets a tolerance on the search for node-to-face interactions. For a given node, only those faces within the distance set by the `search_tolerance`

parameter will be searched to determine whether the node should be welded to the face.

Each section of the line weld has its own local coordinate system (r, s, t). The r-direction lies along a one-dimensional element (and hence on the surface). The s-direction lies on the surface and is tangential to the one-dimensional element. The t-direction lies normal to the face and is orthogonal to the r- and s-directions. Force-displacement functions and moment-rotation functions may be specified for all axes in the local coordinate system. If one of the functions is left out, the resistance is zero for that axis. These functions are similar to the ones used for the spot weld (see Figure 6.2).

The force-displacement function in the r-direction represents shear resistance in the direction of the weld; this function is specified by a SIERRA function name on the `R DISPLACEMENT FUNCTION` command line. The force-displacement in the s-direction represents shear resistance tangential to the weld; this function is specified by a SIERRA function name on the `S DISPLACEMENT FUNCTION` command line. The force-displacement in the t-direction function represents tearing resistance normal to the surface; this function is specified by a SIERRA function name on the `T DISPLACEMENT FUNCTION` command line. The moment-rotation about the r-axis represents a rotational tearing resistance; this is specified by a SIERRA function name on the `R ROTATION FUNCTION` command line. The rotational resistances about the s-direction and the t-direction are likely not very meaningful, as rotations along these axes should be well constrained by the normal and tangential displacement relations. These two rotational resistances, if used, are defined with SIERRA function names on the `S ROTATION FUNCTION` and `T ROTATION FUNCTION` command lines. Note that each SIERRA function used in this command block is defined via a `DEFINITION FOR FUNCTION` command block in the SIERRA scope.

Any of the above functions can be scaled by using a corresponding scale factor. For example, the force-displacement function on the `R DISPLACEMENT FUNCTION` command line can be scaled by the parameter `r_disp_scale` on the `R DISPLACEMENT SCALE FACTOR` command line. Only the force values of the force-displacement curve will be scaled.

The failure function for the line weld is similar to that for the spot weld. Denote the displacement or rotation associated with a line weld as δ. Suppose that δ_i is a displacement in the r-direction. The force-displacement curve specified on the `R DISPLACEMENT FUNCTION` command line has a maximum value η. This is the maximum displacement the weld can endure in the r-direction before breaking. Associate this value of η with δ_i by designating it as η_i. Repeat this pairing process for all the displacements and rotations defining the line weld. Each displacement component in the line weld will be paired with one of the three maximum displacement values associated with the line weld. Each rotation component in the line weld will be paired with one of the three maximum rotation values associated with the line weld. Breaking of the weld under combined loading is calculated the same as the spot weld. The weld breaks under the following condition:

$$\sqrt[k]{\sum \left(\frac{\delta_i}{\eta_i}\right)^k} > 1 \,. \tag{6.5}$$

In the above equation, the parameter k is set by the user. A typical value for k is 2. The summation takes place over all the failure functions (force-displacement and moment-rotation) for all the nodes. (The value for k is specified on the `FAILURE ENVELOPE EXPONENT` command line.)

For an explicit, transient dynamics code like Presto, it is better to remove the forces for the line weld over several time steps rather than over a single time step once the failure criterion is exceeded. The `FAILURE DECAY CYCLES` command line controls the number of time steps over which the final force is removed. To remove the final force at a line weld over five time steps, the integer specified by `number_decay_cycles` would be set to 5. Once the force in the line weld is reduced to zero, it remains zero for all subsequent time.

The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines provide an additional option for the boundary condition. These command lines are used to activate or deactivate the boundary condition for certain time periods. See Section 2.5 for more information about these command lines.

6.10.6 Viscous Damping

```
BEGIN VISCOUS DAMPING <string>damp_name
  #
  # block set commands
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE BLOCK = <string list>block_names
  #
  MASS DAMPING COEFFICIENT = <real>mass_damping
  STIFFNESS DAMPING COEFFICIENT = <real>stiff_damping
  #
  # additional command
  ACTIVE PERIODS = <string list>period names
  INACTIVE PERIODS = <string list>period_names
END [VISCOUS DAMPING <string>damp_name]
```

The `VISCOUS DAMPING` command block adds simple Rayleigh viscous damping to mesh nodes. At each node, Presto computes a damping coefficient, which is then multiplied by the node velocity to create a damping force. The damping coefficient is the sum of the mass times a mass damping coefficient and the nodal stiffness times a stiffness damping coefficient. In general, the mass damping portion damps out low-frequency modes in the mesh, while the stiffness damping portion damps out higher-frequency terms. Appropriate values for the damping coefficients depend on the frequencies of interest in the mesh. The general expression for the critical damping fraction, c_d, for a given frequency is

$$c_d = (k_d * \omega + m_d/\omega)/2\,, \tag{6.6}$$

where k_d is the stiffness damping coefficient, m_d is the mass damping coefficient, and ω is the frequency of interest. The stiffness damping portion must be used with caution. Because this term depends on the stiffness, it can affect the critical time step. Thus certain ranges of values for the stiffness damping coefficient can change the critical time step for the mesh. As Presto does not currently modify the critical time step based on the selected values for this coefficient, some choices for this parameter can cause solution instability.

6.10.6.1 Block Set Commands

The `block set commands` portion of the `VISCOUS DAMPING` command block defines a set of element blocks associated with the viscous damping and can include some combination of the following command lines:

```
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of element blocks. See Section 6.1.1 for more information about the use of these command

lines for creating a set of element blocks used by viscous damping. There must be at least one `BLOCK` or `INCLUDE ALL BLOCKS` command line in the command block.

All the nodes associated with the elements specified by the block set commands will have viscous damping forces applied.

6.10.6.2 Viscous Damping Coefficient

The mass damping coefficient, m_d, in Equation 6.6 is specified using the parameter `mass_damping` on the command line:

```
MASS DAMPING COEFFICIENT = <real>mass_damping
```

Mass damping most strongly damps the low-frequency modes, and in Presto, is applied as a boundary condition which does not affect the critical time step.

The stiffness damping coefficient, k_d, in Equation 6.6, is specified as the parameter `stiff_damping` on the command line:

```
STIFFNESS DAMPING COEFFICIENT = <real>stiff_damping
```

Stiffness damping most strongly damps high-frequency modes and is applied through a stress correction of the pressure term at the element level. Because this type of damping is done at the element level, it has a direct effect on the critical time step as seen in Equation 6.7, where $\epsilon = \frac{k_d \omega}{2}$ in the absence of mass damping and $\frac{2}{\omega} \approx \frac{m}{\kappa}$.

$$\Delta t \leq \frac{2}{\omega}\left(\sqrt{1+\epsilon^2} - \epsilon\right) \tag{6.7}$$

6.10.6.3 Additional Command

The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines can optionally appear in the `VISCOUS DAMPING` command block:

```
ACTIVE PERIODS = <string list>period_names
INACTIVE PERIODS = <string list>period_names
```

This command line can activate or deactivate the viscous damping for certain time periods. See Section 2.5 for more information about this command line.

6.10.7 Volume Repulsion Old

```
BEGIN VOLUME REPULSION OLD <string>repulsion
  FRICTION COEFFICIENT = <real>fric_coeff
  SCALE FACTOR = <real>scale_factor
  OVERLAP TYPE = [NODAL|VOLUMETRIC]

  BEGIN BLOCK SET <string>set
    BLOCK = <string list>block_names
    INCLUDE ALL BLOCKS
    REMOVE BLOCK = <string list>block_names
    #
    SURFACE = <string list>surface_names
    REMOVE SURFACE = <string list>surface_names
    #
    ACTIVE PERIODS = <string list>period_names
    INACTIVE PERIODS = <string list>period_names
    #
    LINE CYLINDER RADIUS = <real>cylinder_radius
    ELEMENT REPRESENTATION = [BEAM_ELEMENT_CYLINDERS|
      TRUE_SOLID_VOLUME|NODES]
  END [BLOCK SET <string>set]
END [VOLUME REPULSION OLD <string>repulsion]
```

The `VOLUME REPULSION OLD` command block is used to create a cylindrical volume around beam elements that is used as a frictional contact surface. Because beam elements are represented as line elements, there is no volume associated with the elements that can be used for contact. This command will generate nodal forces based on interpenetrations of a prescribed set of nodes with the cylindrical contact surfaces. The force is generated using a penalty stiffness method where the magnitude of the force depends on the mass of the node and the current time step. This command will be replaced by Dash contact in the future.

Definition of the coefficient of friction for the cylindrical surface is defined through the `FRICTION COEFFICIENT` command line.

The `SCALE FACTOR` command line specifies a scale factor that scales the force produced from node-surface interactions.

The `OVERLAP TYPE` command line must always be set to `VOLUMETRIC`.

6.10.7.1 Block Set

Complete definition of the contact surfaces and node sets are completely defined within multiple `BLOCK SET` command blocks. At least two `BLOCK SET` command blocks must be defined, one that defines the beam element blocks to wrap in cylinders by setting the `ELEMENT REPRESENTATION` command line to `BEAM_ELEMENT_CYLINDERS`. The second `BLOCK SET` command block defines the node set used to contact the cylindrical surfaces by setting the

`ELEMENT REPRESENTATION` to `NODES`.

The `BLOCK`, `INCLUDE ALL BLOCKS` and `REMOVE BLOCK` command lines must be used when defining the beam element blocks, while a combination of these block command lines and the following surface command lines, `SURFACE` and `REMOVE SURFACE`, must be used to define the node set used for contact.

`ACTIVE PERIODS`command line defined the time periods in which this boundary condition is active, whereas the `INACTIVE PERIODS` command line defines when this boundary condition is inactive.

The `LINE CYLINDER RADIUS` command line specifies the radius of the cylindrical surface around the beam elements.

6.10.8 General Multi-Point Constraints

```
BEGIN MPC
  #
  # Master/Slave MPC commands
  MASTER NODE SET = <string list>master_nset
  MASTER NODES = <integer list>master_nodes
  MASTER SURFACE = <string list>master_surf
  MASTER BLOCK = <string list>master_block
  SLAVE NODE SET = <string list>slave_nset
  SLAVE NODES = <integer list>slave_nodes
  SLAVE SURFACE = <string list>slave_surf
  SLAVE BLOCK = <string list>slave_block
  #
  # Tied contact search commands
  SEARCH TOLERANCE = <real>tolerance
  VOLUMETRIC SEARCH TOLERANCE = <real>vtolerance
  #
  # Tied MPC commands
  TIED NODES = <integer list>tied_nodes
  TIED NODE SET = <string list>tied_nset
  #
  # DOF subset selection
  COMPONENTS = <enum>X|Y|Z|RX|RY|RZ
END [MPC]

# Control handling of multiple MPCs
RESOLVE MULTIPLE MPCS = ERROR|FIRST WINS|LAST WINS(ERROR)
```

Presto provides a general multi-point constraint (MPC) capability that allows a code user to specify arbitrary constraints between sets of nodes. The commands to define a MPC are all listed within a `MPC` command block. There are three types of MPCs: master/slave, tied contact, and tied. All of these types of MPCs are defined within the `MPC` command block, but different commands are used within that block for each case. The commands for each of these types of MPCs are described in detail below.

MPCs can potentially be in conflict with other constraints. Refer to Appendix D for information on how conflicting constraints are handled.

6.10.8.1 Master/Slave Multi-Point Constraints

The master/slave type of MPC imposes a constraint between a set of master nodes and a set of slave nodes. The motion of the three translational degrees of freedom of the slave nodes is constrained to be equal to the average motion of the master nodes. This type of MPC is typically most useful if there is either a single master node and one or more slave nodes, or multiple master nodes and a single slave node. If there are multiple slave nodes, they are constrained to move together as a set.

The sets of master and slave nodes used in the MPC can be defined by using a node set on the mesh file, a list of nodes provided in the input file, or a surface on the mesh file from which a list of nodes is extracted. This can be done for the set of master nodes using one or more of the following commands:

```
MASTER NODE SET = <string list>master_nset
MASTER NODES = <integer list>master_nodes
MASTER SURFACE = <string list>master_surf
MASTER BLOCK = <string list>master_block
SLAVE NODE SET = <string list>slave_nset
SLAVE NODES = <integer list>slave_nodes
SLAVE SURFACE = <string list>slave_surf
SLAVE BLOCK = <string list>slave_block
```

The `MASTER NODE SET` and `SLAVE NODE SET` command lines specify the names of node sets in the mesh file. The nodes in these node sets are included in the sets of master or slave nodes for the constraint.

The `MASTER NODES` and `SLAVE NODES` command lines specify lists of integer IDs of nodes to be included in the sets of master or slave nodes for the constraint.

The `MASTER SURFACE` and `SLAVE SURFACE` command lines specify the name of a surface in the mesh file. The nodes contained in this surface are included in the sets of master or slave nodes for the constraint.

The `MASTER BLOCK` and `SLAVE BLOCK` command lines specify the names of a block in the mesh file. The nodes contained in these blocks are included in the sets of master or slave nodes for the constraint.

6.10.8.2 Tied Contact

A proximity search can optionally be performed to create a set of MPCs that act as tied contact constraints. If the MPCs are created in this way, the search is performed at the time of initialization to find pairings of slave nodes to master faces. A separate constraint is created for each slave node. This is equivalent to using pure master/slave tied contact, and is significantly faster than Presto's standard tied contact for explicit dynamics.

```
SEARCH TOLERANCE = <real> tolerance
```

The `SEARCH TOLERANCE` command line is used to request that a search be performed to create node/face constraints. This line must be present to use MPCs for tied contact. The tolerance value given on the line specifies the maximum distance between a node and a face to create an MPC. This has a similar meaning to the search tolerance used in standard tied contact.

Warning: The `SEARCH TOLERANCE` command line must be present to use MPCs for tied contact. If this command is not present in the `MPC` command block, a master/slave MPC as described in Section 6.10.8.1 will result. All slave nodes would be tied to all master nodes, which is very different from tied contact.

```
VOLUMETRIC SEARCH TOLERANCE = <real> vtolerance
```

In addition to creating node/face constraints, a search can be used to create volumetric constraints, in which a slave node is constrained to a volume bounded by master faces. The `VOLUMETRIC SEARCH TOLERANCE` command is used to enable volumetric constraints and sets the tolerance used for the search. The slave node is constrained to all nodes on the master surface that are within the volumetric search tolerance, `vtolerance`.

Currently the primary usage of volumetric constraints is to constrain a meshed void placed inside another mesh. The volumetric search is used in conjunction with the node/face search. A set of node/face constraints is first created for slave nodes within the standard search tolerance of any master face. Next, a volumetric constraint is created for any remaining unconstrained slave node within the volumetric search tolerance of the node/face constrained nodes. The volumetric constraint is formulated in a way that approximates an isoparametric map.

To use MPCs for tied contact, the master and slave surfaces must be defined. These may be defined using the `MASTER SURFACE`, `MASTER BLOCK`, `SLAVE NODE SET`, `SLAVE SURFACE`, and `SLAVE BLOCK` line commands. These are a subset of the commands available to define master/slave MPCs, as described in Section 6.10.8.1. It is important to note that the `MASTER NODE SET` can not be used to use MPCs for tied contact. The master surface must have information about faces, and this is not available with a node set.

The following example demonstrates how to use MPCs for tied contact between two surfaces:

```
BEGIN MPC
  MASTER SURFACE = surface_10
  SLAVE SURFACE = surface_11
  SEARCH TOLERANCE = 0.0001
END MPC
```

The following example demonstrates the usage of MPCs for both tied and volumetric constraints. Assuming that `surface_10` surrounds the exterior surface of `block_1`, this block would result in tied contact between the nodes on the exterior of `block_1` and `surface_10`, and volumetric constraints between the nodes on the interior of `block_1` and `surface_1`.

```
BEGIN MPC
  MASTER SURFACE = surface_10
  SLAVE BLOCK = block_1
  SEARCH TOLERANCE = 0.0001
  VOLUMETRIC SEARCH TOLERANCE = 3.0
END MPC
```

6.10.8.3 Tied Multi-Point Constraints

The tied type of MPC imposes a constraint that ties together the motion of the three translational degrees of freedom for a set of nodes. Nodes are not specified as being masters or slaves for this type of constraint. The set of nodes to be tied together can be specified as either a list of node IDs or with a node set by using the `TIED NODES` or `TIED NODE SET` command.

```
TIED NODES = <integer list>tied_nodes
TIED NODE SET = <string list>tied_nset
```

The `TIED NODES` command line is used to specify an integer list of IDs of the nodes to be tied together. The `TIED NODE SET` can be used to specify the name of a node set that contains the nodes to be tied together. Only one of these commands can be used in a given `MPC` command block.

Warning: The tied MPC described here does not do a contact search. For the MPC to behave like tied contact, use the commands described in Section 6.10.8.2.

6.10.8.4 Resolve Multiple MPCs

The behavior of multi-point constraints is ill-defined when a master node is constrained to more than one set of slave nodes. Presto's MPC capability can handle chained MPCs, where a master node is a slave node in another constraint, but it cannot simultaneously enforce multiple MPCs that have the same master.

```
RESOLVE MULTIPLE MPCS = ERROR|FIRST WINS|LAST WINS(ERROR)
```

The `RESOLVE MULTIPLE MPCS` command line, used within the region scope, controls how to resolve cases where a slave node is constrained to more than one set of master nodes. Although multiple MPCs cannot be simultaneously enforced, this command provides ways to work around this problem that may be acceptable in many situations. The default option is `ERROR`, which results in an error message and terminates the code if this occurs. Alternatively, this command can be set to `FIRST WINS` to keep the first MPC found for a given slave node or `LAST WINS` to keep the last MPC found. This command line controls the behavior of all MPCs in the model.

6.10.8.5 Constraining a Subset of all DOFs

By default, multi-point constraints are applied to all degrees of freedom of the nodes involved. For nodes that only have translational degrees of freedom, all three components (X, Y and Z) are constrained. Likewise, for nodes that have both translational and rotational degrees of freedom, all six components (X, Y, Z, RX, RY and RZ) are constrained. The `COMPONENTS` command line can be used to enforce the constraint on a subset of the degrees of freedom. If the `COMPONENTS` command line is included in a `MPC` command block, only the components listed would be constrained.

6.10.9 Submodel

```
BEGIN SUBMODEL
  #
  EMBEDDED BLOCKS = <string list>embedded_block
  ENCLOSING BLOCKS = <string list>enclosing_block
END [SUBMODEL]
```

Presto provides a method to embed a submodel in a larger finite element model. The element blocks for both the submodel and the larger system model should exist in the same mesh file. The space occupied by the embedded blocks should also be occupied by the enclosing blocks.

This capability ties each node of the submodel to an element in the larger finite element model. The code makes no correction for mass due to volume overlap. However, this correction in many cases can be done easily by hand simply by adjusting the density of the submodel block so that it is the difference between the density of the submodel block and the enclosing block.

The embedded blocks (the submodel blocks) and the enclosing blocks (the system model blocks) are specified using the following two line commands:

```
  EMBEDDED BLOCKS = <string list>embedded_block
  ENCLOSING BLOCKS = <string list>enclosing_block
```

For example, to embed `block_7` and `block_8` inside a system model where the embedded blocks are within `block_2`, `block_3`, and `block_5`, the following can be used:

```
BEGIN SUBMODEL
  EMBEDDED BLOCKS = block_7 block_8
  ENCLOSING BLOCKS = block2 block_3 block_5
END
```

6.11 References

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2. Kingery, C. N. and Bulmash, G. *Airblast Parameters from TNT Spherical Air Burst and Hemispherical Surface Burst,* Technical Report ARBBRL-TR-02555, Aberdeen Proving Ground, MD: Ballistic Research Laboratory, April 1984.

3. Randers-Pehrson, G. and Bannister, K. A. *Airblast Loading Model for DYNA2D and DYNA3D,* ARL-TR-1310, Army Research Laboratory, March 1997.

4. Protective Design Center, United States Army Corps of Engineers, *ConWep 2.1.0.8.* link.

5. Lysmer, J., and R. L. Kuhlmeyer. "Finite Dynamic Model for Infinite Media." *Journal of the Engineering Mechanics Division, Proceedings of the American Society of Civil Engineers* (August 1979): 859–877.

6. Cook, R. D., Malkus, D. S., and Plesha, M. E. *Concepts and Applications of Finite Element Analysis, Third Edition.* New York: John Wiley and Sons, 1989.

Chapter 7

Contact

This chapter describes the input syntax for defining interactions of contact surfaces in a Presto analysis. For more information on contact and its computational details, consult References 1 and 2.

Contact constraints can potentially be in conflict with other constraints. Refer to Appendix D for information on how conflicting constraints are handled.

Contact refers to the interaction of bodies when they physically touch. This can include the interaction of one part of a surface against another part of the same surface, the surface of one body against the surface of another body, and so forth. The contact algorithms within Presto are designed to ensure that surfaces do not interpenetrate in a nonphysical way, and that the interface behavior is computed correctly according to any user-specified surface-physics models (e.g., energy dissipation from a friction model). Presto uses a kinematic approach rather than a penalty approach to eliminate the interpenetration of surfaces. In the kinematic approach, a series of constraint equations that remove interpenetration are satisfied. A penalty approach can be thought of as introducing "stiff" springs between contact surfaces as a means of preventing interpenetration.

Contact between surfaces is enforced as node-face interactionsor face-face interactions if the dash contact algorithm is used. Consider the two-dimensional contact problem shown in Figure 7.1. Block a is enclosed by surface a, and block b is enclosed by surface b. A surface is defined by a collection of finite element faces. The surface of a block of hexahedral elements, for example, is a collection of quadrilateral faces on the surface of the block. For this two-dimensional drawing, the faces are straight lines between two nodes. Only the faces on the portions of the surfaces that will come into contact are shown.

Figure 7.1 shows the two blocks at time step n. Figure 7.2 shows the blocks at time step $n + 1$ when the blocks have moved and deformed under the influence of external forces. Before contact is taken into account, the two blocks interpenetrate one another. This interpenetration is removed by applying the contact algorithm.

For interpenetration to occur as shown in Figure 7.2, any node on surface a that penetrates surface b must pass through some face on surface b. Likewise, each node on surface b that penetrates surface a must pass through some face on surface a. All the nodes on surface a could be forced to lie on surface b, where surface b has the configuration shown in Figure 7.2. In this case, surface b

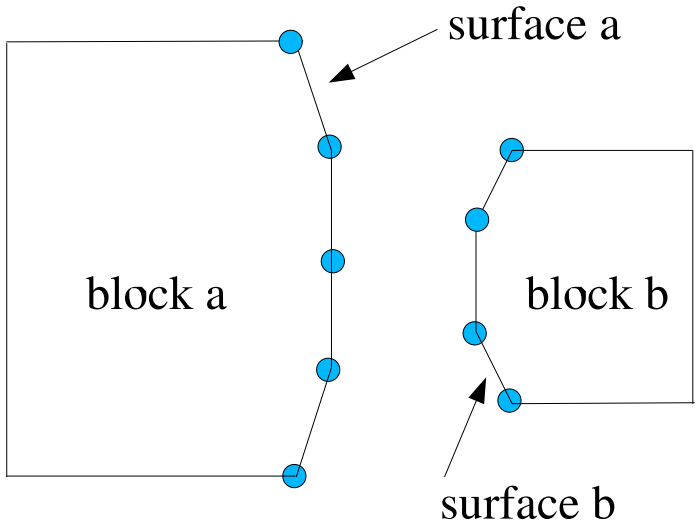

Figure 7.1: Two blocks at time step n before contact.

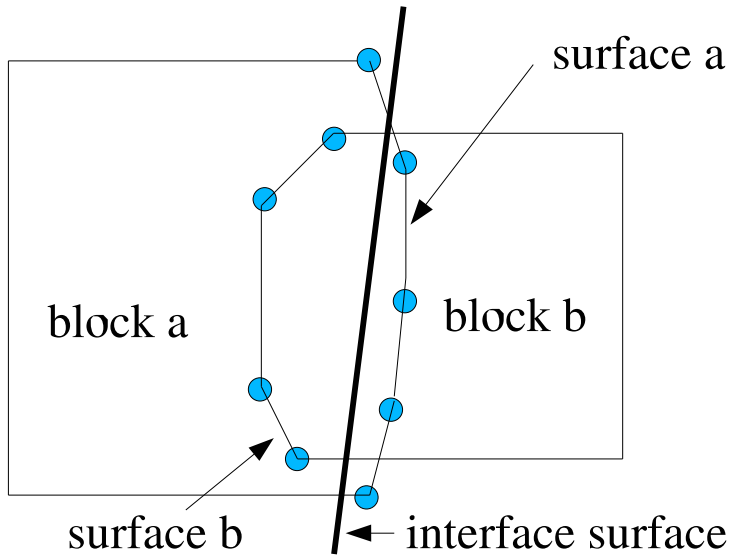

Figure 7.2: Two blocks at time step $n + 1$, after penetration.

would be a master surface and surface a would be a slave surface. Or all nodes on surface b could be forced to lie on surface a, in which case surface a is a master surface and surface b is the slave. More typically, nodes on both surfaces are moved to what can be described as an interface surface, which is shown by a thick black line in Figure 7.2. The interface surface is shown here as a straight line, but it would actually be a curved line in almost all cases.

For the typical case, for each node on surface a that has penetrated some face on surface b, forces based on the amount of node penetration are placed on both the node on a and the nodes associated with the face on b to remove "some part" of the interpenetration. Likewise, forces are computed

for each node on surface *b* that has penetrated some face on surface *a* and for the nodes associated with the penetrated face on surface *a* to remove "another part" of the interpenetration. This node-face interaction from both contact surfaces is typically what is encountered in Presto, and it is referred to as "symmetric" contact. After the nodes on both surfaces, *a* and *b*, have been moved, we have defined an interface surface. A more detailed discussion of how we move the nodes on both surfaces is given in those sections related to kinematic partitioning, Section 7.15.4 and Section 7.16.2.

The preceding two-dimensional example is analogous to much of the contact that is encountered when contact is used in an analysis. Surfaces are generated that consist of a collection of faces, each face being defined by a nodal connectivity. Node-face interactions from both contact surfaces (symmetric contact) are used to move nodes to account for any interpenetration of the surfaces. Presto will also handle variations of the node-face contact described as follows:

- In some cases, you may want one surface of a surface pair to determine the interface surface. One surface will be designated as the master surface. The opposing surface will be designated as the slave surface. The nodes on the slave surface will be moved to the master surface. The master surface sets the interface surface. This arrangement would be a pure master-slave situation. You might want to use this arrangement if you had a very stiff surface like steel contacting a very weak surface like foam.

- In some cases, you may want one surface of a surface pair to be more influential in determining the interface surface than its opposing surface. This arrangement is done by "weighting" the more influential surface and involves a concept called kinematic partitioning. The above case of pure master-slave represents the limiting case for kinematic partitioning.

- A special case of contact called "tied contact" allows you to tie two surfaces on different objects together. The two surfaces that are tied together share a coincident surface or are in very close proximity at time 0.0. The initial point of contact between a tied node and an opposing face at time 0.0 is maintained for all times. At each time step, the node is moved so that it as the same point on the face regardless of where the faces move or how the face deforms.

- One of the surfaces in a contact pair can be an analytic surface. An analytic surface is defined by an algebraic expression, not by a collection of faces derived from elements. The algebraic expression that defines the surface of a cylinder is an example of an analytic surface. The nodes on the opposing surface cannot penetrate the analytic surface.

- Instead of having two surfaces in contact, you can have a set of nodes not associated with faces that contacts a surface. We refer to this set of nodes as a "contact node set." The nodes in the contact node set can contact a surface that is a collection of faces (the usual surface definition) or an analytic surface. The nodes in the contact node set cannot penetrate the surface.

- A mesh could have an initial interpenetration of two surfaces due to the meshing process. We refer to this situation as "initial overlap." You have the option of removing this initial overlap.

- An element block can contact itself. A block of elements may deform to such an extent that a part of the surface of the block comes into contact with another part of the surface of the block. This is referred to as "self-contact." For self-contact, a node that is part of an element block can contact a face that is exterior to the same element block.

There are some special considerations for contact with structural elements (i.e. shells, springs, trusses, beams) with the current implementation of contact. A shell element has both a top face and a bottom face that are defined by the same geometric entity. One-dimensional elements (springs, trusses, and beams) have no faces.

Shell elements are handled by the contact algorithm, but they are much more difficult to handle than solid elements. Determining whether a node has penetrated a shell element is more difficult than determining whether a node has penetrated a solid. For a solid element with an external face, there is only one normal for the face. For a shell element, there are two faces—one on each side of the geometric entity that defines the shell. Each face has a normal, and the two normals for the shell element point in opposite directions. For shell elements, two faces are constructed for the element within the contact algorithm. The faces, each with a unique outward normal, can be coincident, or they can be separated by the thickness of the shell. Separating the two shell faces that are originally coincident at the geometric plane of the shell by the thickness of the shell is referred to as "lofting." To implement lofting, we need information about the thickness of the shell. This information is specified in the `SHELL SECTION` command block described in Section 5.2.4. For more information on lofting, see Section 7.9.

Contact for shell elements is only considered on shell faces; shell edges are currently not considered. The contact of a shell edge with another shell edge is not detected, and the contact of a shell edge with a continuum element edge is not detected. A shell element can coincide with the face of a continuum element. The contact algorithm will properly account for this situation. Two shell elements can also overlay each other, i.e., share the same set of nodes. The contact algorithm will also properly account for this situation. For a block of shell elements, two surfaces are created in contact.

Contact for one-dimensional elements (springs, trusses, beams) is currently implemented only for one-dimensional elements contacting a surface. The contact algorithm will not detect contact of a one-dimensional element with the edge of a continuum element, with the edge of a shell element, or with another one-dimensional element. Contact of one-dimensional elements is discussed in Section 7.2.4.

Contact in Presto is implemented in two distinct phases: a search algorithm and an enforcement algorithm. The search algorithm identifies nodes that have penetrated a face, while the enforcement algorithm computes the forces to remove penetration and the forces that observe the user-specified surface physics. The contact search within Presto focuses on large-scale global contact in a massively parallel environment. This processing step can be quite expensive, taking upwards of 60% of the analysis time, especially on multiprocessor analyses. The search algorithm relies on normal and tangential tolerances to describe a region around each face within which any nodes found are identified as potential interactions. The size of these tolerances is problem dependent.

The enforcement algorithm is based on a kinematic approach that satisfies momentum balance. A kinematic approach with momentum balance enforcement, where iterations are used to ensure

normal impact momentum balance and frictional response, is always more accurate than a penalty approach. Consequently, when the surface interaction involves a frictional response, the kinematic approach with momentum balance is recommended.

A number of friction models are available to describe the surface interactions. In this chapter on contact, we will use the term *friction model* for what is really a surface-physics model.

Contact within a Presto analysis is defined within a `CONTACT DEFINITION` command block. Within the contact definition scope, there are command lines and command blocks that define the specifics for the interaction of surfaces via the contact algorithm. Some of the command lines and command blocks within the contact scope set up default parameters that affect all contact calculations. Some of the command blocks in the contact scope affect only the interaction between a pair of surfaces.

There are three approaches that can be used to define a contact problem:

1. Accept all the Presto default parameters for a problem.
2. Accept the Presto default parameters for some of the contact surfaces. For the rest of the contact surfaces, the user can set values in interactions.
3. Define all surface-pair interactions separately.

Note that the speed of contact is based primarily on the number of nodes and faces in the contact surfaces and, to a much lesser extent, on the number of interactions specified. Consequently, choosing the third approach above is not likely to reduce the run time significantly.

The general pattern of syntax for describing contact is as follows:

- Identify all surfaces that need to be considered for contact. This is done with command lines (or command blocks) within the contact scope.
- Specify any analytic surface used for contact. Analytic surfaces are described with a command block.
- Specify any special contact options such as initial overlap removal or angle for multiple interactions. This is done with command lines within the contact scope.
- Describe friction models used in the surface interactions for this analysis. Currently, there are 11 types of friction models. user subroutines can also be used as friction models. A friction model is described with a command block.
- Set contact enforcement options that will apply to all the surface interactions. These values are set in the `ENFORCEMENT OPTIONS` command block.
- Set contact search options that will serve as defaults for all the surface interactions. These values are set in the `SEARCH OPTIONS` command block.
- Set default interaction values that apply to all the surface interactions. These values are set in the `INTERACTION DEFAULTS` command block.

- Specify values for interactions between specific contact surfaces. This is done within an `INTERACTION` command block. Values specified in this command block override the defaults for the particular pair of surface interactions.

7.1 Contact Definition Block

All commands for contact occur within a `CONTACT DEFINITION` command block. A summary of these commands follows.

```
BEGIN CONTACT DEFINITION <string>name
  #
  CONTACT SURFACE <string>name
    CONTAINS <string list>surface_names
  #
  SKIN ALL BLOCKS = <string>ON|OFF(OFF)
    [EXCLUDE <string list> block_names]
  #
  BEGIN CONTACT SURFACE <string>name
    BLOCK = <string list>block_names
    SURFACE = <string list>surface_names
    NODE SET = <string list>node_set_names
    REMOVE BLOCK = <string list>block_names
    REMOVE SURFACE = <string list>surface_names
    REMOVE NODE SET = <string list>nodelist_names
  END [CONTACT SURFACE <string>name]
  #
  CONTACT NODE SET <string>surface_name
    CONTAINS <string>nodelist_names
  #
  CONTACT FORMULATION TYPE = <string>ACME|DASH(ACME)
  #
  BEGIN ANALYTIC PLANE <string>name
    NORMAL = <string>defined_direction
    POINT = <string>defined_point
    REFERENCE RIGID BODY = <string>rb_name
  END [ANALYTIC PLANE <string>name]
  #
  BEGIN ANALYTIC CYLINDER <string>name
    CENTER = <string>defined_point
    AXIAL DIRECTION = <string>defined_axis
    RADIUS = <real>cylinder_radius
    LENGTH = <real>cylinder_length
    CONTACT NORMAL = <string>OUTSIDE|INSIDE
  END [ANALYTIC CYLINDER <string>name]
  #
  BEGIN ANALYTIC SPHERE <string>name
    CENTER = <string>defined_point
    RADIUS = <real>sphere_radius
  END [ANALYTIC SPHERE <string>name]
  #
  UPDATE ALL SURFACES FOR ELEMENT DEATH = <string>ON|OFF(ON)
```

```
#
BEGIN REMOVE INITIAL OVERLAP
  OVERLAP NORMAL TOLERANCE = <real>over_norm_tol
  OVERLAP TANGENTIAL TOLERANCE = <real>over_tang_tol
  SHELL OVERLAP ITERATIONS = <integer>max_iter(10)
  SHELL OVERLAP TOLERANCE = <real>shell_over_tol(0.0)
END [REMOVE INITIAL OVERLAP]
#
MULTIPLE INTERACTIONS = <string>ON|OFF(ON)
MULTIPLE INTERACTIONS WITH ANGLE = <real>angle_in_deg(60.0)
#
BEGIN SURFACE NORMAL SMOOTHING
  ANGLE = <real>angle_in_deg
  DISTANCE = <real>distance
  RESOLUTION = <string>NODE|EDGE
END [SURFACE NORMAL SMOOTHING]
#
ERODED FACE TREATMENT = <string>NONE|ALL(ALL)
#
BEGIN SHELL LOFTING
  SURFACE = <string_list>surface_names
  REMOVE SURFACE = <string_list>removed_surface_names
  LOFTING ALGORITHM = <string>ON|OFF(ON)
  COINCIDENT SHELL TREATMENT = <string>DISALLOW|IGNORE|
    SIMPLE(DISALLOW)
  COINCIDENT SHELL HEX TREATMENT = <string>DISALLOW|
    IGNORE|TAPERED|EMBEDDED(DISALLOW)
  CONTACT SHELL THICKNESS =
    ACTUAL_THICKNESS|LET_CONTACT_CHOOSE(ACTUAL_THICKNESS)
  ALLOWABLE SHELL THICKNESS TO ELEMENT SIZE RATIOS =
    <real>lower_bound(0.1) TO <real>upper_bound(1.0)
END [SHELL LOFTING]
#
BEGIN FRICTIONLESS MODEL <string>name
END [FRICTIONLESS MODEL <string>name]
#
BEGIN CONSTANT FRICTION MODEL <string>name
  FRICTION COEFFICIENT = <real>coeff
END [CONSTANT FRICTION MODEL <string>name]
#
BEGIN TIED MODEL <string>name
END [TIED MODEL <string>name]
#
BEGIN GLUED MODEL <string>name
END [GLUED MODEL <string>name]
#
BEGIN SPRING WELD MODEL <string>name
```

```
  NORMAL DISPLACEMENT FUNCTION = <string>func_name
  NORMAL DISPLACEMENT SCALE FACTOR =
    <real>scale_factor(1.0)
  TANGENTIAL DISPLACEMENT FUNCTION = <string>func_name
  TANGENTIAL DISPLACEMENT SCALE FACTOR =
    <real>scale_factor(1.0)
  FAILURE ENVELOPE EXPONENT = <real>exponent(2.0)
  FAILURE DECAY CYCLES = <integer>num_cycles(1)
  FAILED MODEL = <string>failed_model_name|FRICTIONLESS
    (FRICTIONLESS)
END [SPRING WELD MODEL <string>name]
#
BEGIN SURFACE WELD MODEL <string>name
  NORMAL CAPACITY = <real>normal_cap
  TANGENTIAL CAPACITY = <real>tangential_cap
  FAILURE DECAY CYCLES = <integer>num_cycles(1)
  FAILED MODEL = <string>failed_model_name|FRICTIONLESS
    (FRICTIONLESS)
END [SURFACE WELD MODEL <string>name]
#
BEGIN AREA WELD MODEL <string>name
  NORMAL CAPACITY = <real>normal_cap
  TANGENTIAL CAPACITY = <real>tangential_cap
  FAILURE DECAY CYCLES = <integer>num_cycles(1)
  FAILED MODEL = <string>failed_model_name|FRICTIONLESS
    (FRICTIONLESS)
END [AREA WELD MODEL <string>name]
#
BEGIN ADHESION MODEL <string>name
  ADHESION FUNCTION = <string>func_name
  ADHESION SCALE FACTOR = <real>scale_factor(1.0)
END [ADHESION MODEL <string>name]
#
BEGIN COMPLIANT JOINT MODEL <string>name
  NORMAL MODULUS = <real>norm_mod
  SHEAR MODULUS = <real>shear_mod
  APERTURE = <real>aperture
  APERTURE LIMIT = <real>aperture_limit
  FRICTION COEFFICIENT = <real>fric_coef
  COHESION = <real>cohesion
END [COMPLIANT JOINT MODEL <string>name]
#
BEGIN COHESIVE ZONE MODEL <string>name
  TRACTION DISPLACEMENT FUNCTION = <string>func_name
  TRACTION DISPLACEMENT SCALE FACTOR = <real>scale_factor(1.0)
  CRITICAL NORMAL GAP = <real>crit_norm_gap
  CRITICAL TANGENTIAL GAP = <real>crit_tangential_gap
```

```
END [COHESIVE ZONE MODEL <string>name]
#
BEGIN JUNCTION MODEL <string>name
  NORMAL TRACTION FUNCTION = <string>func_name
  NORMAL TRACTION SCALE FACTOR = <real>scale_factor(1.0)
  TANGENTIAL TRACTION FUNCTION = <string>func_name
  TANGENTIAL TRACTION SCALE FACTOR = <real>scale_factor(1.0)
  NORMAL CUTOFF DISTANCE FOR TANGENTIAL TRACTION =
    <real>distance
END [JUNCTION MODEL <string>name]
#
BEGIN THREADED MODEL <string>name
  NORMAL TRACTION FUNCTION = <string>func_name
  NORMAL TRACTION SCALE FACTOR = <real>scale_factor(1.0)
  TANGENTIAL TRACTION FUNCTION = <string>func_name
  TANGENTIAL TRACTION SCALE FACTOR =
    <real>scale_factor(1.0)
  TANGENTIAL TRACTION GAP FUNCTION = <string>func_name
  TANGENTIAL TRACTION GAP SCALE FACTOR = <real>scale_factor(1.0)
  NORMAL CAPACITY = <real>normal_cap
  TANGENTIAL CAPACITY = <real>tangential_cap
  FAILURE ENVELOPE EXPONENT = <real>exponent(2.0)
  FAILURE DECAY CYCLES = <integer>num_cycles(1)
  FAILED MODEL = <string>failed_model_name|FRICTIONLESS
    (FRICTIONLESS)
END [THREADED MODEL <string>name]
#
BEGIN PV_DEPENDENT MODEL <string>name
  STATIC COEFFICIENT = <real>stat_coeff
  DYNAMIC COEFFICIENT = <real>dyn_coeff
  VELOCITY DECAY = <real>vel_decay
  REFERENCE PRESSURE = <real>p_ref
  OFFSET PRESSURE = <real>p_off
  PRESSURE EXPONENT = <real>p_exp
END [PV_DEPENDENT MODEL <string>name]
#
BEGIN TIME VARIANT MODEL <string>name
  MODEL = <string>model DURING PERIODS <string_list>time_periods
END [TIME VARIANT MODEL]
#
BEGIN USER SUBROUTINE MODEL <string>name
  INITIALIZE MODEL SUBROUTINE = <string>init_model_name
  INITIALIZE TIME STEP SUBROUTINE = <string>init_ts_name
  INITIALIZE NODE STATE DATA SUBROUTINE =
    <string>init_node_data_name
  LIMIT FORCE SUBROUTINE = <string>limit_force_name
  ACTIVE SUBROUTINE = <string>active_name
```

```
  INTERACTION TYPE SUBROUTINE = <string>interaction_name
END [USER SUBROUTINE MODEL <string>name]
#
BEGIN SEARCH OPTIONS [<string>name]
  GLOBAL SEARCH INCREMENT = <integer>num_steps(1)
  GLOBAL SEARCH ONCE = <string>ON|OFF(OFF)
  SEARCH TOLERANCE = <string>AUTOMATIC|USER_DEFINED(AUTOMATIC)
  NORMAL TOLERANCE = <real>norm_tol
  TANGENTIAL TOLERANCE = <real>tang_tol
  FACE MULTIPLIER = <real>face_multiplier(0.1)
  SECONDARY DECOMPOSITION = <string>ON|OFF(OFF)
END [SEARCH OPTIONS <string>name]
#
BEGIN USER SEARCH BOX <string>name
  CENTER = <string>center_point
  X DISPLACEMENT FUNCTION = <string>x_disp_function_name
  Y DISPLACEMENT FUNCTION = <string>y_disp_function_name
  Z DISPLACEMENT FUNCTION = <string>z_disp_function_name
  X DISPLACEMENT SCALE FACTOR = <real>x_disp_scale_factor
  Y DISPLACEMENT SCALE FACTOR = <real>y_disp_scale_factor
  Z DISPLACEMENT SCALE FACTOR = <real>z_disp_scale_factor
END [SEARCH OPTIONS <string>name]
#
BEGIN ENFORCEMENT OPTIONS [<string>name]
  MOMENTUM BALANCE ITERATIONS = <integer>num_iter(5)
  NUM GEOMETRY UPDATE ITERATIONS = <integer>num_iter(5)
END [ENFORCEMENT OPTIONS <string>name]
#
BEGIN INTERACTION DEFAULTS [<string>name]
  CONTACT SURFACES = <string list>surface_names
  SELF CONTACT = <string>ON|OFF(OFF)
  GENERAL CONTACT = <string>ON|OFF(OFF)
  AUTOMATIC KINEMATIC PARTITION = <string>ON|OFF(OFF)
  INTERACTION BEHAVIOR = <string>SLIDING|
    INFINITESIMAL_SLIDING|NO_INTERACTION(SLIDING)
  FRICTION MODEL = <string>friction_model_name|
    FRICTIONLESS(FRICTIONLESS)
  CONSTRAINT FORMULATION = <string>NODE_FACE|FACE_FACE
END [INTERACTION DEFAULTS <string>name]
#
BEGIN INTERACTION [<string>name]
  SURFACES = <string>surface1 <string>surface2
  MASTER = <string>surface
  SLAVE = <string>surface
  KINEMATIC PARTITION = <real>kin_part
  NORMAL TOLERANCE = <real>norm_tol
  TANGENTIAL TOLERANCE = <real>tang_tol
```

```
    FACE MULTIPLIER = <real>face_multiplier(0.1)
    OVERLAP NORMAL TOLERANCE = <real>over_norm_tol
    OVERLAP TANGENTIAL TOLERANCE = <real>over_tang_tol
    FRICTION MODEL = <string>friction_model_name|
      FRICTIONLESS(FRICTIONLESS)
    AUTOMATIC KINEMATIC PARTITION
    INTERACTION BEHAVIOR = <string>SLIDING|
      INFINITESIMAL_SLIDING|NO_INTERACTION(SLIDING)
    CONSTRAINT FORMULATION = <string>NODE_FACE|FACE_FACE
  END [INTERACTION <string>name]
  #
  BEGIN DASH OPTIONS
    SCALE FACTOR = <real>factor(1.0)
    ENFORCEMENT CONVERGENCE TOLERANCE = <real>1.0e-05
    HIDDEN SELF CONTACT = <string>TRUE|FALSE(TRUE)
    LOFTED SPHERE REPRESENTATION =
      TETRAHEDRON|OCTAHEDRON|CUBE|ICOSAHEDRON(ICOSAHEDRON)
  END
  #
END [CONTACT DEFINITION <string>name]
```

The command block begins with the input line:

```
BEGIN CONTACT DEFINITION <string>name
```

and is terminated with the input line:

```
END [CONTACT DEFINITION <string>name]
```

where `name` is a name for this contact definition. The name should be unique among all the contact definitions in an analysis. All other contact commands are encapsulated within this command block, as shown in the summary of the block presented previously. These other contact commands are described in Section 7.2through Section 7.16. Section 7.17 explains how to implement contact for several example problems.

A typical analysis will have only one `CONTACT DEFINITION` command block. However, more than one contact definition can be used. As each `CONTACT DEFINITION` command block creates its own contact entity, fewer of these command blocks provide more efficient contact processing.

7.2 Descriptions of Contact Surfaces

Contact determines whether two surfaces, each defined by either an analytic representation or a collection of finite element faces, have interpenetrated. This section describes how to define a surface composed of finite element faces. It also describes how to define a set of nodes (zero-dimensional entities) not associated with faces that can contact a surface, the surface being composed of finite element faces or the surface being an analytic surface. This latter case (a node not associated with a face contacting a surface) is useful for models where, for example, we have both continuum and SPH elements. (We will refer to nodes not associated with faces as "unassociated" nodes.) Defining rigid analytic surfaces is discussed in Section 7.3.

A surface is defined as a collection of finite element faces. Both continuum elements and shell elements have faces. For a continuum element, any face that is not shared with another element can be considered for contact. On the other hand, a shell element has both a top face and a bottom face. Top and bottom surfaces are automatically created for the contact algorithm and may be lofted by a user-specified thickness. Shell contact is done by computing the contact forces on the top and bottom surfaces of the shells and then moving the resulting forces back to the original shell nodes.

A contact surface can be generated from a block of continuum elements by "skinning" the block of elements. All exterior faces (any face not shared by two elements) are associated with the surface for that block when the block is skinned. If two blocks of continuum elements are connected (some of the element faces in one block are shared by the element faces in the other block) and both of these blocks are skinned, two surfaces with unique names will be generated. The resulting skinned surface for each block will consist only of faces that are exterior to both blocks. Any face shared by the two blocks will not be in either of the surfaces derived by skinning the two blocks. See Section 7.9 for more information about skinning with shells.

The contact enforcement algorithm only allows for a face to be associated with a single contact surface. If a face were allowed to belong to more than one surface involved in contact, ambiguities would arise in determining the interaction properties for that face. This situation could occur if multiple sidesets used in contact overlap. It could also occur if a sideset used in contact included the surface of a skinned block.

If a face is part of more than one contact surface, the face is included in the first contact surface to which it belongs that is listed in the `CONTACT DEFINITION` block. If it belongs to any other contact surface listed later in that block, it is excluded from that surface for the purpose of contact enforcement, and a warning message is generated.

To enforce contact between unassociated nodes and a surface, a contact node set must be defined. SPH particles contacting a surface is an example of nodes contacting a surface.The contact of one-dimensional elements (springs, trusses, beams) with a surface can be modeled as unassociated nodes contacting a surface, although, as in the case of shells, there are some limitations.

Surfaces involved in contact can be defined using the `CONTACT SURFACE` command line, the `CONTACT SURFACE` command block, or the `SKIN ALL BLOCKS` command line. Unassociated nodes involved in contact can be defined using the `CONTACT NODE SET` command line or the `CONTACT SURFACE` command block. The `CONTACT DEFINITION` command block can contain

any combination of these command lines and command blocks provided that contact surface names are not duplicated. The CONTACT DEFINITION command block must include some type of surface definition. Any element faces or unassociated nodes for use in a contact interaction must be identified as contact surfaces or contact node sets, respectively.

Section 7.2.1 through Section 7.2.4 describe the command lines and command blocks for defining contact surfaces composed of finite element faces and node sets that can contact surfaces.

7.2.1 Contact Surface Command Line

```
CONTACT SURFACE <string>name CONTAINS <string list>surface_names
```

This command line identifies a set of surfaces (specified as side sets) and element blocks that will be considered as a single contact surface; the string name is the unique name for this contact surface. The list denoted by surfaces_names is a list of strings identifying surfaces that are to be associated with this contact surface name. The surfaces can be side sets, element blocks, or any combination of the two as defined in the exodus file. These are not names of analytic surfaces. Any specified element blocks are "skinned," i.e., a surface is created from the exterior of the element block. See the previous discussion on skinning. Blocks of shell elements will be skinned, and the shell surfaces generated from a CONTACT SURFACE command line will be lofted for contact if the lofting algorithm is ON in the SHELL LOFTING command block.

If a block of one-dimensional elements (springs, trusses, beams) is included in the list of surface_names, the element block will be ignored. Thus, to include the one-dimensional elements for contact, a CONTACT NODE SET command line should be used. See Section 7.2.4.

The name you create for a surface can be referenced in command blocks that specify how that surface will interact with another contact surface or with itself. See Section 7.15.1 andSection 7.16.1.

The surfaces can contain a heterogeneous set of face types as well as any number of side sets and element blocks.

If a face appears in a side set and also in a set of faces generated by the skinning of an element block, that face will produce an error. As indicated previously, a given face may not appear in more than one contact surface.

7.2.2 Skin All Blocks

```
SKIN ALL BLOCKS = <string>ON|OFF(OFF)
  [EXCLUDE <string list>block_names]
```

You may wish to consider contact between the external surfaces of all the element blocks in the mesh. The SKIN ALL BLOCKS command line causes all element blocks to be "skinned," i.e., a surface is created from the exterior of each element block. The skinned surfaces are then given contact surface names identical to the name of the element block. For instance, if a mesh contained the element blocks block_1, block_10, and block_11, then SKIN ALL BLOCKS would create

three contact surfaces from these blocks with the names `block_1`, `block_10`, and `block_11`, respectively.

You can selectively delete some blocks from skinning by using the `EXCLUDE` option. Any blocks you do not want to be skinned will be included in a list of block names following `EXCLUDE`.

The `SKIN ALL BLOCKS` is useful for large models in which the individual specification of contact surfaces would be unwieldy.

If the `SKIN ALL BLOCKS` command line is used without the `EXCLUDE` option, contact surfaces cannot be defined by the above `CONTACT SURFACE` command line or the `CONTACT SURFACE` command block. The use of the `SKIN ALL BLOCKS` command line without the `EXCLUDE` option would include all exterior faces for all element blocks in the set of contact surfaces generated by the `SKIN ALL BLOCKS` command line. The added use of a `CONTACT SURFACE` command line or `CONTACT SURFACE` command block would then generate a new surface that would have to include at least one exterior face. But all exterior faces have been included in the surfaces generated by the `SKIN ALL BLOCKS` command line (without the `EXCLUDE` option). This creates a situation where we have the same face in two different surfaces. Specifying the same face in two different contact surfaces is not allowed. See the example discussed in the introductory part of Section 7.2.

If you use the `EXCLUDE` option, you can use a `CONTACT SURFACE` command line or the `CONTACT SURFACE` command block as long as you do not reference the same face on different surfaces when defining the various contact surfaces.

The `CONTACT SURFACE` command block, if it is used to defined a set of unassociated nodes for a contact node set, and the `CONTACT NODE SET` command line can be used with the `SKIN ALL BLOCKS` command line regardless of whether or not it uses the `EXCLUDE` option.

If the mesh includes blocks of shell elements, the shell surfaces generated from a `SKIN ALL BLOCKS` command line will be lofted for contact according to the lofting algorithm specified in the `SHELL LOFTING` command block.

If the mesh includes blocks of one-dimensional elements (beams, trusses), the element blocks with one-dimensional elements are ignored in contact. Thus, to include the one-dimensional elements for contact, a `CONTACT NODE SET` command line should be used. See Section 7.2.4.

7.2.3 Contact Surface Command Block

```
BEGIN CONTACT SURFACE <string>name
  BLOCK = <string list>block_names
  SURFACE = <string list>surface_names
  NODE SET = <string list>node_set_names
  REMOVE BLOCK = <string list>block_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE NODE SET = <string list>node_set_names
END [CONTACT SURFACE <string>name]
```

The `CONTACT SURFACE` command block can be used to define a contact surface consisting of a collection of finite element faces or a set of unassociated nodes that will be a contact node set. We

can use some combinations of the above command lines as a set of Boolean operations to define our collection of faces or collection of unassociated nodes. The result of this command block must be either a set of faces or a set of nodes.

If you want to define a surface named `name` that is a set of faces, you can use some combination of the command lines `BLOCK`, `SURFACE`, `REMOVE BLOCK`, and `REMOVE SURFACE`. For this case, however, the `BLOCK` and `REMOVE BLOCK` command lines must refer to element blocks that are continuum or shell elements. If the element block referred to is a block of continuum elements, the block is skinned. If the element block referred to is a block of shell elements, the top and bottom faces of the shell elements will form the contact faces.

Suppose you specify a `BLOCK` command line that references several continuum blocks. The set of faces defining the surface will consist of the exterior faces for all the element blocks. If you want to preserve the list of element blocks on the `BLOCK` command line while removing the exterior faces associated with one or more of the blocks, you could simply add a `REMOVE BLOCK` command line listing only those blocks whose associated faces are to be removed from the contact surface.

Suppose you specify a `BLOCK` command line that references a block of continuum elements and a `SURFACE` command line that references a side set. Then the contact surface produced by the command block will be the union of the faces defined by the skinning of the block of continuum elements and the faces defined in the side set.

Suppose you specify a `BLOCK` command line that references a block of continuum elements and a `REMOVE SURFACE` command line that references a side set. Furthermore, suppose that the side set is a set of faces that is a subset of the set of faces obtained from skinning the continuum block. Then the contact surface produced by the command block will be the set of faces obtained by skinning the continuum block minus the faces in the side set.

As can be seen from the above examples, we can use the command lines `BLOCK`, `SURFACE`, `REMOVE BLOCK`, and `REMOVE SURFACE` as Boolean operators to construct a set of finite element faces defining a surface. The `BLOCK` and `REMOVE BLOCK` command lines should produce (or remove) faces, however, so that we are performing the Boolean operations on like topological entities. See Section 7.2.4 for further information about using a node set that contacts a surface.

If you want to define a set of unassociated nodes for contact with a surface, you can use some combination of the command lines `BLOCK`, `NODE SET`, `REMOVE BLOCK`, and `REMOVE NODE SET`. For this case, however, the `BLOCK` and `REMOVE BLOCK` command lines must refer to element blocks that are SPH elements, which are topologically equivalent to a node.

Suppose you specify a `BLOCK` command line that references a block of SPH elements and a `NODE SET` command line that references a node set within a command block. Then the node set produced by the command block will be the union of the nodes defined by the SPH elements and the nodes defined in the node set.

Suppose you specify a `BLOCK` command line that references a block of SPH elements and a `REMOVE NODE SET` command line that references a node set. Furthermore, suppose that the node set is a set of nodes that is a subset of the set of nodes in the SPH block. Then the set of nodes produced by the command block will be the set of nodes obtained from the SPH block minus the nodes in the node set.

There must be at least one BLOCK, SURFACE, or NODE SET command line in the command block.

7.2.4 Contact Node Set

```
CONTACT NODE SET <string>surface_name
  CONTAINS <string list>nodelist_names
```

As indicated previously, contact interactions may also be defined between a surface and a set of nodes. The CONTACT NODE SET command line names a set of nodes (the parameter surface_name in the above command line) as a collection of nodes in various node sets specified by the string list nodelist_names. All the nodes in the node set can then interact with a contact surface. If a node in the node set defined as surface_name attempts to penetrate a contact surface, the node will be moved to the surface through the contact calculations.

The node defined by the CONTACT NODE SET command line will be paired with either a mesh surface or an analytic surface when contact interactions are defined. In defining interactions between a contact node set and another surface, the interaction must be defined as a pure master-slave interaction, where the nodes in the contact node set are the slave nodes. The master-slave interaction is defined in the INTERACTION command block (see Section 7.16).The easiest way to define the correct relation between the nodes in the node set and the faces in the actual surface is to pair the surface with the MASTER command line and the node set with the SLAVE command line. Suppose the set of nodes is named beam_nodes on the CONTACT NODE SET command line and the surface these nodes are paired with is named plate. Then the INTERACTION command block for the interaction of the node set and surface would contain the command lines below.

```
MASTER = plate
SLAVE = beam_nodes
```

Presto will not detect whether or not you have specified a master-slave relation between a surface and a set of nodes. If the interaction between a surface and a set of nodes defaults to a kinematic partition value of 0.5 and there is only one enforcement iteration, then any nodes that have penetrated the surface will only be moved one-half the penetration distance. Therefore, you should check your input carefully if you have an interaction between a surface and a node set to make sure that the master-slave relation has been properly defined for this interaction.

The CONTACT NODE SET command line is used to define contact interactions between SPH particles and other contact surfaces—faces on solid elements, shell/membrane faces, and analytic surfaces. The CONTACT NODE SET command line also presents a simple approach for contact between one-dimensional elements (beams, trusses) and other contact surfaces—faces on solid elements, shell/membrane faces, and analytic surfaces. In this case, contact processing will seek to remove interpenetration of the nodes of the one-dimensional elements into the other contact surfaces. The contact capabilities in Presto will not currently handle any contact between two one-dimensional elements.

7.3 Analytic Contact Surfaces

Presto permits the definition of rigid analytic surfaces for use in contact. Contact evaluation between a deformable body and a rigid analytic surface is much faster than contact evaluation between two deformable bodies. Therefore, using a rigid analytic surface is more efficient than using a very stiff deformable body to try to approximate a rigid surface. The commands for defining the rigid analytic surfaces currently available in Presto–plane, cylinder, and sphere—are described next.

7.3.1 Plane

```
BEGIN ANALYTIC PLANE <string>name
  NORMAL = <string>defined_direction
  POINT = <string>defined_point
  REFERENCE RIGID BODY = <string>rb_name
END [ANALYTIC PLANE <string>name]
```

Analytic planes are not deformable, they cannot be moved, and two analytic planes will not interact with each other. The `ANALYTIC PLANE` command block for defining an analytic plane begins with the input line:

```
BEGIN ANALYTIC PLANE <string>name
```

and is terminated with the input line:

```
END [ANALYTIC PLANE <string>name]
```

where the string `name` is some user-selected name for this particular plane. This name is used to identify the surface in the interaction definitions. The string `defined_direction` in the `NORMAL` command line refers to a vector that has been defined with a `DEFINE DIRECTION` command line; this vector defines the outward normal to the plane. The string `defined_point` in the `POINT` command line refers to a point in a plane that has been defined with a `DEFINE POINT` command line. The deformable body should initially be on the side of the plane defined by the outward normal.

If the `REFERENCE RIGID BODY` command can be used to connect the analytic plane to the named rigid body block. If the rigid body block rotates or translates, the plane will move with it. The reference rigid body option only works when the `CONTACT FORMULATION TYPE = DASH` option is used.

7.3.2 Cylinder

```
BEGIN ANALYTIC CYLINDER <string>name
```

```
  CENTER = <string>defined_point
  AXIAL DIRECTION = <string>defined_axis
  RADIUS = <real>cylinder_radius
  LENGTH = <real>cylinder_length
  CONTACT NORMAL = <string>OUTSIDE|INSIDE
END [ANALYTIC CYLINDER <string>name]
```

Analytic cylindrical surfaces are not deformable, they cannot be moved, and two analytic cylindrical surfaces will not interact with each other. The `ANALYTIC CYLINDER` command block for defining an analytic cylindrical surface begins with the command line:

```
BEGIN ANALYTIC CYLINDER <string>name
```

and is terminated with the command line:

```
END [ANALYTIC CYLINDER <string>name]
```

where the string `name` is some user-selected name for this particular cylindrical surface. This name is used to identify the surface in the interaction definitions. The cylindrical surface has a finite length; the cylindrical surface is not an infinitely long surface. To fully specify the location of the cylindrical surface, therefore, you must specify the center point of the cylindrical surface in addition to the axial direction of the cylinder. These quantities, center point and direction, are defined by the `CENTER` and `AXIAL DIRECTION` command lines, respectively. The string `defined_point` in the `CENTER` command line refers to a point that has been defined with a `DEFINE POINT` command line; the string `defined_axis` in the `AXIAL DIRECTION` command line refers to a vector that has been defined with a `DEFINE DIRECTION` command line. The radius of the cylinder is the real value `cylinder_radius` specified with the `RADIUS` command line, and the length of the cylinder is the real value `cylinder_length` specified by the `LENGTH` command line. The length of the cylinder (`cylinder_length`) extends a distance of `cylinder_length` divided by 2 along the cylinder axis in both directions from the center point. If the rigid surface is the outside of the cylinder, you should specify:

```
CONTACT NORMAL = OUTSIDE
```

If the rigid surface is the inside of the cylinder, you should specify:

```
CONTACT NORMAL = INSIDE
```

7.3.3 Sphere

```
BEGIN ANALYTIC SPHERE <string>name
  CENTER = <string>defined_point
  RADIUS = <real>sphere_radius
END [ANALYTIC SPHERE <string>name]
```

Analytic spherical surfaces are not deformable, they cannot be moved, and two analytic spherical surfaces will not interact with each other. The `ANALYTIC SPHERE` command block for defining an analytic spherical surface begins with the input line:

```
BEGIN ANALYTIC SPHERE <string>name
```

and is terminated with the input line:

```
END [ANALYTIC SPHERE <string>name]
```

where the string `name` is some user-selected name for this particular spherical surface. This name is used to identify the surface in the interaction definitions. The center point of the sphere is defined by the `CENTER` command line, which references a point, `defined_point`, specified by a `DEFINE POINT` command line. The radius of the sphere is the real value `sphere_radius` specified with the `RADIUS` command line.

7.4 Update All Surfaces for Element Death

```
UPDATE ALL SURFACES FOR ELEMENT DEATH = <string>ON|OFF(ON)
```

When elements are killed in an analysis, contact surfaces may need to be updated to account for the removal of faces attached to killed elements or the addition of faces exposed by element death. The command line `UPDATE ALL SURFACES FOR ELEMENT DEATH` permits contact surfaces to be updated based on all the `ELEMENT DEATH` command block(s) specified in the input file (see Section 5.5). This update of contact surfaces is controlled by the command line being set to `ON`, the default. The update encompasses the full reinitialization of contact. Thus, surface-physics models that involve state data may lose some information when the new contact surfaces are created. If the command line is set to `OFF`, an element associated with a face on the contact surface could be killed, but the face would remain in the list of faces defining the contact surface, which may be unacceptable for your analysis.

7.5 Remove Initial Overlap

```
BEGIN REMOVE INITIAL OVERLAP
  OVERLAP NORMAL TOLERANCE = <real>over_norm_tol
  OVERLAP TANGENTIAL TOLERANCE = <real>over_tang_tol
  SHELL OVERLAP ITERATIONS = <integer>max_iter(10)
  SHELL OVERLAP TOLERANCE = <real>shell_over_tol(0.0)
END REMOVE INITIAL OVERLAP
```

Meshes supplied for finite element analyses frequently have some level of initial mesh overlap, where finite element nodes rest inside the volume of elements. This can cause problems with contact; overlaps may cause initial forces that are nonphysical and produce erroneous stress waves. Presto provides a mechanism to modify the initial mesh to attempt to remove overlaps in surfaces defined for contact via the `REMOVE INITIAL OVERLAP` command block.

The process used to remove the initial overlap for three-dimensional solid elements involves changing the original coordinates of nodes on contact surfaces. Changing the coordinates yields a new mesh with the overlap removed; the overlap removal adds no initial stresses. Normal and tangential tolerances are specified by the user for all the contact surfaces in the `REMOVE INITIAL OVERLAP` command block. It is also possible to specify overlap normal and tangential tolerances on each surface pairing separately in the `INTERACTION` command block. In other words, overlap removal tolerances specified in `INTERACTION` command blocks will overwrite the tolerances specified in the `REMOVE INITIAL OVERLAP` command block. See Section 7.16 for details. The `REMOVE INITIAL OVERLAP` command block only removes overlaps that are detected along the surfaces defined for contact and not all surfaces in the mesh.

Overlap tolerances are used to designate a box around each surface pair to search for overlaps. If the overlap of the mesh is larger than the box defined by the tolerances, then the overlap will not be found and thus will not be removed. However, if the specified tolerances are larger than an element length in the analysis, the overlap removal mechanism may invert elements, leading to analysis failure. This has two ramifications. First, the tolerances must be carefully specified to correct mesh overlaps and to not invert elements. Second, this mechanism is unable to remove initial overlaps that are greater than an element length. In such cases, the overlap must be removed manually using a meshing tool. The mesh modification done by the `REMOVE INITIAL OVERLAP` feature changes the meshed geometry, and thus can change the mass and time step of affected elements. The mesh returned in the results file includes the changed coordinates and should be checked to ensure that the modifications are acceptable. A summary of the overlap that is removed is reported in the log file. (See Section 1.7 for a discussion of the log file.) The log file lists each block in which the initial overlap has been removed as well as the maximum amount of overlap for each of these blocks. Additionally, you can request that a nodal variable called `REMOVED_OVERLAP` be written to the results file. See Section 8.2.1.1 for a discussion of the output of nodal variables to the results file.

For contact between shell elements, a slightly different approach is used. Because the thickness of a shell must be preserved when shell lofting is requested, removing the initial overlap between nested shells becomes an iterative process whereby shell locations are adjusted to remove the overlap. This process is approximate and may not remove all the overlap in all cases. It is advised

to check the corrected mesh to make sure that the mesh modifications are acceptable. In the input, two additional input lines, `SHELL OVERLAP ITERATIONS` and `SHELL OVERLAP TOLERANCE`, may be needed to properly remove the initial overlap.

Note, if automatic kinematic partitioning is being used, the overlap algorithm will use the symmetric kinematic partition value of 0.5.

- The `SHELL OVERLAP ITERATIONS` command line controls the maximum number of iterations that will be used by the overlap removal mechanism to resolve nested shells. By default, the value of `max_iter` is 10. If the mesh has only a few layers of shells that may overlap, a value of 10 should suffice. However, if the mesh has a number of layers of shells that may overlap, this value may need to be much larger.

- The `SHELL OVERLAP TOLERANCE` command line specifies an amount of overlap, `shell_over_tol`, that is permitted to be left in the shell elements. This helps to limit the actual number of iterations required to remove the shell overlap, and to spread any remaining overlap over a number of shells instead of concentrating it all in a single shell. If the default value of 0.0 for the shell overlap tolerance is used, iteration continues until either all the overlap is removed or the maximum number of iterations is reached. If a nonzero value for the shell overlap tolerance is used, iteration continues until the tolerance is reached or the maximum number of iterations is reached. Note that the overlap removal process is only done once during an analysis, so a large number of iterations will only affect the first time step, not every time step.

The `SHELL OVERLAP ITERATIONS` and `SHELL OVERLAP TOLERANCE` commands have no meaning for analyses that do not have shell elements.

7.6 Angle for Multiple Interactions

```
MULTIPLE INTERACTIONS = <string>ON|OFF(ON)
MULTIPLE INTERACTIONS WITH ANGLE = <real>angle_in_deg(60.0)
```

When a node lies on the edge of a body, that node may need to support contact interactions with more than one face at the same time. For instance, see Figure 7.3. In Figure 7.3a, three blocks are shown, with a single node identified. Through contact, this node can interact with both the block on the upper right and the block on the bottom. If the node only supports a single interaction, then it will be arbitrarily considered for contact between one of the blocks, but not the other, as in Figure 7.3b. In this case, contact enforcement will prevent penetration into the lower block, but may permit penetration into the upper right block. The proper way to deal with this case is shown in Figure 7.3c, where multiple interactions are considered at the node.

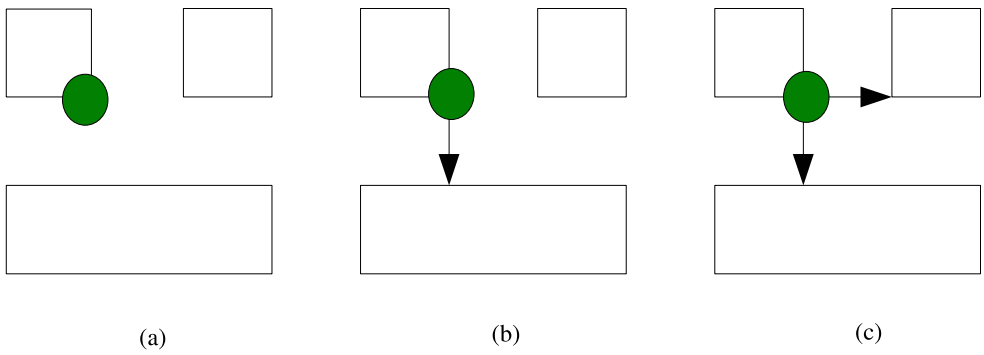

Figure 7.3: Illustrations of multiple interactions at a node: (a) initial configuration, with node of interest identified; (b) single interaction; and (c) multiple interactions.

By default, Presto permits multiple interactions at a node. However, these multiple interactions may incur extra cost in the contact algorithm by increasing the number of interactions in enforcement. Also, a local search algorithm (see Section 7.12), which uses various contact tracking approaches, may operate more efficiently when the node can only have one interaction. Finally, multiple interactions may lead to instabilities that can be eliminated by switching to single interactions. For these reasons, the `MULTIPLE INTERACTIONS` command line allows the user to choose whether multiple interactions should be considered at a node. A value of `OFF` indicates that a node can have only one interaction. This value affects all interactions in a contact definition. Presto does not currently have the capability to force single interactions for some surface pairs while allowing multiple interactions for other surface pairs.

When the `MULTIPLE INTERACTIONS` command line is `ON`, the number of interactions that can be considered at a node is dependent on the measure of curvature of those faces that are connected to the node. If the angle between two faces on which the node is attached is small, then only one interaction is allowed. However, in cases where the angle between the faces is large enough such that they form a discrete corner, multiple interactions are considered. The contact algorithms can

properly handle only a limited number of interactions per node (currently three), so it is generally feasible to properly define interactions at a node, e.g., at the corner of a block.

The critical angle for multiple interactions is set with the `MULTIPLE INTERACTIONS WITH ANGLE` command line, where `angle` is the angle over which an edge is considered sharp. If the angle between adjoining faces is greater than this critical angle, multiple interactions can be created. By default, this critical angle is 60 degrees, which works well for most analyses. This value can be changed in the contact input if needed.

7.7 Surface Normal Smoothing

```
BEGIN SURFACE NORMAL SMOOTHING
  ANGLE = <real>angle_in_deg(60.0)
  DISTANCE = <real>distance(0.01)
  RESOLUTION = <string>NODE|EDGE(NODE)
END SURFACE NORMAL SMOOTHING
```

Surface normal smoothing is a feature that is primarily used in Adagio.

Finite element discretization often results in models with faceted edges, while the true geometry of the part is actually smoothly curved. If the faces of adjacent finite elements on a surface have differing normals, the discontinuities at the edges between those faces can cause problems with contact. These discontinuities in the face normals are particularly troublesome with an implicit code such as Adagio, which uses an iterative solver to obtain a converged solution at every step. If a node is in contact near an edge with a normal discontinuity, the node may slide back and forth between the two neighboring faces during the iterations. Because the normal directions of the two faces differ, this can make it difficult to converge on a solution to this discontinuous contact problem.

Surface normal smoothing is a technique that creates a smooth variation in the normal near edges. The normal varies linearly from the value on one face to the value on the other face over a distance that spans the edge. A smoothly varying normal at the edge makes it much easier for an iterative solver to obtain a converged solution in the case where a node has penetrated near the edge of a face.

Presto does not use an iterative solver and thus does not encounter the difficulties associated with face normal discontinuities. Consequently, the `SURFACE NORMAL SMOOTHING` command block is not typically useful for Presto models. It is provided in both Presto and Adagio, however, to provide a consistent transition between the two codes if they are used together in a coupled analysis.

If the `SURFACE NORMAL SMOOTHING` command block is present, this feature is activated. There are three optional commands that can be used within this block to control the behavior of normal smoothing.

- The `ANGLE` command is used to control whether smoothing should occur between neighboring faces. If the angle between two faces is less than the specified angle (given in degrees), smoothing is activated between them. Otherwise, the discontinuity is considered to be a feature of the model rather than an artifact of meshing, and they are not smoothed. The default value for `angle` is 60.
- The `DISTANCE` command specifies the distance as a fraction of the face size over which smoothing should occur. The specified value can vary from 0 to 1. The default value for `distance` is 0.01.
- The `RESOLUTION` command specifies the method used to determine the smoothed normal direction. The default `NODE` option uses a node-based algorithm to fit a smooth curve, while the `EDGE` option uses an edge-based algorithm.

7.8 Eroded Face Treatment

```
ERODED FACE TREATMENT = <string>ALL|NONE(ALL)
```

The `ERODED FACE TREATMENT` command line is used to define what happens to newly exposed element faces when a contact surface erodes because of element death. This command line applies to the case in which a contact surface has been generated by the skinning of an element block (Section 7.2). Suppose we have a contact block that has been skinned to create a contact surface, and let us consider an element that contributes a face to the original contact surface. If this element is killed at some point by element death, the death of this element exposes new faces. If the `ALL` option in the command line has been selected, any newly exposed faces will be included in the updated contact definition. If the `NONE` option is used, the faces exposed by element death will not be included in the updated contact surface. Both options will remove any faces on killed elements from the contact definition, though the `NONE` option tends to be more robust on complex geometries, such as those containing equivalenced elements, shell elements sandwiched between solid elements, and degenerate elements.

The default option is `ALL`.

7.9 Shell Lofting

```
BEGIN SHELL LOFTING
  SURFACE = <string_list>surface_names
  REMOVE SURFACE = <string_list>removed_surface_names
  LOFTING ALGORITHM = <string>ON|OFF(ON)
  COINCIDENT SHELL TREATMENT = <string>DISALLOW|IGNORE|
    SIMPLE(DISALLOW)
  COINCIDENT SHELL HEX TREATMENT = <string>DISALLOW|
    IGNORE|TAPERED|EMBEDDED(DISALLOW)
  CONTACT SHELL THICKNESS =
    ACTUAL_THICKNESS|LET_CONTACT_CHOOSE(ACTUAL_THICKNESS)
  ALLOWABLE SHELL THICKNESS TO ELEMENT SIZE RATIOS =
    <real>lower_bound(0.1) TO <real>upper_bound(1.0)
END [SHELL LOFTING]
```

Presto can also assess contact on shell elements. Shell elements can interact with other shell elements, faces of solid elements, and contact node sets (such as SPH). Contact on shell elements can occur on either the meshed shell geometry, i.e., ignoring any shell thickness, or on the "lofted" geometry, i.e., a geometry that includes the thickness of the shell. Currently, contact appears to be more robust on the non-lofted geometry; however, for simulations in which the thickness is important, the lofted geometry can provide more-reasonable results. Also critical to shell contact is how shells that are fully coincident with other elements (i.e., share all their nodes with another element) are treated. These options are controlled by the user in the `SHELL LOFTING` command block.

The `SURFACE` and `REMOVE SURFACE` command lines allow for the specification of a subset of shell contact surfaces to be lofted. These command lines are optional and by default, all shell surfaces are lofted. If the `SURFACE` command line is used by itself, only those surfaces listed will be lofted. If the `REMOVE SURFACE` command line is used by itself, all contact surfaces except those listed will be lofted.

The `LOFTING ALGORITHM` command line determines whether contact on a shell should be done on the lofted geometry or on the original shell geometry. If the value of the `LOFTING ALGORITHM` command line is set to `ON`, shell contact uses the lofted geometry; if it set to `OFF`, shell contact uses the original shell geometry.

The `COINCIDENT SHELL TREATMENT` command line identifies how shells that share the same nodes should be treated. If the `DISALLOW` option is selected, (the default), then any time that shells in contact are detected to share all the same nodes, the code will abort with an error message indicating which elements were found to be coincident. The `DISALLOW` option should be used if you do not want any coincident shells to be considered in the analysis. The option operates essentially as a check on the mesh. If the `IGNORE` option is selected, any contact faces attached to coincident shells are ignored for contact. This option is only provided as a backup approach if undiagnosed code problems arise from coincident shells. If such a case occurs, the `IGNORE` option may permit the user to continue with an analysis while the code team diagnoses the problem. The `SIMPLE` option enables coincident shells to be processed correctly. If lofting has been enabled

and the SIMPLE option is selected, the thickness of the lofted coincident shell is taken as the largest thickness of all the coincident shells. If lofting is off and the SIMPLE option is selected, the coincident shell is treated as if only one of the shells is present.

The COINCIDENT SHELL HEX TREATMENT command line has a function similar to that of the COINCIDENT SHELL TREATMENT command line. The COINCIDENT SHELL HEX TREATMENT command line, however, identifies how shells that are fully coincident with the hex elements are treated. If the DISALLOW option is selected (the default), then any time that a shell in contact is detected to share all the same nodes with the face of a continuum element, the code will abort with an error message indicating which elements were found to be coincident. The DISALLOW option should be used if you do not want any shells coincident with hexes to be considered in the analysis. The option operates essentially as a check on the mesh. If the IGNORE option is selected, any contact faces attached to shells that are coincident with faces of continuum elements are ignored for contact. This option is only provided as a backup approach if undiagnosed code problems arise from coincident shells and continuum elements. If such a case occurs, the IGNORE option may permit the user to continue with an analysis while the code team diagnoses the problem. The TAPERED and EMBEDDED options permit shells that are coincident with faces of continuum elements to be processed in contact. The TAPERED option does two things: it includes for contact any faces that are on the free surface and ignores faces sandwiched between the shell and the continuum element, and it automatically adjusts the lofting of the surfaces to provide a smooth transition between shells that are not coincident with the faces of the continuum elements and those that are coincident with the faces of the continuum elements. The EMBEDDED option includes for contact both free surface faces and those that are between the coincident shells and faces of the continuum elements; the option does not adjust thicknesses to make smooth transitions between shells that are not coincident with faces of continuum elements and those that are coincident with faces of continuum elements. In general, the TAPERED option is preferred; only use the EMBEDDED option if the TAPERED option causes a code problem.

The CONTACT SHELL THICKNESS command line controls whether contact should be enforced using the actual thickness of elements, or using a pseudo thickness that is computed by the contact algorithm. The default option to this command, ACTUAL_THICKNESS, causes the actual element thickness to be used.

The LET_CONTACT_CHOOSE option to the CONTACT SHELL THICKNESS command tells the contact algorithm to create lofted geometries out of the shells that are more appropriate for contact. Shells that are very thick or very thin in relation to their in-plane dimension can be problematic in contact. Thin shells may require a large number of time sub-steps in the contact algorithm to ensure that objects do not pass completely through one another. Shells that are thick in relation to their in-plane dimension can produce ill-defined geometries as seen in Figure 7.4. The LET_CONTACT_CHOOSE option can help alleviate these problems. The CONTACT SHELL THICKNESS command is functional only in Dash contact.

By default, when the LET_CONTACT_CHOOSE option is used, lofted geometry thicknesses are ensured to be within 0.1 and 1.0 times the in-plane dimension of the shell. If the contact-appropriate thickness already lies within those bounds, the lofted thickness will not be changed. The permissible bounds for the ratios of contact-appropriate thickness to actual thickness can be set using the lower_bound and upper_bound parameters in the ALLOWABLE SHELL THICKNESS TO

`ELEMENT SIZE RATIOS` command. The `ALLOWABLE SHELL THICKNESS` command is functional only in Dash contact.

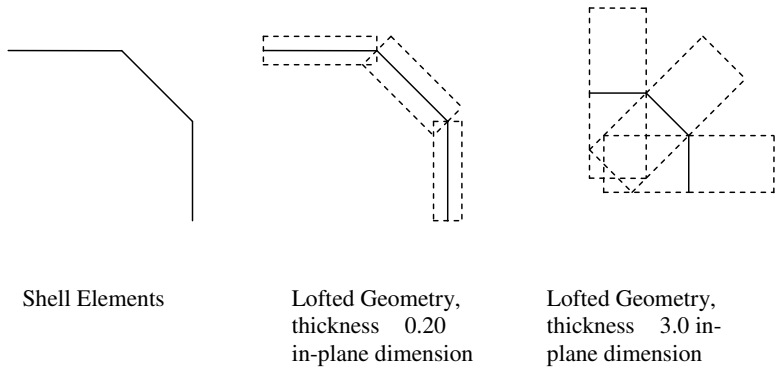

Figure 7.4: Example lofted geometries produced by shell lofting.

7.10 Contact Output Variables

Contact variables can be output to provide information about enforcement of contact interactions. Currently, information on only one interaction at each node is provided. If a node has more than one interaction, the last one in its internal interaction list is reported.

Nodal contact variables that can be output are listed in Table 8.7. Where applicable, names of the equivalent variables in JAS3D are given in parentheses at the end of the description. The variables can be output in history files or results files; see Chapter 8 for more information on outputting nodal variables. Note that currently the variables cannot be calculated at output time so the first time they are output a request is made to calculate them. This means that the first output step where they are to appear the data will be all zero. A work around for this is to have at least one output step in which these variables appear before their values are needed.

7.11 Friction Models

To describe the physics of interactions that occur between contact surfaces, the Presto input for contact relies upon the definition of friction models. The user then relates these friction models to pairs of interactions in the interaction-definition blocks (see Section 7.15 and Section 7.16). During the search phase of contact, node-face interactions are identified, and the designated friction model is used to determine how the resulting contact forces are resolved between these pairs.

The following friction models are currently available: frictionless contact, constant coulomb friction, tied contact, glued contact, spring weld, surface weld, area weld, adhesion, cohesive zone, junction, threaded joint, and pressure-velocity–dependent friction. In addition, models defined by user subroutines can be used as friction models. By default, interactions between contact surfaces that have not had friction models assigned are treated as frictionless. All friction models are command blocks, although some of the models do not have any command lines inside the command block. The commands for defining the available friction models are described next. Friction models are associated with specific pairings of contact surfaces through the interaction-definition blocks in Section 7.15 and Section 7.16. Presto uses the ACME library for contact enforcement. See the documentation for ACME to obtain a more in-depth description of the implementation and usage for the various friction models.

7.11.1 Frictionless Model

```
BEGIN FRICTIONLESS MODEL <string>name
END [FRICTIONLESS MODEL <string>name]
```

The `FRICTIONLESS MODEL` command block defines frictionless contact between surfaces. In frictionless contact, contact forces are computed normal to the contact surfaces to prevent penetration, but no forces are computed tangential to the contact surfaces. The string `name` is a user-selected name for this friction model that is used when identifying this model in the interaction definitions. No command lines are needed inside the command block. A default named frictionless model named `frictionless` can be used without defining this command block.

7.11.2 Constant Friction Model

```
BEGIN CONSTANT FRICTION MODEL <string>name
  FRICTION COEFFICIENT = <real>coeff
END [CONSTANT FRICTION MODEL <string>name]
```

The `CONSTANT FRICTION MODEL` command block defines a constant coulomb friction coefficient between two surfaces as they slide past each other in contact. No resistance is provided to keep the surfaces together if they start to separate. The string `name` is a user-selected name for this friction model that is used to identify this model in the interaction definitions, and `coeff` is the constant coulomb friction coefficient. There is no default value for the friction coefficient.

7.11.3 Tied Model

```
BEGIN TIED MODEL <string>name
END [TIED MODEL <string>name]
```

The `TIED MODEL` command block restricts nodes found in initial contact with faces to stay in the same relative location to the faces throughout the analysis. The string `name` is a user-selected name for this friction model that is used to identify this model in the interaction definitions. No command lines are needed inside the command block. A default named tied model named `tied` can be used without defining this command block.

7.11.4 Glued Model

```
BEGIN GLUED MODEL <string>name
END [GLUED MODEL <string>name]
```

The `GLUED MODEL` command block defines a contact interaction that allows the interacting faces to move independently until they come into contact, but once they come into contact, they behave as a tied contact interaction, with no relative normal or tangential motion for the rest of the analysis. The string `name` is a user-specified name for this friction model that is used to reference this model in the interaction definitions. No command lines are needed inside the command block. A default named glued model named `glued` can be used without defining this command block.

7.11.5 Spring Weld Model

```
BEGIN SPRING WELD MODEL <string>name
  NORMAL DISPLACEMENT FUNCTION = <string>func_name
  NORMAL DISPLACEMENT SCALE FACTOR = <real>scale_factor(1.0)
  TANGENTIAL DISPLACEMENT FUNCTION = <string>func_name
  TANGENTIAL DISPLACEMENT SCALE FACTOR =
    <real>scale_factor(1.0)
  FAILURE ENVELOPE EXPONENT = <real>exponent(2.0)
  FAILURE DECAY CYCLES = <integer> num_cycles(1)
  FAILED MODEL = <string>failed_model_name|FRICTIONLESS
    (FRICTIONLESS)
 END [SPRING WELD MODEL <string>name]
```

The `SPRING WELD MODEL` command block defines a contact friction model that, when applied between two contact surfaces, connects a slave node to the nearest point of a corresponding master face with a spring. The spring behavior is defined by a force-displacement curve in the normal and tangential directions. If the motion of the problem generates displacement between the slave node and its corresponding master face and this motion is in purely the normal or tangential direction, the spring will fail once it passes the maximum displacement in the normal and tangential

force-displacement curves, respectively. For displacements that include both normal and tangential components, the spring fails according to a failure criterion defined as the sum of the ratios of the normal and tangential components to their maximum values, raised to a power. If the criterion is greater than 1.0, the spring fails. Once the spring fails, its contact forces reduce over a number of load steps, and the contact evaluation reverts to another user-specified friction model (or frictionless contact if not specified).

In the above command block:

- The string `name` is a user-selected name for this friction model that is used to identify this model in the interaction definitions.
- The normal force-displacement curve is specified by the `NORMAL DISPLACEMENT FUNCTION` command line, where the string `func_name` is the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope. This function can be scaled by the real value `scale_factor` in the `NORMAL DISPLACEMENT SCALE FACTOR` command line; the default for this factor is 1.0
- The tangential force-displacement curve is specified by the `TANGENTIAL DISPLACEMENT FUNCTION` command line, where the string `func_name` is the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the SIERRA scope. This function can be scaled by the real value `scale_factor` in the `TANGENTIAL DISPLACEMENT SCALE FACTOR` command line; the default for this factor is 1.0.
- The real value `exponent` in the `FAILURE ENVELOPE EXPONENT` command line specifies how normal and tangential failure criteria may be combined to yield failure of the weld, as described above. The default value for this exponent is 2.0.
- The `FAILURE DECAY CYCLES` command line describes how many cycles to ramp down the load in the spring weld after it fails through the integer value `num_cycles`. The default value for the number of decay cycles is 1.
- When the spring weld breaks, the friction model that contact reverts to when evaluating future node-face interactions between the surfaces is identified in the `FAILED MODEL` command line with the string `failed_model_name`. The friction model listed in this command must have been previously defined in the input file. The default value for the model used after failure is the frictionless model.

The `SPRING WELD MODEL` command block is very similar to the Presto `SPOT WELD` command block, but permits greater flexibility in specifying a different friction model to be applied after failure.

7.11.6 Surface Weld Model

```
BEGIN SURFACE WELD MODEL <string>name
  NORMAL CAPACITY = <real>normal_cap
```

```
  TANGENTIAL CAPACITY = <real>tangential_cap
  FAILURE DECAY CYCLES = <integer>num_cycles(1)
  FAILED MODEL = <string>failed_model_name|FRICTIONLESS
    (FRICTIONLESS)
END [SURFACE WELD MODEL <string>name]
```

The `SURFACE WELD MODEL` command block defines a contact friction model that behaves identically to the `TIED MODEL` until a maximum force between the node and face of an interaction is reached in the normal direction or the tangential direction. Once this maximum force is reached, the tied contact "fails" and the friction model switches to a different friction model, as specified by the user.

In the above command block, the string `name` is a user-selected name for this friction model that is used to identify this model in the interaction definitions. The maximum allowed force in the normal direction is specified by the real value `normal_cap` in the `NORMAL CAPACITY` command line. The maximum allowed force in the tangential direction is specified by the real value `tangential_cap` in the `TANGENTIAL CAPACITY` command line. There are no defaults for these values. The surface weld will break when either the specified normal or tangential capacity is reached. Once the model fails, the applied forces decrease to zero over a number of time steps defined through the integer value `num_cycles` in the `FAILURE DECAY CYCLES` command line. The default for `num_cycles` is 1. The friction model that should be used after the weld fails is identified in the `FAILED MODEL` command line with the string `failed_model_name`. The friction model designated in the `FAILED MODEL` command line must be defined within the `CONTACT DEFINITION` command block. The default model after failure is the frictionless contact model.

7.11.7 Area Weld Model

```
BEGIN AREA WELD MODEL <string>name
  NORMAL CAPACITY = <real>normal_cap
  TANGENTIAL CAPACITY = <real>tangential_cap
  FAILURE DECAY CYCLES = <integer> num_cycles(1)
  FAILED MODEL = <string>failed_model_name|FRICTIONLESS
    (FRICTIONLESS)
END [AREA WELD MODEL <string>name]
```

The `AREA WELD MODEL` command block defines a contact friction model that behaves identically to the `TIED MODEL` until a maximum traction between a node and face in an interaction is reached in the normal direction or the tangential direction. Once this maximum traction is reached, the tied contact "fails" and the friction model switches to a different friction model, as specified by the user. This model is identical to the `SURFACE WELD MODEL` command block, except that tractions are used instead of forces.

In the above command block, the string `name` is a user-selected name for this friction model that is used to identify this model in the interaction definitions. The maximum allowed traction in the normal direction is specified by the real value `normal_cap` in the `NORMAL CAPACITY` command line. The maximum allowed traction in the tangential direction is specified by the real

value tangential_cap in the TANGENTIAL CAPACITY command line. There are no defaults for these values. The area weld will break when either the specified normal or tangential capacity is reached. Once the model fails, the applied tractions decrease to zero over a number of time steps defined through the integer value num_cycles in the FAILURE DECAY CYCLES command line. The default for num_cycles is 1. The friction model that should be used after the weld fails is identified in the FAILED MODEL command line with the string failed_model_name. The friction model designated in the FAILED MODEL command line must be defined within the CONTACT DEFINITION command block. The default model after failure is the frictionless contact model.

7.11.8 Adhesion Model

```
BEGIN ADHESION MODEL <string>name
  ADHESION FUNCTION = <string>func_name
  ADHESION SCALE FACTOR = <real>scale_factor(1.0)
END [ADHESION MODEL <string>name]
```

The ADHESION MODEL command block defines a friction model that behaves like frictionless contact when two surfaces are in contact, but computes an additional force between the surfaces when they are not touching. The value of the additional force is given by a user-specified function of force versus distance, where the distance is the distance between a node and the closest point on the opposing surface.

In the above command block, the string name is a user-selected name for this friction model that is used to identify this model in the interaction definitions. The force between surfaces that are not touching is given by the ADHESION FUNCTION command line, where the string func_name is the name of a function defined in a DEFINITION FOR FUNCTION command block in the SIERRA scope. The values of this function are expected to be non-negative. The function can be scaled by the real value scale_factor in the ADHESION SCALE FACTOR command line; the default for this factor is 1.0. Because contact forces are typically only given to node-face interactions if they touching, the contact search requires appropriate tolerances when this model is used. The normal and tangential tolerances specified in the interaction definitions should be set to the maximum distance at which the adhesion model should be applying force. However, setting this distance to be very large may cause excessive numbers of interactions to be identified in the search phase, causing the contact processing to be very slow and/or generate erroneous interactions.

7.11.9 Compliant Joint Model

```
BEGIN COMPLIANT JOINT MODEL <string>name
  NORMAL MODULUS = <real>norm_mod
  SHEAR MODULUS = <real>shear_mod
  APERTURE = <real>aperture
  APERTURE LIMIT = <real>aperture_limit
  FRICTION COEFFICIENT = <real>fric_coef
```

```
  COHESION = <real>cohesion
END [COMPLIANT JOINT MODEL <string>name]
```

The compliant joint model is formulated for use in modeling of geologic faults and joints. The joint has an elastic response when both opening and closing defined by `norm_mod` and `shear_mod`. Normal and shear modulus have units of stress.

When the joint is closing, the modulus of the joint varies from `norm_mod` to infinity over a gap distance of `aperture`. The `aperture_limit` is a number between 0.0 and 1.0 that defines how far along the aperture curve the model will go while still increasing the stiffness. A small value causes the model to have a nearly constant stiffness during joint closing. A larger number causes more stiffening of the joint as the overclosure approaches the aperture. A value of 1.0 allows the normal stiffness to go all the way to infinity. Values of aperture limit near one are not recommended as they tend to cause the joint model to become extremely stiff and cause the model to be unstable. The aperture has units of length, while the aperture limit is a dimensionless constant.

When the joint is open, it has a shear stiffness specified by `shear_mod`. When the joint is closing, Coulomb frictional effects are added to the shear force. These are computed as `fric_coef` times the compressive force, where `fric_coef` is a dimensionless friction coefficient.

Additional cohesive resistance to joint opening is provided by `cohesion`. This parameter has units of stress.

The compliant joint model is only available when using the Dash contact formulation. Additionally, due to the need to store state variables, the compliant joint model may only be used on interfaces that use node-face contact interactions.

The stiffness of the compliant joint model changes over time based on the loading history of the joint. This stiffness is not explicitly taken into account by the critical time step estimate. Thus, if the critical time step of the contact joint is lower than the critical time step used by the analysis, the analysis may become unstable. If this occurs, the user will need to either manually drop the integration time step used by the code or change parameters in this model to decrease the stiffness of the joint.

7.11.10 Cohesive Zone Model

```
BEGIN COHESIVE ZONE MODEL <string>name
  TRACTION DISPLACEMENT FUNCTION = <string>func_name
  TRACTION DISPLACEMENT SCALE FACTOR = <real>scale_factor(1.0)
  CRITICAL NORMAL GAP = <real>crit_norm_gap
  CRITICAL TANGENTIAL GAP = <real>crit_tangential_gap
END [COHESIVE ZONE MODEL <string>name]
```

The `COHESIVE ZONE MODEL` command block defines a friction model that prevents penetration when contact surfaces are touching, but provides an additional force when the distance between the node and face in an interaction increases. This force is determined by a user-specified function. Once the distance exceeds a user-specified value in the normal direction or the tangential direction,

the force is no longer applied. This model can be used to mimic the energy required to separate two surfaces that are initially touching.

In the above command block, the string `name` is a user-selected name for this friction model that is used to identify this model in the interaction definitions. The displacement function for traction is given by the `TRACTION DISPLACEMENT FUNCTION` command line, where the string `func_name` is the name of a function defined in a `DEFINITION FOR FUNCTION` command block in the SIERRA scope. This function can be scaled by the real value `scale_factor` in the `TRACTION DISPLACEMENT SCALE FACTOR` command line; the default for this factor is 1.0. In the `CRITICAL NORMAL GAP` command line, the real value `crit_norm_gap` specifies the normal distance between the node and face past which the cohesive zone no longer provides a force. In the `CRITICAL TANGENTIAL GAP` command line, the real value `crit_tangential_gap` specifies the tangential distance between the node and face past which the cohesive zone no longer provides a force.

7.11.11 Junction Model

```
BEGIN JUNCTION MODEL <string>name
  NORMAL TRACTION FUNCTION = <string>func_name
  NORMAL TRACTION SCALE FACTOR = <real>scale_factor(1.0)
  TANGENTIAL TRACTION FUNCTION = <string>func_name
  TANGENTIAL TRACTION SCALE FACTOR = <real>scale_factor(1.0)
  NORMAL CUTOFF DISTANCE FOR TANGENTIAL TRACTION = <real>distance
END [JUNCTION MODEL <string>name]
```

The `JUNCTION MODEL` command block defines a model that prevents the interpenetration of contact surfaces and that also provides normal and tangential tractions to a node-face interaction when the surfaces are not touching. The normal tractions are defined as a function of the normal distance between the node and face of an interaction, while the tangential traction is given as a function of the relative tangential velocity. The tractions are defined by user-specified functions, and the tangential tractions from this model drop to zero once the normal distance between the node and the face exceeds a critical value. This friction model provides a simple way to model threaded connections, though the `THREADED MODEL` defined in Section 7.11.12 has more flexibility.

In the above command block, the string `name` is a user-selected name for this friction model that is used to identify this model in the interaction blocks. The normal traction curve is specified by the `NORMAL TRACTION FUNCTION` command line, where the string `func_name` is the name of a function defined in a `DEFINITION FOR FUNCTION` command block in the SIERRA scope. This function defines a relation between the traction and the distance between the node and the face in the normal direction. This function can be scaled by the real value `scale_factor` in the `NORMAL TRACTION SCALE FACTOR` command line; the default for this factor is 1.0. Similarly, the tangential traction curve is specified by the `TANGENTIAL TRACTION FUNCTION` command line, where the string `func_name` is the name of a function defined in a `DEFINITION FOR FUNCTION` command block in the SIERRA scope. This function defines a relation between the traction and the relative velocity of the node and face in the tangential direction. This function can be scaled by the real value `scale_factor` in the `TANGENTIAL TRACTION SCALE FACTOR` command line; the

default for this factor is 1.0. Once the normal distance between a node and a face using this model reaches a critical distance, the tangential traction drops to zero; this distance is specified with the real value `distance` in the `NORMAL CUTOFF DISTANCE FOR TANGENTIAL TRACTION` command line.

7.11.12 Threaded Model

```
BEGIN THREADED MODEL <string>name
  NORMAL TRACTION FUNCTION = <string>func_name
  NORMAL TRACTION SCALE FACTOR = <real>scale_factor(1.0)
  TANGENTIAL TRACTION FUNCTION = <string>func_name
  TANGENTIAL TRACTION SCALE FACTOR = <real>scale_factor(1.0)
  TANGENTIAL TRACTION GAP FUNCTION = <string>func_name
  TANGENTIAL TRACTION GAP SCALE FACTOR = <real>scale_factor(1.0)
  NORMAL CAPACITY = <real>normal_cap
  TANGENTIAL CAPACITY = <real>tangential_cap
  FAILURE ENVELOPE EXPONENT = <real>exponent(2.0)
  FAILURE DECAY CYCLES = <integer>num_cycles(1)
  FAILED MODEL = <string>failed_model_name|FRICTIONLESS
    (FRICTIONLESS)
END [THREADED MODEL <string>name]
```

The `THREADED MODEL` command block defines a friction model that is designed to mimic a threaded interface. This model prevents interpenetration of contact surfaces, and also supplies additional tractions when the surfaces are not touching. Tensile tractions in the normal direction are given by a user-specified function of force versus distance between the node and face. Tensile tractions in the tangential direction are computed as the product of a traction tangential-displacement curve and a scaling curve that is a function of the normal displacement. Maximum normal and tangential tractions are input such that the model "fails" at a node-face interaction once they are reached. For interactions that include both normal and tangential displacements, the model failure is defined according to a failure criterion defined as the sum of the ratios of the normal and tangential traction components to their maximum capacity values, raised to a power. After failure, interactions shift to a different user-specified friction model.

In the above command block:

- The string `name` is a user-selected name for this friction model that is used to identify the model in the interaction definitions.

- The traction-displacement relation in the normal direction is specified by the `NORMAL TRACTION FUNCTION` command line, where the string `func_name` is the name of a function defined in a `DEFINITION FOR FUNCTION` command block in the SIERRA scope. This function can be scaled by the real value `scale_factor` in the `NORMAL TRACTION SCALE FACTOR` command line; the default for this factor is 1.0.

- The traction-displacement relation in the tangential direction is specified by two curves. The traction-displacement relation in the tangential direction when there is no displacement in the normal direction is defined by the `TANGENTIAL TRACTION FUNCTION` command line, where the string `func_name` is the name of a function defined in a `DEFINITION FOR FUNCTION` command block in the SIERRA scope. This function can be scaled by the real value `scale_factor` in the `TANGENTIAL TRACTION SCALE FACTOR` command line; the default for this factor is 1.0. When the distance in the normal direction is greater than zero, the tangential traction is scaled by a function specified in the `TANGENTIAL TRACTION GAP FUNCTION` command line, where the string `func_name` is the name of a function defined in a `DEFINITION FOR FUNCTION` command block in the SIERRA scope. This function defines a scaling factor as a function of the normal displacement. The function can be scaled by the real value `scale_factor` in the `TANGENTIAL TRACTION GAP SCALE FACTOR` command line; the default for this factor is 1.0.

- The threaded model "fails" once the normal and tangential tractions reach a critical capacity value. The normal capacity is specified by the real value `normal_cap` in the `NORMAL CAPACITY` command line. The tangential capacity is specified by the real value `tangential_cap` in the `TANGENTIAL CAPACITY` command line. There are no default values for these parameters. These capacities are defined for pure normal or tangential displacements. In cases where there is a combination of tangential and normal displacements, a failure curve is used to determine the combination of tangential and normal tractions that determines model failure. This curve is defined as the sum of the ratios of the normal and tangential traction components to their maximum capacity values, raised to a power. The power in the function is defined by the real value exponent in the `FAILURE ENVELOPE EXPONENT` command line. The default value of the exponent is 2.0. Once the model fails, the applied tractions decrease to zero over a number of time steps defined through the integer value `num_cycles` in the `FAILURE DECAY CYCLES` command line. The default for `num_cycles` is 1. When the model exceeds the designated capacity, the contact surfaces using this model switch to a different friction model as identified in the `FAILED MODEL` command line with the string `failed_model_name`. The friction model designated in the `FAILED MODEL` command line must be defined within the `CONTACT DEFINITION` command block. The default model is the frictionless model.

7.11.13 PV_Dependent Model

```
BEGIN PV_DEPENDENT MODEL <string>name
  STATIC COEFFICIENT = <real>stat_coeff
  DYNAMIC COEFFICIENT = <real>dyn_coeff
  VELOCITY DECAY = <real>vel_decay
  REFERENCE PRESSURE = <real>p_ref
  OFFSET PRESSURE = <real>p_off
  PRESSURE EXPONENT = <real>p_exp
END [PV_DEPENDENT MODEL <string> name]
```

The `PV_DEPENDENT MODEL` command block defines a friction model similar to a coulomb fric-

tion model, but which provides a frictional response that is dependent on the pressure and the velocity. The pressure-dependent portion of the model behaves similarly to the constant friction model except that the tangential traction is given by

$$\left[\frac{p + \text{p_off}}{\text{p_ref}}\right]^{\text{p_exp}}. \tag{7.1}$$

The velocity-dependent part is given by

$$\left(\text{stat_coeff} - \text{dyn_coeff}\right) e^{\left(-\text{vel_decay}\|v\|\right)} + \text{dyn_coeff}. \tag{7.2}$$

The `PV_DEPENDENT MODEL` command block multiplies the pressure and velocity effects together.

In the above command block:

- The string `name` is a name assigned to this friction model that is used to identify the model in the interaction definitions.
- The real value `p_ref` in the pressure-dependent part given in Equation (7.1) is specified with the `REFERENCE PRESSURE` command line.
- The real value `p_off` in the pressure-dependent part given in Equation (7.1) is specified with the `OFFSET PRESSURE` command line.
- The real value `p_exp` in the pressure-dependent part given in Equation (7.1) is specified with the `PRESSURE EXPONENT` command line.
- The real value `stat_coeff` in the velocity-dependent part given in Equation (7.2) is specified with the `STATIC COEFFICIENT` command line.
- The real value `dyn_coeff` in the velocity-dependent part given in Equation (7.2) is specified with the `DYNAMIC COEFFICIENT` command line.
- The real value `vel_decay` in the velocity-dependent part given in Equation (7.2) is specified with the `VELOCITY DECAY` command line.

7.11.14 Time Variant Model

```
BEGIN TIME VARIANT MODEL <string>name
  MODEL = <string>model DURING PERIODS <string_list>time_periods
END [TIME VARIANT MODEL]
```

The `TIME VARIANT MODEL` command block does not directly define a friction model, but provides a mechanism to switch between separately defined friction models between time periods. The only command line in the block is the `MODEL` command, which is used to reference a separately-defined friction model `model` and provide a list of time periods during which that model is active.

Multiple MODEL commands may be used to activate different friction models throughout the analysis. See Section 2.5 for more information on controlling functionality by time period. This feature is only available for Dash contact.

7.11.15 User Subroutine Friction Models

```
BEGIN USER SUBROUTINE MODEL <string>name
  INITIALIZE MODEL SUBROUTINE = <string>init_model_name
  INITIALIZE TIME STEP SUBROUTINE = <string>init_ts_name
  INITIALIZE NODE STATE DATA SUBROUTINE =
    <string>init_node_data_name
  LIMIT FORCE SUBROUTINE = <string>limit_force_name
  ACTIVE SUBROUTINE = <string>active_name
  INTERACTION TYPE SUBROUTINE = <string>interaction_name
END [USER SUBROUTINE MODEL <string>name]
```

The USER SUBROUTINE MODEL command blocks permit contact to use a user subroutine to define a friction model between surfaces. This capability is in a test phase at this time; please contact a Presto developer for more information.

In this command block:

- The string name is a user-specified name that is used to identify this model in the interaction definitions.
- The command line INITIALIZE MODEL SUBROUTINE specifies a user subroutine to initialize the friction model. The name of the subroutine is given by init_model_name.
- The command line INITIALIZE TIME STEP SUBROUTINE specifies a user subroutine to initialize the time step. The name of the subroutine is given by init_ts_name.
- The command line INITIALIZE NODE STATE DATA SUBROUTINE specifies a user subroutine to initialize the node state data. The name of the subroutine is given by init_node_data_name.
- The command line LIMIT FORCE SUBROUTINE specifies a user subroutine to provide the limit force for the friction model. The name of the subroutine is given by limit_force_name.
- The command line ACTIVE SUBROUTINE specifies a user subroutine to compute forces for an active node-face interaction. The name of the subroutine is given by active_name.
- The command line INTERACTION TYPE SUBROUTINE specifies a user subroutine to define the interaction type. The name of the subroutine is given by interaction_name.

7.12 Search Options

```
BEGIN SEARCH OPTIONS [<string>name]
  #
  # search algorithms
  GLOBAL SEARCH INCREMENT = <integer>num_steps(1)
  GLOBAL SEARCH ONCE = <string>ON|OFF(OFF)
  #
  # search tolerances
  SEARCH TOLERANCE = <string>AUTOMATIC|USER_DEFINED(AUTOMATIC)
  NORMAL TOLERANCE = <real>norm_tol
  TANGENTIAL TOLERANCE = <real>tang_tol
  FACE MULTIPLIER = <real>face_multiplier(0.1)
  #
  # secondary decomposition
  SECONDARY DECOMPOSITION = <string>ON|OFF(OFF)
END [SEARCH OPTIONS <string>name]
```

Contact involves a search phase and an enforcement phase. The contact search algorithm used to detect interactions between contact surfaces is often the most computationally expensive part of an analysis. The user can exert some control over how the search phase is carried out via the `SEARCH OPTIONS` command block. By selecting different options in this command block, the user can make trade-offs between the accuracy of the search and computing time.

The most accurate approach to the search phase is a global search at every time step. For a global search, a box is drawn around each face. The box depends on the shape of the face, the location of the face in space, and search tolerances. Now suppose we want to determine whether some node has penetrated that face. We must first determine if the node lies in one or more boxes that surround a face. This search, although done with an optimal algorithm, is still time consuming. The search must be done for all nodes that may be in contact with a face. A less accurate approach for the search phase is to use what is called a local tracking algorithm. For the tracking algorithm approach, we first do a global search. When a node has contacted a face in the global search, we record the face (or faces) contacted by the node. Instead of using the global search on subsequent time steps, we simply rely on the record of the node-face interactions to compute the contact forces. The last face contacted by a node in the global search is assumed to remain in contact with that node for subsequent time steps. In actuality, the node may slide off the face it was contacting at the time of the global search. In this case, faces that share an edge with the original contact face are searched to determine whether they (the edge adjacent faces) are in contact with the node. If the node moves across a corner of the face (rather than an edge), we may lose the contact interaction for the node until the next global search. If we lose the contact interaction, we lose some of the accuracy in the contact calculations until we do the next global search. Furthermore, it is possible that additional nodes may actually come into contact in the time steps between global searches. These nodes are typically caught during the next global search, but inaccuracies can result from missing the exact time of contact. The tracking algorithm, under certain circumstances, can work quite well even though it is less accurate. We can encounter analyses where we can set the number of intervals (time steps) between global searches to a relatively small number (5) and lose only

a few or none of the node-to-face contacts between global searches. Likewise, we can encounter analyses where we can set the interval between global searches to a large number (100 or more) and lose only a few or none of the node-to-face contacts between global searches. Finally, we can encounter problems where we may only have to do one global search at the beginning and rely solely on the tracking information for the rest of the problem (without losing any contact). What search approach is best for your problem depends on the geometry of your structure, the loads on your structure, and the amount of deformation of your structure. This section tells you how to control the search phase for your specific problem.

The `SEARCH OPTIONS` command block begins with the input line:

```
BEGIN SEARCH OPTIONS [<string>name]
```

and ends with:

```
END [SEARCH OPTIONS <string>name]
```

The `name` for the command block is optional.

Without a `SEARCH OPTIONS` command block, the default search with associated default search parameters is used for all contact pairs. If you want to override the default search method for all contact pairs, you should add a `SEARCH OPTIONS` command block. By adding a `SEARCH OPTIONS` command block, you establish a new set of global defaults for the search for all contact pairs. The default for the search is that tracking is turned on and the number of intervals (time steps) between a global search is one (`GLOBAL SEARCH INCREMENT = 1` and `GLOBAL SEARCH ONCE = OFF`).

The valid command lines within a `SEARCH OPTIONS` command block are described in Section 7.12.1, Section 7.12.2, and Section 7.12.3. The values specified by these commands are applied by default to all interaction contact surfaces, unless overridden by a specific interaction definition.

7.12.1 Search Algorithms

```
GLOBAL SEARCH INCREMENT = <integer>num_steps(1)
GLOBAL SEARCH ONCE = <string>ON|OFF(OFF)
```

Known Issue: Attempting to use `GLOBAL SEARCH INCREMENT` with a value greater than 1, especially in a problem that contains shells and/or restart, will, in most cases, cause code failure. A `GLOBAL SEARCH INCREMENT` value greater than 1 will, under the best circumstances, give only a marginal improvement in speed.

The above two command lines let you determine the frequency of the global search. Although these command lines are mutually exclusive, they provide for three search options:

1. If you want to do only one global search and have all subsequent searches be tracking searches, then you should use the `GLOBAL SEARCH ONCE` command line with the string parameter set to `ON`. By default, the `GLOBAL SEARCH ONCE` option is `OFF`. If you set `GLOBAL SEARCH ONCE` to `ON`, then this should be the only command line for the search algorithms in the command block. The `GLOBAL SEARCH INCREMENT` command line should not be used.

2. If you want to use the global search only intermittently, with the tracking search in between the global search, you should use the `GLOBAL SEARCH INCREMENT` set to some integer value greater than 1. The integer value `num_steps` determines the number of time steps between global searches. The `GLOBAL SEARCH ONCE` command line should not be used.

3. If you want to do a global search at every time step, you should use the `GLOBAL SEARCH INCREMENT` command line with `num_steps` set to `1` or just simply omit this line since the default for the search increment is `1`. The `GLOBAL SEARCH ONCE` command line should not be used.

In summary, you have three options for the global search. You can do a global search only once (the first time step), and do a tracking search for all subsequent searches by setting `GLOBAL SEARCH ONCE` to `ON`. You can do a global search for the beginning time step and intermittently thereafter; the time steps between the global searches will use a tracking search. For this approach, you will need only the `GLOBAL SEARCH INCREMENT` command line. Finally, you can set `GLOBAL SEARCH INCREMENT` to `1` and do a global search at every time step.

7.12.2 Search Tolerances

```
SEARCH TOLERANCE = <string>AUTOMATIC|USER_DEFINED(AUTOMATIC)
NORMAL TOLERANCE = <real>norm_tol
TANGENTIAL TOLERANCE = <real>tang_tol
FACE MULTIPLIER = <real>face_multiplier(0.1)
```

As indicated previously, the contact functionality in Presto uses a box defined around each face to locate nodes that may potentially contact the face. This box is defined by a tolerance normal to the face and another tolerance tangential to the face (see Figure 7.5). The code adds to these tolerances the maximum motion over a time step when identifying interactions. In the above command lines, the parameter `norm_tol` is the normal tolerance (defined on the `NORMAL TOLERANCE` command line) for the search box and the parameter `tang_tol` is the tangential tolerance (defined on the `TANGENTIAL TOLERANCE` command line) for the search box.

By default, Presto will automatically calculate normal and tangential tolerances based on the minimum characteristic length multiplied by the value input by the `FACE MULTIPLIER` command. The face multiplier is 0.1. The automatic tolerances add the maximum motion over a time step just like the user defined tolerances. If you leave automatic search on and also specify normal and/or tangential tolerances with the `NORMAL TOLERANCE` and `TANGENTIAL TOLERANCE` command lines, the larger of the two (automatic or user specified) tolerances will be used. For example, suppose

you specify a normal tolerance of 1.0×10^{-3} and the automatic tolerancing computes a normal tolerance of 1.05×10^{-3}. Then Presto will use a normal tolerance of 1.05×10^{-3}.

When the `USER_DEFINED` option is specified for the `SEARCH TOLERANCE` command line, these normal and tangential tolerances must be specified. If these tolerances are not specified, code execution will be terminated with an error.

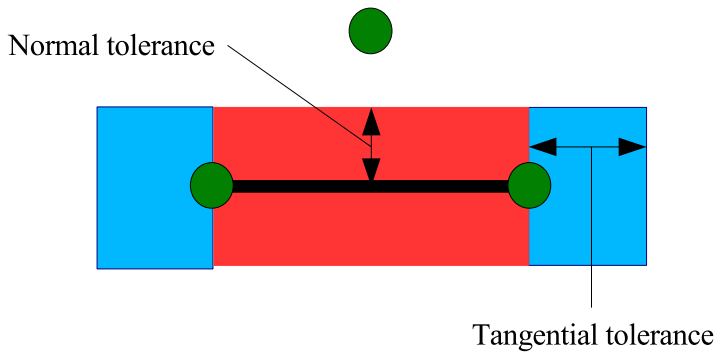

Figure 7.5: Illustration of normal and tangential tolerances.

Both of these tolerances are absolute distances in the same units as the analysis. The proper tolerances are problem dependent. If a normal or tangential tolerance is specified in the `SEARCH OPTIONS` command block, they apply to all interactions. These default search tolerances can be overwritten for a specific interaction by specifying a value for the normal tolerance and/or tangential tolerance for that interaction inside the `INTERACTION` command block (see Section 7.16).

7.12.3 Secondary Decomposition

```
SECONDARY DECOMPOSITION = <string>ON|OFF(ON)
```

The `SECONDARY DECOMPOSITION` command line controls internal options used by the ACME contact search algorithm. Computational results for secondary decomposition `ON` should be identical to those for secondary decomposition `OFF`. However, the computational time for these two distinct options may vary significantly.

When a mesh is divided for parallel processing, it is usually divided such that each processor has the same number of elements. The element-based load balance needs to achieve good parallel performance for element and material calculations. It is possible to have the number of elements per processor balanced but the number of contact faces per processor highly unbalanced. If contact is highly localized in one region of the model, it may happen that a small subset of the processors contains most of the contact interactions. A secondary decomposition is a parallel decomposition that balances the number of contact faces. When secondary decomposition is on, the contact algorithm first moves all data to the secondary decomposition and then it runs the contact calculations. When the secondary decomposition is off, all contact calculations are done in the primary decomposition.

The computational effort to move data to the secondary decomposition can be quite large. Thus, if the contact surfaces are well balanced in the primary decomposition, a large cost savings can be realized by turning off the secondary decomposition. Three conditions must be met for turning off the secondary decomposition to achieve cost savings. First, the number of contact faces per processor must be somewhat balanced in the primary decomposition. Second, faces in contact should be on the same processor as much as possible. Inertial and RCB decomposition tend to meet this condition of having contact faces in proximity on the same processor, while Multi-KL does not. Third, conditions one and two must persist throughout the entire analysis. An initially well balanced, well distributed mesh may become poorly balanced through element death or large deformations.

7.13 User Search Box

```
BEGIN USER SEARCH BOX <string>name
  #
  # box center point
  CENTER = <string>center_point
  X DISPLACEMENT FUNCTION = <string>x_disp_function_name
  Y DISPLACEMENT FUNCTION = <string>y_disp_function_name
  Z DISPLACEMENT FUNCTION = <string>z_disp_function_name
  X DISPLACEMENT SCALE FACTOR = <real>x_disp_scale_factor
  Y DISPLACEMENT SCALE FACTOR = <real>y_disp_scale_factor
  Z DISPLACEMENT SCALE FACTOR = <real>z_disp_scale_factor
  #
  # box lengths
  X EXTENT FUNCTION = <string>x_extent_function_name
  Y EXTENT FUNCTION = <string>y_extent_function_name
  Z EXTENT FUNCTION = <string>z_extent_function_name
  #
END [USER SEARCH BOX <string>name]
```

When using Dash contact, user-defined search boxes can be used to improve the efficiency of the contact search in some situations. The `USER SEARCH BOX` command can be used to define the coordinates of a rectangular box aligned with the global coordinate system that contains the regions where contact will be enforced. Multiple user search boxes can be defined.

Commands used within the `USER SEARCH BOX` command block define the location of the center of the box, a prescribed displacement of the center, and the size of the box in the three global coordinate directions. These are documented in the following sections.

If the `USER SEARCH BOX` command is used, contact will not be enforced outside the set of user-defined search boxes specified by the user. These search boxes should be defined over an area larger than the actual contact zone to handle cases of large motion.

In general, problems having a large area in which the analyst wishes to ignore contact (such as an area of particle collisions outside the scope of interest) or in which the area of contact is a known patch that encompasses a small subset of the faces in the contact surfaces are the most likely to experience enhanced performance with user-defined search boxes.

7.13.1 Search Box Location

```
  CENTER = <string>center_point
  X DISPLACEMENT FUNCTION = <string>x_disp_function_name
  Y DISPLACEMENT FUNCTION = <string>y_disp_function_name
  Z DISPLACEMENT FUNCTION = <string>z_disp_function_name
  X DISPLACEMENT SCALE FACTOR = <real>x_disp_scale_factor
  Y DISPLACEMENT SCALE FACTOR = <real>y_disp_scale_factor
  Z DISPLACEMENT SCALE FACTOR = <real>z_disp_scale_factor
```

The location of a user search box is specified by a combination of a center point location and a set of extents in the global coordinates. The commands listed here define the location of the center of the search box as a function of time.

The `CENTER` command is used to specify a point, where `center_point` is the name of a point that is defined externally to this command block using the `DEFINE POINT` command (See Section 2.1.6).

The `X DISPLACEMENT FUNCTION`, `Y DISPLACEMENT FUNCTION`, and `Z DISPLACEMENT FUNCTION` command lines refer to functions that define the motion of the search box center in the X, Y, and Z directions as a function of time. These commands are required.

The `X DISPLACEMENT SCALE FACTOR`, `Y DISPLACEMENT SCALE FACTOR`, and `Z DISPLACEMENT SCALE FACTOR` command lines are optional, and can be used to provide scale factors that are multiplied by the corresponding displacement functions.

7.13.2 Search Box Size

```
X EXTENT FUNCTION = <string>x_extent_function_name
Y EXTENT FUNCTION = <string>y_extent_function_name
Z EXTENT FUNCTION = <string>z_extent_function_name
```

The size of the user search box is defined by the X, Y, and Z extent functions, which are required. These are specified using the `X EXTENT FUNCTION`, `Y EXTENT FUNCTION`, and `Z EXTENT FUNCTION` command lines. Each of these functions defines the total length of the box in the respective coordinate direction as a function in time. The search box extends half the distance in the negative and positive directions from the center point.

7.14 Enforcement Options

Options

```
BEGIN ENFORCEMENT OPTIONS [<string>name]
  MOMENTUM BALANCE ITERATIONS = <integer>num_iterations(5)
END [ENFORCEMENT OPTIONS <string>name]
```

Contact, as previously indicated, involves a search phase and an enforcement phase. The user can exert some control over how the enforcement phase is carried out via the `ENFORCEMENT OPTIONS` command block. By selecting different options in this command block, the user can make trade-offs between solution accuracy and computing time. The `ENFORCEMENT OPTIONS` command block begins with the input line:

```
BEGIN ENFORCEMENT OPTIONS [<string>name]
```

and is terminated with the input line:

```
END [ENFORCEMENT OPTIONS <string>name]
```

The name for the command block, `name`, is optional

Only a single `ENFORCEMENT OPTIONS` command block is permitted within a `CONTACT DEFINITION` command block. Without an `ENFORCEMENT OPTIONS` command block, the default enforcement algorithm with associated default enforcement options is used for all contact pairs. If you want to override the defaults for enforcement for all contact pairs, you should add an `ENFORCEMENT OPTIONS` command block. By adding this command block, you establish a new set of global defaults for enforcement for all contact pairs. You can override some of these global defaults for enforcement for a contact pair by inserting certain command lines in the `INTERACTION` command block (see Section 7.16) for that contact pair. It is possible, therefore to tailor the enforcement approach for individual contact pairs.

Currently, the enforcement option is of limited use. Options for user control will be expanded in future versions of Presto.

The momentum balance algorithm for enforcement of the contact constraints uses an iterative process to ensure incremental momentum balance over a time step. Rather than making one pass to compute contact forces for node push-back, several passes are made to more accurately compute the normal contact force and, subsequently, the tangential (frictional) contact forces. The number of passes (iterations) is set by the value `num_iterations` in the `MOMENTUM BALANCE ITERATIONS` command line. The default value for the number of iterations is 5. This value is generally acceptable for removing overlap in the mesh. To get accurate results in a global sense in analyses that use friction, a value of 10 is more appropriate. To get accurate contact response at individual points in analyses with friction, a value of 20 or greater may be needed. Note that as the number of iterations increases, the expense of enforcement increases.

Thus a user can balance execution speed and accuracy with this command line, though care must be taken to ensure that the appropriate level of accuracy is attained. This command line affects only the enforcement phase of the contact. A single search phase is used for contact detection, but the enforcement phase uses an iterative process.

7.15 Default Values for Interactions

```
BEGIN INTERACTION DEFAULTS
  CONTACT SURFACES = <string list>surface_names
  SELF CONTACT = <string>ON|OFF(OFF)
  GENERAL CONTACT = <string>ON|OFF(OFF)
  AUTOMATIC KINEMATIC PARTITION = <string>ON|OFF(OFF)
  FRICTION MODEL = <string>friction_model_name|FRICTIONLESS
    (FRICTIONLESS)
  INTERACTION BEHAVIOR = <string>SLIDING|
    INFINITESIMAL_SLIDING|NO_INTERACTION(SLIDING)
  CONSTRAINT FORMULATION = <string>NODE_FACE|FACE_FACE
END [INTERACTION DEFAULTS]
```

This section discusses the `INTERACTION DEFAULTS` command block. This command block enables contact enforcement either on all contact surfaces or on a subset of the contact surfaces. It is also used to set default parameters for contact interactions. Those defaults can be overridden for specific interactions by specifying them separately in `INTERACTION` blocks.

It is important to note that unless some combination of the `INTERACTION DEFAULTS` command block and `INTERACTION` command blocks (Section 7.16) exists in the `CONTACT DEFINITION` command block, enforcement will not take place. Up to this point, all command lines and command blocks have provided information to set up the search phase and have provided details for surface interaction. However, contact enforcement for surfaces—the actual removal of interpenetration between surfaces and the calculation of surface forces consistent with friction models—will not take place unless some combination of the `INTERACTION DEFAULTS` command block and `INTERACTION` command blocks is used to set up surface interactions.

Contact between surfaces requires data to describe the interaction between these surfaces. You may specify defaults for the surface interactions for some or all surface pairs by using the `INTERACTION DEFAULTS` command block. Within this command block, you can provide a list of surfaces that are a subset of the contact surfaces. Any pair of surfaces listed in the `INTERACTION DEFAULTS` command block will acquire the default values that are defined within the `INTERACTION DEFAULTS` command block. If you omit the `CONTACT SURFACES` command line, defaults in the `INTERACTION DEFAULTS` command block are applied to all surfaces. Any default set within an `INTERACTION DEFAULTS` command block can be overridden by commands in an `INTERACTION` command block. See Section 7.16.

If you consider only the use of the `INTERACTION DEFAULTS` command block (and not the use of the `INTERACTION` command block), you have three options for the surface interaction values:

- You can specify default surface interaction values for all the contact surface pairs by specifying all the contact surfaces in an `INTERACTION DEFAULTS` command block.

- You can specify default surface interaction values for some of the contact surface pairs by specifying a subset of the contact surfaces in an `INTERACTION DEFAULTS` command block.

- You can leave all interactions off by default by not specifying an INTERACTION DEFAULTS command block.

The values specified by the command lines in the INTERACTION DEFAULTS command block are applied by default to all interaction contact surfaces unless overridden by a specific interaction definition.

7.15.1 Surface Identification

```
CONTACT SURFACES = <string list>surface_names
```

This command line identifies the contact surfaces to which the surface interaction values defined in the INTERACTION DEFAULTS command block will apply. The string list on the CONTACT SURFACES command line specifies the names of these contact surfaces. The CONTACT SURFACES command line can include any surface specified in a CONTACT SURFACE command line, a CONTACT SURFACE command block, or a SKIN ALL BLOCKS command line.

The SURFACES command line is optional. If you want the defaults to apply to all the surfaces you have defined, you will NOT use the SURFACES command line in this command block. If you want the defaults to apply to a subset of all contact surfaces, then you will list the specific set of surfaces on a SURFACES command line. The names of all the surfaces with the default values will be listed in the string list designated as surface_names.

7.15.2 Self-Contact and General Contact

```
SELF CONTACT = <string>ON|OFF(OFF)
GENERAL CONTACT = <string>ON|OFF(OFF)
```

The SELF CONTACT command line, if set to ON, specifies that the default values set in the command lines of the command block will apply to self-contact between the listed surfaces (or all surfaces if no surfaces are listed). The GENERAL CONTACT command line, if set to ON, specifies that the default values set in the command lines of this command block apply to contact between the listed surfaces (or all surfaces if no surfaces are listed) excluding self-contact. The default values for both of these command lines is OFF. To enforce general contact between all surfaces specified in the INTERACTION DEFAULTS command block but no self-contact, this line must be present:

```
GENERAL CONTACT = ON
```

To enforce self-contact for all surfaces specified in the INTERACTION DEFAULTS command block, this line must be present:

```
SELF CONTACT = ON
```

If no individual contact interactions have been specified with INTERACTION command blocks, contact will only be enforced if either general contact or self-contact (or both) are enabled.

If general contact or self-contact is enabled, contact enforcement may be disabled for individual surfaces (for self-contact) or pairs of surfaces (for general contact) by using the INTERACTION BEHAVIOR = NO_INTERACTION in the INTERACTION command block.

7.15.3 Friction Model

```
FRICTION MODEL = <string>friction_model_name|FRICTIONLESS
  (FRICTIONLESS)
```

The FRICTION MODEL command line permits the description of how surfaces interact with each other using a friction model defined in a friction-model command block (see Section 7.11). In the above command line, the string friction_model_name should match the name assigned to some friction model command block. For example, if you specified the name of an AREA WELD command block as AW1 and wanted to reference that name in the FRICTION MODEL command line, the value of friction_model_name would be AW1.

The default interaction is frictionless contact.

7.15.4 Automatic Kinematic Partition

```
AUTOMATIC KINEMATIC PARTITION
```

If the AUTOMATIC KINEMATIC PARTITION command line is used, Presto will automatically compute the kinematic partition factors for pairs of surfaces. (See Section 7.16.2 for more information on kinematic partitioning.) The automatic kinematic partitions are computed from the impedance of each surface based on nodal average density and wave speed. Automatic computation of kinematic partition factors provides the best approach to exact enforcement of symmetric contact of opposing surfaces provided that these surfaces have the same mesh resolution. If the mesh resolution is disparate, you can specify the coarser meshed body as master, but generally it is better to use more contact iterations to deal with this case of a fine mesh contacting a coarse mesh.

For the interaction of any two surfaces, the sum of the partition factors for the surfaces must be 1.0. This is automatically taken care of when the AUTOMATIC KINEMATIC PARTITION command line is used. The default value for kinematic partition factors for all surfaces is 0.5.

The AUTOMATIC KINEMATIC PARTITION command line can be used to set the kinematic partitions for all interactions or to set the kinematic partitions for specific interactions. Thus the command line can appear in two different scopes:

1. The command line can be used within the INTERACTION DEFAULTS command block. In this case, all contact surface interactions defined in the command block will use the automatic kinematic partitioning scheme by default. This will override the default case that assigns a

kinematic partition factor of 0.5 to all surfaces. For particular interactions, it is possible to override the use of the automatic kinematic partition factors by specifying kinematic partition values (with the KINEMATIC PARTITION command line) within the INTERACTION command blocks for those interactions.

2. The command line can be used inside an INTERACTION command block. If the automatic partitioning command line appears inside an INTERACTION command block, the kinematic partition factors for that particular interaction will be calculated by the automatic kinematic partition scheme.

Automatic kinematic partitioning is not currently operational for shell elements. If it is enabled, the kinematic partitioning factor is set to 0.5 for all contact interactions involving shell elements.

7.15.5 Interaction Behavior

```
INTERACTION BEHAVIOR = <string>SLIDING|
  INFINITESIMAL_SLIDING|NO_INTERACTION(SLIDING)
```

The INTERACTION BEHAVIOR command line specifies how the search will be done. For SLIDING contact, the search algorithm is constantly updating information that lets the code accurately track the sliding of the node over the face and any adjacent faces. The SLIDING option, which is the default, lets us handle the case where we have large relative sliding between a face and a node. A node contacting a face can slide over time by a significant amount over the face. The node can slide onto an adjacent face or onto a face on a nearby surface. For the case of INFINITESIMAL_SLIDING, search information is not updated to the extent that it is with the SLIDING option. In the case of INFINITESIMAL_SLIDING, it is assumed that there is very little slip over time of a node relative to its initial contact point on a face. Furthermore, it is assumed a node will not slide off the face that it initially contacts. The INFINITESIMAL_SLIDING option is not as accurate as the SLIDING option, but neither is it as expensive as the SLIDING option. For some cases, however, the INFINITESIMAL_SLIDING option may work quite well even though it is not as accurate as the SLIDING option. Finally, you may turn off the search completely by using the NO_INTERACTION option.

With the third option, NO_INTERACTION, you could turn off the search for all surfaces specified in the INTERACTION DEFAULTS command block. You could then turn on the search on a case-by-case basis for various contact pairs or for the self-contact of surfaces by using INTERACTION command blocks. This is a convenient way to set defaults for the friction model and automatic kinematic partitioning without turning on all the interactions. More likely, you will set contact interactions to default to the SLIDING option in the INTERACTION DEFAULTS command block, and then turn off specific contact interactions through INTERACTION command blocks.

Using the INTERACTION BEHAVIOR command line in the INTERACTION DEFAULTS command block represents a sophisticated application of this command line. Consult with Presto developers for more information about this command line used in an INTERACTION DEFAULTS command block.

7.15.6 Constraint Formulation

```
CONSTRAINT FORMULATION = NODE_FACE|FACE_FACE
```

The `CONSTRAINT FORMULATION` command is used to switch between node/face and face/face enforcement for contact constraints. If the `NODE_FACE` option is selected, node/face contact is used, and if the `FACE_FACE` option is selected, face/face contact is used. This command only has an effect when Dash contact is used. ACME only supports node/face contact. With Dash contact, face/face contact is used by default, except for the case where one of the surfaces is explicitly defined by a node set, in which case node/face contact is used.

7.16 Values for Specific Interactions

```
BEGIN INTERACTION [<string>name]
  SURFACES = <string_list>surfaces [EXCLUDE <string_list>surfaces]
  MASTER   = <string_list>surfaces [EXCLUDE <string_list>surfaces]
  SLAVE    = <string_list>surfaces [EXCLUDE <string_list>surfaces]
  KINEMATIC PARTITION = <real>kin_part
  NORMAL TOLERANCE = <real>norm_tol
  TANGENTIAL TOLERANCE = <real>tang_tol
  FACE MULTIPLIER = <real>face_multiplier(0.1)
  OVERLAP NORMAL TOLERANCE = <real>over_norm_tol
  OVERLAP TANGENTIAL TOLERANCE = <real>over_tang_tol
  FRICTION MODEL = <string>friction_model_name|FRICTIONLESS
    (FRICTIONLESS)
  AUTOMATIC KINEMATIC PARTITION
  INTERACTION BEHAVIOR = <string>SLIDING|
    INFINITESIMAL_SLIDING|NO_INTERACTION(SLIDING)
  CONSTRAINT FORMULATION = <string>NODE_FACE|FACE_FACE
END [INTERACTION <string>name]
```

The Presto contact input also permits the setting of values for specific interactions using the `INTERACTION` command block. If an `INTERACTION DEFAULTS` command block is present within a `CONTACT DEFINITION` command block, the values provided by an `INTERACTION` command block override the defined defaults. If an `INTERACTION DEFAULTS` command block is not present, only those interactions defined by `INTERACTION` command blocks are searched for contact, and values without system defaults must be specified.

The `INTERACTION` command block begins with:

```
BEGIN INTERACTION [<string>name]
```

and ends with:

```
END [INTERACTION <string>name]
```

where `name` is a name for the interaction. Note that this name is currently used only for informational output purposes and is not required.

The valid commands within an `INTERACTION` command block are described in Section 7.16.1 through Section 7.16.6.

7.16.1 Surface Identification

```
SURFACES = <string_list>surfaces [EXCLUDE <string_list>surfaces]
MASTER   = <string_list>surfaces [EXCLUDE <string_list>surfaces]
SLAVE    = <string_list>surfaces [EXCLUDE <string_list>surfaces]
```

There are two methods to identify the surfaces described by a specific interaction.

One method is to identify all surfaces in a single line with the `SURFACES` command line. For explicit dynamics, the surface list must contain at least two surfaces. This command will define a symmetric two-way contact interaction between each surface on the command line and every other surface on the command line. If a contact `KINEMATIC PARTITION` is also specified, the surface list must contain only two surfaces (see Section 7.16.2).

To specify self contact, the surface must appear in the `SURFACES` command line twice. Each surface specified on the `SURFACES` command line interacts with each other surface on that line. If a surface is specified on the line twice, it indicates that a surface will also interact with itself.

The second method to identify contact surfaces is to use the `MASTER` and `SLAVE` command lines. The nodes of the slave surfaces are searched against the faces of the master surfaces. Each of these command lines takes as input a list of names of contact surfaces defined in the contact block. A master slave interaction will be defined between each surface in the master list and each surface in the slave list. A surface may not be present in both the master and the slave list.

Master/Slave contact always uses a kinematic partition of 1.0 thus the `KINEMATIC PARTITION` command may not be used with master/slave contact.

The surface named `all_surfaces` is a special reserved word that is equivalent to typing all contact surfaces known by the contact block into the string list. Optionally, the `EXCLUDE` keyword can be placed on the command line and followed by a list of surface names to exclude from the list. If the `SURFACES`, `MASTER`, or `SLAVE` command lines appear multiple times within a `CONTACT INTERACTION` block, their surface lists will be concatenated. The effect is equivalent to specifying all of the surface names on a single line. The `SURFACES` command line cannot be used simultaneously with the `MASTER` and `SLAVE` command lines.

The following examples demonstrate ways to identify contact surfaces involved in an interaction:

This command defines a symmetric interaction between `s1` and `s2`:

```
SURFACES = s1 s2
```

This defines a symmetric self contact interaction between `s1` and itself:

```
SURFACES = s1 s1
```

This defines a set of symmetric interactions between `s1` and `s2`, `s1` and `s3`, `s2` and `s3`:

```
SURFACES = s1 s2 s3
```

This defines a full set of symmetric interactions between `s1` and itself, `s2` and itself, `s1` and `s2`:

```
SURFACES = s1 s1 s2 s2
```

This command defines a set of interactions between all pairs of defined surfaces in the model, with the exception of surfaces `s7` and `s8`, which have no interactions:

```
SURFACES = all_surfaces exclude s7 s8
```

This command defines a set of interactions between all pairs of defined surfaces in the model, as well interactions between each surface and itself, with the exception of surfaces `s7` and `s8`, which have no interactions:

```
SURFACES = all_surfaces all_surfaces exclude s7 s8
```

These commands define a one-way interaction between the nodes of `s1` and the faces of `m1`:

```
MASTER = m1
SLAVE = s1
```

These commands define a set of one-way interactions between the nodes of `s1` and the faces of `m1`, the nodes of `s1` and the faces of `m2`, the nodes of `s2` and the faces of `m1`, the nodes of `s2` and the faces of `m2`.

```
MASTER = m1 m2
SLAVE = s1 s2
```

These commands define that the nodes of surface `s1` are slaved to all other contact faces in the contact definition block.

```
MASTER = all_surfaces exclude s1
SLAVE = s1
```

7.16.2 Kinematic Partition

```
KINEMATIC PARTITION = <real>kin_part
```

To provide accurate contact evaluation, Presto typically computes two-way contact between two surfaces, where interactions are defined between the nodes of the first surface and the faces of the second surface, and also between the nodes of the second surface and the faces of the first surface. If the two surfaces have penetrated each other by a distance δ, then each of the contact evaluations will compute forces to move the surface a distance δ, so that the total resulting displacement would be 2δ if both sets of contact computations were fully applied. The `KINEMATIC PARTITION` command line defines a kinematic partition scaling factor, `kin_part`, for the two contact computations so that the total contact motion is correct. The kinematic partition factor, `kin_part`, is a value between 0.0 and 1.0. The factor scales the relative motion of the first surface, where `kin_part` = 0.0 means the first surface will move none of δ, while `kin_part` = 1.0 means the surface moves all of δ. The second surface moves the portion of δ that remains after the motion of the first surface (i.e., δ for second surface = 1.0 – `kin_part`). For instance, if `kin_part` is 0.2, the first surface will move 20% of the penetration distance (0.2δ in our example), and the second surface would move the remaining 80% (0.8δ in our example). The default value is 0.5, so that each surface would move half of the penetration distance. If `kin_part` is 0.0, the first surface does not move

at all, and the second surface moves the full distance. This is exactly equivalent to a one-way master-slave contact definition, where the first surface is the master and the second is the slave. If `kin_part` is 1.0, the second surface is the master, and the first surface is the slave. Figure 7.6 illustrates how the kinematic partition factor varies from 0.0 to 1.0, with the specific example of `kin_part` being set to 0.2.

```
begin interaction
 surfaces = <first_surface> <second_surface>
 kinematic partition = 0.2
end
```

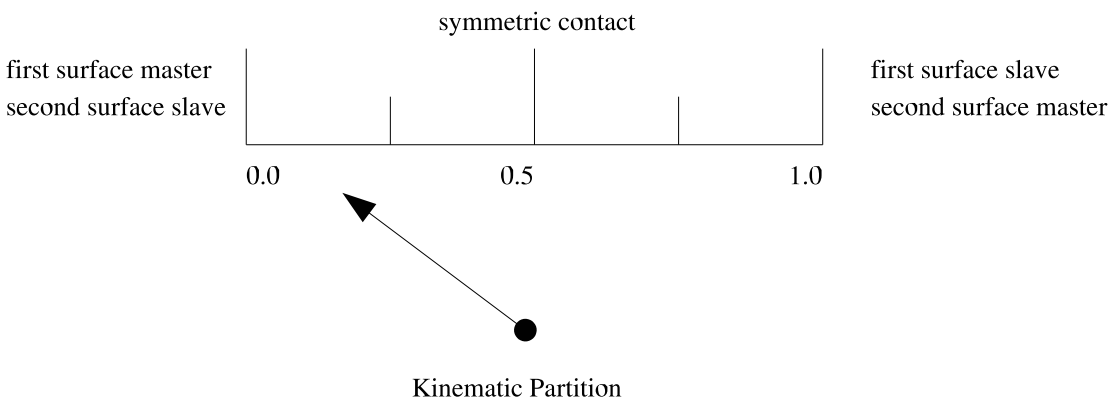

Figure 7.6: Illustration of kinematic partition values.

The capability provided by the `KINEMATIC PARTITION` command line is important in cases where contact occurs between two materials of disparate stiffness. Physically, we would expect a material with a higher stiffness to have more of an effect in determining the position of the contact surface than a more compliant material. In this case, we want the softer material to move more of the distance, and thus it should have a higher kinematic partition factor. The appropriate kinematic partition factor can be determined in closed form; see the ACME contact library reference [1] for more information. Alternately, the `AUTOMATIC KINEMATIC PARTITION` capability can automatically calculate the proper kinematic partition based on the stiffness of the materials.

Another case where the kinematic partition factor has traditionally been used is when meshes with dissimilar resolutions contact each other. If an interaction is defined with a fine mesh as the master surface and a coarse mesh as a slave surface, the contact algorithms will permit nodes on the master surface to penetrate the slave surface. In these cases, such problems can be alleviated by making the coarse mesh the master surface. However, the iterative approach implemented in the enforcement can also take care of this problem and is advised. If very few iterations are chosen, an appropriate kinematic partition factor may be needed to prevent unintentional penetration due to mesh discretization.

For self-contact, the kinematic partition factor should be 0.5.

A kinematic partition factor cannot be defined for interactions that use the pure master-slave syntax (see Section 7.16.1).

In general, it is best to use the automatic kinematic partition option to properly compute the kinematic partition for a pair of surfaces. However, in a few cases, master-slave interactions are preferred. These cases consist of (1) interaction between an analytic surface and a deformable body, where the analytic body should be the master surface; and (2) contact between shells and solids, where the solid should be the master surface.

7.16.3 Tolerances

```
NORMAL TOLERANCE = <real>norm_tol
TANGENTIAL TOLERANCE = <real>tang_tol
FACE MULTIPLIER = <real>face_multiplier(0.1)
OVERLAP NORMAL TOLERANCE = <real>over_norm_tol
OVERLAP TANGENTIAL TOLERANCE = <real>over_tang_tol
```

You can set tolerances for the interaction for a specific contact surface pair or for self-contact of a surface by using the above tolerance-related command lines in an `INTERACTION` command block. See Section 7.12.2 on search tolerances and Section 7.5 on overlap tolerances for a complete discussion of tolerances for contact.

7.16.4 Friction Model

```
FRICTION MODEL = <string>friction_model_name|FRICTIONLESS
  (FRICTIONLESS)
```

You can set the friction model for the interaction for a specific contact surface pair or for self-contact of a surface by using the above command line in an `INTERACTION` command block. See Section 7.15.3 for a discussion of this command line.

7.16.5 Automatic Kinematic Partition

```
AUTOMATIC KINEMATIC PARTITION
```

You can turn on (or off) automatic kinematic partitioning for a specific contact surface pair by using the above command line in an `INTERACTION` command block. See Section 7.15.4 for a discussion of automatic kinematic partitioning.

7.16.6 Interaction Behavior

```
INTERACTION BEHAVIOR = <string>SLIDING|
  INFINITESIMAL_SLIDING|NO_INTERACTION(SLIDING)
```

You can set the search behavior for a specific contact surface pair or for self-contact of a surface by using the above command line in an `INTERACTION` command block. See Section 7.15.5 for a discussion of this command line.

A particular use of this command line in this particular command block is to set the interaction behavior to `NO_INTERACTION`. This deactivates enforcement between the surfaces specified in the `INTERACTION` command block.

7.16.7 Constraint Formulation

```
CONSTRAINT FORMULATION = NODE_FACE|FACE_FACE
```

The `CONSTRAINT FORMULATION` command is used to switch between node/face and face/face enforcement for contact constraints. See Section 7.16.7 for a discussion of this command line.

7.17 Examples

This section has several example problems. We present the geometric configuration for the problems and the appropriate command lines to describe contact for the problems.

7.17.1 Example 1

Our first example problem has two blocks that come into contact due to initial velocity conditions. Block 1 has an initial velocity equal to $v1$, and block 2 has an initial velocity equal to $v2$. The geometric configuration for this problem is shown in Figure 7.7.

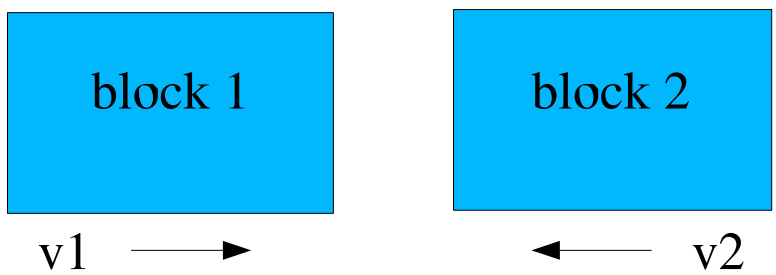

Figure 7.7: Problem with two blocks coming into contact.

The simplest input for this problem will be named `EXAMPLE1` and is shown as follows:

```
BEGIN CONTACT DEFINITION EXAMPLE1

  # define contact surfaces
  SKIN ALL BLOCKS = ON

  # set interactions
  BEGIN INTERACTION DEFAULTS
    GENERAL CONTACT = ON
  END INTERACTION DEFAULTS
END
```

In our example, the `SKIN ALL BLOCKS` command line with its parameter set to `ON` will create a surface named `surface_1` (from the skinning of `block_1` and a surface named `surface_2` (from the skinning of `block_2`).

All the normal and tangential tolerances will be set automatically in the above example. Frictionless contact is assumed. The kinematic partition factor defaults to 0.5 for both surfaces, `surface_1` and `surface_2`.

If you omitted the `INTERACTION DEFAULTS` command block with `GENERAL CONTACT` set to `ON`, then contact enforcement would not take place.

Now, let us consider the same problem (two blocks coming into contact) in which the contact definition for the problem is not defined simply by using all the default settings. The input for this variation of our two-block problem will be named EXAMPLE1A and is shown as follows:

```
BEGIN CONTACT DEFINITION EXAMPLE1A

  # define contact surfaces
  SKIN ALL BLOCKS = ON

  # friction model
  BEGIN CONSTANT FRICTION MODEL ROUGH
    FRICTION COEFFICIENT = 0.5
  END CONSTANT FRICTION MODEL ROUGH
  # search options
  BEGIN SEARCH OPTIONS
    GLOBAL SEARCH INCREMENT = 10
    NORMAL TOLERANCE = 1.0E-3
    TANGENTIAL TOLERANCE = 1.0E-3
  END SEARCH OPTIONS

  # set interactions
  BEGIN INTERACTION DEFAULTS
    FRICTION MODEL = ROUGH
    GENERAL CONTACT = ON
  END INTERACTION DEFAULTS
END
```

As is the case of the EXAMPLE1 command block, the SKIN ALL BLOCKS command line with its parameter set to ON will create a surface named surface_1 (from the skinning of block_1) and a surface named surface_2 (from the skinning of block_2).

For EXAMPLE1A, we want to have frictional contact between the two blocks. For the frictional contact, we define a constant friction model with a CONSTANT FRICTION MODEL command block. We name this model ROUGH.

The SEARCH OPTIONS command block sets the interval between global searches to 10; the default value is 5. Also, in this command block, we have set values for the normal and tangential tolerances. The option to compute the search tolerance automatically has been left on. The larger of the two values—an automatically computed tolerance or the user-specified tolerance—will be selected as the search tolerance during the search phase.

In the INTERACTION DEFAULTS command block, we select the friction model ROUGH on the FRICTION MODEL command line. As in the case of the EXAMPLE1 command block, if you omitted the INTERACTION DEFAULTS command block with GENERAL CONTACT set to ON, contact enforcement would not take place.

7.17.2 Example 2

Our second example problem has three blocks that come into contact due to initial velocity conditions. Block 1 has an initial velocity equal to $v1$, and block 3 has an initial velocity equal to $v3$. The geometric configuration for this problem is shown in Figure 7.8.

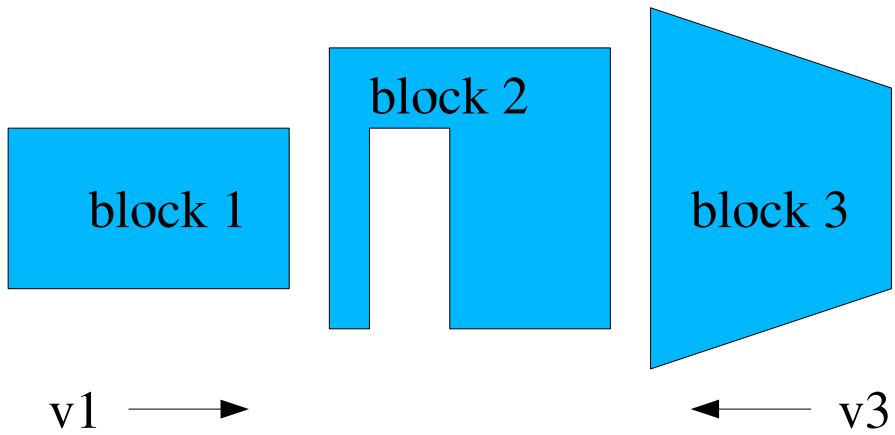

Figure 7.8: Problem with three blocks coming into contact.

The input for this three-block problem will be named `EXAMPLE2` and is shown as follows:

```
BEGIN CONTACT DEFINITION EXAMPLE2

  # define contact surfaces
  CONTACT SURFACE surface_1 CONTAINS block_1
  CONTACT SURFACE surface_2 CONTAINS block_2
  CONTACT SURFACE surf_3 CONTAINS surface_3

  # friction model
  BEGIN CONSTANT FRICTION MODEL ROUGH
    FRICTION COEFFICIENT = 0.5
  END CONSTANT FRICTION MODEL ROUGH

  # search options
  BEGIN SEARCH OPTIONS
    GLOBAL SEARCH INCREMENT = 10
    NORMAL TOLERANCE = 1.0E-3
    TANGENTIAL TOLERANCE = 1.0E-3
  END SEARCH OPTIONS

  # set interactions
  BEGIN INTERACTION DEFAULTS
    FRICTION MODEL = ROUGH
    GENERAL CONTACT = ON
```

```
    SELF CONTACT = ON
  END INTERACTION DEFAULTS

  # set specific interaction
  BEGIN INTERACTION S2TOS3
    SURFACES = surface_2 surf_3
    KINEMATIC PARTITION = 0.4
    NORMAL TOLERANCE = 0.5E-3
    TANGENTIAL TOLERANCE = 0.5E-3
    FRICTION MODEL = FRICTIONLESS
  END INTERACTION S2TOS3
END
```

For the EXAMPLE2 command block, we have defined three surfaces. The first surface, surface_1, is obtained by skinning block_1. The second surface, surface_2 is obtained by skinning block_2. The third surface, surf_3, is the user-defined surface surface_3. The user-defined surface, surface_3, can contain a subset of the external element faces that define block_3 or all the external element faces that define block_3.

The SEARCH OPTIONS command block sets the interval between global searches to 10; the default value is 5. Also, in this command block, we have set values for the normal and tangential tolerances. The option to compute the search tolerance automatically has been left on. The larger of the two values—an automatically computed tolerance or the user-specified tolerance—will be selected as the search tolerance during the search phase.

In the INTERACTION DEFAULTS command block, we select the friction model ROUGH on the FRICTION MODEL command line. Both GENERAL CONTACT and SELF CONTACT are set to ON in the EXAMPLE2 command block. For this problem, block_2 can undergo self-contact. Setting GENERAL CONTACT to ON will enforce contact between surface_1 and surface_2, surface_2 and surf_3, and surface_1 and surf_3. Setting SELF CONTACT to ON will enforce self-contact for all three of the surfaces.

For this particular example, we want to override some of the Presto default values for surface interaction and some of the default values for surface interaction set by the INTERACTION DEFAULTS command block for the interaction between surface_2 and surf_3. To override default values, we use an INTERACTION command block and indicate that it applies to surface_2 and surf_3 with a SURFACES command line. We override the Presto default for the kinematic partition factor by using a KINEMATIC PARTITION command line with the kinematic partition parameter set to a value of 0.4. We override the normal and tangential tolerances and the friction model set in the INTERACTION command block. The normal and tangential tolerances for interaction between surface_2 and surf_3 is set to 0.5E-3 rather than the global value of 1.0E-3. The friction model for interaction between surface_2 and surf_3 is set to FRICTIONLESS rather than the default value of ROUGH.

7.18 Dash Contact

```
CONTACT FORMULATION TYPE = ACME|DASH(ACME)
```

Dash is an alternative contact algorithm that is a replacement for the ACME explicit dynamics contact algorithm. The Dash algorithm is selected with the contact formulation type command. Generally any existing ACME contact command block may be converted to a Dash command block simply by using this one command. However, Dash will ignore some ACME options so is only applicable on a subset of problems that ACME can run.

7.18.1 How Dash is Different from ACME

Dash is a facet-based enforcement algorithm. Dash attempts to compute the total volume of overlap between two facet sets and remove the overlap. In contrast, ACME only removes the gap between nodes and faces. Dash uses a reduced order area integration scheme for calculation and removal of volumetric overlaps.

In some cases, Dash is more robust than ACME and can more accurately solve certain classes of problems. Dash often works better than ACME for problems with high loading rates and stiffening materials. ACME contact enforcement tends to aggravate hourglass modes when used on these types of problems. Additionally, problems in which tolerancing issues, multiple interaction issues, or topology restrictions cause ACME to perform poorly may be run more robustly with Dash.

For frictional behavior, however, Dash is generally less accurate than ACME. Dash is less able to exactly capture the transition from sticking to slipping behavior and other such frictional details than is ACME.

Dash is designed to work correctly for a wide variety of problems with minimal user tweaking. It is generally recommended that Dash be used with a minimal set of inputs, for example 'skin all blocks', 'self and/or general contact = on', and interaction friction models. Dash has no tolerances, kinematic partitions, or any other such inputs.

Dash uses an iterative penalty based enforcement scheme. Dash enforcement explicitly balances Momentum by always applying equal and opposite forces.

7.18.2 Interaction Behavior for Particle Element Blocks

Element blocks containing particle elements (SPH, Mass Particle, or peridynamics) undergo special treatment, as described below.

Because the SPH and peridynamics algorithms define interactions between elements, it is typically not desirable to enforce self-contact within those element blocks. Self-contact is thus disabled by default for SPH and peridynamics blocks.

In addition, contact between blocks of SPH elements is also disabled by default. The SPH algorithm contains its own contact-like algorithm to govern interactions between SPH particles, even in different element blocks.

Elements that are converted to particles are placed in a new element block. The name of the new element block is the name of the parent block, with `_particles` appended. For example, the particles created from `block_1` are placed in a new element block named `block_1_particles`. The `SKIN ALL BLOCKS` command creates a new contact surface containing the particles that has the same name as the particle block (`block_1_particles` in this example). By default, the contact surface for the particles has the same interactions as does the parent block, subject to the exceptions listed above for interactions between particle blocks.

Any of the above defaults can be overridden by defining individual interactions. For example, if `block_1` and `block_2` are SPH particle blocks, they will not interact though contact by default. However, the following command block can be included to cause contact to be enforced between them.

```
BEGIN INTERACTION
  SURFACES = block_1 block_2
END
```

If a single contact surface is defined by combining multiple types of objects, the special particle-specific default behavior described in this section is disabled. For example, the following command block will turn on self-contact for all entities within the surface `s1`, including between the particles in `block_2_particles`.

```
BEGIN INTERACTION DEFAULTS
  SELF CONTACT = ON
END
CONTACT SURFACE s1 CONTAINS block_1 block_2_particles surface_3
```

7.18.3 Current Dash Usage Guidelines

Use Dash for remeshing problems. ACME does not perform well on changing topologies. Dash may also be useful for problems with element death. ACME often must artificially kill a large number of additional elements other than those which have reached a user defined death criteria. ACME requires these additional element removals in order to work around certain ACME surface topology restrictions. Dash has no topology restrictions so does not need to kill any extra elements to maintain a valid contact topology.

Dash is often significantly faster than ACME, particularly on parallel problems. Speedups from 1.5 to 4 times have been observed on a wide range of problems when using Dash as compared to ACME.

When performing contact involving shells, Dash turns the shells into lofted volumes. The volume thickness is stored in the `shell_thickness` element variable and is used within the shell lofting algorithm as the offset to use in contact enforcement.

The following ACME capabilities are not currently supported by Dash:

- 8 and 10 node tetrahedron contact

- Complex friction models (anything other than frictionless, constant friction, glued, and tied)
- Tied contact at a distance. Dash assumes all contact occurs at a nominal gap of zero. Tolerances specified in the input deck are currently ignored.

Additionally avoid using side set contact with Dash and prefer block skinning. Dash contains ray tracing algorithms to determine if certain contact points are inside or outside of bodies. If the surfaces Dash is using do not define fully enclosed bodies Dash may become confused and think a point inside the body is actually outside the body or vice versa.

Dash can also perform node-face contact by defining a contact node set in the same fashion as is done in ACME. The nodes defined in a node-face interaction must be the slave object to correctly compute contact. Node normals used to determine tied contact are computed by averaging the normals of the faces connected to that node. In addition, it is recommended to use node-face contact when using Dash with rigid body contact.

Dash accepts the same surface definitions as does ACME. Dash also uses identical syntax for interaction definition. The relevant contact block options for Dash are:

```
CONTACT SURFACE <name> CONTAINS <surface_name>
CONTACT SURFACE <name> CONTAINS <block_name>
CONTACT NODE SET <name> CONTAINS <nodelist_name>

BEGIN INTERACTION DEFAULTS
  GENERAL CONTACT = ON|OFF (OFF)
  SELF CONTACT = ON|OFF (OFF)
  DEFAULT FRICTION MODEL = <string>(default_frictionless)
END [INTERACTION DEFAULTS]

BEGIN FRICTIONLESS MODEL <string>name
END [FRICTIONLESS MODEL <string>name]

BEGIN CONSTANT FRICTION MODEL <string>name
  FRICTION COEFFICIENT = <real>coeff
END [CONSTANT FRICTION MODEL <string>name]

BEGIN TIED MODEL <string>name
END [TIED MODEL <string>name]

BEGIN GLUED FRICTION MODEL <string>name
END [GLUED FRICTION MODEL <string>name]

BEGIN INTERACTION <string>name
  SURFACES = <string>surface1 <string>surface2
  MASTER = <string>surface
  SLAVE = <string>surface
  FRICTION MODEL = <string>friction_model_name
END [INTERACTION <string>name]
```

```
BEGIN ENFORCEMENT OPTIONS
  MOMENTUM BALANCE ITERATIONS = <integer>(5)
  NUM GEOMETRY UPDATE ITERATIONS = <integer>(1)
END [ENFORCEMENT OPTIONS]

BEGIN REMOVE INITIAL OVERLAP
END [REMOVE INITIAL OVERLAP]

BEGIN DASH OPTIONS
  SCALE FACTOR = <real>factor(1.0)
  INTERACTION DEFINITION SCHEME = <string>DASH_DEFAULT|EXPLICIT
    (DASH_DEFAULT)
  SEARCH LENGTH SCALING = <real>factor(0.15)
  LOFTED SPHERE REPRESENTATION =
    TETRAHEDRON|OCTAHEDRON|CUBE|ICOSAHEDRON(ICOSAHEDRON)
END [DASH OPTIONS]

BEGIN DEBUG
  OUTPUT LEVEL = <integer>(0)
  VISUALIZE CONTACT FACETS = OFF|ON (OFF)
END [DEBUG]
```

All contact definition block commands not listed above are ignored by Dash. This includes contact tolerances, kinematic partitions, ACME performance options, etc. The contact surface definition, interaction definition, and friction model specification commands work identically to their ACME counterparts. The four supported friction models also behave identically to the ACME versions of those friction models.

The `MOMENTUM BALANCE ITERATIONS` command controls how many iterative enforcement passes Dash will perform. For Dash these are not really momentum balance iterations as Dash explicitly balances momentum at every iteration. Increasing the number of momentum balance iterations will increase result accuracy, minimizing overlap and better conserving energy terms.

`NUM GEOMETRY UPDATE ITERATIONS` is unique to Dash. This command allows the contact search geometry to be updated multiple times per search step. Larger values for this command yield better enforcement, but at significantly increased cost.

The `DASH OPTIONS` command block contains a few options unique to Dash. Generally Dash is designed to run accurately with as few user specified parameters as possible; however, a few options do exist.

The `SCALE FACTOR` command defines the final scaling factor to apply to contact forces. This is mostly a developer option to help debug certain contact pathologies.

The `INTERACTION DEFINITION SCHEME`, command controls how contact interactions are defined. By default all Dash interactions are one sided. As the full volume of overlap is removed there is really no concept of master face or slave face. By default Dash picks an optimal enforcement order for each interaction pair based on face size. However, the ability exists to explicitly

use the potentially symmetric interactions defined in the input deck by supplying the `EXPLICIT` option to this command. This may allow better enforcement in some circumstances, particularly tied contact.

The `SEARCH LENGTH SCALING` command defines how far into a body Dash will search for potentially interacting faces. The search tolerance is a multiplier on the face characteristic length. If faces move farther than the factor supplied in the `SEARCH LENGTH SCALING` command line times the face characteristic length in a single time step, contact could be lost. Thus, extremely high velocity contacts may require use of higher values of this parameter. Note that the default values used should be sufficient for impact speeds below the material sound speed.

The `LOFTED SPHERE REPRESENTATION` command defines how sphere elements are represented in contact. When a sphere element block is skinned for contact it is turned into a set of faceted spheres. The type of faceting used on the spheres is controlled by the option to this command, and can be either `TETRAHEDRON`, `OCTAHEDRON`, `CUBE`, or `ICOSAHEDRON`. The `ICOSAHEDRON` option is the default. The radius of the spheres is given by half of the particle radius, which is stored in the `sph_radius` nodal variable. Lower order geometries are generally slightly faster, but may be significantly less accurate.

The `DEBUG` command block contains commands that can be used to control the output of debugging information by the contact algorithm. The `OUTPUT LEVEL` command in the `DEBUG` block controls the amount of information written to the log file. At the default level of zero, only minimal information is included. At level 1 or greater, more information is printed to the log file such as the composition of the different contact surfaces and friction model matrices.

The `VISUALIZE CONTACT FACETS` command in the `DEBUG` command block can be used to plot the actual contact surfaces and lofted contact geometries in the results output file. Extra element blocks and node blocks will be added to the output mesh to represent the contact geometries. Note that use of this option will significantly increase the size of the results file and moderately increase the run time.

Dash represents lofted structural elements slightly differently than ACME. Dash can only represent shells via lofted geometry and has no option to handle zero thickness shells. Dash adds the edge faces to lofted shells allowing edge and edge to face contact to function correctly on shell elements. Dash also handles beam on beam contact via lofted geometry. Beam objects are turned into a representative hexagonal prism that has roughly the same cross sectional area of the beam element. Beam contact is functional for edge-on or end-on cases.

7.19 References

1. Brown, K. H., R. M. Summers, M. W. Glass, A. S. Gullerud, M. W. Heinstein, and R. E. Jones. *ACME: Algorithms for Contact in a Multiphysics Environment*, API Version, 2.2, SAND2004-5486. Albuquerque, NM: Sandia National Laboratories, October 2001. pdf.

2. Heinstein, M. W., and T. E. Voth. *Contact Enforcement for Explicit Transient Dynamics*, Draft SAND report. Albuquerque, NM: Sandia National Laboratories, 2005.

Chapter 8

Output

Presto produces a variety of output. This chapter discusses how to control the four major types of output: results output, history output, heartbeat output, and restart output. Results output lets the user select a set of variables (internal, user-defined, or some combination thereof). If the user selects a nodal variable such as displacement for results output, the displacements for all the nodes in a model will be output to a results file. If the user selects an element variable such as stress for results output, the stress for all elements in the model that calculate this quantity (stress) will be output. The history output option lets the user select a very specific set of information for output. For example, if you know that the displacement at a particular node is critical, then you can select only the displacement at that particular node as history output. The heartbeat output is similar to the history output except that the output is written to a text file instead of to a binary (exodusII [1]) file. The restart output is written so that any calculation can be halted at some arbitrary analysis time and then restarted at this time. The user has no control over what is written to the restart file. When a restart file is written, it must be a complete state description of the calculations at some given time. A restart file contains a great deal of information and is typically much larger than a results file. You need to carefully limit how often a restart file is written.

Section 8.2 describes the results output. Included in the results output is a description of commands for user-defined output (Section 8.2.2). User-defined output lets the user postprocess analysis results as the code is running to produce a reduced set of output information. Section 8.3 describes the history output, Section 8.4 describes the heartbeat output, and Section 8.5 describes the restart output. All four types of output (results, history, heartbeat, and restart) can be synchronized for analyses with multiple regions. This scheduling functionality is discussed in Section 8.6. In Section 8.9, there is a list of key variables.

Unless otherwise noted, the command blocks and command lines discussed in Chapter 8 appear in the region scope.

8.1 Syntax for Requesting Variables

Variables may be accessed in the code either in whole or by component. Values at specific components or integration points of multi-component variables may be accessed via parenthesis syntax. Parenthesis syntax may be applied to results output, history output, element death, or any other command where variable names are specified. Values of single-component variables indexed in some other way may be accessed with underscore syntax, which is primarily applicable to rigid body fields as discussed in Section 8.1.4.

Parenthesis syntax is a variable name of the form:

```
<string>var_name[(<index>component[,<integer>integration_point)]]
```

For a variable named `var`, a variable name of the form `var(A,B)` asks for the `A` component of the variable at integration point `B`. If a variable is a vector, `x`, `y`, or `z` may be specified as the component. If a variable is 3x3 tensor, `xx`, `yy`, `zz`, `xy`, `xz`, `yz`, `yx`, `zx`, or `zy` may be specified as the component. For other types of variables components of the variable may be requested through an integer index.

The characters `:` and `*` are wild cards if used for specifying either the component or the integration point. `var(:,B)` asks for all components of var at integration point B. `var(A,:)` asks for component A of var at all integration points. `var(:,:)` asks for all components of var at all integration points. `var` is shorthand for `var(:,:)`.

`var(A)` will behave slightly differently depending on the nature of the variable. If the variable has multiple components, then `Var(A)` is treated like `var(A,:)`. If a variable has one and only one component then it is assumed that A refers to the integration point number rather than the component number and `Var(A)` is treated like `var(1,A)`.

8.1.1 Example 1

Let stress be a tensor defined on a single integration point element and a displacement vector be defined at all model nodes. The following output variable specification:

```
element stress as str
nodal displacement as disp
```

asks for all the components of the stress tensor on elements and all components of the displacement vector on nodes. The code would write the following variables to the output file:

```
str_xx
str_yy
str_zz
str_xy
str_xz
```

```
str_yz
disp_x
disp_y
disp_z
```

If only the `yy` component of stress is desired, either of the following could be used:

```
element stress(yy) as my_yy_str1
element stress(2) as my_yy_str2
```

If only the `z` component of displacement is desired either of the following could be specified:

```
nodal displacement(z) as my_z_disp1
nodal displacement(3) as my_z_disp2
```

Note, index 2 of a tensor corresponds to the `yy` component of the tensor and index 3 of a vector corresponds to the `z` component of the vector.

8.1.2 Example 2

Let stress be a tensor defined on each integration point of a three integration point element. Let eqps be a scalar material state variable also defined at each element integration point. To ask for all stress components on all integration points and all eqps data at all integration points the following could be specified:

```
element stress as str
element eqps as eqps
```

Which would output the variables:

```
str_xx_1, str_yy_1, str_zz_1, str_xy_1, str_xz_1, str_yz_1
str_xx_2, str_yy_2, str_zz_2, str_xy_2, str_xz_2, str_yz_2
str_xx_3, str_yy_3, str_zz_3, str_xy_3, str_xz_3, str_yz_3
eqps_1, eqps_2, eqps_2
```

To ask for just the stress tensor and eqps value on the second integration point the following syntax can be used:

```
element stress(:,2) as str_intg2
element eqps(2) as eqps_intg2
```

This would output the variables:

```
str_intg2_xx
str_intg2_yy
str_intg2_zz
str_intg2_xy
str_intg2_xz
str_intg2_yz
eqps_intg2
```

To ask for the `xy` component of stress on all integration points any of the following could be used:

```
element  stress(xy,*) as str_xy_all
element  stress(xy,:) as str_xy_all
element  stress(xy)   as str_xy_all
```

Any of the above would output:

```
str_xy_all_1
str_xy_all_2
str_xy_all_3
```

8.1.3 Other command blocks

The parenthesis syntax described above for results output can also be used in most other commands involving variable names. For example, to kill elements based on yy stress or z displacement the following could be specified:

```
begin element death
  criterion is element value of stress(yy) > 1000
  criterion is average nodal value of displacement(z) > 3.0
end
```

8.1.4 Rigid Body Variables

Variables of rigid bodies are provided as separate components of the rigid body fields. To access variables of rigid bodies you must output the desired field component(s), and to access the field component of individual rigid bodies an underscore syntax is employed (the parenthesis syntax applies to multi-component fields and integration points). The underscore syntax simply takes the desired field component and appends it with an underscore and the desired rigid body name.

For example the following lines in a history output block (see Section 8.3)

```
global ax_rb1
global displz_rb4
```

would output to the history file the variables

```
ax_rb1
displz_rb4
```

which are the translational acceleration in the x-direction of rigid body rb1 and the translational displacement in the z-direction of rigid body rb4, respectively (see Table 8.2).

8.2 Results Output

The results output capability lets you select some set of variables that will be written to a file at various intervals. As previously indicated, all the values for each selected variable will be written to the results file. (The interval at which information is written can be changed throughout the analysis time.) The name of the results file is set in the `RESULTS OUTPUT` command block.

8.2.1 Exodus Results Output File

```
BEGIN RESULTS OUTPUT <string>results_name
  DATABASE NAME = <string>results_file_name
  DATABASE TYPE = <string>database_type(exodusII)
  OVERWRITE = <string>OFF|ON|TRUE|FALSE|YES|NO
    (ON|TRUE|YES)
  TITLE <string>user_title
  NODE  <string>variable_name
    [AS <string>dbase_variable_name] ...
    <string>variable_name [AS
    <string>dbase_variable_name]
    | NODAL  <string>variable_name
        [AS <string>dbase_variable_name] ...
        <string>variable_name [AS
        <string>dbase_variable_name]
  NODESET  <string>variable_name
    [AS <string>dbase_variable_name] ...
    <string>variable_name [AS
    <string>dbase_variable_name]
    | NODESET  <string>variable_name
        [AS <string>dbase_variable_name]
        INCLUDE|ON|EXCLUDE <string list>nodelist_names
        ... <string>variable_name
        [AS <string>dbase_variable_name] INCLUDE|ON|EXCLUDE
        <string list>nodelist_names
  FACE  <string>variable_name
    [AS <string>dbase_variable_name] ...
    <string>variable_name [AS
    <string>dbase_variable_name]
    | FACE  <string>variable_name
        [AS <string>dbase_variable_name]
        INCLUDE|ON|EXCLUDE <string list>surface_names
        ...  <string>variable_name
        [AS <string>dbase_variable_name] INCLUDE|ON|EXCLUDE
        <string list>surface_names
  ELEMENT  <string>variable_name
    [AS <string>dbase_variable_name] ...
    <string>variable_name [AS
    <string>dbase_variable_name]
    | ELEMENT  <string>variable_name
        [AS <string>dbase_variable_name]
        INCLUDE|ON|EXCLUDE <string list>block_names
        ... <string>variable_name
        [AS dbase_variable_name] INCLUDE|ON|EXCLUDE
        <string list>block_names
  GLOBAL  <string>variable_name
```

```
    [AS <string>dbase_variable_name] ...
    <string>variable_name [AS
    <string>dbase_variable_name]
  OUTPUT MESH = EXPOSED_SURFACE|BLOCK_SURFACE
  COMPONENT SEPARATOR CHARACTER = <string>character|NONE
  EXCLUDE = <string>list_of_excluded_element_blocks
  INCLUDE = <string>list_of_included_element_blocks
  START TIME = <real>output_start_time
  TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
  AT TIME <real>time_begin INCREMENT =
    <real>time_increment_dt
  ADDITIONAL TIMES = <real>output_time1
    <real>output_time2 ...
  AT STEP <integer>step_begin INCREMENT =
    <integer>step_increment
  ADDITIONAL STEPS = <integer>output_step1
    <integer>output_step2 ...
  TERMINATION TIME = <real>termination_time_value
  SYNCHRONIZE_OUTPUT
  USE OUTPUT SCHEDULER <string>scheduler name
  OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|SIGHUP|SIGINT|
    SIGPIPE|SIGQUIT|SIGTERM|SIGUSR1|SIGUSR2|SIGABRT|
    SIGKILL|SIGILL|SIGSEGV
END [RESULTS OUTPUT <string>results_name]
```

You can specify a results file, the results to be included in this file, and the frequency at which results are written by using a `RESULTS OUTPUT` command block. The command block appears inside the region scope.

More than one results file can be specified for an analysis. Thus for each results file, there will be one `RESULTS OUTPUT` command block. The command block begins with:

```
BEGIN RESULTS OUTPUT <string>results_name
```

and is terminated with:

```
END [RESULTS OUTPUT <string>results_name]
```

where `results_name` is a user-selected name for the command block. Nested within the `RESULTS OUTPUT` command block is a set of command lines, as shown in the block summary given above. The first two command lines listed (`DATABASE NAME` and `DATABASE TYPE`) give pertinent information about the results file. The command line

```
DATABASE NAME = <string>results_file_name
```

gives the name of the results file with the string `results_file_name`. If the results file is to appear in the current directory and is named `job.e`, this command line would appear as:

```
DATABASE NAME = job.e
```

If the results file is to be created in some other directory the command line must include the path to that directory.

Two metacharacters can appear in the name of the results file. If the `%P` character is found in the name, it will be replaced with the number processors being used for the run. For example, if you are running on 1024 processors and use the name `results-%P/job.e`, then the name would be expanded to `results-1024/job.e` and the actual results files would be `results-1024/job.e.1024.0000` to `results-1024/job.g.1024.1023`. The other recognized metacharacter is `%B` which is replaced with the base name of the input file containing the input commands. For example, if the commands are in the file `my_analysis_run.i` and the results database name is specified as `%B.e`, then the results would be written to the file `my_analysis_run.e`.

If the results file does not use the Exodus II format [1], you must specify the format for the results file using the command line:

```
DATABASE TYPE = <string>database_type(exodusII)
```

Currently, both the Exodus II database and the XDMF database [2] are supported in Presto and Adagio. Exodus II is more commonly used than XDMF. Other options may be added in the future.

The `OVERWRITE` command line can be used to prevent the overwriting of existing results files.

```
OVERWRITE = <string>OFF|ON|TRUE|FALSE|YES|NO
     (ON|TRUE|YES)
```

The `OVERWRITE` command line allows only a single value. If you set the value to `FALSE`, `NO`, or `OFF`, the code will terminate before existing results files can be overwritten. If you set the value to `TRUE`, `YES`, or `ON`, then existing results files can be overwritten (the default status). Suppose, for example, that we have an existing results file named `job21.e`. Suppose also that we have an input file with a `RESULTS OUTPUT` command block that contains the `OVERWRITE` command line set to `ON` and the `DATABASE NAME` command line set to:

```
DATABASE NAME = job21.e
```

If you run the code under these conditions, the existing results file `job21.e` will be overwritten.

Whether or not results files are overwritten is also impacted by the use of the automatic read and write option for restart files described in Section 8.5.1.1. If you use the automatic read and write option for restart files, the results files, like the restart files, are automatically managed. The automatic read and write option in restart adds extensions to file names and prevents the overwriting of any existing restart or results files. For the case of a user-controlled read and write of restart files (Section 8.5.1.2) or of no restart, however, the `OVERWRITE` command line is useful for preventing the overwriting of results files.

You may add a title to the results file by using the `TITLE` command line. Whatever you specify for the `user_title` will be written to the results file. Some of the programs that process the results file (such as various SEACAS programs [3]) can read and display this information.

The other command lines that appear in the `RESULTS OUTPUT` command block determine the type and frequency of information that is output. Descriptions of these command lines follow in Section 8.2.1.1 through Section 8.2.1.18.

8.2.1.1 Output Nodal Variables

```
NODE  <string>variable_name
  [AS <string>dbase_variable_name] ...
  <string>variable_name [AS <string>dbase_variable_name]
  | NODAL  <string>variable_name
    [AS <string>dbase_variable_name] ...
    <string>variable_name [AS <string>dbase_variable_name]
```

Any nodal variable in Presto can be selected for output in the results file by using a command line in one of the two forms shown above. The only difference between the two forms is the use of `NODE` or `NODAL`. The string `variable_name` is the name of the nodal variable to output. The string `variable_name` can be either a variable listed in Section 8.9 or a user-defined variable (see Section 8.2.2 and Section 10.2.4).

For the above two command lines, any nodal variable requested for output is output for all nodes.

It is possible to specify an alias for any of the nodal variables by using the `AS` specification. Suppose, for example, you wanted to output the external forces in Presto, which are defined as `force_external`, with the alias `f_ext`. You would then enter the command line:

```
NODE force_external AS f_ext
```

In this example, the external force is a vector quantity. For a vector quantity at a node, suffixes are appended to the variable name (or alias name) to denote each vector component. The results database would have three variable names associated with the external force: `f_ext_x`, `f_ext_y`, and `f_ext_z`. You can change the component separator, an underscore in this example, by using the `COMPONENT SEPARATOR CHARACTER` command line (see Section 8.2.1.7).

The `NODE` command line can be used an arbitrary number of times within a `RESULTS OUTPUT` command block. It is also possible to specify more than one nodal variable for output on a command line, as indicated by the ellipsis in the command line format. In the following example, two nodal variables are specified for output. Note that the internal forces are defined as `force_internal`.

```
NODE force_external force_internal
```

Aliases can be specified for each of the variables in a single command line. Thus, If you wanted to output the alias `f_ext` for external forces and also wanted to output the alias `f_int` for internal forces, you would enter the command line:

```
NODE force_external AS f_ext
     force_internal AS f_int
```

The specification of an alias is optional.

8.2.1.2 Output Node Set Variables

```
NODESET  <string>variable_name
  [AS <string>dbase_variable_name] ...
```

```
<string>variable_name [AS <string>dbase_variable_name]
| NODESET  <string>variable_name
    [AS <string>dbase_variable_name]
    INCLUDE|ON|EXCLUDE <string list>nodelist_names
    ... <string>variable_name [AS <string>dbase_variable_name]
    INCLUDE|ON|EXCLUDE <string list>nodelist_names
```

A nodal variable may be defined on a subset of the total set of nodes defining a model. A nodal variable that is defined only on a subset of nodes is referred to as a node set variable. The `NODESET` command line lets you specify a node set variable for output to the results file.

There are two forms of the `NODESET` command line. Either form will let you output a node set variable.

The first form of the command line is as follows:

```
NODESET  <string>variable_name
  [AS <string>dbase_variable_name] ...
  <string>variable_name [AS <string>dbase_variable_name]
```

Here, the string `variable_name` is a node set variable associated with one or more node sets. In this form, the node set variable is output for all node sets associated with that node set variable.

It is possible to specify an alias in the results file for any of the node set variables by using the `AS` option. Suppose, for example, you wanted to output the node set variable `force_nsetype`, but have that variable have the name `fnsetype` in the results file. You would then enter the command line:

```
NODESET force_nsetype AS fnsetype
```

The `NODESET` command line can be used an arbitrary number of times within a `RESULTS OUTPUT` command block. It is also possible to specify more than one node set variable for output on a command line, as indicated by the ellipsis in the command line format. In the following example, two node set variables are specified for output. Here, the second node set variable is defined as `force_nsetype2`.

```
NODESET force_nsetype force_nsetype2
```

Aliases can be specified for each of the variables in a single command line. Thus, if you wanted to output the alias `fnsetype` for node set variable `force_nsetype` and also wanted to output the alias `fnsetype2` for node set variable `force_nsetype2`, you would enter the command line:

```
NODESET force_nsetype AS fnsetype
     force_nsetype2 AS fnsetype2
```

The specification of an alias is optional.

The second form of the command line is as follows:

```
NODESET  <string>variable_name
  [AS <string>dbase_variable_name]
```

```
INCLUDE|ON|EXCLUDE <string list>nodelist_names
... <string>variable_name [AS <string>dbase_variable_name]
INCLUDE|ON|EXCLUDE <string list>nodelist_names
```

This form of the NODESET command line is similar to the first, except that the user can control which node sets are used for output. The user can include a specific list of node sets for output by using the INCLUDE option or the ON option. (The keyword INCLUDE is synonymous with the keyword ON.) Alternatively, the user can exclude a specific list of node sets for output by using the EXCLUDE option.

Suppose that the node set variable force_nsetype from the above example has been defined for nodelist_10, nodelist_11, nodelist_20, and nodelist_21. If we only want to output the node set variable for node sets nodelist_10, nodelist_11, and nodelist_21, then we could specify the NODESET command line as follows:

```
NODESET force_nsetype AS fnsetype
     INCLUDE nodelist_10, nodelist_11, nodelist_21
```

(In the above command line, the keyword ON could be substituted for INCLUDE.) Alternatively, we could use the command line:

```
NODESET force_nsetype AS fnsetype
     EXCLUDE nodelist_20
```

In the above command lines, an alias for a node set can be substituted for a node set identifier. For example, if center_case is an alias for nodelist_10, then the string center_case could be substituted for nodelist_10 in the above command lines. Because a node set identifier is a mesh entity, the alias for the node set identifier would be defined via an ALIAS command line in a FINITE ELEMENT MODEL command block.

Note that the list of identifiers uses a comma to separate one node set identifier from the next node set identifier.

8.2.1.3 Output Face Variables

```
FACE  <string>variable_name
  [AS <string>dbase_variable_name] ...
  <string>variable_name [AS <string>dbase_variable_name]
  | FACE  <string>variable_name
      [AS <string>dbase_variable_name]
      INCLUDE|ON|EXCLUDE <string list>surface_names
      ...  <string>variable_name [AS <string>dbase_variable_name]
      INCLUDE|ON|EXCLUDE <string list>surface_names
```

A variable may be defined on some set of faces that constitute a surface. A variable defined on a set of faces is referred to as a face variable. The FACE command line lets you specify a face variable for output to the results file.

There are two forms of the FACE command line. Either form will let you output a face variable.

The first form of the command line is as follows:

```
FACE  <string>variable_name
  [AS <string>dbase_variable_name] ...
  <string>variable_name [AS
  <string>dbase_variable_name]
```

Here, the string `variable_name` is a face variable associated with one or more surfaces. In this form, the face variable is output for all surfaces associated with that face variable.

It is possible to specify an alias in the results file for any face variable by using the `AS` option. Suppose, for example, you wanted to output a face variable `pressure_face`, but have that variable have the name `pressuref` in the results file. You would then enter the command line:

```
FACE pressure_face AS pressuref
```

The `FACE` command line can be used an arbitrary number of times within a `RESULTS OUTPUT` command block. It is also possible to specify more than one face variable for output on a command line, as indicated by the ellipsis in the command line format. In the following example, two face variables are specified for output. Here, the second face variable is defined as `scalar_face2`.

```
FACE pressure_face scalar_face2
```

Aliases can be specified for each of the variables in a single command line. Thus, If you wanted to output the alias `pressuref` for face variable `pressure_face` and also wanted to output the alias `scalarf2` for face variable `scalar_face2`, you would enter the command line:

```
FACE pressure_face AS pressuref
     scalar_face2 AS scalarf2
```

The specification of an alias is optional.

The second form of the command line is as follows:

```
FACE  <string>variable_name
  [AS <string>dbase_variable_name]
  INCLUDE|ON|EXCLUDE <string list>surface_names
  ...  <string>variable_name
  [AS <string>dbase_variable_name] INCLUDE|ON|EXCLUDE
  <string list>surface_names
```

This form of the `FACE` command line is similar to the first, except that the user can control which surfaces are used for output. The user can include a specific list of surfaces for output by using the `INCLUDE` option or the `ON` option. (The keyword `INCLUDE` is synonymous with the keyword `ON`.) Alternatively, the user can exclude a specific list of surfaces for output by using the `EXCLUDE` option.

Suppose that the face variable `pressure_face` from the above example has been defined for `surface_10`, `surface_11`, `surface_20`, and `surface_21`. If we only want to output the face variable for `surface_10`, `surface_11`, and `surface_21`, then we could specify the `FACE` command line as follows:

```
FACE pressure_face AS pressuref
     INCLUDE surface_10, surface_11,
     surface_21
```

(In the above command line, the keyword `ON` could be substituted for `INCLUDE`.) Alternatively, we could use the command line:

```
FACE pressure_face AS pressuref
     EXCLUDE surface_20
```

In the above command lines, an alias for a surface can be substituted for a surface identifier. For example, if `center_case` is an alias for `surface_10`, then the string `center_case` could be substituted for `surface_10` in the above command lines. Because a surface identifier is a mesh entity, the alias for the surface identifier would be defined via an `ALIAS` command line in a `FINITE ELEMENT MODEL` command block.

Note that the list of identifiers uses a comma to separate one surface identifier from the next surface identifier.

8.2.1.4 Output Element Variables

```
ELEMENT  <string>variable_name
  [AS <string>dbase_variable_name] ...
  <string>variable_name [AS
  <string>dbase_variable_name]
  | ELEMENT  <string>variable_name
      [AS <string>dbase_variable_name]
      INCLUDE|ON|EXCLUDE <string list>block_names
      ... <string>variable_name
      [AS dbase_variable_name] INCLUDE|ON|EXCLUDE
      <string list>block_names
```

Any element variable in Presto can be selected for output in the results file by using the `ELEMENT` command line.

There are two forms of the `ELEMENT` command line. Either form will let you output an element variable.

The first form of the command line is as follows:

```
ELEMENT  <string>variable_name
  [AS <string>dbase_variable_name] ...
  <string>variable_name [AS
  <string>dbase_variable_name]
```

Here, the string `variable_name` is the name of the element variable to output. The string `variable_name` can be a variable listed in Section 8.9 or a user-defined variable (see Section 8.2.2 and Section 10.2.4).

In the first form of the ELEMENT command line, the element variable is output for all element blocks that have the element variable as a defined variable. For example, all the solid elements have stress as a defined variable. If you had a mesh consisting of hexahedral and tetrahedral elements and requested output of the element variable stress, then stress would be output for all element blocks consisting of hexahedral and tetrahedral elements.

It is possible to specify an alias for any of the element variables by using the AS specification. Suppose, for example, you wanted to output the stress in Presto, which is defined as stress, with the alias str. You would then enter the command line:

```
ELEMENT stress AS str
```

In this example, stress is a symmetric tensor quantity. For a symmetric tensor quantity, suffixes are appended to the variable name (or alias name) to denote each symmetric tensor component. The results database would have six variable names associated with the stress: stress_xx, stress_yy, stress_zz, stress_xy, stress_xz, and stress_yz. You can change the tensor component separator, an underscore in this example, by using the COMPONENT SEPARATOR CHARACTER command line (see Section 8.2.1.7).

The ELEMENT command line can be used an arbitrary number of times within a RESULTS OUTPUT command block. It is also possible to specify more than one element variable for output on a command line, as indicated by the ellipsis in the command line format. In the following example, two element variables are specified for output. Here, the second element variable is defined as left_stretch.

```
ELEMENT stress left_stretch
```

Aliases can be specified for each of the variables in a single command line. Thus, If you wanted to output the alias str for element variable stress and also wanted to output the alias strch for face variable lseft_stretch, you would enter the command line:

```
ELEMENT stress AS str
     left_stretch AS strch
```

The specification of an alias is optional.

The second form of the command line is as follows:

```
ELEMENT  <string>variable_name
  [AS <string>dbase_variable_name]
  INCLUDE|ON|EXCLUDE <string list>block_names
  ... <string>variable_name
  [AS dbase_variable_name] INCLUDE|ON|EXCLUDE
  <string list>block_names
```

This form of the ELEMENT command line is similar to the first, except that the user can control which element blocks are used for output. The user can include a specific list of element blocks for output by using the INCLUDE option or the ON option. (The keyword INCLUDE is synonymous with the keyword ON.) Alternatively, the user can exclude a specific list of element blocks for output by using the EXCLUDE option.

Suppose that the element variable stress from the above example exists for element blocks block_10, block_11, block_20, and block_21. If we only want to output the element variable for block_10, block_11, and block_21, then we could specify the ELEMENT command line as follows:

```
ELEMENT stress AS str
     INCLUDE block_10, block_11,
     block_21
```

(In the above command line, the keyword ON could be substituted for INCLUDE.) Alternatively, we could use the command line:

```
ELEMENT stress AS str
     EXCLUDE block_20
```

In the above command lines, an alias for an element block can be substituted for an element block identifier. For example, if center_case is an alias for block_10, then the string center_case could be substituted for block_10 in the above command lines. Because an element block identifier is a mesh entity, the alias for the element block identifier would be defined via an ALIAS command line in a FINITE ELEMENT MODEL command block. Note that the list of identifiers uses a comma to separate one element block identifier from the next element block identifier.

For multi-integration point elements, quantities from the integration points are appended with a numerical index indicating the integration point. A suffix ranging from 1 to the number of integration points is attached to the quantity to indicate the corresponding integration point. The suffix is padded with leading zeros. If the number of integration points is less than 10, the suffix has the form _*i*, where *i* ranges from 1 to the number of integration points. If the number of integration points is greater than or equal to 10 and less than 100, the sequence of suffixes takes the form _01, _02, _03, and so forth. Finally, if the number of integration points is greater than or equal to 100, the sequence of suffixes takes the form _001, _002, _003, and so forth. As an example, if the von Mises stress is requested for a shell element with 15 integration points, then the quantities von_mises_01, von_mises_02, ..., von_mises_15 are output for the shell element.

In the above discussion concerning the format for output at multiple integration points, the underscore character preceding the integration point number can be replaced by another delimiter or the underscore character can be eliminated by use of the COMPONENT SEPARATOR CHARACTER command line (see Section 8.2.1.7).

Shell tensor quantities transform_shell_stress, transform_shell_strain and transform_shell_rate_of_deformation may be transformed to a user specified shell local co-rotational coordinate system (i.e. an in-plane coordinate system that rotates with the shell element) for output using the ORIENTATION shell section command. If no orientation is specified, these in-plane stresses and strains are output in the default orientation. See Section 5.2.4 for more details.

8.2.1.5 Subsetting of Output Mesh

A specified subset of the element blocks in the mesh can be output to the results database using the `INCLUDE` or `EXCLUDE` commands. The syntax is:

```
INCLUDE = <string>list_of_included_element_blocks
EXCLUDE = <string>list_of_excluded_element_blocks
```

Either command can appear multiple times within the results output block, but the two cannot be mixed within a single results output block. If the `INCLUDE` command is specified, the results database will only contain the listed element blocks; if the `EXCLUDE` command is specified, the results database will contain all element blocks except for the listed element blocks. If the model has surfaces or nodesets, only the portion of the surfaces or nodesets on the selected element blocks will be output.

8.2.1.6 Output Mesh Selection

```
OUTPUT MESH = EXPOSED_SURFACE|BLOCK_SURFACE
```

The `OUTPUT MESH` command provides a way to reduce the amount of data that is written to the results database. There are two options that can be selected:

`EXPOSED_SURFACE` Only output the element faces that make up the "skin" of the finite element model; no internal nodes or elements will be written to the results database. The element results variables will be applied to the skin faces. If the mesh is visualized without any cutting planes, the display should look the same as if the original full mesh were visualized; however, the amount of data written to the output file can be much less than is needed if the full mesh were output.

`BLOCK_SURFACE` This option is similar to the `EXPOSED_SURFACE` option except that the skinning process is done an element block at a time instead of for the full model. In this option, faces shared between element blocks will appear in the output model.

8.2.1.7 Component Separator Character

```
COMPONENT SEPARATOR CHARACTER = <string>character|NONE
```

The component separator character is used to separate an output-variable base name from any suffixes. For example, the variable `stress` can have the suffixes `xx`, `yy`, etc. By default, the base name is separated from the suffixes with an underscore character so that we have `stress_xx`, `stress_yy`, etc. in the results output file.

You can replace the underscore as the default separator by using the above command line. If you wanted to use the period as the separator, then you would use the following command line:

```
COMPONENT SEPARATOR CHARACTER = .
```

For our example with stress, the stress components would then appear in the results output file as `stress.xx`, `stress.yy`, etc. If the stress is for a shell element, there is also an integration point suffix preceded, by default, with an underscore. The above command line also resets the underscore character that precedes the integration point suffix. For our example with the `stress` base name and the underscore replaced by the period, the results file would have `stress.xx.01`, `stress.xx.02`, etc., for the shell elements.

You can eliminate the separator with an empty string or `NONE`.

8.2.1.8 Output Global Variables

```
GLOBAL  <string>variable_name
  [AS <string>dbase_variable_name
  <string>variable_name AS <string>dbase_variable_name ...]
```

Any global variable in Presto can be selected for output in the results file by using the `GLOBAL` command line. The string `variable_name` is the name of the global variable. The string `variable_name` can be either a variable listed in Section 8.9 or a user-defined variable (see Section 8.2.2 and Section 10.2.4).

Kinetic, external, hourglass, and internal energies can be requested as the sum over the entire mesh or as sums over individual element blocks as noted in Section 8.9. For example, if the mesh contains element blocks with IDs 100 and 200, the kinetic and hourglass energy summed over each of these blocks individually can be requested with the commands

```
GLOBAL  ke_block100 as ke100
GLOBAL  ke_block200 as ke200
GLOBAL  hge_block100 as hge100
GLOBAL  hge_block200 as hge200
```

and the total kinetic energy as

```
GLOBAL  kinetic_energy as ke
```

Kinetic, internal, and external energies are computed as nodal values. Since nodes may be shared by element blocks, the total sum of an energy quantity over individual element blocks will not necessarily be equal to the global sum requested using the `kinetic_energy`, `internal_energy`, or `external_energy` variable names.

With the `AS` specification, you can specify the variable and select an alias for this variable in the results file. Suppose, for example, you wanted to output the time steps in Presto, which are identified as `timestep`, with the alias `tstep`. You would then enter the command line:

```
GLOBAL timestep AS tstep
```

The GLOBAL command line can be used an arbitrary number of times within a RESULTS OUTPUT command block. It is also possible to specify more than one global variable for output on a command line. If you also wanted to output the kinetic energy , which is defined as KineticEnergy , with the alias ke , you would enter the command line:

```
GLOBAL timestep as tstep
     KineticEnergy as ke
```

The specification of an alias is optional.

8.2.1.9 Set Begin Time for Results Output

```
START TIME = <real>output_start_time
```

Using the START TIME command line, you can write output to the results file beginning at time output_start_time. No results will be written before this time. If other commands set times for results (AT TIME, ADDITIONAL TIMES) that are less than output_start_time, those times will be ignored, and results will not be written at those times.

8.2.1.10 Adjust Interval for Time Steps

```
TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
```

This command line is used to specify that the output will be at exactly the times specified. To hit the output times exactly in an explicit, transient dynamics code, it is necessary to adjust the time step as the time approaches an output time. The integer value steps in the TIMESTEP ADJUSTMENT INTERVAL command line specifies the number of time steps to look ahead in order to adjust the time step.

If this command line does not appear, results are output at times closest to the specified output times.

8.2.1.11 Output Interval Specified by Time Increment

```
AT TIME <real>time_begin INCREMENT = <real>time_increment_dt
```

At the time specified by time_begin, results will be output every time increment given by the real value time_increment_dt.

8.2.1.12 Additional Times for Output

```
ADDITIONAL TIMES = <real>output_time1 <real>output_time2 ...
```

In addition to any times specified by the command line in Section 8.2.1.11, you can use the ADDITIONAL TIMES command line to specify an arbitrary number of additional output times.

8.2.1.13 Output Interval Specified by Step Increment

```
AT STEP <integer>step_begin INCREMENT =
  <integer>step_increment
```

At the step specified by `step_begin`, results will be output every step increment given by the integer value `step_increment`.

8.2.1.14 Additional Steps for Output

```
ADDITIONAL STEPS = <integer>output_step1
  <integer>output_step2 ...
```

In addition to any steps specified by the command line in Section 8.2.1.13, you can use the `ADDITIONAL STEPS` command line to specify an arbitrary number of additional output steps.

8.2.1.15 Set End Time for Results Output

```
TERMINATION TIME = <real>termination_time_value
```

Results will not be written to the results file after time `termination_time_value`. If other commands set times for results (`AT TIME`, `ADDITIONAL TIMES`) that are greater than `termination_time_value`, those times will be ignored, and results will not be written at those times.

8.2.1.16 Synchronize Output

```
SYNCHRONIZE OUTPUT
```

In an analysis with multiple regions, it is sometimes desirable to synchronize the output of results data between the regions. This can be done by adding the `SYNCHRONIZE OUTPUT` command line to the results output block. If a results block has this set, then it will write output whenever a previous region writes output. The ordering of regions is based on the order in the input file, algorithmic considerations, or by solution control specifications.

Although the `USE OUTPUT SCHEDULER` command line can also synchronize output between regions, the `SYNCHRONIZE OUTPUT` command line will synchronize the output with regions where the output frequency is not under the direct control of the Sierra IO system. Examples of this are typically coupled applications where one or more of the codes are not Sierra-based applications such as Alegra and CTH. A results block with `SYNCHRONIZE OUTPUT` specified will also synchronize its output with the output of the external code.

The `SYNCHRONIZE OUTPUT` command can be used with other output scheduling commands such as time-based or step-based output specifications.

8.2.1.17 Use Output Scheduler

```
USE OUTPUT SCHEDULER <string>scheduler_name
```

In an analysis with multiple regions, it can be difficult to synchronize output such as results files. To help synchronize output for analyses with multiple regions, you can define an `OUTPUT SCHEDULER` command block at the SIERRA scope. The scheduler can then be referenced in the `RESULTS OUTPUT` command block via the `USE OUTPUT SCHEDULER` command line. The string `scheduler_name` must match a name used in an `OUTPUT SCHEDULER` command block. See Section 8.6 for a description of using this command block and the `USE OUTPUT SCHEDULER` command line.

8.2.1.18 Write Results If System Error Encountered

```
OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|SIGHUP|SIGINT|
  SIGPIPE|SIGQUIT|SIGTERM|SIGUSR1|SIGUSR2|SIGABRT|
  SIGKILL|SIGILL|SIGSEGV
```

The `OUTPUT ON SIGNAL` command line is used to initiate the writing of a results file when the system encounters a type of system error. Only one error type in the list of error types should be entered for this command line. Generally, these system errors cause the code to terminate before the code can add any current results output (results output past the last results output time step) to the results output file. If the code encounters the specified type of error during execution, a results file will be written before execution is terminated.

This command line can also be used to force the writing of a results file at some point during execution of the code. Suppose the command line

```
OUTPUT ON SIGNAL = SIGUSR2
```

is included in the input file. While the code is running, a user can execute (from the keyboard) the system command line

`kill -s SIGUSR2` *pid*

to terminate execution and force the writing of a results file. In the above system command line, *pid* is the process identifier, which is an integer.

Note that the `OUTPUT ON SIGNAL` command line is primarily a debugging tool for code developers.

8.2.2 User-Defined Output

```
BEGIN FILTER <string>filter_name
  ACOEFF = <real_list>a_coeff
  BCOEFF = <real_list>b_coeff
  INTERPOLATION TIME STEP = <real>ts
END [FILTER]

BEGIN USER OUTPUT
  # mesh-entity set commands
  NODE SET = <string_list>nodelist_names
  SURFACE = <string_list>surface_names
  BLOCK = <string_list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list> surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # compute result commands
  COMPUTE GLOBAL <string>result_var_name AS
    SUM|AVERAGE|MAX|MIN OF NODAL|ELEMENT <string>value_var_name
  COMPUTE NODAL <string>result_var_name AS
    MAX OVER TIME|MIN OVER TIME|ABSOLUTE VALUE MAX
    OVER TIME OF NODAL <string>value_var_name
  COMPUTE ELEMENT <string>result_var_name AS
    MAX OVER TIME|MIN OVER TIME|ABSOLUTE VALUE MAX
    OVER TIME OF ELEMENT <string>value_var_name
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name |
    SURFACE SUBROUTINE = <string>subroutine_name |
    ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # copy command
  COPY ELEMENT VARIABLE <string>ev_name TO NODAL VARIABLE
    <string>nv_name

  # variable transformation command
  TRANSFORM NODAL|ELEMENT VARIABLE <string>variable_name
    TO COORDINATE SYSTEM <string>coord_sys_name
```

```
    AS <string> transformed_name
  #
  # Data filtering
  FILTER <string>new_var FROM NODAL|ELEMENT <string>source_var
    USING <string>filter_name


  #
  # compute for element death
  COMPUTE AT EVERY TIME STEP

  #
  # additional command
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [USER OUTPUT]
```

The USER OUTPUT command block lets the user generate specialized output information derived from analysis results such as element stresses, displacements, and velocities. For example, the USER OUTPUT command block could be used to sum the contact forces in a particular direction in the global axes and on a certain surface to give a net resultant contact force on that surface. In this example, we essentially postprocess contact information and reduce it to a single value for a surface (or set of surfaces). This, then, is one of the purposes of the USER OUTPUT command block—to postprocess analysis results as the code is running and produce a reduced set of specialized output information. The USER OUTPUT command block offers an alternative to writing out large quantities of data and then postprocessing them with an external code to produce specialized output results. Another use of the USER OUTPUT command block is to generate variables that can be used for element death. An element can be killed by using a criterion based on a user variable defined in the USER OUTPUT command block.

There are three options for calculating user-defined quantities. In the first option, a single command line in the command block is used to compute reductions of variables on subsets of the mesh. This option makes use of one of the compute result command lines. For instance, the above example of the contact force is a case where we can accomplish the desired result simply by using the COMPUTE GLOBAL command line. In the second option, the command block specifies a user subroutine to run immediately preceding output to calculate any desired variable. This option makes use of a NODE SET, SURFACE, or ELEMENT BLOCK SUBROUTINE command line. Finally, there is an option to copy an element variable for an element to the nodes associated with the element, via the COPY ELEMENT VARIABLE command line. This copy option is a specialized option that has been made available primarily for creating results files for some of the postprocessing tools used with Presto. You can use only one of the three options—compute global result, user subroutine, or copy—in a given command block.

For the compute result option, a user-defined variable is automatically generated. This user-defined variable is given whatever name the user selects for results_var_name in the above specification for any of the three compute result command lines. Parenthesis syntax (Section 8.1) may be used to define reductions on specific integration points or components of a variable. By default, a

reduction operation operates on each integration point. For example, if the compute global command was used to average values of element stress it would average the values of stress at all integration points of all elements. If the command was used to average `stress(:,1)`, the result would only be the average of stress on the first integration points.

If the user subroutine or copy option is used, the user will need to define some type of user variable with the `USER VARIABLE` command block described in Section 10.2.4.

User-defined variables, whether they are generated via the compute result option or the `USER VARIABLE` command block, are not automatically written to a results or history file. If the user wants to output any user-defined variables, these variables must be referenced in a results or history output specification (see Section 8.2.1 and Section 8.3, which describe the output of variables to results files and history files, respectively). If the user wants to use any user-defined variable for element death, the user must include the `COMPUTE AT EVERY TIME STEP` command line.

The `USER OUTPUT` command block contains five groups of commands—mesh-entity set, compute result, user subroutine, copy, and compute for element death. Each of these command groups is basically independent of the others. In addition to the command lines in the five command groups, there is an additional command line: `ACTIVE PERIODS`. The following sections provide descriptions of the different command groups and the `ACTIVE PERIODS` command line.

8.2.2.1 Mesh-Entity Set Commands

The `mesh-entity set commands` portion of the `USER OUTPUT` command block specifies the nodes, element faces, or elements associated with the variable to be output. This portion of the command block can include some combination of the following command lines:

```
NODE SET = <string_list>nodelist_names
SURFACE = <string_list>surface_names
BLOCK = <string_list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list> surface_names
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes, element faces, or elements. See Section 6.1.1 for more information about the use of these command lines for mesh entities. There must be at least one `NODE SET`, `SURFACE`, `BLOCK`, or `INCLUDE ALL BLOCKS` command line in the command block.

8.2.2.2 Compute Result Commands

The compute result commands are used to compute new variables by performing operations on an existing variable. Currently three general forms of the compute results command are supported:

```
COMPUTE GLOBAL result_var_name AS SUM|AVERAGE|MAX|MIN
```

```
  OF NODAL|ELEMENT source_var_name
COMPUTE NODAL result_var_name AS
  MAX OVER TIME|MIN OVER TIME|ABSOLUTE VALUE MAX OVER TIME
   OF NODAL source_var_name
COMPUTE ELEMENT result_var_name AS
  MAX OVER TIME|MIN OVER TIME|ABSOLUTE VALUE MAX OVER TIME
   OF ELEMENT source_var_name
```

The compute global result command returns a single global value or a set of global values by examining the current values for a named nodal or element variable and then calculating the output according to a user-specified operation. A single global value, for example, might be the maximum value of one of the stress components of all the elements in our specified set; a set of global values would be the maximum value of each stress component of all elements in our specified set.

The compute nodal and element variable commands compute a new nodal or element field by operating on an existing field. These commands can be used for computing such things as the maximum stress in each element over the course of the analysis.

In the above command lines, the following definitions apply:

- The string `result_var_name` is the name of a new variable in which the computed results are stored. To output this variable in a results file, a heartbeat file, or a history file, you will simply use whatever you have selected for `results_var_name` as the variable name in the output block.
- Four different global reduction methods are available for computing global variables: `SUM`, `AVERAGE`, `MAX`, and `MIN`. `SUM` adds the variable value of all included mesh entities. `AVERAGE` takes the average value of the variable over all included mesh entities. `MAX` finds the maximum value over all included mesh entities. `MIN` finds the minimum value over all included mesh entities.
- Three different over time methods are available for computing nodal or element variables: `MAX OVER TIME`, `MIN OVER TIME`, and `ABSOLUTE VALUE MAX OVER TIME`. These options compute the max, min, or absolute max over time of values in the source variable.
- The source variable used to compute a global variable must be either a nodal quantity or an element quantity, as specified by the `NODAL` or `ELEMENT` option. The variable source variable used to compute a nodal or element variable must be of the same type as the result variable.
- The string `source_var_name` is the name of the variable used to compute the result variable. (see Section 8.9 for a listing of available code variables).
- Standard component syntax may also be used in the `source_variable_name` to specify operating on sub-components of a given variable (such as only `stress(xx)`).

The following is an example of using the `COMPUTE` command line to compute the net x-direction reaction force:

```
COMPUTE GLOBAL wall_x_reaction AS SUM OF NODAL reaction(x)
```

The following is an example of using the COMPUTE command line to compute the maximum force seen by the spot welds.

```
COMPUTE NODAL max_spotn AS MAXIMUM OVER TIME OF NODAL spot_weld_
normal_force
```

8.2.2.3 User Subroutine Commands

If the user subroutine option is used, the user-defined output quantities will be calculated by a subroutine that is written by the user explicitly for this purpose. The subroutine will be called by Presto at the appropriate time to perform the calculations. User subroutines allow for more generality in computing user-defined results than the COMPUTE GLOBAL command line. Suppose, for example, you had an analytic solution for a problem and wanted to compute the difference between some analytic value and a corresponding computed value throughout an analysis. The user subroutine option would allow you to make this comparison. The full details for user subroutines are given in Chapter 10.

The following command lines are related to the user subroutine option:

```
NODE SET SUBROUTINE = <string>subroutine_name |
  SURFACE SUBROUTINE = <string>subroutine_name |
  ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value
```

The user subroutine option is invoked by using the NODE SET SUBROUTINE command line, the SURFACE SUBROUTINE command line, or the ELEMENT BLOCK SUBROUTINE command line. The particular command line selected depends on the mesh-entity type of the variable for which the result quantities are being calculated. For example, variables associated with nodes would be calculated by using a NODE SET SUBROUTINE command line, variables associated with faces by using a SURFACE SUBROUTINE command line, and variables associated with elements by using the ELEMENT BLOCK SUBROUTINE command line. The string subroutine_name is the name of a FORTRAN subroutine that is written by the user. A user subroutine in the USER OUTPUT command block returns no values. Instead, it performs its operations directly with commands such as aupst_put_nodal_var, aupst_put_elem_var, and aupst_put_global_var. See Chapter 10 for further discussion of these various put commands.

Following the selected command line (NODE SET SUBROUTINE, SURFACE SUBROUTINE, or ELEMENT BLOCK SUBROUTINE) are other command lines that may be used to implement

the user subroutine option. These command lines are described in Section 10.2.2 and consist of SUBROUTINE DEBUGGING OFF, SUBROUTINE DEBUGGING ON, SUBROUTINE REAL PARAMETER, SUBROUTINE INTEGER PARAMETER, and SUBROUTINE STRING PARAMETER. Examples of using these command lines are provided in Chapter 10.

Importantly, to implement the user subroutine option and output the calculated information, you would also need to do the following:

1. Create the user-defined variable with a USER VARIABLE command block.

2. Calculate the results for the user-defined variable in the user subroutine.

3. Write the results for the user-defined variable to an output file by referencing it in a RESULTS OUTPUT command block and/or a HISTORY OUTPUT command block and/or a HEARTBEAT OUTPUT command block. In the RESULTS OUTPUT command block, you would use a NODAL command line, an ELEMENT command line, or a GLOBAL command line, depending on how you defined the variable in the USER VARIABLE command block. Similarly, in the HISTORY OUTPUT or HEARTBEAT OUTPUT command block, you would use the applicable form of the variable command line, depending on how you defined the variable in the USER VARIABLE command block.

8.2.2.4 Copy Command

```
COPY ELEMENT VARIABLE <string>ev_name TO NODAL VARIABLE
  <string>nv_name
```

The COPY ELEMENT VARIABLE command line copies the value of an element variable to a node associated with the element. The element variable to be copied is specified by ev_name; the name of the nodal variable to which the value is being transferred is nv_name. The nodal variable must be specified as a user-defined variable.

8.2.2.5 Variable Transformation Command

```
TRANSFORM NODAL|ELEMENT VARIABLE <string>variable_name
  TO COORDINATE SYSTEM <string>coord_sys_name
  AS <string> transformed_name
```

The TRANSFORM NODAL|ELEMENT VARIABLE command line transforms a nodal vector (displacement, velocity, acceleration, etc) or an element tensor (stress, strain, etc.) from components in the global coordinate system to components in the coordinate system defined in a BEGIN COORDINATE SYSTEM command block having the name coord_sys_name (see Section 2.1.8). The transformed variables will be output to the results file as transformed_name.

Warning: This command cannot be used to transform shell element tensors which are not computed in the global coordinate system. Output of shell stress and strain components in a user-defined, local co-rotational coordinate system are obtained with the element variables `transform_shell_stress` and `transform_shell_strain` as described in Section 8.2.1.

8.2.2.6 Data Filtering Commands

```
BEGIN FILTER <string>filter_name
  ACOEFF = <real_list>a_coeff
  BCOEFF = <real_list>b_coeff
  INTERPOLATION TIME STEP = <real>ts
END [FILTER]


BEGIN USER OUTPUT
  FILTER <string>new_var FROM NODAL|ELEMENT <string>source_var
    USING <string>filter_name
END
```

The user output `FILTER` command creates a new variable "new_var" by performing an on-the-fly frequency filter of the named element or nodal variable "source_var". The `BEGIN FILTER` command block defines a filter with the name "filter_name". The filter defined by the begin filter command block is then referenced by the `USER OUTPUT` filter command.

In the `BEGIN FILTER` command block the A and B filtering coefficients are defined with the `ACOEFF` and `BCOEFF` command lines. The filter must define at least one A and one B coefficient, there is no maximum number coefficients and the length of A and B do not need to match.

Filter operations assume that the data given at a constant time step. The explicit dynamics time step will tend to vary during the analysis. The `INTERPOLATION TIME STEP` command is used to linearly interpolate the data that is being produced at a non-constant time step down to some specified constant time step. The interpolation time step must be larger than zero and ideally should be specified such that it is smaller than the smallest time step with which the computations will iterate.

One way to obtain the filtering coefficients is with MATLAB. The following is an example of defining a third order Butterworth filter with a pass frequency of 100Hz at data interpolated to a time step of 1.0e-5 seconds. The filter is then used to filter acceleration histories of the nodes to 100Hz. The MATLAB code below will give the desired filtering coefficients. Note that the full 16-digit precision of the coefficients returned by MATLAB should be used. If truncated precision numbers are used, the filters can potentially be unstable.

```
clear;
format long e;
```

```
passFrequency = 100;
interp_ts = 1.0e-5;
butterCoeff = 2.0*interp_ts*passFrequency;
[bcoeff,acoeff] = butter(3,butterCoeff);
acoeff
bcoeff
```

The computed filtering coefficients can be used in a `USER OUTPUT` block as show below. If the analysis time step always remains above 1.0e-5 the filter will be valid. If the analysis time step drops below 1.0e-5 there could be aliasing issues, and a smaller interpolation time step should be specified.

```
BEGIN FILTER filt_100Hz
  ACOEFF = 1.000000000000000e+00 -2.987433650055722e+00 $
           2.974946132665442e+00 -9.875122361107358e-01
  BCOEFF = 3.081237301416628e-08  9.243711904249885e-08 $
           9.243711904249885e-08  3.081237301416628e-08
  INTERPOLATION TIME STEP = 1.0e-5
END
BEGIN USER OUTPUT
  FILTER ax100Hz FROM NODAL acceleration(x) USING filt_100Hz
  FILTER ay100Hz FROM NODAL acceleration(y) USING filt_100Hz
  FILTER az100Hz FROM NODAL acceleration(z) USING filt_100Hz
END
```

8.2.2.7 Compute at Every Step Command

```
COMPUTE AT EVERY TIME STEP
```

If this command line appears in the `USER OUTPUT` command block, a user-defined variable in the command block will be written at every time step. The `COMPUTE AT EVERY TIME STEP` command line is required if a user-defined variable is used in a criterion for element death. (Section 10.2.4 discusses user-defined variables, and Section 5.5 discusses element death.) For element death, a user-defined variable must be calculated at every time step.

8.2.2.8 Additional Command

The `ACTIVE PERIODS` or `INACTIVE PERIODS` command lines can appear as an option in the `USER OUTPUT` command block:

```
ACTIVE PERIODS = <string list>period_names
INACTIVE PERIODS = <string list>period_names
```

These command lines determine when the boundary condition is active. See Section 2.5 for more information about this optional command line.

8.3 History Output

```
BEGIN HISTORY OUTPUT <string>history_name
  DATABASE NAME = <string>history_file_name
  DATABASE TYPE = <string>database_type(exodusII)
  OVERWRITE = <string>OFF|ON|TRUE|FALSE|YES|NO
    (ON|TRUE|YES)
  TITLE <string>user_title
  #
  # for global variables
  GLOBAL <string>variable_name
    [AS <string>history_variable_name]
  #
  # for mesh entity - node, edge, face,
  # element - variables
  NODE|NODAL|EDGE|FACE|ELEMENT <string>variable_name
    AT NODE|NODAL|EDGE|FACE|ELEMENT <integer>entity_id
    AS <string>history_variable_name
  #
  # for nearest point output of mesh entity - node,
  # edge, face, element - variables
  NODE|NODAL|EDGE|FACE|ELEMENT <string>variable_name
    NEAREST LOCATION <real>global_x,
      <real>global_y>, <real>global_z
    AS <string>history_variable_name
  START TIME = <real>output_start_time
  TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
  AT TIME <real>time_begin INCREMENT =
    <real>time_increment_dt
  ADDITIONAL TIMES = <real>output_time1
    <real>output_time2 ...
  AT STEP <integer>step_begin INCREMENT =
    <integer>step_increment
  ADDITIONAL STEPS = <integer>output_step1
    <integer>output_step2 ...
  TERMINATION TIME = <real>termination_time_value
  SYNCHRONIZE_OUTPUT
  USE OUTPUT SCHEDULER <string>scheduler_name
  OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|SIGHUP|SIGINT|
    SIGPIPE|SIGQUIT|SIGTERM|SIGUSR1|SIGUSR2|SIGABRT|
    SIGKILL|SIGILL|SIGSEGV
END [HISTORY OUTPUT <string>history_name]
```

A history file gives nodal variable results (displacements, forces, etc.) for specific nodes, edge variable results for specific edges, face variable results for specific faces, element results (stress, strain, etc.) for specific elements, and global results at specified times. You can specify a history file, the results to be included in this file, and the frequency at which results are written by using

a HISTORY OUTPUT command block. The command block appears inside the region scope. For history output, you will typically work with node and element variables, and, on some occasions, face variables.

More than one history file can be specified for an analysis. For each history file, there will be one HISTORY OUTPUT command block. The command block for a history file description begins with:

```
BEGIN HISTORY OUTPUT <string>history_name
```

and is terminated with:

```
END [HISTORY OUTPUT <string>history_name]
```

where history_name is a user-selected name for the command block. Nested within the HISTORY OUTPUT command block are a set of command lines, as shown in the block summary given above. The first two command lines listed (DATABASE NAME and DATABASE TYPE) give pertinent information about the history file. The command line

```
DATABASE NAME = <string>history_file_name
```

gives the name of the history file with the string history_file_name. If the history file is to appear in the current directory and is named job.h, this command line would appear as:

```
DATABASE NAME = job.h
```

If the history file is to be created in some other directory, the command line would have to show the path to that directory.

Two metacharacters can appear in the name of the history file. If the %P character is found in the name, it will be replaced with the number processors being used for the run. For example, if you are running on 1024 processors and use the name history-%P/job.h, then the name would be expanded to history-1024/job.h. The other recognized metacharacter is %B which is replaced with the base name of the input file containing the input commands. For example, if the commands are in the file my_analysis_run.i and the history database name is specified as %B.h, then the history would be written to the file my_analysis_run.h.

If the history file does not use the Exodus II format [1], you must specify the format for the history file using the command line:

```
DATABASE TYPE = <string>database_type(exodusII)
```

Currently, both the Exodus II database and the XDMF database [2] are supported in Presto and Adagio. Exodus II is more commonly used than XDMF. Other options may be added in the future.

The OVERWRITE command line can be used to prevent the overwriting of existing history files.

```
OVERWRITE = <string>OFF|ON|TRUE|FALSE|YES|NO
     (ON|TRUE|YES)
```

The OVERWRITE command line allows only a single value. If you set the value to FALSE, NO, or OFF, the code will terminate before existing history files can be overwritten. If you set the value to TRUE, YES, or ON, then existing history files can be overwritten (the default status). Suppose, for example, that we have an existing history file named job21.h. Suppose also that we have an

input file with a HISTORY OUTPUT command block that contains the OVERWRITE command line set to ON and the DATABASE NAME command line set to:

```
DATABASE NAME = job21.h
```

If you run the code under these conditions, the existing history file job21.h will be overwritten.

Whether or not history files are overwritten is also impacted by the use of the automatic read and write option for restart files described in Section 8.5.1.1. If you use the automatic read and write option for restart files, the history files, like the restart files, are automatically managed. The automatic read and write option in restart adds extensions to file names and prevents the overwriting of any existing restart or history files. For the case of a user-controlled read and write of restart files (Section 8.5.1.2) or of no restart, however, the OVERWRITE command line is useful for preventing the overwriting of history files.

You may add a title to the history file by using the TITLE command line. Whatever you specify for the user_title will be written to the history file. Some of the programs that process the history file (such as various SEACAS programs [3]) can read and display this information.

The other command lines that appear in the HISTORY OUTPUT command block determine the type and frequency of information that is output. Descriptions of these command lines follow in Section 8.3.1 through Section 8.3.12. Note that the command lines for controlling the frequency of history output (in Section 8.3.1 through Section 8.3.12) are the same as those for controlling the frequency of results output. These frequency-related command lines are repeated here for convenience.

8.3.1 Output Variables

The GLOBAL, NODE (or NODAL), EDGE, FACE, or ELEMENT command line is used to select variables for output in the history file. One of several types of variables can be selected for output. The form of the command line varies depending on the type of variable that is selected for output.

8.3.1.1 Global Output Variables

```
GLOBAL <string>variable_name
  [AS <string>history_variable_name]
```

This form of the command line lets you select any global variable for output in the history file. The variable is selected with the string variable_name. The string variable_name is the name of the global variable and can be either a variable listed in Section 8.9 or a user-defined variable (see Section 8.2.2 and Section 10.2.4).

You can also specify a name, history_variable_name, for the selected entity following the AS keyword. For example, suppose you want to output the kinetic energy (KineticEnergy) as KE. The command line to obtain the kinetic energyin the history file would be

```
GLOBAL KineticEnergy AS KE
```

The specification of an alias is optional for output of a global variable.

8.3.1.2 Mesh Entity Output Variables

```
NODE|NODAL|EDGE|FACE|ELEMENT <string>variable_name
  AT NODE|NODAL|EDGE|FACE|ELEMENT <integer>entity_id
  AS <string>history_variable_name
```

This form of the command line lets you select any nodal, edge, face, or element variable for a specific mesh entity for output in the history file. For example, this form of the command line will let you pick the displacement at a specific node and output the displacement to the history file using an alias that you have chosen.

For this form of the command line, the mesh entity type is set to `NODE` (or `NODAL`), `EDGE`, `FACE`, or `ELEMENT` depending on the variable (set by `variable_name`) to be output. If the mesh entity type is set to `NODE` (or `NODAL`), `EDGE`, or `FACE`, the string `variable_name` can be either a variable listed in Section 8.9 or a user-defined variable (see Section 8.2.2 and Section 10.2.4). If the mesh entity type is set to `ELEMENT`, the string `variable_name` can be a variable listed in Section 8.9 or a user-defined variable (see Section 8.2.2 and Section 10.2.4.

Selection of a specific mesh entity follows the `AT` keyword. You select a mesh entity type (`NODE` [or `NODAL`], `EDGE`, `FACE`, or `ELEMENT`) followed by the specific integer identifier, `entity_id`, for the mesh entity. You must specify a name, `history_variable_name`, for the selected entity following the `AS` keyword. For example, suppose you want to output the accelerations at node 88. The command line to obtain the accelerations at node 88 for the history file would be:

```
NODE ACCELERATION AT NODE 88 AS accel_88
```

where `accel_88` is the name that will be used for this history variable in the history file.

Note that either the keyword `NODE` or `NODAL` can be used for nodal quantities.

As an example, the command line to obtain the von Mises stress for element 1024 for the history file would be:

```
ELEMENT VON_MISES AT ELEMENT 1024 AS vm_1024
```

where `vm_1024` is the name that will be used for this history variable in the history file.

8.3.1.3 Nearest Point Output Variables

```
NODE|NODAL|EDGE|FACE|ELEMENT <string>variable_name
  NEAREST LOCATION <real>global_x,
    real<global_y>, real<global_z>
  AS <string>history_variable_name
```

This form of the command line lets you select any nodal, edge, face, or element variable for output in the history file using a nearest point criterion. The command line described in this subsection is an alternative to the command line described in the preceding section, Section 8.3.1.2, for obtaining history output. The command line in this section or the command line in Section 8.3.1.2 produces history files with variable information. The difference in these two command lines (Section 8.3.1.3 and Section 8.3.1.2) is simply in how the variable information is selected.

For the above form of the command line, the mesh entity type is set to NODE (or NODAL), EDGE, FACE, or ELEMENT depending on the variable (set by variable_name) to be output. If the mesh entity type is set to NODE (or NODAL), EDGE, or FACE, the string variable_name can be either a variable listed in Section 8.9 or a user-defined variable (see Section 8.2.2 and Section 10.2.4). If the mesh entity type is set to ELEMENT, the string variable_name can be a variable listed in Section 8.9 or a user-defined variable (see Section 8.2.2 and Section 10.2.4).

The specific mesh entity used for output is determined by global coordinates specified by the NEAREST LOCATION keyword and its associated input parameters—global_x, global_y, global_z. The specific mesh entity chosen for output is as follows:

- If the mesh entity has been set to NODE (or NODAL), the node in the mesh selected for output is the node whose initial position is nearest the input global X, Y, and Z coordinates specified with the parameters global_x, global_y, and global_z.
- If the mesh entity has been set to EDGE, the edge in the mesh selected for output is the edge with a center point (the average location of the two end points of the edge) whose initial position is nearest the input global X, Y, and Z coordinates specified with the parameters global_x, global_y, and global_z.
- If the mesh entity has been set to FACE, the face in the mesh selected for output is the face with a centroid whose initial position is nearest the input global X, Y, and Z coordinates specified with the parameters global_x, global_y, and global_z.
- If the mesh entity has been set to ELEMENT, the element in the mesh selected for output is the element with a centroid whose initial position is nearest the input global X, Y, and Z coordinates specified with the parameters global_x, global_y, and global_z.

Note that, in all the above cases, the original model coordinates are used when selecting the nearest entity, not the current coordinates.

You must specify a name, history_variable_name, for the selected entity following the AS keyword. As an example, suppose you want to output the accelerations at a node closest to the point with global coordinates (1012.0, 54.86, 103.3141). The command line to obtain the accelerations at the node closest to this location for the history file would be:

```
NODE ACCELERATION
     NEAREST LOCATION 1012.0, 54.86, 103.3141 AS accel_near
```

where accel_near is the name that will be used for this history variable in the history file.

Note that either the keyword NODE or NODAL can be used for nodal quantities.

8.3.2 Outputting History Data on a Node Set

It is commonly desired to output history data on a single-node node set. If a mesh file is slightly modified, the node and element numbers will completely change. The node associated with a node set, however, remains the same, i.e., the node in the node set retains the same initial geometric

location with the same connectivity to other elements even when its node number changes. Therefore, we might want to specify the history output for a node set with a single node rather than with the global identifier for a node. This can easily be accomplished, as follows:

```
 begin user output
   node set = nodelist_1
   compute global disp_ns_1 as average of nodal displacement
 end

begin history output
  global disp_ns_1
end
```

If `nodelist_1` contains only a single node, the history output variable `disp_ns_1` will contain the displacement for the single node in the node set. If `nodelist_1` contains multiple nodes, the average displacement of the nodes will be output.

8.3.3 Set Begin Time for History Output

```
START TIME = <real>output_start_time
```

Using the `START TIME` command line, you can write history variables to the history file beginning at time `output_start_time`. No history variables will be written before this time. If other commands set times for history output (`AT TIME`, `ADDITIONAL TIMES`) that are less than `output_start_time`, those times will be ignored, and history output will not be written at those times.

8.3.4 Adjust Interval for Time Steps

```
TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
```

This command line is used to specify that the output will be at exactly the times specified. To hit the output times exactly in an explicit, transient dynamics code, it is necessary to adjust the time step as the time approaches an output time. The integer value `steps` in the `TIMESTEP ADJUSTMENT INTERVAL` command line specifies the number of time steps to look ahead in order to adjust the time step.

If this command line does not appear, history variables are output at times closest to the specified output times.

8.3.5 Output Interval Specified by Time Increment

```
AT TIME <real>time_begin INCREMENT = <real>time_increment_dt
```

At the time specified by `time_begin`, history variables will be output every time increment given by the real value `time_increment_dt`.

8.3.6 Additional Times for Output

```
ADDITIONAL TIMES = <real>output_time1 <real>output_time2 ...
```

In addition to any times specified by the command line in Section 8.3.5, you can use the `ADDITIONAL TIMES` command line to specify an arbitrary number of additional output times.

8.3.7 Output Interval Specified by Step Increment

```
AT STEP <integer>step_begin INCREMENT =
  <integer>step_increment
```

At the step specified by `step_begin`, history variables will be output every step increment given by the integer value `step_increment`.

8.3.8 Additional Steps for Output

```
ADDITIONAL STEPS = <integer>output_step1
  <integer>output_step2 ...
```

In addition to any steps specified by the command line in Section 8.3.7, you can use the `ADDITIONAL STEPS` command line to specify an arbitrary number of g

8.3.9 Set End Time for History Output

```
TERMINATION TIME = <real>termination_time_value
```

History output will not be written to the history file after time `termination_time_value`. If other commands set times for history output (`AT TIME`, `ADDITIONAL TIMES`) that are greater than `termination_time_value`, those times will be ignored, and history output will not be written at those times.

8.3.10 Synchronize Output

```
SYNCHRONIZE OUTPUT
```

In an analysis with multiple regions, it is sometimes desirable to synchronize the output of history data between the regions. This can be done by adding the `SYNCHRONIZE OUTPUT` command line to the history output block. If a history block has this set, then it will write output whenever a previous region writes output. The ordering of regions is based on the order in the input file, algorithmic considerations, or by solution control specifications.

Although the `USE OUTPUT SCHEDULER` command line can also synchronize output between regions, the `SYNCHRONIZE OUTPUT` will synchronize the output with regions where the output frequency is not under the direct control of the Sierra IO system. Examples of this are typically coupled applications where one or more of the codes are not Sierra-based applications such as Alegra and CTH. A history block with `SYNCHRONIZE OUTPUT` specified will also synchronize its output with the output of the external code.

The `SYNCHRONIZE OUTPUT` command can be used with other output scheduling commands such as time-based or step-based output specifications.

8.3.11 Use Output Scheduler

```
USE OUTPUT SCHEDULER <string>scheduler_name
```

In an analysis with multiple regions, it can be difficult to synchronize output such as history files. To help synchronize output for analyses with multiple regions, you can define an `OUTPUT SCHEDULER` command block at the SIERRA scope. The scheduler can then be referenced in the `HISTORY OUTPUT` command block via the `USE OUTPUT SCHEDULER` command line. The string `scheduler_name` must match a name used in an `OUTPUT SCHEDULER` command block. See Section 8.6 for a description of using this command block and the `USE OUTPUT SCHEDULER` command line.

8.3.12 Write History If System Error Encountered

```
OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|SIGHUP|SIGINT|
  SIGPIPE|SIGQUIT|SIGTERM|SIGUSR1|SIGUSR2|SIGABRT|
  SIGKILL|SIGILL|SIGSEGV
```

The `OUTPUT ON SIGNAL` command line is used to initiate the writing of a history file when the system encounters a type of system error. Only one error type in the list of error types should be entered for this command line. Generally, these system errors cause the code to terminate before the code can add any current history output (history output past the last history output time step) to the history file. If the code encounters the specified type of error during execution, a history file will be written before execution is terminated.

This command line can also be used to force the writing of a history file at some point during execution of the code. Suppose the command line

```
OUTPUT ON SIGNAL = SIGUSR2
```

is included in the input file. While the code is running, a user can execute (from the keyboard) the system command line

`kill -s SIGUSR2` *pid*

to terminate execution and force the writing of a results file. In the above system command line, *pid* is the process identifier, which is an integer.

Note that the `OUTPUT ON SIGNAL` command line is primarily a debugging tool for code developers.

8.4 Heartbeat Output

```
BEGIN HEARTBEAT OUTPUT <string>heartbeat_name
  # Can also use predefined streams "cout", "stdout",
  # "cerr", "clog", "log", "output", or "outputP0"
  STREAM NAME = <string>heartbeat_file_name
  #
  # Specify whether heartbeat file will be in spyhis (cth)
  # format, or default format
  FORMAT = SPYHIS|DEFAULT
  #
  # for global variables
  GLOBAL <string>variable_name
    [AS <string>heartbeat_variable_name]
  #
  # for mesh entity - node, edge, face,
  # element - variables
  NODE|NODAL|EDGE|FACE|ELEMENT <string>variable_name
    AT NODE|NODAL|EDGE|FACE|ELEMENT <integer>entity_id
    AS <string>heartbeat_variable_name
  #
  # for nearest point output of mesh entity - node,
  # edge, face, element - variables
  NODE|NODAL|EDGE|FACE|ELEMENT <string>variable_name
    NEAREST LOCATION <real>global_x,
      <real>global_y>, <real>global_z
    AS <string>heartbeat_variable_name
  START TIME = <real>output_start_time
  TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
  AT TIME <real>time_begin INCREMENT =
    <real>time_increment_dt
  ADDITIONAL TIMES = <real>output_time1
    <real>output_time2 ...
  AT STEP <integer>step_begin INCREMENT =
    <integer>step_increment
  ADDITIONAL STEPS = <integer>output_step1
    <integer>output_step2 ...
  TERMINATION TIME = <real>termination_time_value
  SYNCHRONIZE_OUTPUT
  USE OUTPUT SCHEDULER <string>scheduler_name
  OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|SIGHUP|SIGINT|
    SIGPIPE|SIGQUIT|SIGTERM|SIGUSR1|SIGUSR2|SIGABRT|
    SIGKILL|SIGILL|SIGSEGV
  PRECISION = <integer>precision
  LABELS = <string>OFF|ON
  LEGEND = <string>OFF|ON
  TIMESTAMP FORMAT <string>timestamp_format
```

```
  MONITOR = <string>RESULTS|RESTART|HISTORY
END [HEARTBEAT OUTPUT <string>heartbeat_name]
```

The heartbeat output is text output file that gives:

- nodal variable results (displacements, forces, etc.) for specific nodes,
- edge variable results for specific edges,
- face variable results for specific faces,
- element results (stress, strain, etc.) for specific elements, and
- global results

at specified times.

Known Issue: User defined variables (see Section 10.2.4) are not currently supported with heartbeat output.

The output is written as text instead of the binary history output. You can specify a heartbeat file, the results to be included in this file, the formatting of the output, and the frequency at which results are written by using a `HEARTBEAT OUTPUT` command block. The command block appears inside the region scope. For heartbeat output, you will typically work with global, node, and element variables, and, on some occasions, face variables.

More than one heartbeat file can be specified for an analysis. For each heartbeat file, there will be one `HEARTBEAT OUTPUT` command block. The command block for a heartbeat file description begins with

```
BEGIN HEARTBEAT OUTPUT <string>heartbeat_name
```

and is terminated with

```
END [HEARTBEAT OUTPUT <string>heartbeat_name]
```

where `heartbeat_name` is a user-selected name for the command block. Nested within the `HEARTBEAT OUTPUT` command block are a set of command lines, as shown in the block summary given above. The first command line listed (`STREAM NAME`) gives pertinent information about the heartbeat file. The command line

```
STREAM NAME = <string>heartbeat_file_name
```

gives the name of the heartbeat file with the string `heartbeat_file_name`. If the file already exists, it is overwritten. If the heartbeat file is to appear in the current directory and is named `job.h`, this command line would appear as

```
STREAM NAME = job.h
```

If the heartbeat file is to be created in some other directory, the command line would have to show the absolute path to that directory.

In addition to specifying a specific filename, there are several predefined streams that can be specified. The predefined streams are:

- 'cout' or 'stdout' specifies standard output;
- 'cerr', 'stderr', 'clog', or 'log' specifies standard error;
- 'output' or 'outputP0' specifies Sierra's standard output which is redirected to the file specified by the '-o' option on the command line.

Two metacharacters can appear in the name of the heartbeat file. If the `%P` character is found in the name, it will be replaced with the number processors being used for the run. For example, if you are running on 1024 processors and use the name `heartbeat-%P/job.h`, then the name would be expanded to `heartbeat-1024/job.h`. The other recognized metacharacter is `%B` which is replaced with the base name of the input file containing the input commands. For example, if the commands are in the file `my_analysis_run.i` and the heartbeat stream name is specified as `%B.h`, then the heartbeat data would be written to the file `my_analysis_run.h`.

The other command lines that appear in the `HEARTBEAT OUTPUT` command block determine the type, frequency, and format of information that is output. Descriptions of these command lines follow in Section 8.4.1 through Section 8.4.14. Note that the command lines for controlling the frequency of heartbeat output (in Section 8.4.3 through Section 8.4.12) are the same as those for controlling the frequency of results and history output. These frequency-related command lines are repeated here for convenience.

8.4.1 Output Variables

The `GLOBAL`, `NODE` (or `NODAL`), `EDGE`, `FACE`, or `ELEMENT` command line is used to select variables for output in the heartbeat file. One of several types of variables can be selected for output. The form of the command line varies depending on the type of variable that is selected for output.

8.4.1.1 Global Output Variables

```
GLOBAL <string>variable_name
  [AS <string>heartbeat_variable_name]
```

This form of the command lets you select any global variable for output in the heartbeat file. The variable is selected with the string `variable_name`. The string `variable_name` is the name of the global variable and can be either a variable listed in Section 8.9 or a user-defined variable (see Section 8.2.2 and Section 10.2.4). The `variable_name` can also specify `time`, `timestep`, or `step` to output the current simulation time, timestep, or execution step, respectively.

You can also specify a name, `heartbeat_variable_name`, for the selected entity following the `AS` keyword. For example, suppose you want to output the kinetic energy (KineticEnergy) as KE. The command line to obtain the kinetic energyin the heartbeat file would be:

```
GLOBAL KineticEnergy AS KE
```

The specification of an alias is optional for a global variable.

8.4.1.2 Mesh Entity Output Variables

```
NODE|NODAL|EDGE|FACE|ELEMENT <string>variable_name
  AT NODE|NODAL|EDGE|FACE|ELEMENT <integer>entity_id
  AS <string>heartbeat_variable_name
```

This form of the command lets you select any nodal, edge, face, or element variable for a specific mesh entity for output in the heartbeat file. For example, this command line will let you pick the displacement at a specific node and output the displacement to the heartbeat file using an alias that you have chosen.

For this form of the command, the mesh entity type is set to `NODE` (or `NODAL`), `EDGE`, `FACE`, or `ELEMENT` depending on the variable (set by `variable_name`) to be output. If the mesh entity type is set to `NODE` (or `NODAL`), `EDGE`, or `FACE`, the string `variable_name` can be either a variable listed in Section 8.9 or a user-defined variable (see Section 8.2.2 and Section 10.2.4). If the mesh entity type is set to `ELEMENT`, the string `variable_name` can be a variable listed in Section 8.9 or a user-defined variable (see Section 8.2.2 and Section 10.2.4).

Selection of a specific mesh entity follows the `AT` keyword. You select a mesh entity type (`NODE` [or `NODAL`], `EDGE`, `FACE`, or `ELEMENT`) followed by the specific integer identifier, `entity_id`, for the mesh entity. You must specify a name, `heartbeat_variable_name`, for the selected entity following the `AS` keyword. For example, suppose you want to output the accelerations at node 88. The command line to obtain the accelerations at node 88 for the heartbeat file would be:

```
NODE ACCELERATION AT NODE 88 AS accel_88
```

where `accel_88` is the name that will be used for this heartbeat variable in the heartbeat file.

Note that either the keyword `NODE` or `NODAL` can be used for nodal quantities.

As an example, the command line to obtain the von Mises stress for element 1024 for the heartbeat file would be:

```
ELEMENT VON_MISES AT ELEMENT 1024 AS vm_1024
```

where `vm_1024` is the name that will be used for this heartbeat variable in the heartbeat file.

8.4.1.3 Nearest Point Output Variables

```
NODE|NODAL|EDGE|FACE|ELEMENT <string>variable_name
  NEAREST LOCATION <real>global_x,
    real<global_y>, real<global_z>
  AS <string>heartbeat_variable_name
```

This form of the command lets you select any nodal, edge, face, or element variable for output in the heartbeat file using a nearest point criterion. The command line described in this subsection

is an alternative to the command line described in the preceding section, Section 8.4.1.2, for obtaining heartbeat output. The command line in this section or the command line in Section 8.4.1.2 produces heartbeat files with variable information. The difference in these two command lines (Section 8.4.1.3 and Section 8.4.1.2) is simply in how the variable information is selected.

For the above form of the command, the mesh entity type is set to `NODE` (or `NODAL`), `EDGE`, `FACE`, or `ELEMENT` depending on the variable (set by `variable_name`) to be output. If the mesh entity type is set to `NODE` (or `NODAL`), `EDGE`, or `FACE`, the string `variable_name` can be either a variable listed in Section 8.9 or a user-defined variable (see Section 8.2.2 and Section 10.2.4). If the mesh entity type is set to `ELEMENT`, the string `variable_name` can be a variable listed in Section 8.9 or a user-defined variable (see Section 8.2.2 and Section 10.2.4).

The specific mesh entity used for output is determined by global coordinates specified by the `NEAREST LOCATION` keyword and its associated input parameters—`global_x`, `global_y`, `global_z`. The specific mesh entity chosen for output is as follows:

- If the mesh entity has been set to `NODE` (or `NODAL`), the node in the mesh selected for output is the node whose initial position is nearest the input global X, Y, and Z coordinates specified with the parameters `global_x`, `global_y`, and `global_z`.

- If the mesh entity has been set to `EDGE`, the edge in the mesh selected for output is the edge with a center point (the average location of the two end points of the edge) whose initial position is nearest the input global X, Y, and Z coordinates specified with the parameters `global_x`, `global_y`, and `global_z`.

- If the mesh entity has been set to `FACE`, the face in the mesh selected for output is the face with a centroid whose initial position is nearest the input global X, Y, and Z coordinates specified with the parameters `global_x`, `global_y`, and `global_z`.

- If the mesh entity has been set to `ELEMENT`, the element in the mesh selected for output is the element with a centroid whose initial position is nearest the input global X, Y, and Z coordinates specified with the parameters `global_x`, `global_y`, and `global_z`.

Note that, in all the above cases, the original model coordinates are used when selecting the nearest entity, not the current coordinates.

You must specify a name, `heartbeat_variable_name`, for the selected entity following the `AS` keyword. As an example, suppose you want to output the accelerations at a node closest to the point with global coordinates (1012.0, 54.86, 103.3141). The command line to obtain the accelerations at the node closest to this location for the heartbeat file would be:

```
NODE ACCELERATION
     NEAREST LOCATION 1012.0, 54.86, 103.3141 AS accel_near
```

where `accel_near` is the name that will be used for this heartbeat variable in the heartbeat file.

Note that either the keyword `NODE` or `NODAL` can be used for nodal quantities.

8.4.2 Outputting Heartbeat Data on a Node Set

It is commonly desired to output heartbeat data on a single-node node set. If a mesh file is slightly modified, the node and element numbers will completely change. The node associated with a node set, however, remains the same, i.e., the node in the node set retains the same initial geometric location with the same connectivity to other elements even when its node number changes. Therefore, we might want to specify the heartbeat output for a node set with a single node rather than with the global identifier for a node. This can easily be accomplished, as follows:

```
 begin user output
   node set = nodelist_1
   compute global disp_ns_1 as average of nodal displacement
 end

begin heartbeat output
  global disp_ns_1
end
```

If `nodelist_1` contains only a single node, the heartbeat output variable `disp_ns_1` will contain the displacement for the single node in the node set. If `nodelist_1` contains multiple nodes, the average displacement of the nodes will be output.

8.4.3 Set Begin Time for Heartbeat Output

```
START TIME = <real>output_start_time
```

Using the `START TIME` command line, you can write heartbeat variables to the heartbeat file beginning at time `output_start_time`. No heartbeat variables will be written before this time. If other commands set times for heartbeat output (`AT TIME`, `ADDITIONAL TIMES`) that are less than `output_start_time`, those times will be ignored, and heartbeat output will not be written at those times.

8.4.4 Adjust Interval for Time Steps

```
TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
```

This command line is used to specify that the output will be at exactly the times specified. To hit the output times exactly in an explicit, transient dynamics code, it is necessary to adjust the time step as the time approaches an output time. The integer value `steps` in the `TIMESTEP ADJUSTMENT INTERVAL` command line specifies the number of time steps to look ahead in order to adjust the time step.

If this command line does not appear, heartbeat variables are output at times closest to the specified output times.

8.4.5 Output Interval Specified by Time Increment

```
AT TIME <real>time_begin INCREMENT = <real>time_increment_dt
```

At the time specified by `time_begin`, heartbeat variables will be output every time increment given by the real value `time_increment_dt`.

8.4.6 Additional Times for Output

```
ADDITIONAL TIMES = <real>output_time1 <real>output_time2 ...
```

In addition to any times specified by the command line in Section 8.4.5, you can use the `ADDITIONAL TIMES` command line to specify an arbitrary number of additional output times.

8.4.7 Output Interval Specified by Step Increment

```
AT STEP <integer>step_begin INCREMENT =
  <integer>step_increment
```

At the step specified by `step_begin`, heartbeat variables will be output every step increment given by the integer value `step_increment`.

8.4.8 Additional Steps for Output

```
ADDITIONAL STEPS = <integer>output_step1
  <integer>output_step2 ...
```

In addition to any steps specified by the command line in Section 8.3.7, you can use the `ADDITIONAL STEPS` command line to specify an arbitrary number of g

8.4.9 Set End Time for Heartbeat Output

```
TERMINATION TIME = <real>termination_time_value
```

Heartbeat output will not be written to the heartbeat file after time `termination_time_value`. If other commands set times for heartbeat output (`AT TIME`, `ADDITIONAL TIMES`) that are greater than `termination_time_value`, those times will be ignored, and heartbeat output will not be written at those times.

8.4.10 Synchronize Output

```
SYNCHRONIZE OUTPUT
```

In an analysis with multiple regions, it is sometimes desirable to synchronize the output of heartbeat data between the regions. This can be done by adding the `SYNCHRONIZE OUTPUT` command line to the heartbeat output block. If a heartbeat block has this set, then it will write output whenever a previous region writes output. The ordering of regions is based on the order in the input file, algorithmic considerations, or by solution control specifications.

Although the `USE OUTPUT SCHEDULER` command line can also synchronize output between regions, the `SYNCHRONIZE OUTPUT` will synchronize the output with regions where the output frequency is not under the direct control of the Sierra IO system. Examples of this are typically coupled applications where one or more of the codes are not Sierra-based applications such as Alegra and CTH. A heartbeat block with `SYNCHRONIZE OUTPUT` specified will also synchronize its output with the output of the external code.

The `SYNCHRONIZE OUTPUT` command can be used with other output scheduling commands such as time-based or step-based output specifications.

8.4.11 Use Output Scheduler

```
USE OUTPUT SCHEDULER <string>scheduler_name
```

In an analysis with multiple regions, it can be difficult to synchronize output such as heartbeat files. To help synchronize output for analyses with multiple regions, you can define an `OUTPUT SCHEDULER` command block at the SIERRA scope. The scheduler can then be referenced in the `HEARTBEAT OUTPUT` command block via the `USE OUTPUT SCHEDULER` command line. The string `scheduler_name` must match a name used in an `OUTPUT SCHEDULER` command block. See Section 8.6 for a description of using this command block and the `USE OUTPUT SCHEDULER` command line.

8.4.12 Write Heartbeat On Signal

```
OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|SIGHUP|SIGINT|
  SIGPIPE|SIGQUIT|SIGTERM|SIGUSR1|SIGUSR2|SIGABRT|
  SIGKILL|SIGILL|SIGSEGV
```

The `OUTPUT ON SIGNAL` command line is used to initiate the writing of a heartbeat file when the system encounters the specified signal. The signal can either occur as the result of a system error, or the user can explicitly send the specified signal to the application (See the system documentation man pages for “signal” or “kill” for more information). Only one signal type in the list of signal types should be entered for this command line. Generally, these signals cause the code to terminate before the code can add any current heartbeat output (heartbeat output past the last heartbeat output

time step) to the heartbeat file. If the code encounters the specified type of error during execution, a heartbeat file will be written before execution is terminated.

This command line can also be used to force the writing of a heartbeat file at some point during execution of the code. Suppose the command line

```
OUTPUT ON SIGNAL = SIGUSR2
```

is included in the input file. While the code is running, a user can execute (from the keyboard) the system command line

`kill -s SIGUSR2` *pid*

to force the writing of a results file. In the above system command line, *pid* is the process identifier, which is an integer.

Note that the `OUTPUT ON SIGNAL` command line is primarily a debugging tool for code developers.

8.4.13 Heartbeat Output Formatting Commands

There are several command lines for the heartbeat section that modify the formatting of the heartbeat text output. The default output for the heartbeat data consists of a line beginning with a timestamp showing the current wall-clock time followed by multiple columns of data, for example:

```
Begin HeartBeat Region_1_Heartbeat
  Stream Name = output
  At Step 0, Increment = 10

  precision is 5

  global step
  global timestep as dt
  global time
  global total_energy as te
End
```

```
+[12:18:51] step=240, dt=3.13933e-04, time=7.56578e-02, te=4.02795e-06
+[12:18:51] step=250, dt=3.13933e-04, time=7.87971e-02, te=1.32125e-06
+[12:18:51] step=260, dt=3.13933e-04, time=8.19365e-02, te=6.88142e-07
+[12:18:51] step=270, dt=3.13933e-04, time=8.50758e-02, te=3.93574e-06
+[12:18:52] step=280, dt=3.13933e-04, time=8.82151e-02, te=7.46609e-06
+[12:18:52] step=290, dt=3.13933e-04, time=9.13545e-02, te=1.03856e-05
+[12:18:52] step=300, dt=3.13933e-04, time=9.44938e-02, te=1.36822e-05
+[12:18:52] step=310, dt=3.13933e-04, time=9.76331e-02, te=1.64630e-05
```

The above example begins each line with a timestamp followed by five labeled data columns. The precision of the real data is 5. There is no legend in the above example. This format can be modified with the following commands.

8.4.13.1 CTH SpyHis output format

```
FORMAT = SPYHIS|DEFAULT
```

If the `FORMAT=SPYHIS` is specified, then the heartbeat output will be formatted such that it can be processed with the CTH spyhis application which is a post-processor for time-history data.

8.4.13.2 Specify floating point precision

```
PRECISION = <integer>precision
```

By default, the real data is written with a precision of 5 which gives 5 digits following the decimal point. This can be altered with the `PRECISION` command. If the command line `PRECISION = 2` is specified, then the above data would look like:

```
Begin HeartBeat Region_1_Heartbeat
  ...
  precision = 2
  ...
End
```

```
+[12:18:51] step=240, dt=3.14e-04, time=7.57e-02, te=4.03e-06
+[12:18:51] step=250, dt=3.14e-04, time=7.88e-02, te=1.32e-06
+[12:18:51] step=260, dt=3.14e-04, time=8.19e-02, te=6.88e-07
```

Note that the precision applies to all real data; it is not possible to specify a different precision for each variable.

8.4.13.3 Specify Labeling of Heartbeat Data

```
LABELS = <string>OFF|ON
```

The above example shows the default output which consists of a label and the data separated by "=". The existence of the labels is controlled with the `LABELS` command. If `LABELS = OFF` is specified, then the above data would look like:

```
Begin HeartBeat Region_1_Heartbeat
  ...
  labels = off
  precision = 2
  ...
End
```

```
+[12:17:37] 240, 3.14e-04, 7.57e-02, 4.03e-06
+[12:17:37] 250, 3.14e-04, 7.88e-02, 1.32e-06
+[12:17:38] 260, 3.14e-04, 8.19e-02, 6.88e-07
```

8.4.13.4 Specify Existence of Legend for Heartbeat Data

```
LEGEND = <string>OFF|ON
```

Outputting the data without labels can make it easier to work with the data in a spreadsheet program or other data manipulation program, but with no labels, it is difficult to determine what the data really represents. The `LEGEND` output will print a line at the beginning of the heartbeat output identifying the data in each column. For example:

```
     Begin HeartBeat Region_1_Heartbeat
       ...
       legend = on
       labels = off
       precision = 2
       ...
     End

+[12:17:37] Legend: step, dt, time, te
+[12:17:37] 240, 3.14e-04, 7.57e-02, 4.03e-06
+[12:17:37] 250, 3.14e-04, 7.88e-02, 1.32e-06
+[12:17:38] 260, 3.14e-04, 8.19e-02, 6.88e-07
```

8.4.13.5 Specify format of timestamp

```
TIMESTAMP FORMAT <string>"timestamp_format"
```

Each line of the heartbeat output is preceded by a timestamp which shows the wall-clock time at the time that the line was output. This can be useful to verify that the code is still running and producing output and to determine how fast the code is running. The default timestamp is in the format "[12:34:56]" which is specified by the format [%H:%M:%S]. If a different format is desired, it can be specified with the `TIMESTAMP FORMAT` command line. The format must be surrounded by double or single quotes and the format is defined to be the string between the first single or double quote and the last matching quote type. If you want to modify the format, see the documentation for the UNIX `strftime` command for details on how to specify the format. The example below shows a timestamp format delimited by "`{`" and "`}`". The timestamp consists of a ISO-8601 date format followed by the current time.

```
...
     timestamp format "{%F %H:%M:%S}"
...
+{2008-03-17 09:26:17} 2212, 1.34244e-06, 2.96948e-03, 2.96948e-03
+{2008-03-17 09:26:17} 2213, 1.34244e-06, 2.97082e-03, 2.97082e-03
+{2008-03-17 09:26:17} 2214, 1.34244e-06, 2.97216e-03, 2.97216e-03
+{2008-03-17 09:26:17} 2215, 1.34244e-06, 2.97350e-03, 2.97350e-03
+{2008-03-17 09:26:17} 2216, 1.34244e-06, 2.97485e-03, 2.97485e-03
```

8.4.14 Monitor Output Events

```
MONITOR = <string>RESULTS|RESTART|HISTORY
```

It is sometimes a benefit to know when the code has written a new set of data to one of the other output files (restart output, history output, or results output). The heartbeat output will report this data if the `MONITOR` command line is specified. Each time output is performed to any of the monitored output types, a line will be written to the heartbeat file specifying the timestamp, the simulation time and step, and the label name of the output type. For example:

```
begin results output my_results
  at step 0, increment = 10
...
end results output results

begin heartbeat data hb
  stream name = stdout
  monitor = results
  labels = off
  legend = on
  timestamp format "%F %H:%M:%S "
  at step 0, increment = 2
  global step
  global timestep as dt
  global time
  element spring_engineering_strain at \#
      element 1 as sp1
 end
```

Will give the following output:

```
....
+2008-03-17 10:03:22  718, 1.34244e-06, 9.63871e-04, 9.63871e-04
-2008-03-17 10:03:22  Results data written at time = 0.00096656,
step = 720. my_results
+2008-03-17 10:03:22  720, 1.34244e-06, 9.66556e-04, 9.66556e-04
+2008-03-17 10:03:22  722, 1.34244e-06, 9.69241e-04, 9.69241e-04
+2008-03-17 10:03:22  724, 1.34244e-06, 9.71926e-04, 9.71926e-04
+2008-03-17 10:03:22  726, 1.34244e-06, 9.74611e-04, 9.74611e-04
+2008-03-17 10:03:22  728, 1.34244e-06, 9.77296e-04, 9.77296e-04
-2008-03-17 10:03:22  Results data written at time = 0.00097998,
step = 730. my_results
+2008-03-17 10:03:22  730, 1.34244e-06, 9.79981e-04, 9.79981e-04
....
```

8.5 Restart Data

```
BEGIN RESTART DATA <string>restart_name
  DATABASE NAME = <string>restart_file
  INPUT DATABASE NAME = <string>restart_input_file
  OUTPUT DATABASE NAME = <string>restart_output_file
  DATABASE TYPE = <string>database_type(exodusII)
  OVERWRITE = <string>OFF|ON|TRUE|FALSE|YES|NO
    (ON|TRUE|YES)
  START TIME = <real>restart_start_time
  TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
  AT TIME <real>time_begin INCREMENT =
    <real>time_increment_dt
  ADDITIONAL TIMES = <real>output_time1
    <real>output_time2 ...
  AT STEP <integer>step_begin INCREMENT =
    <integer>step_increment
  ADDITIONAL STEPS = <integer>output_step1
    <integer>output_step2 ...
  TERMINATION TIME = <real>termination_time_value
  OVERLAY COUNT = <integer>overlay_count
  CYCLE COUNT = <integer>cycle_count
  SYNCHRONIZE_OUTPUT
  USE OUTPUT SCHEDULER <string>scheduler_name
  OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|SIGHUP|SIGINT|
    SIGPIPE|SIGQUIT|SIGTERM|SIGUSR1|SIGUSR2|SIGABRT|
    SIGKILL|SIGILL|SIGSEGV
  OPTIONAL
END [RESTART DATA <string>restart_name]
```

You can specify restart files, either to be written to or read from, and the frequency at which restarts are written by using a `RESTART DATA` command block. The command block appears inside the region scope. To initiate a restart, the `RESTART TIME` command line (see Section 2.1.3.1) or the `RESTART` command line (see Section 2.1.3.2) must also be used. These command lines appear in the SIERRA scope.

NOTE: In addition to the times at which you request restart information to be written, restart information is automatically written when an element inverts.

The `RESTART DATA` command block begins with the input line:

```
BEGIN RESTART DATA <string>restart_name
```

and is terminated with:

```
END [RESTART DATA <string>restart_name]
```

where `restart_name` is a user-selected name for the `RESTART DATA` command block.

Nested within the `RESTART DATA` command block are a set of command lines, as shown in the

block summary given above.

We begin the discussion of the RESTART DATA command block with various options regarding the use of restart in general. In Section 8.5.1, you will learn how to use the DATABASE NAME, INPUT DATABASE NAME, OUTPUT DATABASE NAME, DATABASE TYPE, and OPTIONAL command lines. Usage of the first three of these command lines is tied to the two restart-related command lines RESTART and RESTART TIME, which are found in the SIERRA scope.

Section 8.5.2 discusses use of the OVERWRITE command line, which will prevent or allow the overwriting of existing restart files. (Note that this command line also appears in the command blocks for results output and history output.)

The other command lines that appear in the RESTART DATA command block determine the frequency at which restarts are written. Descriptions of these command lines follow in Section 8.5.3 through Section 8.5.14. Note that the command lines for controlling the frequency of restart output are the same as those for controlling the frequency of results output and history output. These frequency-related command lines are repeated here for convenience.

8.5.1 Restart Options

```
DATABASE NAME = <string>restart_file
INPUT DATABASE NAME = <string>restart_input_file
OUTPUT DATABASE NAME = <string>restart_output_file
DATABASE TYPE = <string>database_type(exodusII)
OPTIONAL
```

You can read from and create restart files in an automated fashion, the preferred method, or you can carefully control how you read from and create restart files. In our discussion of the overall options for the use of restart, we begin with the first three command lines listed above (DATABASE NAME, INPUT DATABASE NAME, and OUTPUT DATABASE NAME). All three of these command lines specify a parameter that is a file name or a directory path and file name. If the parameter begins with the "/" character, it is an absolute path; otherwise, the path to the current directory will be prepended to the parameter on the command line. Suppose, for example, that we want to work with a restart file named component.rst in the current directory. If we are using the DATABASE NAME command line, then this command line would appear as:

```
DATABASE NAME = component.rst
```

To read or create files in some other directory, the command line must include the path to that directory. The directory must exist, it will not be created.

The DATABASE NAME command line will let you read restart information and write restart information to the same file. Section 8.5.1.1 through Section 8.5.1.4 show how this command line is used in particular instances.

You can specify a restart file to read from by using the command line:

```
INPUT DATABASE NAME = <string>restart_input_file
```

You can specify a restart file to write to by using the command line:

```
OUTPUT DATABASE NAME = <string>restart_output_file
```

Note that you must use either a `DATABASE NAME` command line or the `INPUT DATABASE NAME` command line/`OUTPUT DATABASE NAME` command line pair, but not both, in a `RESTART DATA` command block.

Two metacharacters can appear in the name of the restart file. If the `%P` character is found in the name, it will be replaced with the number processors being used for the run. For example, if you are running on 1024 processors and use the name `restart-%P/job.rs`, then the name would be expanded to `restart-1024/job.rs` and the actual restart files would be `restart-1024/job.rs.1024.0000` to `restart-1024/job.rs.1024.1023`. The other recognized metacharacter is `%B` which is replaced with the base name of the input file containing the input commands. For example, if the commands are in the file `my_analysis_run.i` and the restart database name is specified as `%B.rs`, then the restart data would be written to or read from the file `my_analysis_run.rs`.

If the restart file does not use the Exodus II format [1], you must specify the format for the results file using the `DATABASE TYPE` command line:

```
DATABASE TYPE = <string>database_type(exodusII)
```

Currently, the Exodus II database and the XDMF database [2] are supported in Presto and Adagio. Exodus II is more commonly used than XDMF. Other options may be added in the future.

In certain coupled physics analyses in which there are multiple regions, only a subset of the regions may have a restart database associated with them. The `OPTIONAL` command (Section 8.5.1) is used to tell the application that it is acceptable to restart the analysis even though a region does not have an associated restart database. Note that this is only allowed in analyses containing multiple regions; if there is only a single region, it must have a restart database in order to restart.

8.5.1.1 Automatic Read and Write of Restart Files

You can use the restart option in an automated fashion by using a combination of the `RESTART` command line in the SIERRA scope and the `DATABASE NAME` command line in the `RESTART DATA` command block. This automated use of restart can best be explained by an example. We will use a two-processor example and assume all files will be in our current directory.

The option of automated restart will not only manage the restart files to prevent overwriting, it will also manage the results files and history files to prevent overwriting. In the example we give, we will assume our run includes a `RESULTS OUTPUT` command block with the command line

```
DATABASE NAME = rslt.e
```

to generate results files with the root file name `rslt.e`. We will also assume a run includes a `HISTORY OUTPUT` command block with the command line

```
DATABASE NAME = hist.h
```

to generate history files with the root file name `hist.h`.

For the first run in our restart sequence, we will have the command line

```
RESTART = AUTOMATIC
```

in the SIERRA scope of our input file. In a `TIME STEPPING` command block, which is embedded in a `TIME CONTROL` command block (Section 3.1.1) in the procedure scope of our input file, we will have the command line:

```
START TIME = 0.0
```

In the `TIME CONTROL` command block we will have the command line

```
TERMINATION TIME = 2.5E-3
```

to set the limits for the begin and end times of the first restart run. These time-related command lines should not be confused with the `START TIME` and `TERMINATION TIME` command lines that appear in the `RESTART DATA` command block.

Finally, for the first run in our restart sequence, the `RESTART DATA` command block in our input file will be as follows:

```
BEGIN RESTART DATA RESTART_DATA
  DATABASE NAME = g.rsout
  AT TIME 0.0 INCREMENT = 0.25E-3
END RESTART DATA RESTART_DATA
```

In this block, the `DATABASE NAME` command line specifies a root file name for the restart file. The `AT TIME` command line gives the time when we will start to write the restart information and the interval at which the restart information will be written (see Section 8.5.5).

For our first run, the automatic restart option will generate the following restart files:

```
# restart files
g.rsout.2.0
g.rsout.2.1
# results files
rslt.e.2.0
rslt.e.2.1
# history files
hist.h.2.0
hist.h.2.1
```

For the above files, there are extensions on the file names that indicate we have a two-processor run. The 2.0 and 2.1 extensions associate the restart files with the corresponding individual mesh files on each processor. (If our mesh file is `mesh.g`, then our mesh files on the individual processors will be `mesh.g.2.0` and `mesh.g.2.1`.) All restart information in the above files appears at time intervals of 0.25×10^{-3}, and the last restart information is written at time 2.5×10^{-3}. We have also listed the results and history files that will be generated for this run due to the file definitions in the command blocks for the results and history files.

For the second run in our sequence of restart runs, we want to start at the previous termination time, 2.5×10^{-3}, and terminate at time 5.0×10^{-3}. We leave everything in our input file (including the

START TIME = 0.0 command line in the TIME STEPPING command block, the RESTART command line, and the RESTART DATA command block) the same except for the TERMINATION TIME command line (in the TIME CONTROL command block). The TERMINATION TIME command line will now become:

```
TERMINATION TIME = 5.0E-3
```

It is important to note here that the actual start time for the second run in our analysis is now set by the last time (2.5×10^{-3}) that restart information was written. The command line START TIME = 0.0 in the TIME STEPPING command block is now superseded as the actual starting time for the second run by the restart commands. Any START TIME command line in a TIME STEPPING command block is still valid in terms of defining time stepping blocks (these blocks being used to set activation periods), but the restart process sets the actual start time for our analysis. This pattern of control for setting the actual start time holds for any run in our sequence of restart runs.

For the second run in our sequence of restart runs, the restart files will be from time 2.5×10^{-3} to time 5.0×10^{-3}. The restart files in our current directory after the second run will be as follows:

```
# restart files
g.rsout.2.0
g.rsout.2.1
g.rsout-s0002.2.0
g.rsout-s0002.2.1
# results files
rslt.e.2.0
rslt.e.2.1
rslt.e-s0002.2.0
rslt.e-s0002.2.1
# history files
hist.h.2.0
hist.h.2.1
hist.h-s0002.2.0
hist.h-s0002.2.1
```

Notice that we have generated new restart files with a -s0002 extension in addition to the extension associated with the individual processors. All restart information in the above files with the -s0002 extension appears at time intervals of 0.25×10^{-3}, the restart information is written between time 2.5×10^{-3} and time 5.0×10^{-3}, and the final restart information is written at time 5.0×10^{-3}. The restart files for the first run in our sequence of restart runs, g.rsout.2.0 and g.rsout.2.1, have been preserved. New results and history files have been created using the same extension, -s0002, as that used for the restart files. The original results and history files have been preserved.

Now, we want to do a third run in our sequence of restart runs. For the third run in our sequence of restart runs, we want to start at the previous termination time, 5.0×10^{-3}, and terminate at time 8.5×10^{-3}. We leave everything in our input file (including the START TIME command line, the RESTART command line, and the RESTART DATA command block) the same except for

the TERMINATION TIME command line. The TERMINATION TIME command line (within the TIME CONTROL command block) will now become:

```
TERMINATION TIME = 8.5E-3
```

For the third run in our sequence of restart runs, the restart files will be from time 5.0×10^{-3} to time 8.5×10^{-3}. The restart files in our current directory after the third run will be as follows:

```
# restart files
g.rsout.2.0
g.rsout.2.1
g.rsout-s0002.2.0
g.rsout-s0002.2.1
g.rsout-s0003.2.0
g.rsout-s0003.2.1
# results files
rslt.e.2.0
rslt.e.2.1
rslt.e-s0002.2.0
rslt.e-s0002.2.1
rslt.e-s0003.2.0
rslt.e-s0003.2.1
# history files
hist.h.2.0
hist.h.2.1
hist.h-s0002.2.0
hist.h-s0002.2.1
hist.h-s0003.2.0
hist.h-s0003.2.1
```

Notice that we have generated new restart files with a -s0003 extension in addition to the extension associated with the individual processors. All restart information in the above files with the -s0003 extension appears at time intervals of 0.25×10^{-3}, the restart information is written between time 5.0×10^{-3} and time 8.5×10^{-3}, and the final restart information is written at time 8.5×10^{-3}. The restart files for the first and second runs in our sequence of restart runs have been preserved. New results and history files have been created using the same extension, -s0003, as that used for the restart files. The original results and history files have been preserved.

The process just described can be continued as long as necessary. We will continue the process of generating new restart files with extensions that indicate their place in the sequence of runs.

8.5.1.2 User-Controlled Read and Write of Restart Files

You can use the restart option and select specific restart times and specific restart files to read from and write to by using a combination of the RESTART TIME command line in the SIERRA scope and the INPUT DATABASE NAME and OUTPUT DATABASE NAME command line in the RESTART DATA command block. This "controlled" use of restart can best be explained by an example.

We will use a two-processor example and assume all files will be in our current directory. In this example, we will manage the creation of new restart files so as not to overwrite existing restart files. Unlike the automated option for restart, this controlled use of restart requires that the user manage restart file names so as to prevent overwriting previously generated restart files. The same is true for the results and history files. The user will have to manage the creation of new results and history files so as not to overwrite existing results and history files. Creating new results and history files for each run in the sequence of restart runs requires changing the `DATABASE NAME` command line in the `RESULTS OUTPUT` and `HISTORY OUTPUT` command blocks. We will not show examples for use of the `DATABASE NAME` command line in the `RESULTS OUTPUT` and `HISTORY OUTPUT` command blocks here, as the actual use of the `DATABASE NAME` command line in the results and history command blocks would closely parallel the pattern we see for management of the restart file names.

For the first run in our restart sequence, we will have only a `RESTART DATA` command block in the region; there will be no restart-related command line in the SIERRA scope of our input file. We will, however, have a

```
START TIME = 0.0
```

command line in a `TIME STEPPING` command block (within the `TIME CONTROL` command block) and a

```
TERMINATION TIME = 2.5E-3
```

command line within the `TIME CONTROL` command block to set the limits for the begin and end times. The `RESTART DATA` command block in our input file will be as follows:

```
BEGIN RESTART DATA RESTART_DATA
  OUTPUT DATABASE NAME = RS1.rsout
  AT TIME 0.0 INCREMENT = 0.5E-3
END RESTART DATA RESTART_DATA
```

For our first run, the restart option will generate the following restart files:

```
RS1.rsout.2.0
RS1.rsout.2.1
```

For the above files, the extensions on the file names indicate that we have a two-processor run. The 2.0 and 2.1 extensions associate the restart files with the corresponding individual mesh files on each processor. If our mesh file is `mesh.g`, then our mesh files on the individual processors will be `mesh.g.2.0` and `mesh.g.2.1`. All restart information in the above files appears at time intervals of 0.5×10^{-3}, and the last restart information is written at time 2.5×10^{-3}.

For the second run in our sequence of restart runs, we want to start at the previous termination time, 2.5×10^{-3}, and terminate at time 5.0×10^{-3}. To do this, we must add a

```
RESTART TIME = 2.5E-3
```

command line to the SIERRA scope and set the termination time to 5.0×10^{-3} by using the command line

```
TERMINATION TIME = 5.0E-3 \rm
```

within the `TIME CONTROL` command block.

It is important to note here that the actual start time for the second run in our analysis is now set by the restart time set on the `RESTART TIME` command line, 2.5×10^{-3}. The command line `START TIME = 0.0` in the `TIME STEPPING` command block is now superseded as the actual starting time for the second run by the restart commands. Any `START TIME` command line in a `TIME STEPPING` command block is still valid in terms of defining time stepping blocks (these blocks being used to set activation periods), but the restart process sets the actual start time for our analysis. This pattern of control for setting the actual start time holds for any run in our sequence of restart runs.

We also must change the `RESTART DATA` command block to the following:

```
BEGIN RESTART DATA RESTART_DATA
  INPUT DATABASE NAME = RS1.rsout
  OUTPUT DATABASE NAME = RS2.rsout
  AT TIME 0.0 INCREMENT = 0.5E-3
END RESTART DATA RESTART_DATA
```

For this second run, we will read from the following files:

```
RS1.rsout.2.0
RS1.rsout.2.1
```

And we will write to the following files:

```
RS2.rsout.2.0
RS2.rsout.2.1
```

All restart information in the above output files, `RS2.rsout.2.0` and `RS2.rsout.2.1`, appears at time intervals of 0.5×10^{-3}, restart information is written from time 2.5×10^{-3} to time 5.0×10^{-3}, and the last restart information is written at time 5.0×10^{-3}. Notice that we have preserved the restart files from the first run from our restart sequence of runs because we have specifically given the input and output databases distinct names—`RS2.rsout` for the input file name and `RS1.rsout` for the output file name.

Now, we want to do a third run in our sequence of restart runs. For this third run, we want to start at time 4.5×10^{-3} and terminate at time 8.5×10^{-3}. We do not want to start at the termination time for the previous restart, which is 5.0×10^{-3}; rather, we want to start at time 4.5×10^{-3}. We change the `RESTART TIME` command line to

```
RESTART TIME = 4.5E-3
```

and the `TERMINATION TIME` command line within the `TIME CONTROL` command block to:

```
TERMINATION TIME = 8.5E-3
```

And we change the `RESTART DATA` command block to the following:

```
BEGIN RESTART DATA RESTART_DATA
  INPUT DATABASE NAME = RS2.rsout
  OUTPUT DATABASE NAME = RS3.rsout
  AT TIME 0.0, INCREMENT = 0.5E-3
END RESTART DATA RESTART_DATA
```

For this third run, we will read from the following files:

```
RS2.rsout.2.0
RS2.rsout.2.1
```

And we will write to the following files:

```
RS3.rsout.2.0
RS3.rsout.2.1
```

All restart information in the above output files, `RS3.rsout.2.0` and `RS3.rsout.2.1`, appears at time intervals of 0.5×10^{-3}, restart information is written from time 4.5×10^{-3} to time 8.5×10^{-3}, and the last restart information is written at time 8.5×10^{-3}. Notice that we have preserved all restart files from previous runs in our restart sequence of runs because we have specifically given the input and output databases distinct names for this third run.

8.5.1.3 Overwriting Restart Files

If you use the `RESTART TIME` command line in conjunction with the `DATABASE NAME` command line, you will overwrite restart information (unless you have included an `OVERWRITE` command line set to `ON`). As indicated previously, you will probably want to have a restart file (or files in the case of parallel runs) associated with each run in a sequence of restart runs. The example in this section shows how to overwrite restart files if that is an acceptable approach for a particular analysis.

For our first run, we will set a termination time of 1.0×10^{-3} with the command line

```
TERMINATION TIME = 1.0E-3
```

and set the `RESTART DATA` command block as follows:

```
BEGIN RESTART DATA
  DATABASE NAME = RS.out
  AT TIME 0.0 INTERVAL = 0.25E-3
END RESTART DATA
```

Our first run will generate the following restart files:

```
RS.out.2.0
RS.out.2.1
```

All restart information in the above output files, `RS.out.2.0` and `RS.out.2.1`, appears at time intervals of 0.25×10^{-3}, restart information is written from time 0.0 to time 1.0×10^{-3}, and the last restart information is written at time 1.0×10^{-3}.

Suppose for our second run we set the termination time to 2.0×10^{-3} with the command line

```
TERMINATION TIME = 2.0E-3
```

and add the command line

```
RESTART TIME = 1.0E-3
```

to the SIERRA scope. We leave the `RESTART DATA` command block unchanged.

For our second run, restart information is read from the files `RS.out.2.0` and `RS.out.2.1`. These files are then overwritten with new restart information beginning at time 1.0×10^{-3}. The files `RS.out.2.0` and `RS.out.2.1` will have restart information beginning at time 1.0×10^{-3} in intervals of 0.25×10^{-3}. The restart information will terminate at time 2.0×10^{-3}.

Now we want to do a third run with a termination time of 3.0×10^{-3}. We change the termination time by using the command line:

```
TERMINATION TIME = 3.0E-3
```

And we change the `RESTART TIME` command line so that it is now:

```
RESTART TIME = 3.0E-3
```

For our third run, restart information is read from the files `RS.out.2.0` and `RS.out.2.1`. These files are then overwritten with new restart information beginning at time 2.0×10^{-3}. The files `RS.out.2.0` and `RS.out.2.1` will have restart information beginning at time 2.0×10^{-3} in intervals of 0.25×10^{-3}. The restart information will terminate at time 3.0×10^{-3}.

8.5.1.4 Recovering from a Corrupted Restart

Suppose you are using the automated option for restart and a system crash occurs when the restart file is being written. The restart file contains a corrupted entry for one of the restart times. In this case, you can continue using the automated option for restart. Restart will detect the corrupted entry and then find an entry previous to the corrupted entry that can be used for restart. This previous entry should be the entry prior to the corrupted entry unless something unusual has occurred. If the first intact restart entry is not the previous entry, restart continues to back up until an intact restart entry is found.

You could do a manual recovery. The manual recovery requires the use of a `RESTART TIME` command line to select some intact restart entry. You will have to use the `INPUT DATABASE NAME` and `OUTPUT DATABASE NAME` command lines to avoid overwriting previous restart files (see Section 8.5.1.2). You will also have to change file names in the results and history command blocks to avoid overwriting previous results and history files. Once you have done the manual recovery, you could then revert to the automatic restart option.

8.5.2 Overwrite Command in Restart

```
OVERWRITE = <string>OFF|ON|TRUE|FALSE|YES|NO
  (ON|TRUE|YES)
```

The OVERWRITE command line can be used to prevent the overwriting of existing restart files. The use of the automatic read and write option for restart files as described in Section 8.5.1.1 does not require the OVERWRITE command line. The automatic read and write option adds extensions to file names and prevents the overwriting of any existing restart files. For the case of a user-controlled read and write of restart files (Section 8.5.1.2), however, the OVERWRITE command line is useful for preventing the overwriting of restart files. If the OVERWRITE command line is set to OFF, FALSE, or NO, then existing restart files will not be overwritten. Execution of the code will terminate before existing restart files are overwritten. The default option is to overwrite existing restart files. If the OVERWRITE command line is not included, or the command line is set to ON, TRUE, or YES, then existing files can be overwritten.

8.5.3 Set Begin Time for Restart Writes

```
START TIME = <real>restart_start_time
```

Using the START TIME command line, you can write restarts to the restart file beginning at time restart_start_time. No restarts will be written before this time. If other commands set times for restarts (AT TIME, ADDITIONAL TIMES) that are less than restart_start_time, those times will be ignored, and restarts will not be written at those times.

8.5.4 Adjust Interval for Time Steps

```
TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
```

This command line is used to specify that the restarts will be written at exactly the times specified. To hit the restart times exactly in an explicit transient dynamics code, it is necessary to adjust the time step as the time approaches a restart time. The integer value steps in the TIMESTEP ADJUSTMENT INTERVAL command line specifies the number of time steps to look ahead in order to adjust the time step.

If this command line does not appear, then restarts are written at times closest to the specified restart times.

8.5.5 Restart Interval Specified by Time Increment

```
AT TIME <real>time_begin INCREMENT = <real>time_increment_dt
```

At the time specified by time_begin, restarts will be written every time increment given by the real value time_increment_dt.

8.5.6 Additional Times for Restart

```
ADDITIONAL TIMES = <real>output_time1 <real>output_time2 ...
```

In addition to any restart times specified by the command line in Section 8.5.5, you can use the `ADDITIONAL TIMES` command line to specify an arbitrary number of additional restart times.

8.5.7 Restart Interval Specified by Step Increment

```
AT STEP <integer>step_begin INCREMENT =
  <integer>step_increment
```

At the step specified by `step_begin`, restarts will be written every step increment given by the integer value `step_increment`.

8.5.8 Additional Steps for Restart

```
ADDITIONAL STEPS = <integer>output_step1
  <integer>output_step2 ...
```

In addition to any steps specified by the command line in Section 8.5.7, you can use the `ADDITIONAL STEPS` command line to specify an arbitrary number of additional restart steps.

8.5.9 Set End Time for Restart Writes

```
TERMINATION TIME = <real>termination_time_value
```

Restarts will not be written to the restart file after time `termination_time_value`. If other commands set times for restarts (`AT TIME`, `ADDITIONAL TIMES`) that are greater than `termination_time_value`, those times will be ignored, and restarts will not be written at those times.

8.5.10 Overlay Count

```
OVERLAY COUNT = <integer>overlay_count
```

The `OVERLAY COUNT` command line specifies the number of restart output times that will be overlaid on top of the current step before advancing to the next step. For example, suppose that we set the `overlay_count` parameter to 2, and we request that restart information be written every 0.1 second. At time 0.1 second, restart step 1 will be written to the output restart database. At time 0.2 second, restart information will be written over the step 1 information, which originally contained

restart information at 0.1 second. At time 0.3 second, restart information will be written over the step 1 information, which last contained information at 0.2 second. At time 0.4 second, we will now write step 2 to the output restart database (step 1 has already been written over twice). At time 0.5 second, restart information will be written over the step 2 information, which originally contained information at 0.4 second. At time 0.6 second, restart information will be written over the step 2 information, which last contained information at 0.5 second. At time 0.7 second, restart step 3 will be written to the output restart database (step 2 has already been written over twice). This pattern continues so that we would build up a sequence of restart information at times 0.3, 0.6, 0.9, . . . second until we reach the termination time for the problem. If there was a problem during the analysis, the last step on the output restart database would be whatever had last been written to the database. If, for example, we had set our termination time to 1.0 second and a problem occurred after restart information had been written at 0.7 second but before we completed the time step at 0.8 second, then the last information on the output restart database would be at 0.7 second.

You can use the `OVERLAY COUNT` command line in conjunction with a `CYCLE COUNT` command line. For a description of the `CYCLE COUNT` command line and its use with the `OVERLAY COUNT` command line, see Section 8.5.11.

8.5.11 Cycle Count

```
CYCLE COUNT = <integer>cycle_count
```

The `CYCLE COUNT` command line specifies the number of restart steps that will be written to the output restart database before previously written steps are overwritten. For example, suppose we set the `cycle_count` parameter to 5, and we request that restart information be written every 0.1 second. The restart system will write information to the output restart database at times 0.1, 0.2, 0.3, 0.4, and 0.5 second. At time 0.6 second, the information at step 1, originally written at time 0.1 second, will be overwritten with information at time 0.6 second. At time 0.7 second, the information at step 2, originally written at time 0.2 second, will be overwritten with information at time 0.7 second. At time 0.8 second, the output restart database will contain restart information at times 0.6, 0.7, 0.8, 0.4, and 0.5 second. Time will not necessarily be monotonically increasing on a database that uses a `CYCLE COUNT` command line.

If you only want the last step available on the output restart database, set `cycle_count` equal to 1.

The `CYCLE COUNT` and `OVERLAY COUNT` command lines can be used at the same time. For this example, we will combine our example with an overlay count of 2 as given in Section 8.5.10 with our example of a cycle count of 5 as given in this section (Section 8.5.11). Information is written to the output restart database time step every 0.1 second. The output times at which information is written to the output restart database are 0.1, 0.2, 0.3, . . . second. Each of these times corresponds to an output step. Time 0.1 second corresponds to output step 1, time 0.2 second corresponds to output step 2, time 0.3 corresponds to output step 3, and so forth. An output time of $n \times 0.1$ corresponds to output step n. The overlay command will result in information at time 0.3, 0.6, 0.9, 1.2, and 1.5 seconds written as steps 1, 2, 3, 4, and 5 on the output restart database. For times greater than 1.6 seconds, the cycle command will now take effect because we have five steps written

on the output restart database. Information at times 1.6, 1.7, and 1.8 seconds will now overwrite the information at step 1, which had information at time 0.3 second. Information at times 1.9, 2.0, and 2.1 seconds will now overwrite the information at step 2, which had information at time 0.6 second. For any output step n, its position, step number n_s, in the restart output database is as follows:

$$
\begin{aligned}
&if\, n_s \neq 0 \\
&\quad n_s = int(n/(n_o + 1))\%n_c \\
&else \\
&\quad n_s = n_c \\
&end
\end{aligned}
$$

In the above equations, n_c is the cycle count, and n_o is the overlay count. The expression $int(n/(n_o + 1))$ produces an integer arithmetic result. For example, if n is 4 and n_o is 2, then we have 4 divided by 3, and the integer arithmetic result is 1 (any fractional remainder is discarded). The operator % is the modulus operator; the modulus operator gives the modulus of its first operand with respect to its second operand, i.e., it produces the remainder of dividing the first operand by the second operand. The result of 1 % 5 is 1, for example.

8.5.12 Synchronize Output

```
SYNCHRONIZE OUTPUT
```

In an analysis with multiple regions, it is sometimes desirable to synchronize the output of restart data between the regions. This can be done by adding the `SYNCHRONIZE OUTPUT` command line to the restart output block. If a restart block has this set, then it will write output whenever a previous region writes output. The ordering of regions is based on the order in the input file, algorithmic considerations, or by solution control specifications.

Although the `USE OUTPUT SCHEDULER` command line can also synchronize output between regions, the `SYNCHRONIZE OUTPUT` will synchronize the output with regions where the output frequency is not under the direct control of the Sierra IO system. Examples of this are typically coupled applications where one or more of the codes are not Sierra-based applications such as Alegra and CTH. A restart block with `SYNCHRONIZE OUTPUT` specified will also synchronize its output with the output of the external code.

The `SYNCHRONIZE OUTPUT` command can be used with other output scheduling commands such as time-based or step-based output specifications.

8.5.13 Use Output Scheduler

```
USE OUTPUT SCHEDULER <string>scheduler_name
```

In an analysis with multiple regions, it can be difficult to synchronize output such as restart files. To help synchronize output for analyses with multiple regions, you can define an `OUTPUT SCHEDULER` command block at the SIERRA scope. The scheduler can then be referenced in the `RESTART DATA` command block via the `USE OUTPUT SCHEDULER` command line. The string `scheduler_name` must match a name used in an `RESTART DATA` command block. See Section 8.6 for a description of using this command block and the `USE OUTPUT SCHEDULER` command line.

8.5.14 Write Restart If System Error Encountered

```
OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|SIGHUP|SIGINT|
  SIGPIPE|SIGQUIT|SIGTERM|SIGUSR1|SIGUSR2|SIGABRT|
  SIGKILL|SIGILL|SIGSEGV
```

The `OUTPUT ON SIGNAL` command line is used to initiate the writing of a restart file when the system encounters a type of system error. Only one error type in the list of error types should be entered for this command line. Generally, these system errors cause the code to terminate before the code can add any current restart output (restart output past the last restart output time step) to the restart file. If the code encounters the specified type of error during execution, a restart file will be written before execution is terminated.

This command line can also be used to force the writing of a restart file at some point during execution of the code. Suppose the command line

```
OUTPUT ON SIGNAL = SIGUSR2
```

is included in the input file. While the code is running, a user can execute (from the keyboard) the system command line

`kill -s SIGUSR2` *pid*

to terminate execution and force the writing of a results file. In the above system command line, *pid* is the process identifier, which is an integer.

The most useful application of the command line is to send a signal via a system command line to write a restart file. Note that the `OUTPUT ON SIGNAL` command line is primarily a debugging tool for code developers.

8.6 Output Scheduler

In an analysis with multiple regions, it can be difficult to synchronize output such as results files, history files, and restart files. To help synchronize output for analyses with multiple regions, you can define an `OUTPUT SCHEDULER` command block at the SIERRA scope. This scheduler can then be referenced in several places:

- The scheduler can be referenced in the `RESULTS OUTPUT` command block to control the output of results information.
- The scheduler can be referenced in the `HISTORY OUTPUT` command block to control the output of history information.
- The scheduler can be referenced in the `RESTART DATA` command block to control the writing of restart files.

In summary, the `OUTPUT SCHEDULER` command block is defined in the SIERRA scope. The scheduler is referenced by a `USE OUTPUT SCHEDULER` command line that can appear in a `RESULTS OUTPUT`, `HISTORY OUTPUT`, and `RESTART DATA` command block. Section 8.6.1 describes the `OUTPUT SCHEDULER` command block, and Section 8.6.2 illustrates how this block is referenced with the `USE OUTPUT SCHEDULER` command line.

8.6.1 Output Scheduler Command Block

```
BEGIN OUTPUT SCHEDULER <string>scheduler_name
  START TIME = <real>output_start_time
  TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
  AT TIME <real>time_begin INCREMENT =
    <real>time_increment_dt
  ADDITIONAL TIMES = <real>output_time1
    <real>output_time2 ...
  AT STEP <integer>step_begin INCREMENT =
    <integer>step_increment
  ADDITIONAL STEPS = <integer>output_step1
    <integer>output_step2 ...
  TERMINATION TIME = <real>termination_time_value
END [OUTPUT SCHEDULER <string>scheduler_name]
```

An output scheduler is defined with a command block in the SIERRA scope. The `OUTPUT SCHEDULER` command block begins with the input line:

```
BEGIN OUTPUT SCHEDULER <string>scheduler_name
```

and is terminated with the line:

```
END OUTPUT SCHEDULER <string>scheduler_name
```

where scheduler_name is a user-defined name for the command block. All the normal scheduling command lines are valid in an OUTPUT SCHEDULER command block.

8.6.1.1 Set Begin Time for Output Scheduler

```
START TIME = <real>output_start_time
```

Using the START TIME command line, you can set the start time for a scheduler beginning at time output_start_time. The scheduler will not take effect before this time. If other commands set times for scheduling (AT TIME, ADDITIONAL TIMES) that are less than output_start_time, those times will be ignored.

8.6.1.2 Adjust Interval for Time Steps

```
TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
```

This command line is used to specify that, when the scheduler is in effect, output will be at exactly the times specified. To hit the output times exactly in an explicit, transient dynamics code, it is necessary to adjust the time step as the time approaches an output time. The integer value steps in the TIMESTEP ADJUSTMENT INTERVAL command line specifies the number of time steps to look ahead in order to adjust the time step.

If this command line does not appear, output occurs at times closest to the specified output times.

8.6.1.3 Output Interval Specified by Time Increment

```
AT TIME <real>time_begin INCREMENT = <real>time_increment_dt
```

At the time specified by time_begin, output will be scheduled at every time increment given by the real value time_increment_dt.

8.6.1.4 Additional Times for Output

```
 ADDITIONAL TIMES = <real>output_time1 <real>output_time2 ...
```

In addition to any times specified by the command line in Section 8.6.1.3, you can use the ADDITIONAL TIMES command line to specify an arbitrary number of additional output times.

8.6.1.5 Output Interval Specified by Step Increment

```
AT STEP <integer>step_begin INCREMENT =
  <integer>step_increment
```

At the step specified by `step_begin`, output will be scheduled at every step increment given by the integer value `step_increment`.

8.6.1.6 Additional Steps for Output

```
ADDITIONAL STEPS = <integer>output_step1
  <integer>output_step2 ...
```

In addition to any steps specified by the command line in Section 8.6.1.5, you can use the `ADDITIONAL STEPS` command line to specify an arbitrary number of additional output steps.

8.6.1.7 Set End Time for Output Scheduler

```
TERMINATION TIME = <real>termination_time_value
```

Using the `TERMINATION TIME` command line, you can set the termination time for a scheduler beginning at time `termination_time_value`. The scheduler will not be in effect after this time. If other commands set times for scheduling (`AT TIME`, `ADDITIONAL TIMES`) that are greater than `termination_time_value`, those times will be ignored by the scheduler.

8.6.2 Example of Using the Output Scheduler

Once an output scheduler has been defined via the `OUTPUT SCHEDULER` command block, it can be used by inserting a `USE OUTPUT SCHEDULER` command line in any of the following command blocks: `RESULTS OUTPUT`, `HISTORY OUTPUT`, and `RESTART DATA`. The following paragraph provides an example of using output schedulers.

In the SIERRA scope, we define two output schedulers, `Timer` and `Every_Step`:

```
BEGIN OUTPUT SCHEDULER Timer
  AT TIME 0.0 INCREMENT = 10.0e-6
  TIME STEP ADJUSTMENT INTERVAL = 4
END OUTPUT SCHEDULER Timer
#
BEGIN OUTPUT SCHEDULER Every_Step
  AT STEP 0 INCREMENT = 1
END OUTPUT SCHEDULER Every_Step
```

With the `USE OUTPUT SCHEDULER` command, we reference the scheduler named `Timer` for results output:

```
BEGIN RESULTS OUTPUT Out_Region_1
  .
```

```
  USE OUTPUT SCHEDULER Timer
  .
END RESULTS OUTPUT Out_Region_1
```

With the `USE OUTPUT SCHEDULER` command, we reference the scheduler named `Every_STEP` for history output:

```
BEGIN HISTORY OUTPUT Out_Region_2
  .
  USE OUTPUT SCHEDULER Every_Step
  .
END HISTORY OUTPUT Out_Region_2
```

8.7 Variable Interpolation

```
BEGIN VARIABLE INTERPOLATION [<string>var_interp_name]
  TRANSFER TYPE = INTERPOLATE FROM NEAREST FACE|
    SUM TO NEAREST ELEMENT
  SOURCE VARIABLE = ELEMENT|GLOBAL|NODAL|
    SURFACE NORMAL NODAL <string>source_var_name
  SOURCE ELEMENT BLOCK = <string>source_block
  SOURCE SURFACE = <string>source_surface
  TARGET VARIABLE = ELEMENT|GLOBAL|NODAL
    <string>target_var_name
  TARGET SURFACE = <string>target_surface
  SEARCH TOLERANCE = <real>search_tol
  PROXIMITY SEARCH TYPE = RAY SEARCH|SPHERE SEARCH
  RAY SEARCH DIRECTION = <real>vecx <real>vecy <real>vecz
  RAY SEARCH DIRECTION = ORTHOGONAL TO LINE <real>p1x
    <real>p1y <real>p1z <real>p2x <real>p2y <real>p2z
  RAY SEARCH DIRECTION = TARGET SURFACE NORMAL

  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names

END [VARIABLE INTERPOLATION <string>var_interp_name]
```

The command block for a variable interpolation begins with `BEGIN VARIABLE INTERPOLATION [<string>var_interp_name]` and is terminated with `END [VARIABLE INTERPOLATION <string>var_interp_name]` where `var_interp_name` is an optional user-selected name for the command block.

The command `TRANSFER TYPE` can be set to either `INTERPOLATE FROM NEAREST FACE` or `SUM TO NEAREST ELEMENT`. The `TRANSFER TYPE` restricts the commands that can be used in conjunction with it.

When `TRANSFER TYPE` is set to `INTERPOLATE FROM NEAREST FACE` the available commands are restricted to:

```
BEGIN VARIABLE INTERPOLATION [<string>var_interp_name]
  TRANSFER TYPE = INTERPOLATE FROM NEAREST FACE
  SOURCE VARIABLE = NODAL|SURFACE NORMAL NODAL
    <string>source_var_name
  SOURCE SURFACE = <string>source_surface
  TARGET VARIABLE = NODAL <string>target_var_name
  TARGET SURFACE = <string>target_surface
  SEARCH TOLERANCE = <real>search_tol
  PROXIMITY SEARCH TYPE = RAY SEARCH|SPHERE SEARCH
  RAY SEARCH DIRECTION = <real>vecx <real>vecy <real>vecz
  RAY SEARCH DIRECTION = ORTHOGONAL TO LINE <real>p1x
```

```
    <real>p1y <real>p1z <real>p2x <real>p2y <real>p2z
  RAY SEARCH DIRECTION = TARGET SURFACE NORMAL
END [VARIABLE INTERPOLATION <string>var_interp_name]
```

For `TRANSFER TYPE = INTERPOLATE FROM NEAREST FACE`, a given point on the target surface finds the closest point on the source surface. At that closet point the source variable is interpolated. The interpolated value is then copied to the given point. Optionally if the `SURFACE NORMAL NODAL` component is being used and the variable being transferred is a vector then only the surface normal component of that variable will be transferred. This is useful for several applications involving transferring solid mesh quantities such as velocity to a reference mesh modeling a fluid (e.g., air).

When `TRANSFER TYPE` is set to `SUM TO NEAREST ELEMENT` the available commands are restricted to:

```
BEGIN VARIABLE INTERPOLATION [<string>var_interp_name]
  TRANSFER TYPE = SUM TO NEAREST ELEMENT
  SOURCE VARIABLE = ELEMENT <string>source_var_name
  SOURCE ELEMENT BLOCK = <string>source_block
  TARGET VARIABLE = ELEMENT <string>target_var_name
  TARGET SURFACE = <string>target_surface
  SEARCH TOLERANCE = <real>search_tol
  PROXIMITY SEARCH TYPE = RAY SEARCH|SPHERE SEARCH
  RAY SEARCH DIRECTION = <real>vecx <real>vecy <real>vecz
  RAY SEARCH DIRECTION = ORTHOGONAL TO LINE <real>p1x
    <real>p1y <real>p1z <real>p2x <real>p2y <real>p2z
END [VARIABLE INTERPOLATION <string>var_interp_name]
```

For `TRANSFER TYPE = SUM TO NEAREST ELEMENT`, a given element in the source block computes its centroid. Then the closest face to that centroid on the target surface is found. The source element value is summed to the element associated with the target face.

The command `SOURCE VARIABLE` specifies the type of variable, `ELEMENT`, `GLOBAL`, or `NODAL`, and the name of the source variable `source_var_name`.

The command `SOURCE SURFACE` specifies the name of the source side set `source_surface`.

The command `TARGET VARIABLE` specifies the type of variable, `ELEMENT`, `GLOBAL`, or `NODAL`, and the name of the target variable `target_var_name`. The target variable must exist. If necessary, a target variable can be created using the `BEGIN USER VARIABLE` command block (Section 10.2.4).

The command `TARGET SURFACE` specifies the name of the target side set `target_surface`.

The command `SEARCH TOLERANCE` specifies a search distance for use in the proximity search.

The command `PROXIMITY SEARCH TYPE` can be set to either `RAY SEARCH` or `SPHERE SEARCH`. When `PROXIMITY SEARCH TYPE = SPHERE SEARCH` the `SEARCH TOLERANCE` is used as the radius for closest point searches. When `PROXIMITY SEARCH TYPE = RAY SEARCH` the

SEARCH TOLERANCE and any RAY SEARCH DIRECTION are used together to form rays with lengths equal to the SEARCH TOLERANCE in both the positive and negative directions from an associated RAY SEARCH DIRECTION. Faces penetrated by the ray get included in the set of faces for determining the closest point.

The command RAY SEARCH DIRECTION specifies a search direction for the PROXIMITY SEARCH = RAY SEARCH DIRECTION case. A RAY SEARCH DIRECTION can be specified directly with three values, vecx, vecy, and vecz. Alternatively, RAY SEARCH DIRECTION can be calculated through options ORTHOGONAL TO LINE or TARGET SURFACE NORMAL. For ORTHOGONAL TO LINE the search direction is the vector between a given point and the closest point on the infinite line specified with the two points p1x, p1y, p1z and p2x, p2y, p2z. For TARGET SURFACE NORMAL the search direction is the nodal normal vector calculated from the TARGET SURFACE.

8.8 Global Output Options

The following commands exist at the region scope to control the output of global variables:

```
GLOBAL ENERGY REPORTING = EXACT|APPROXIMATE|OFF (EXACT)
EXTENSIVE RIGID BODY VARS OUTPUT = OFF|HISTORY|RESULTS|ALL (ALL)
```

Through the `GLOBAL ENERGY REPORTING` command line Presto offers three reporting options for global energy variables: `EXACT`, `APPROXIMATE`, and `OFF`. The `EXACT` and `APPROXIMATE` reporting options use different algorithms for tracking the global values of external energy, internal energy, contact energy, and hourglass energy. In many cases, the `APPROXIMATE` reporting option will provide a modest performance improvement with a negligible effect on the reported energy values. The `OFF` option will result in a further performance improvement and will report energy values of zero.

Note that the `GLOBAL ENERGY REPORTING` command has no effect on the analysis itself; the energy values calculated are used only for reporting purposes.

The line command `EXTENSIVE RIGID BODY VARS OUTPUT` controls the default output of global rigid body variables. Regardless of the option choice here, global rigid body variables may be output by name in the history or results output blocks. See Table 8.2 for a list of available variables. The `EXTENSIVE RIGID BODY VARS OUTPUT` options are: `OFF` to specify no default rigid body global variable output; `HISTORY` to specify default rigid body global variable output to the history file(s) only; `RESULTS` to specify default rigid body global variable output to the results file(s) only; `ALL` to specify default rigid body global variable output to both the history and results files. This option defaults to `ALL` so that if this command is not specified both the history and results files will contain the variables listed in Table 8.2 at every output time.

8.9 Variables

This section lists commonly used variables that the user can select as output to the results file and the history file. The first part of this section lists global, nodal, and element variables. The second part of this section lists variables associated with material models.

8.9.1 Global, Nodal, Face, and Element Variables

This section lists commonly used global, nodal, and element variables. The variables are presented in tables based on use, as follows:

- Table 8.1 Global Variables for All Analyses
- Table 8.2 Global Variables for Rigid Bodies
- Table 8.3 Global Variables for J-Integral
- Table 8.4 Nodal Variables for All Analyses
- Table 8.5 Nodal Variables for Shells
- Table 8.6 Nodal Variables for Spot Welds
- Table 8.7 Nodal Variables for Contact
- Table 8.8 Nodal Variables for J-Integral
- Table 8.9 Face Variables for Blast Pressure Boundary Condition
- Table 8.10 Element Variables for All Elements
- Table 8.11 Element Variables for Solid Elements
- Table 8.12 Element Variables for Membranes
- Table 8.13 Element Variables for Shells
- Table 8.14 Element Variables for Trusses
- Table 8.15 Element Variables for Cohesive Elements
- Table 8.16 Element Variables for Beams
- Table 8.17 Element Variables for Springs
- Table 8.18 Element Variables for J-Integral

The tables provide the following information about each variable:

Variable Name. This is the string that will appear on the `GLOBAL`, `NODE`, `FACE`, or `ELEMENT` command line.

Type. This is the variable's type. The various types are denoted with the labels `Integer`, `Integer[]`, `Real`, `Real[]`, `Vector_2D`, `Vector_3D`, `SymTen33`, and `FullTen36`. The type `Integer` indicates the variable is an integer; the type `Integer[]` is an integer array; the type `Real` indicates the variable is a real; the type `Real[]` is a real array. The type `Vector_2D` indicates the variable type is a two-dimensional vector. The type `Vector_3D` indicates the variable is a three-dimensional vector. For a three-dimensional vector, the variable quantities will be output with suffixes of `_x`, `_y`, and `_z`. For example, if the variable displacement is requested to be output as `displ`, the components of the displacement vector on the results file will be `displ_x`, `displ_y`, and `displ_z`. The type `SymTen33` indicates the variable is a symmetric 3×3 tensor. For a 3×3 symmetric tensor, the variable quantities will be output with suffixes of `_xx`, `_yy`, `_zz`, `_xy`, `_yz`, and `_zx`. For example, if the variable `stress` is requested for output as `stress`, the components of the stress tensor on the results file will be `stress_xx`, `stress_yy`, `stress_zz`, `stress_xy`, `stress_yz`, and `stress_zx`. The type `FullTen36` is a full 3×3 tensor with three diagonal terms and six off-diagonal terms.

Derived. Any variable designated with a `yes` in this column must be included in a `BEGIN DERIVED OUTPUT` command block if it is to be transferred to another procedure or region as described in Section 5.7.

For multi-integration point elements, quantities from the element integration points will be appended with a numerical suffix indicating the integration point. A suffix ranging from 1 to the number of integration points is attached to the quantity to indicate the corresponding integration point. The suffix is padded with leading zeros. If the number of integration points is less than 10, the suffix has the form _*i*, where *i* ranges from 1 to the number of integration points. If the number of integration points is greater than or equal to 10 and less than 100, the sequence of suffixes takes the form `_01`, `_02`, `_03`, and so forth. Finally, if the number of integration points is greater than or equal to 100, the sequence of suffixes takes the form `_001`, `_002`, `_003`, and so forth. As an example, if `von_mises` is requested for a shell element with 15 integration points, then the quantities `von_mises_01`, `von_mises_02`, ..., `von_mises_15` are output for the shell element.

The tables of various types of variables follow.

Table 8.1: Global Variables For All Analyses

Variable Name	Type	Comments
artificial_energy	Real	
contact_energy	Real	(A component of external energy)
external_energy	Real	
ke_blockblockID	Real	Kinetic energy sum for block blockID
ee_strain_blockblockID	Real	External energy sum for block blockID
ie_strain_blockblockID	Real	Internal energy sum for block blockID
momentum_blockblockID	Vector_3D	Momentum sum for block blockID
hourglass_energy	Real	(A component of internal energy)
hge_blockblockID	Real	Hourglass energy sum for block blockID
internal_energy	Real	
kinetic_energy	Real	
momentum	Vector_3D	Momentum vector
timestep	Real	Current time step
timestep_element	Real	Time step from element estimator
timestep_nodal	Real	Time step from nodal estimator
timestep_material	Real	Time step from material model
timestep_lanczos	Real	Time step from Lanczos estimator
timestep_powermethod	Real	Time step from power method estimator
wall_clock_time	Real	Accumulated wall clock time
wall_clock_time_per_step	Real	Wall clock time for last time step
cpu_time	Real	Accumulated CPU time
cpu_time_per_step	Real	CPU time for last time step

Table 8.2: Global Variables for Rigid Bodies. (See Section 8.8 for default output options.)

Variable Name	Type	Comments
ax,ay,az	Real	Translational acceleration
velx,vely,velz	Real	Translational velocity
displx,disply,displz	Real	Translational displacement
rotax,rotay,rotaz	Real	Rotational acceleration
rotvx,rotvy,rotvz	Real	Rotational velocity
rotdx,rotdy,rotdz	Real	Rotational displacement
reactx,reacty,reactz	Real	Translational reaction
rreactx,rreacty, rreactz	Real	Rotational reaction
qvec1,qvec2,qvec3, qvec4	Real	Unit quaternion

Table 8.3: Global Variables for J-Integral (See Section 9.2)

Variable Name	Type	Comments
j_average_<jint_name>	Real[]	Average value of the J-integral over the crack. Array sized to number of integration domains and numbered from inner to outer domain. <jint_name> is the name of the J INTEGRAL block.

Table 8.4: Nodal Variables for All Analyses

Variable Name	Type	Comments
model_coordinates	Vector_3D	Original coordinates of nodes
coordinates	Vector_3D	Current coordinates of nodes
displacement	Vector_3D	Total displacement
velocity	Vector_3D	
acceleration	Vector_3D	
force_internal	Vector_3D	
force_external	Vector_3D	
force external_ transferred	Vector_3D	Force transferred from another physics (coupled problems only)
force_contact	Vector_3D	
reaction	Vector_3D	
mass	Real	
nodal_time_step	Real	Nodal stable time step (explicit control modes, coarse mesh only)
hourglass_energy	Real	Nodal integrated energy due to hourglass forces
quaternion	Real	Current quaternion (rigid body reference nodes only)

Table 8.5: Nodal Variables for Shells and Beams

Variable Name	**Type**	**Comments**
`rotational_displacement`	`Vector_3D`	
`rotational_velocity`	`Vector_3D`	
`rotational_acceleration`	`Vector_3D`	
`moment_internal`	`Vector_3D`	
`moment_external`	`Vector_3D`	
`moment external_ transferred`	`Vector_3D`	Moment transferred from another physics (coupled problems only)
`rotational_reaction`	`Vector_3D`	
`rotational_mass`	`Real`	

Table 8.6: Nodal Variables for Spot Welds

Variable Name	Type	Comments
spot_weld_parametric_coordinates	Vector_2D	Coordinates of node on face
spot_weld_normal_force_at_death	Real	Value of force normal to face when spot weld breaks
spot_weld_tangential_force_at_death	Real	Value of force tangential to face when spot weld breaks
spot_weld_death_flag	Integer	alive = 0, dead = FAILURE DECAY CYCLES (default is 10), -1 = no spot weld constructed at this node
spot_weld_scale_factor	Real	Nodal influence area of current node
spot_weld_normal_displacement	Real	Current displacement of weld normal to face
spot_weld_tangential_displacement	Real	Current displacement of weld tangential to face
spot_weld_normal_force	Real	Current force of weld normal to face
spot_weld_tangential_force	Real	Current force of weld tangential to face
spot_weld_stiffness	Real	Current stiffness of weld
spot_weld_norm_stiffness	Real	Current stiffness of weld normal to face
spot_weld_tang_stiffness	Real	Current stiffness of weld tangential to face
spot_weld_initial_offset	Vector_3D	The initial offset of the spot weld node from the spot weld surface. Does not change over time, only output if IGNORE INITIAL OFFSET = YES is specified at input.
spot_weld_initial_normal	Vector_3D	The initial normal of the spot weld surface at the point of interaction. Only output if IGNORE INITIAL OFFSET = YES is specified at input.

Table 8.7: Nodal Variables for Contact (See Section 7.10)

Variable	Type	Description
contact_status	Real	Status of the interactions at the node. Possible values are as follows: 0.0 = Node is not a contact node (not in a defined contact surface) 0.5 = Node is not in contact 1.0 = Node is in contact and is slipping -1.0 = Node is in contact and is sticking (celement).
contact_normal_direction	Vector_3D	Direction of the constraint. This is, in general, the normal of the face in the interaction (cdirnor).
contact_tangential_direction	Vector_3D	Direction of the contact tangential force (cdirtan).
contact_normal_force_magnitude	Real	Magnitude of the contact force at the node in the direction normal to the contact face. Magnitude of contact_normal_direction.
contact_tangential_force_magnitude	Real	Magnitude of the contact force at the node in the plane of the contact face. Magnitude of contact_tangential_direction.
contact_normal_traction_magnitude	Real	Traction normal to the contact face. contact_normal_force_magnitude divided by contact_area. If there are multiple interactions for this node, the traction only for the last interaction is given (cfnor).
contact_tangential_traction_magnitude	Real	Traction in the plane of the contact face. contact_traction_force_magnitude divided by contact_area. If there are multiple interactions for this node, the traction only for the last interaction is given (cftan).

Continued on next page

Table 8.7 – Continued from previous page

Variable	Type	Description
contact_incremental_slip_magnitude	Real	Magnitude of incremental slip over the current time step (cdtan).
contact_incremental_slip_direction	Vector_3D	Normalized direction of incremental slip over the current time step (cdirislp).
contact_accumulated_slip	Real	Magnitude of tangential slip accumulated over the entire analysis. This is the distance along the slip path, and not the magnitude of contact_accumulated_slip_vector (cstan).
contact_accumulated_slip_vector	Vector_3D)	Total accumulated tangential slip over the entire analysis (cdirslp).
contact_frictional_energy	Real	Accumulated amount of frictional energy dissipated over the entire analysis.
contact_frictional_energy_density	Real	Accumulated amount of frictional energy dissipated over the entire analysis, divided by the contact area (cetan).
contact_area	Real	Contact area for the node. This is the tributary area around the node for this interaction. If there are multiple interactions, the reported area is the area associated with the last interaction (carea).
contact_normal_gap	Real	Magnitude of gap in the direction normal to the face (cgnor).
contact_tangential_gap	Real	Magnitude of gap in the direction tangent to the face (only applicable for compliant friction models) (cgtan).

Table 8.8: Nodal Variables for J-Integral (See Section 9.2)

Variable Name	**Type**	**Comments**
`j_<jint_name>`	`Real[]`	Pointwise value of J-integral along crack. Array sized to number of integration domains and numbered from inner to outer domain. `<jint_name>` is the name of the `J INTEGRAL` block.

Table 8.9: Face Variables for Blast Pressure Boundary Condition (See Section 6.10.2)

Variable Name	**Type**	**Comments**
`pressure`	`Real`	Current total pressure. This is the only field for this boundary condition that varies in time.
`normal`	`Vector_3D`	Face normal vector
`incident_pressure`	`Real`	Peak incident pressure
`reflected_pressure`	`Real`	Peak reflected pressure
`alpha`	`Real`	Decay coefficient α
`beta`	`Real`	Decay coefficient β
`cosa`	`Real`	Cosine of θ
`arrival_time`	`Real`	Time for arrival of blast at face
`positive_duration`	`Real`	Duration of blast at face

Table 8.10: Element Variables for All Elements

Variable Name	**Type**	**Derived** (Sec 5.7)	**Comments**
`diagonal_ratio`	`Real`		See Section 2.4
`element_mass`	`Real`		
`perimeter_ratio`	`Real`		See Section 2.4
`solid_angle`	`Real`		See Section 2.4
`timestep`	`Real`		Critical time step for the element. The element in the model with the smallest time step controls the analysis time step.
`von_mises`	`Real`	yes	Von Mises stress norm
`hydrostatic_stress`	`Real`	yes	One-third the trace of the stress sensor
`fluid_pressure`	`Real`	yes	Negative of `hydrostatic_stress`
`stress_invariant_1`	`Real`	yes	Trace of the stress tensor
`stress_invariant_2`	`Real`	yes	Second invariant of the stress tensor
`stress_invariant_3`	`Real`	yes	Third invariant of the stress tensor
`max_principal_stress`	`Real`	yes	Largest eigenvalue of the stress tensor
`intermediate_principal_stress`	`Real`	yes	Middle eigenvalue of the stress tensor
`min_principal_stress`	`Real`	yes	Smallest eigenvalue of the stress tensor
`max_shear_stress`	`Real`	yes	Maximum shear stress from Mohr's circle
`octahedral_shear_stress`	`Real`	yes	Octahedral shear norm of the stress tensor

Table 8.11: Element Variables for Solid Elements

Variable Name	**Type**	**Derived** (Sec 5.7)	**Comments**
aspect_ratio	Real		Tets only. See Section 2.4
dilmod	Real		
left_stretch	SymTen33		
nodal_jacobian_ratio	Real		Hexes only. See Section 2.4
rate_of_deformation	SymTen33		Hexes and node-based tets only.
rotation	FullTen36		
shrmod	Real		
stress	SymTen33		
unrotated_stress	SymTen33		
log_strain	SymTen33		Log strain tensor
unrotated_log_strain	SymTen33		Log strain tensor in unrotated configuration
effective_log_strain	Real	yes	Effective log strain
log_strain_invariant_1	Real	yes	Trace of the log strain tensor
log_strain_invariant_2	Real	yes	Second invariant of the log strain tensor
log_strain_invariant_3	Real	yes	Third invariant of the log strain tensor
max_principal_log_strain	Real	yes	Largest eigenvalue of the log strain tensor
intermediate_principal_log_strain	Real	yes	Middle eigenvalue of the log strain tensor
min_principal_log_strain	Real	yes	Smallest eigenvalue of the log strain tensor
max_shear_log_strain	Real	yes	Maximum shear log strain from Mohr's circle
octahedral_shear_log_strain	Real	yes	Octahedral strain norm of the log strain tensor
volume	Real		

Table 8.12: Element Variables for Membranes

Variable Name	**Type**	**Comments**
memb_stress	SymTen33	
element_area	Real	
element_thickness	Real	

Table 8.13: Element Variables for Shells

Variable Name	**Type**	**Derived** (Sec 5.7)	**Comments**
`memb_stress`	`SymTen33`		Stress at midplane in global X, Y, and Z coordinates
`bottom_stress`	`SymTen33`		Stress at bottom integration point in global X, Y, and Z coordinates
`top_stress`	`SymTen33`		Stress at top integration point in global X, Y, and Z coordinates
`unrotated_stress`	`SymTen33`		
`transform_shell_stress`	`SymTen21`	yes	In-plane shell stress
`strain`	`SymTen33`		Integrated strain at midplane in local shell coordinate system
`effective_strain`	`Real`	yes	Effective strain norm
`strain_invariant_1`	`Real`	yes	Trace of the strain tensor
`strain_invariant_2`	`Real`	yes	Second invariant of the strain tensor
`strain_invariant_3`	`Real`	yes	Third invariant of the strain tensor
`max_principal_strain`	`Real`	yes	Largest eigenvalue of the strain tensor
`intermediate_principal_strain`	`Real`	yes	Middle eigenvalue of the strain tensor
`min_principal_strain`	`Real`	yes	Smallest eigenvalue of the strain tensor
`max_shear_strain`	`Real`	yes	Maximum shear strain from Mohr's circle
`octahedral_shear_strain`	`Real`	yes	Octahedral strain norm of the strain tensor
`transform_shell_strain`	`Real`	yes	In-plane shell strain
`element_area`	`Real`		
`element_thickness`	`Real`		
`rate_of_deformation`	`SymTen33`		Rate of deformation (stretching) tensor

Table 8.14: Element Variables for Trusses

Variable Name	Type	Comments
truss_init_length	Real	
truss_stretch	Real	
stress	SymTen33	Axial stress is stored in stress_xx. All other components are zero. See Section 5.2.7 for more details.
truss_strain_incr	Real	
truss_force	Real	

Table 8.15: Element Variables for Cohesive Elements

Variable Name	Type	Comments
cse_traction	Vector_3D	
cse_separation	Vector_3D	
cse_initial_trac	Vector_3D	Available only if traction initialization is used
cse_activated	Integer	For intrinsic elements
cse_fracture_area	Real	Currently not used

Table 8.16: Element Variables for Beams

Variable Name	Type	Comments
`beam_strain_inc`	`Vector_2D`	Thirty-two strain increment values are output. Some values may be zero depending on section. Axial strains are 01, 03, 05, . . . Shear strains are 02, 04, 06, . . . See Section 5.2.6 for more details.
`stress`	`SymTen33`	Ninety-six stress values are output, although only the first two values per integration point contain actual stress values. Some integration points may not have data depending on the section. Axial stresses are in `stress_xx_01`, `stress_xx_02`, ..., `stress_xx_16`. Shear stresses are in `stress_xy_01`, `stress_xy_02`, ..., `stress_xy_16`, where 01, 02, . . . , 16, refer to the integration points. See Section 5.2.6 for more details.
`beam_stress_axial`	`Real`	Sixteen axial stress values. Some may be zero depending on section.
`beam_stress_shear`	`Real`	Sixteen shear stress values. Some may be zero depending on section.
`beam_axial_force`	`Real`	Axial force at midpoint.
`beam_transverse_force_s`	`Real`	Transverse shear in s-direction at midpoint.
`beam_transverse_force_t`	`Real`	Transverse shear in t-direction at midpoint.
`beam_moment_r`	`Real`	Torsion at midpoint.
`beam_moment_s`	`Real`	Moment about s-direction at midpoint.
`beam_moment_t`	`Real`	Moment about t-direction at midpoint.
`beam_avg_rate_of_def`	`Real`	Average rate of deformation over all integration point.

Table 8.17: Element Variables for Springs

Variable Name	Type	Comments
`spring_force`	`Real`	Magnitude of the internal spring force.
`spring_engineering_strain`	`Real`	Change in length over initial length $\frac{dL}{L_0}$.
`spring_init_length`	`Real`	Initial spring length, L_0.

Table 8.18: Element Variables for J-Integral (See Section 9.2)

Variable Name	**Type**	**Comments**
energy_momentum_tensor	FullTen36	Energy momentum tensor
integration_domains_ <jint_name>	Integer[]	Flag indicating elements in integration domains. Set to 1 if in domain, 0 otherwise. Array sized to number of domains and numbered from inner to outer domain. <jint_name> is the name of the J INTEGRAL block.

8.9.2 Variables for Material Models

It is possible to output the state variables from the material models. Most of the materials, with the exception of simple models such as the elastic model, have state variables that can be output. The method used to output state variables depends on how the model is implemented. There are currently three cases:

- The Strumento version of most of the solid models for which the entire state variable array can be dumped.
- The Strumento version of a few solid models for which state variables are accessed by name
- The versions of the solid models implemented in the LAME library for which state variables are accessed by name

In the future, the implementation of the solid material models in LAME will be used by default, and all state variables will be accessed by name. The following sections describe the different methods required to output material model variables.

8.9.2.1 State Variable Output by Index for Strumento Solid Material Models

To output all of the state variables for a given material model. Use the `ELEMENT` command line in the `RESULTS OUTPUT` command block of the form:

```
ELEMENT state_material_name
```

where `material_name` is the name of the material model, e.g. `state_elastic_plastic`, `state_power_law_hardening`, `state_foam_plasticity`, or `state_orthotropic_rate`. All of the state variables for the material will be output.

Some of the Strumento material models are implemented in a way such that state variables are accessed directly by name rather than by index. For example, to access the `C10` variable in the Mooney-Rivlin material model, one would simply list the name `C10` to obtain that output. The state variables for the Mooney-Rivlin, Swanson, and Orthotropic Crush material models are accessed in this way.

Section 8.9.2.3 provides tables listing the state variables for all solid material models. Models for which state variable output is requested by name have names entered in a column entitled "Name (Strumento Model)".

8.9.2.2 State Variable Output for LAME Solid Material Models

The state variables for material models in LAME are accessible directly by name. For instance, the equivalent plastic strain variable is accessible by the name `EQPS` for all elastic-plastic material models.

Section 8.9.2.3 provides tables listing the state variables for all solid material models. Models that are implemented in LAME have state variable names listed in the column entitled "Name (LAME Model)". If there are no entries in that column for a given material, then that material is not implemented in LAME.

Available LAME state variables for a material will also be listed in the log file from a run that uses the material model.

8.9.2.3 State Variable Tables for Solid Material Models

As explained in the preceding sections, there are three cases to be considered for state variable output from solid material models: Strumento models, Strumento models for which state output is obtained using the variable name, and LAME models, for which state output is also obtained by variable name. Tables of state variables for commonly used material models are provided in Tables 8.23 through 8.45. These tables contain the indices or names used to access the state variables in the Strumento version of the models, as well as the names used to access the LAME versions of the models. If there are no entries in the "Strumento Model" column for a model, that model is only implemented in LAME. Likewise, if there are no entries in the "LAME Model" column, there is no version of that model in LAME.

Table 8.19: State Variables for ELASTIC Model (Section 4.2.1)

This model has no state variables.

Table 8.20: State Variables for ELASTIC FRACTURE Model (Section 4.2.4)

Index (Strumento Model)	**Name (LAME Model)**	**Variable Description**
1	`DEATH_FLAG`	flag for element death
2	`CRACK_OPENING_STRAIN`	critical value of opening strain
3	`FAILURE_DIRECTION_X`	crack opening direction - x component
4	`FAILURE_DIRECTION_Y`	crack opening direction - y component
5	`FAILURE_DIRECTION_Z`	crack opening direction - z component
6	`PRINCIPAL_STRESS`	value of maximum principal stress

Table 8.21: State Variables for ELASTIC PLASTIC Model (Section 4.2.5)

Index (Strumento Model)	**Name (LAME Model)**	**Variable Description**
1	EQPS	equivalent plastic strain
2	BACK_STRESS_XX	back stress - xx component
3	BACK_STRESS_YY	back stress - yy component
4	BACK_STRESS_ZZ	back stress - zz component
5	BACK_STRESS_XY	back stress - xy component
6	BACK_STRESS_YZ	back stress - yz component
7	BACK_STRESS_ZX	back stress - zx component
8	RADIUS	radius of yield surface

Table 8.22: State Variables for EP POWER HARD Model (Section 4.2.6)

Index (Strumento Model)	**Name (LAME Model)**	**Variable Description**
1	EQPS	equivalent plastic strain
2	RADIUS	radius of yield surface

Table 8.23: State Variables for DUCTILE FRACTURE Model (Section 4.2.7)

Index (Strumento Model)	**Name (LAME Model)**	**Variable Description**
1	EQPS	equivalent plastic strain
2	TEARING_ PARAMETER	tearing parameter
3	CRACK_OPENING_ STRAIN	crack opening strain
4	FAILURE_ DIRECTION_X	crack opening direction - x component
5	FAILURE_ DIRECTION_Y	crack opening direction - y component
6	FAILURE_ DIRECTION_Z	crack opening direction - z component
7	DEATH_FLAG	flag for element death
8	RADIUS	radius of yield surface

Table 8.24: State Variables for MULTILINEAR EP Model (Section 4.2.8)

Index (Strumento Model)	**Name (LAME Model)**	**Variable Description**
1	EQPS	equivalent plastic strain
2	RADIUS	radius of yield surface
3	BACK_STRESS_XX	back stress - xx component
4	BACK_STRESS_YY	back stress - yy component
5	BACK_STRESS_ZZ	back stress - zz component
6	BACK_STRESS_XY	back stress - xy component
7	BACK_STRESS_YZ	back stress - yz component
8	BACK_STRESS_ZX	back stress - zx component

Table 8.25: State Variables for ML EP FAIL Model (Section 4.2.9)

Index (Strumento Model)	**Name (LAME Model)**	**Variable Description**
1	EQPS	equivalent plastic strain
2	RADIUS	radius of yield surface
3	BACK_STRESS_XX	back stress - xx component
4	BACK_STRESS_YY	back stress - yy component
5	BACK_STRESS_ZZ	back stress - zz component
6	BACK_STRESS_XY	back stress - xy component
7	BACK_STRESS_YZ	back stress - yz component
8	BACK_STRESS_ZX	back stress - zx component
9	TEARING_ PARAMETER	tearing parameter
10	CRACK_OPENING_ STRAIN	crack opening strain
11	FAILURE_ DIRECTION_X	crack opening direction - x component
12	FAILURE_ DIRECTION_Y	crack opening direction - y component
13	FAILURE_ DIRECTION_Z	crack opening direction - z component
14	CRACK_FLAG	status of the model: 0 for loading, 1 or 2 for initiation of failure, 3 during unloading, 4 for completely unloaded

Table 8.26: State Variables for FOAM PLASTICITY Model (Section 4.2.15)

Index (Strumento Model)	**Name (LAME Model)**	**Variable Description**
1	`ITER`	iterations
2	`EVOL`	volumetric strain
3	`PHI`	phi
4	`EQPS`	equivalent plastic strain
5	`PA`	A
6	`PB`	B

Table 8.27: State Variables for WIRE MESH Model (Section 4.2.18)

Index (Strumento Model)	**Name (LAME Model)**	**Variable Description**
1	`EVOL`	engineering volumetric strain
2	`PHI`	current yield strength in compression

Table 8.28: State Variables for HONEYCOMB Model

Index (Strumento Model)	**Name (LAME Model)**	**Variable Description**
1	`CRUSH`	minimum volume ratio
2	`EQDOT`	effective strain rate
3	`RMULT`	rate multiplier
5	`ITER`	iterations
6	`EVOL`	volumetric strain

Table 8.29: State Variables for HYPERFOAM Model

This model has no state variables.

Table 8.30: State Variables for JOHNSON COOK Model (Section 4.2.10)

Index (Strumento Model)	**Name (LAME Model)**	**Variable Description**
1	`RADIUS`	radius of yield surface
2	`EQPS`	equivalent plastic strain
3	`THETA`	temperature
4	`EQDOT`	effective total strain rate

Table 8.31: State Variables for LOW DENSITY FOAM Model (Section 4.2.16)

Index (Strumento Model)	**Name (LAME Model)**	**Variable Description**
	`PAIR`	air pressure

Table 8.32: State Variables for MOONEY RIVLIN Model (Section 4.2.24)

Name (Strumento Model)	**Name (LAME Model)**	**Variable Description**
C10	C10	
C01	C01	
RK	K	
SFJth	SFJTH	
RJTH	JTH	
V_MECH	VMECH_XX	
	VMECH_YY	
	VMECH_ZZ	
	VMECH_XY	
	VMECH_YZ	
	VMECH_ZX	
	SFJTH_FLAG	

Table 8.33: State Variables for NEO HOOKEAN Model (Section 4.2.3)

This model has no state variables.

Table 8.34: State Variables for ORTHOTROPIC CRUSH Model (Section 4.2.19)

Name (Strumento Model)	**Name (LAME Model)**	**Variable Description**
CRUSH	CRUSH	minimum volume ratio, crush is unrecoverable

Table 8.35: State Variables for ORTHOTROPIC RATE Model (Section 4.2.20)

Index (Strumento Model)	**Name (LAME Model)**	**Variable Description**
	CRUSH	minimum volume ratio, crush is unrecoverable

Table 8.36: State Variables for PIEZO Model

Index (Strumento Model)	**Name (LAME Model)**	**Variable Description**
	STATE	

Table 8.37: State Variables for POWER LAW CREEP Model (Section 4.2.12)

Index (Strumento Model)	**Name (LAME Model)**	**Variable Description**
1	ECREEP	equivalent creep strain
2	SEQDOT	equivalent stress rate

Table 8.38: State Variables for SHAPE MEMORY Model

Index (Strumento Model)	**Name (LAME Model)**	**Variable Description**
	STATE	

Table 8.39: State Variables for SOIL FOAM Model (Section 4.2.13)

Index (Strumento Model)	**Name (LAME Model)**	**Variable Description**
	EVOL	

Table 8.40: State Variables for SWANSON Model (Section 4.2.27)

Name (Strumento Model)	**Name (LAME Model)**	**Variable Description**
SFJTH	SFJTH	
RJTH	RJTH	
V_MECH	VMECHXX	
	VMECHYY	
	VMECHZZ	
	VMECHXY	
	VMECHYZ	
	VMECHZX	
	SFJTH_FLAG	

Table 8.41: State Variables for VISCOELASTIC SWANSON Model (Section 4.2.28)

Index (Strumento Model)	**Name (LAME Model)**	**Variable Description**
	SFJTH	
	JTH	
	VMECHXX	
	VMECHYY	
	VMECHZZ	
	VMECHXY	
	VMECHYZ	
	VMECHZX	
	VSXXDEV1 – VSXXDEV10	
	VSYYDEV1 – VSYYDEV10	
	VSZZDEV1 – VSZZDEV10	
	VSXYDEV1 – VSXYDEV10	
	VSYZDEV1 – VSYZDEV10	
	VSZXDEV1 – VSZXDEV10	
	SOXXDEV	
	SOYYDEV	
	SOZZDEV	
	SOXYDEV	
	SOYZDEV	
	SOZXDEV	

Table 8.42: State Variables for THERMO EP POWER Model

Index (Strumento Model)	**Name (LAME Model)**	**Variable Description**
1	EQPS	equivalent plastic strain
2	RADIUS	radius of yield surface
3	BACK_STRESS_XX	back stress - xx component
4	BACK_STRESS_YY	back stress - yy component
5	BACK_STRESS_ZZ	back stress - zz component
6	BACK_STRESS_XY	back stress - xy component
7	BACK_STRESS_YZ	back stress - yz component
8	BACK_STRESS_ZX	back stress - zx component

Table 8.43: State Variables for THERMO EP POWER WELD Model

Index (Strumento Model)	**Name (LAME Model)**	**Variable Description**
	EQPS	equivalent plastic strain
	RADIUS	radius of yield surface
	BACK_STRESS_XX	back stress - xx component
	BACK_STRESS_YY	back stress - yy component
	BACK_STRESS_ZZ	back stress - zz component
	BACK_STRESS_XY	back stress - xy component
	BACK_STRESS_YZ	back stress - yz component
	BACK_STRESS_ZX	back stress - zx component
	WELD_FLAG	

Table 8.44: State Variables for UNIVERSAL POLYMER Model

Index (Strumento Model)	**Name (LAME Model)**	**Variable Description**
	AEND	
	IGXX1 - IGXX20	
	IGYY1 - IGYY20	
	IGZZ1 - IGZZ20	
	IGXY1 - IGXY20	
	IGYZ1 - IGYZ20	
	IGZX1 - IGZX20	
	IKI11 - IKI120	
	IKAT1 - IKAT20	
	IF1P1 - IF1P20	
	IF2J1 - IF2J20	
	EPSXX	
	EPSYY	
	EPSZZ	
	EPSXY	
	EPSYZ	
	EPSZX	
	LOGA	

Table 8.45: State Variables for VISCOPLASTIC Model

Index (Strumento Model)	**Name (LAME Model)**	**Variable Description**
	SVBXX	
	SVBYY	
	SVBZZ	
	SVBXY	
	SVBYZ	
	SVBZX	
	EQDOT	
	COUNT	
	SHEAR	
	BULK	
	RATE	
	EXP	
	ALPHA	
	A1	
	A2	
	A4	
	A5	

8.9.2.4 Variables for Shell/Membrane Material Models

Shell and membrane material models also make their state variables available through direct naming of the variables. Tables 8.46 through 8.49 indicate the names of the state variables for the shell material models.

Table 8.46: State Variables for ELASTIC PLASTIC Model for Shells (Section 4.2.5)

Variable Name	Variable Description
`eqps`	Equivalent plastic strain
`back_stress`	Back stress
`radius`	Radius of the yield surface

Table 8.47: State Variables for EP POWER HARD Model for Shells (Section 4.2.6)

Variable Name	Variable Description
`eqps`	Equivalent plastic strain
`radius`	Radius of yield surface

Table 8.48: State Variables for MULTILINEAR EP Model for Shells (Section 4.2.8)

Variable Name	Variable Description
`eqps`	Equivalent plastic strain
`tensile_eqps`	Equivalent plastic strain only accumulated in tension
`back_stress`	Back stress
`radius`	Radius of the yield surface

Table 8.49: State Variables for ML EP FAIL Model for Shells (Section 4.2.9)

Variable Name	**Variable Description**
`eqps`	Equivalent plastic strain
`back_stress`	Back stress
`radius`	Radius of the yield surface
`tearing_parameter`	The current value of the tearing parameter
`crack_opening_strain`	The value of the crack opening strain during the failure process
`crack_flag`	Status of the model: 0 for loading, 1 or 2 for initiation of failure, 3 during unloading, 4 for completely unloaded

8.9.3 Variables for Surface Models

It is possible to output the state variables from the surface models. The element state variables are output using the variable name by use of following line command:

```
ELEMENT surface_model_state_name
```

Section 8.9.3.1 provides tables listing the state variables for all surface models.

8.9.3.1 State Variable Tables for Surface Models

Table 8.50: State Variables for TRACTION DECAY Surface Model (Section 4.3.1)

Index	Name	Variable Description
0	MAX_ SEPARATION_S	maximum separation in the first tangential direction
1	MAX_ SEPARATION_T	maximum separation in the second tangential direction
2	MAX_ SEPARATION_N	maximum separation in the normal direction

Table 8.51: State Variables for TVERGAARD HUTCHINSON Surface Model (Section 4.3.2)

Index	Name	Variable Description
0	PEAK_TRACTION	maximum traction the model can experience
1	LAMBDA_MAX	maximum lambda the model has experienced
2	TRACTION_AT_ LAMBDA_MAX	traction at LAMBDA_MAX

Table 8.52: State Variables for THOULESS PARMIGIANI Surface Model (Section 4.3.3)

Index	**Name**	**Variable Description**
0	FRACTION_OF_FAILURE	current fraction of failure
1	PEAK_TRACTION_N	maximum normal traction the model can experience
2	PEAK_TRACTION_T	maximum tangential traction the model can experience
3	LAMBDA_MAX_N	maximum normal lambda the model has experienced
4	TRACTION_AT_LAMBDA_MAX_N	normal traction at LAMBDA_MAX_N
5	LAMBDA_MAX_T	maximum tangential lambda the model has experienced
6	TRACTION_AT_LAMBDA_MAX_T	tangential traction at LAMBDA_MAX_T
7	G_AT_LAMBDA_MAX_N	the area under the normal traction separation curve up to LAMBDA_MAX_N
8	G_AT_LAMBDA_MAX_T	the area under the tangential traction separation curve up to LAMBDA_MAX_T

8.10 References

1. Larry A. Schoof, Victor R. Yarberry, *EXODUS II: A Finite Element Data Model*, SAND92-2137, Sandia National Laboratories, September 1994. pdf. See also documentation available at EXODUS II sourceforge page. link.

2. The eXtensible Data Model and Format (XDMF). link.

3. Sjaardema, G. D. *Overview of the Sandia National Laboratories Engineering Analysis Code Access System*, SAND92-2292. Albuquerque, NM: Sandia National Laboratories, January 1993. pdf.

Chapter 9

Special Modeling Techniques

This chapter describes techniques useful for performing special types of analyses:

- Section 9.1 describes the Representative Volume Element (RVE) capability, which is a multiscale technique that uses a separate finite element model to represent the material response at a point.
- Section 9.2 describes the capability to compute J-Integrals as a criterion for fracture growth.
- Section 9.3 describes the peridynamics functionality available in Presto. Peridynamics is a nonlocal formulation of continuum mechanics that is well-suited for modeling material discontinuities such as cracks.

9.1 Representative Volume Elements

The use of representative volume elements (RVEs) is a multiscale technique in which the material response at element integration points in a reference mesh is computed using an RVE that is itself discretized with finite elements. RVEs are typically used to represent local, periodic material inhomogeneities such as fibers or random microstructures to avoid the requirement of a global mesh with elements small enough to capture local material phenomena.

This capability is currently implemented only for uniform gradient hex elements in the reference mesh. In the current implementation of RVEs, periodic boundary conditions are applied to each RVE representing the deformation of a parent element and the stresses are computed in the elements of the RVE. These stresses are then volume-averaged over the RVE and the resulting homogenized stresses are passed back to the parent element.

This chapter explains how to use the RVE capability. Section 9.1.1 gives a detailed description of how RVEs are incorporated into an analysis. Details of the mesh requirements are delineated in Section 9.1.2 and the commands needed in an input file are described in Section 9.1.3.

9.1.1 RVE Processing

The use of the RVE capability requires two regions, each with its own mesh file. One region processes the reference mesh and the other processes all the RVEs. The commands used in the input file for the reference mesh region are the same as any other Presto region with the exception that a special RVE material model is used for any element blocks that use an RVE. The RVE region is also very similar to an ordinary region. The only differences are that an RVE region has a line command for defining the RVEs' relationship to parent elements in the reference region and has restrictions on the use of boundary conditions.

The processing of an RVE essentially replaces the constitutive model of the parent element in the reference mesh. The steps followed at each iteration/time step of the reference mesh during an analysis using RVEs are:

1. Internal force algorithm is called in the reference region to compute rate of deformation.
2. Each RVE gets the rate of deformation from its parent element in the reference region.
3. The rate of deformation is applied to each RVE as a periodic boundary condition using prescribed velocity.
4. The RVE region is solved to obtain the stress in each element of each RVE.
5. The stresses in the elements of an RVE are volume-averaged over the RVE.
6. Each RVE passes its homogenized (i.e. volume-averaged) stress tensor back to its parent element in the reference mesh.
7. The reference region computes internal force again. Element blocks whose elements have associated RVEs do not compute a stress; they simply use the stress passed to them from their RVE.

9.1.2 Mesh Requirements

Two mesh files, one each for the reference region and the RVE region, are required for an RVE analysis. Figure 9.1 shows an example of the two meshes. The reference mesh of a bar with six elements is shown on the upper left. On the lower right is the mesh for the RVE region containing six RVEs, one for each element of the reference region. In this case, the first five RVEs each consist of two element blocks and the last RVE has four.

In general, each RVE should be a cube with any discretization the user desires. All RVEs must be aligned with the global x, y, and z axes. For stress computations, these axes are rotated into a local coordinate system that can be specified on the reference mesh elements. In other words, if a local coordinate system is specified on a reference mesh element, the RVE global axes will be rotated internally in Presto to align with the local system on the associated parent element. So the global X axis for an RVE is actually the local X' axis in the parent element.

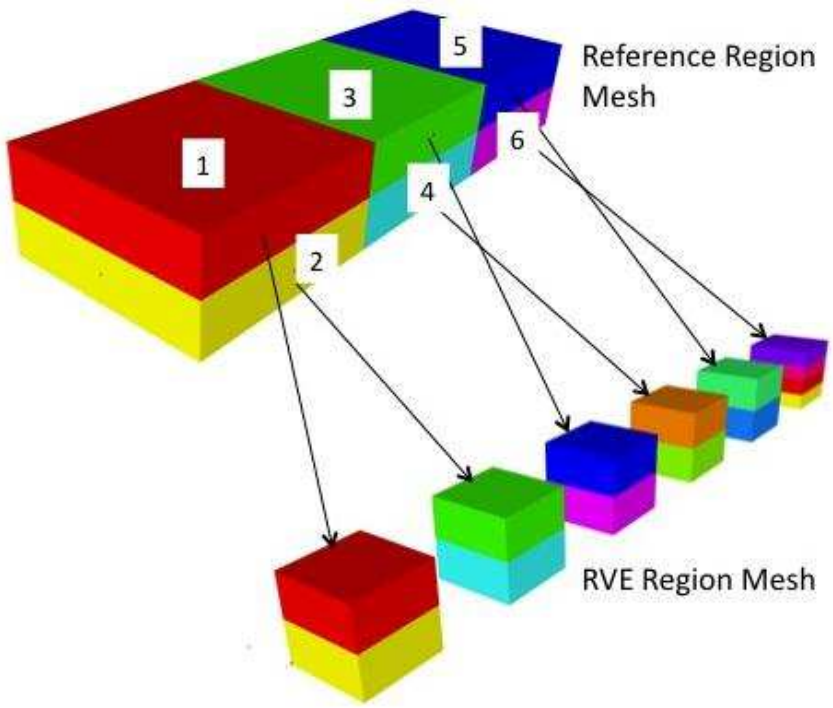

Figure 9.1: Example of meshes for RVE analysis

Additional mesh requirements apply if the mesh does not match across opposing surfaces of the RVE. In this case, the RVE must include a block of membrane elements on the exterior surfaces with matching discretization on opposing surfaces (+x/-x, +y/-y, +z/-z). In order the minimize the effects of this membrane layer on the RVE response, it should be made as thin as possible. This membrane layer then must be tied to the underlying nonmatching RVE surfaces.

The RVE mesh must contain sidesets or nodesets on each surface of every RVE. The RVE may be enclosed with one sideset that spans all six surfaces of the curb, or the user may specify individual sidesets or nodesets on each face. These sidesets/nodesets are used to apply the periodic boundary conditions on the RVE. Presto generates the boundary conditions internally so the user does not have to include them in the input file. However, this assumes that the sidesets/nodesets exist in the mesh file numbered in a specified order. If individual sidesets/nodesets are used on each face of the RVE, the six sidesets/nodesets must be numbered consecutively, starting with the positive-x face, followed by the negative-x face, positive-y face, negative-y face, positive-z face, and ending with the negative-z face. The beginning sideset id (for the positive-x face) is set by the user in the input file.

9.1.3 Input Commands

There are several input commands that are relevant to RVEs. In the reference region, these commands include a special RVE material model and commands to define and use a local coordinate system along which an associated RVE will be aligned. In addition to the reference region, an RVE region is needed using the `BEGIN RVE REGION` command block. The RVE region com-

mand block uses the same nested commands as any other Presto region (with some restrictions as explained in this section) and an additional line command that relates the RVEs to their parent elements in the reference region.

9.1.3.1 RVE Material Model

In an RVE analysis, any elements of the reference mesh that use an RVE must use the RVE material model. This model is defined similar to other material models as described in Chapter 4 but uses the RVE keyword on the `BEGIN PARAMETERS FOR MODEL` command line as follows:

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  #
  DENSITY = <real>density_value
  #
  BEGIN PARAMETERS FOR MODEL RVE
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
  END PARAMETERS FOR MODEL RVE
  #
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

Currently, the RVE material model tells the reference element not to perform a constitutive evaluation but to instead accept the stress tensor obtained from computation on an RVE. However, the use of an RVE material model still requires the input of Young's modulus and Poissons ratio. These values may be used for time time step estimation and hourglass computations even though they are not used in a constitutive evaluation.

Element blocks in the RVE region can use any material model that is supported in Presto other than RVE.

9.1.3.2 Embedded Coordinate System

The finite element model of an element block in the reference mesh that uses RVEs can use an embedded coordinate system to orient the RVE relative to the reference element. A coordinate system is defined in the sierra scope as described in Section 2.1.8. A local coordinate system is then associated with an element block through the use of a `COORDINATE SYSTEM` command line within a `BEGIN SOLID SECTION` command block.

```
BEGIN SOLID SECTION <string>section_name
  #
  COORDINATE SYSTEM = <string>coord_sys_name
  #
END [SOLID SECTION <string>section_name]
```

The string `coord_sys_name` must be a name associated in the input file with a `BEGIN COORDINATE SYSTEM` command block in the sierra scope. This coordinate system will then be used on all elements of a block associated with a `BEGIN PARAMETERS FOR BLOCK` command block that includes the command line specifying this solid section.

9.1.3.3 RVE Region

A representative volume element (RVE) region must be a quasistatic region specified with the RVE keyword in the `BEGIN RVE REGION` command line. The RVE region uses the same block commands and line commands as any other quasistatic region with the addition of line commands that define which element blocks of the reference region are associated with RVEs. There are also some restrictions on boundary conditions as described in Section 9.1.3.6.

```
BEGIN RVE REGION <string>rve_region_name
  #
  # Definition of RVEs
  ELEMENTS <integer>elem_i:<integer>elem_j
    BLOCKS <integer>blk_i:<integer>blk_j
    SURFACE|NODESET <integer>start_id INCREMENT <integer>k
  #
  # Boundary Conditions
  #
  # Results Output Definition
  #
  # Solver Definition
  #
END [RVE REGION <string>rve_region_name]
```

9.1.3.4 Definition of RVEs

One or more `ELEMENTS` command lines are used to associate elements of the reference region mesh with RVEs in the RVE region. In the

```
ELEMENTS <integer>elem_i:<integer>elem_j
  BLOCKS <integer>blk_i:<integer>blk_j
  SURFACE|NODESET <integer>start_id INCREMENT <integer>incr
```

command line, elements numbered `elem_i` through `elem_j` of the reference mesh will be associated with RVEs (for a total number of RVEs equal to `elem_j` - `elem_i` + 1), and each RVE will consist of `blk_i` - `blk_j` + 1 element blocks. The block ids of the first RVE must be `blk_i` through `blk_j` and subsequent RVEs (if `elem_j` is greater than `elem_i`) must have consecutively increasing numbers for their block ids.

Similarly `start_id` gives the `surface_id` of the first RVE if a single, encompassing surface is used, or the first `surface_id` or `nodelist_id` of the first RVE (the positive x surface as

explained in Section 9.1.2) if six individual sidesets/nodeset are used. The remaining surfaces (nodesets) of the first RVE and all the surfaces of the following RVEs must be consecutively numbered following `start_id` in the mesh file as explained in Section 9.1.2.

The increment value `incr` indicates the number of sidesets present on the exterior of the RVEs. This is used to determine how to increment the IDs of the sidesets from one RVE to the next, as well as to determine how to prescribe periodic boundary conditions on the RVE. The increment can have a value of either one or six. A value of one indicates that each RVE has one sideset that encompasses all six faces, while a value of six specifies that six sidesets or nodesets are present, one on each face. Note that nodesets are not allowed for the case where `incr` is one.

The following example shows the use of the `ELEMENTS` command line:

```
elements 1:5 blocks 1:2 surface 7 increment 6
elements 6:6 blocks 11:14 nodeset 15 increment 6
```

These commands generate the RVEs shown in Figure 9.1.

The first `ELEMENTS` command line specifies that elements with element ids 1 through 5 in the parent region mesh each have an RVE with two element blocks. The RVE associated with element 1 of the parent region will have two element blocks starting with `block_id` of 1 and ending with a `block_id` of 2. Subsequent RVEs will have consecutively numbered element blocks. That is, parent element 2 will be associated with an RVE that consists of element blocks 3 and 4 in the RVE region, parent element 3 will be associated with the RVE that has element blocks 5 and 6, etc., for the first five elements of the parent region mesh. The keyword `SURFACE` specifies that all the periodic boundary conditions generated by the code for the RVEs for elements 1 to 5 will use sidesets in the RVE region mesh. These sidesets will start with id 7 for the positive-x face of the RVE associated with parent element 1 and continue consecutively for the other faces of the RVE and the RVEs associated with parent elements 2 through 5 in the order specified in Section 9.1.2. In other words, the positive-x face of the RVE for parent element 1 is sideset 7, negative-x is sideset 8, positive-y is sideset 9, negative-y is sideset 10, positive-z is sideset 11, and negative-z is sideset 12. The sidesets for the RVE for parent element 2 will start with id 13 and continue consecutively in the same face order. The process continues for all five RVEs specified in this command line.

The second `ELEMENTS` line specifies that element 6 of the parent region mesh will be associated with the RVE that consists of element blocks 11, 12, 13, and 14. The `NODESET` keyword says this RVE has a nodeset associated with each face of the RVE, starting with nodeset id 15 on the positive-x face, with id's increasing consecutively for the other five faces in the same order described in the paragraph above.

Note that the six elements specified in these command lines must be in element blocks of the reference region mesh that use the RVE material model.

9.1.3.5 Multi-Point Constraints

In the case in which the RVE has nonmatching surfaces, and therefore includes a block of membrane elements on the exterior surfaces, the user must specify a set of multi-point constraints

(MPCs) to tie the membranes to the surface. This is done in the input file through use of an MPC command block:

```
RESOLVE MULTIPLE MPCS = ERROR
BEGIN MPC
  MASTER SURFACE = <string>membrane_surface_id
  SLAVE SURFACE  = <string>RVE_surface_id
  SEARCH TOLERANCE = <real>tolerance
END
```

In this case, the membrane_surface_id corresponds to the single sideset that encompasses the membrane block is the master and the single sideset that encompasses the exterior surfaces of the RVE is the slave. While the underlying RVE may have nonmatching exterior surfaces, the opposing surfaces of the membrane block must have matching discretizations. For more information on the use of MPCs, see Section 6.10.8.1 and the RESOLVE MULTIPLE MPCS command line is discussed in Section 6.10.8.4.

9.1.3.6 RVE Boundary Conditions

Strain rates computed by elements in the reference region are applied through periodic prescribed velocity boundary conditions on the faces of the associated RVEs. These are generated internally by Presto so the periodic boundary conditions do not need to be in the user's input file. However, because the RVE region is quasistatic, each of the RVEs must be fixed against rigid body motion. This must be done in the input file through use of the prescribed velocity boundary conditions:

```
BEGIN PRESCRIBED VELOCITY pres_vel_name
  NODE SET = <string>nodelist_name
  FUNCTION = <string>function_name
  SCALE FACTOR = <real>scale_factor
  COMPONENT = <string>X|Y|Z
END [PRESCRIBED VELOCITY pres_vel_name]
```

This type of boundary condition is described in detail in Chapter 6 but the use for RVEs is restricted. First, either the function must always evaluate to 0.0 or the scale_factor must have a value of 0. This is essentially a way of using the prescribed velocity boundary condition to fix the nodes in nodelist_name. However, in order for these conditions to work with the periodic boundary conditions which are used to apply the strain rate, PRESCRIBED VELOCITY must be used rather than FIXED DISPLACEMENT or PRESCRIBED DISPLACEMENT boundary conditions.

Generally, three BEGIN PRESCRIBED VELOCITY command blocks will be needed, one each for X, Y, and Z components. In order to eliminate rigid body motion without over constraining the motion, each BEGIN PRESCRIBED VELOCITY block should constrain exactly one node of an RVE in one component direction. (However, nodelist_name may contain nodes from multiple RVEs. Separate boundary condition blocks are not required for each RVE.). To prevent rigid body rotations, the three constrained nodes on each RVE should not be collinear.

9.2 J-Integrals

Presto provides a capability to compute the J-integral via a a domain integral.

Known Issue: Currently, the J-Integral evaluation capability is based on assumptions of elastostatics and a stationary crack, and is only implemented for uniform gradient hex elements.

J is analogous to G from linear elastic fracture mechanics ($-\delta\pi/\delta a$) and is the driving force on the crack tip a [1,2]. Crack propagation occurs when $J \geq R$, where R is the material resistance and is often referred to as the critical energy release rate J_{1c}. In the reference configuration, the vectorial form of the J-integral in finite deformation [4] is

$$\boldsymbol{J} = \int_{\Gamma_0} \boldsymbol{\Sigma} \boldsymbol{N} dA \tag{9.1}$$

where $\boldsymbol{\Sigma} = W\boldsymbol{I} - \boldsymbol{F}^T\boldsymbol{P}$ is referred to as the Eshelby energy-momentum tensor [3]. W is the stored energy density in the reference configuration and $\boldsymbol{F}$ and $\boldsymbol{P}$ are the deformation gradient and first Piola-Kirchhoff stress, respectively. Rice [2] realized that because $\boldsymbol{\Sigma}$ is divergence-free in the absence of body forces, one can examine $\boldsymbol{J}$ in the direction of the defect $\boldsymbol{L}$ (unit vector) and obtain a path-independent integral for traction-free crack faces. J can be written as

$$J = \int_{\Gamma_0} \boldsymbol{L} \cdot \boldsymbol{\Sigma} \boldsymbol{N} dA \tag{9.2}$$

and interpreted as a path-independent driving force in the direction of the defect. We note that one can also express $\boldsymbol{\Sigma}$ in terms of $\bar{\boldsymbol{\Sigma}}$, where $\bar{\boldsymbol{\Sigma}} = W\boldsymbol{I} - \boldsymbol{H}^T\boldsymbol{P}$ and $\boldsymbol{H} = \mathrm{Grad}\,\boldsymbol{u}$. Although $\boldsymbol{\Sigma}$ is symmetric and $\bar{\boldsymbol{\Sigma}}$ is not symmetric, they are equivalent when integrated over the body ($\mathrm{Div}\boldsymbol{P} = \boldsymbol{0}$). In fact, differences in the energy-momentum tensor stem from the functional dependence of the stored energy function W. $\boldsymbol{\Sigma}$ and $\bar{\boldsymbol{\Sigma}}$ derive from $W(\boldsymbol{F})$ and $W(\boldsymbol{H})$, respectively. When integrated, both collapse to the familiar 2-D relation for infinitesimal deformations.

$$J = \int_{\Gamma} \boldsymbol{e}_1 \cdot \boldsymbol{\Sigma} \boldsymbol{n} ds = \int_{\Gamma} (W n_1 - u_{i,1}\sigma_{ij} n_j) \mathrm{d}s \tag{9.3}$$

9.2.1 Technique for Computing J

J is often expressed as a line (2D) or surface (3D) integral on a ring surrounding the crack tip. Defining a smooth ring over which to compute this surface integral and performing projections of the required field values onto that ring presents a number of difficulties in the context of a finite element code.

To compute the J-integral in a finite element code, it is more convenient to perform a volume integral over a domain surrounding the crack tip. We can then leverage the information at integration points rather than rely on less accurate projections. To do this, we follow the method described in

[5]. We replace $\boldsymbol{L}$ with a smooth function $\boldsymbol{q}$. On the inner contour of the domain Γ_0, $\boldsymbol{q} = \boldsymbol{L}$. On the outer contour of the domain C_0, $\boldsymbol{q} = \boldsymbol{0}$. Because the outer normal of the domain $\boldsymbol{M}$ is equal and opposite of the normal $\boldsymbol{N}$ on Γ_0, there is a change of sign. For traction-free surfaces, we can apply the divergence theorem, enforce $\mathrm{Div}\boldsymbol{\Sigma} = \boldsymbol{0}$, and find that the energy per unit length $\bar{J}$ is

$$\bar{J} = -\int_{\Omega_0} (\boldsymbol{\Sigma} : \mathrm{Grad}\, \boldsymbol{q})\mathrm{d}V. \tag{9.4}$$

We note that the all the field quantities are given via simulation and we choose to define $\boldsymbol{q}$ on the nodes of the domain $\boldsymbol{q}^I$ and employ the standard finite element shape functions to calculate the gradient. We can specify the crack direction $\boldsymbol{L}$ or assume that the crack will propagate in the direction normal to the crack front $-\boldsymbol{M}$. For a "straight" crack front, $\boldsymbol{L} = -\boldsymbol{M}$. If $\boldsymbol{S}$ is is tangent to the crack front and $\boldsymbol{T}$ is normal to the lower crack surface, $\boldsymbol{S} \times \boldsymbol{M} = \boldsymbol{T}$. We note that for non-planar, curving cracks, $\boldsymbol{M}$, $\boldsymbol{S}$, and $\boldsymbol{T}$ are functions of the arc length S. For ease, we employ the notation $\boldsymbol{N}$ rather than $-\boldsymbol{M}$. For a crack front S_0, we can define the average driving force J_{avg} as

$$J_{avg} = \frac{\bar{J}}{\int_{S_0} \boldsymbol{L} \cdot \boldsymbol{N}\mathrm{d}S}. \tag{9.5}$$

While the average driving force is useful for interpreting experimental findings and obtaining a macroscopic representation of the driving force, we also seek to examine the local driving force $J(S)$. Using the finite element interpolation functions to discretize $\boldsymbol{L}$ through the smooth function $\boldsymbol{q}$, we find $\boldsymbol{q} = \lambda^I \boldsymbol{q}^I$. For a specific node K, we can define $|\boldsymbol{q}^K| = 1$ and $\boldsymbol{q}^I = \boldsymbol{0}$ for all other $I \neq K$ on S_0. Note that we still need to specify the function $\boldsymbol{q}$ in the $\boldsymbol{S} - \boldsymbol{T}$ plane from the inner contour Γ_0 to the outer contour C_0. The resulting expression for the approximate, pointwise driving force at node K on the crack front is

$$J^K = \frac{\bar{J}}{\int_{S_0} \lambda^K \boldsymbol{q}^K \cdot \boldsymbol{N}\mathrm{d}S}. \tag{9.6}$$

Again, we note that if the direction of propagation $\boldsymbol{L}$ is taken in the direction of the normal $\boldsymbol{N}$, the denominator is $\int_{S_0} \lambda^K \mathrm{d}S$. More information regarding the pointwise approximation of J^K can be found in [6,7].

9.2.2 Input Commands

A user can request that J-integrals be computed during the analysis by including one or more `J INTEGRAL` command blocks in the `REGION` scope. This block can contain the following commands:

```
BEGIN J INTEGRAL <jint_name>
  #
  # integral parameter specification commands
  CRACK DIRECTION = <real>dir_x <real>dir_y <real>dir_z
  CRACK PLANE SIDE SET = <string list>side_sets
  CRACK TIP NODE SET = <string list>node_sets
  INTEGRATION RADIUS = <real>int_radius
```

```
  NUMBER OF DOMAINS = <integer>num_domains
  FUNCTION = PLATEAU|PLATEAU_RAMP|LINEAR(PLATEAU)
  SYMMETRY = OFF|ON(OFF)
  #
  # time period selection commands
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END J INTEGRAL <jint_name>
```

A set of parameters must be provided to define the crack geometry and the integration domains used in the calculation of the J-integral. The model must be set up so that there is a sideset on one surface of the crack plane behind the crack tip and a nodeset containing the nodes on the crack tip. Both the `CRACK PLANE SIDE SET` and `CRACK TIP NODE SET` commands must be used to specify the names of the sideset behind the crack tip and the nodeset on the crack tip, respectively.

By default, the direction of crack propagation is computed from the geometry of the crack plane and tip as provided in the crack plane sideset and crack tip nodeset ($\boldsymbol{L} = \boldsymbol{N}$). The `CRACK DIRECTION` command can optionally be used to override the direction of crack propagation ($\boldsymbol{L}$) computed from the geometry. This command takes three real numbers that define the three components of the crack direction vector as arguments.

To fully define the domains used for the domain integrals, the radius of the domains and the number of domains must also be specified. A series of disc-shaped integration domains are formed with varying radii going out from the crack tip. The `INTEGRATION RADIUS` command is used to specify the radius of the outermost domain. The number of integration domains is specified using the `NUMBER OF DOMAINS` command. The radii of the domains increase linearly going from the innermost to the outermost domain.

The weight function $\boldsymbol{q}$ used to calculate the J-integral is specified by use of the option `FUNCTION` command line. The `LINEAR` function set the weight function to 1.0 on the crack front Γ_0 and 0.0 at the edge of the domain C_0, `int_radius` away from the crack tip. The `PLATEAU` function, which is the default behavior, sets all values of the weight function to 1.0 that lie within the domain of integration and all values outside of the domain are set to 0.0. This allows for integration over a single ring of elements at the edge of the domain. The third option for the `FUNCTION` command is `PLATEAU_RAMP`, which for a single domain will take on the same values as the `LINEAR` function. However, when there are multiple domains over the radius `int_radius`, the nth domain will have weight function values of 1.0 over the inner (n-1) domains and will vary from 1.0 to 0.0 over the outer n^{th} ring of the domain. These functions can be seen graphically in Figure 9.2.

We note that in employing both the `PLATEAU` and the `PLATEAU_RAMP` functions, one is effectively taking a line integral at finite radius (albeit different radii). In contrast, the `LINEAR` option can be viewed as taking the $lim\ \Gamma_0 \rightarrow 0^+$. If the model is a half symmetry model with the symmetry plane on the plane of the crack, the optional `SYMMETRY` command can be used to specify that the symmetry conditions be accounted for in the formation of the integration domains and in the evaluation of the integral. The default behavior is for symmetry to not be used.

The user may optionally specify the time periods during which the J-integral is computed. The `ACTIVE PERIODS` and `INACTIVE PERIODS` command lines are used for this purpose. See Sec-

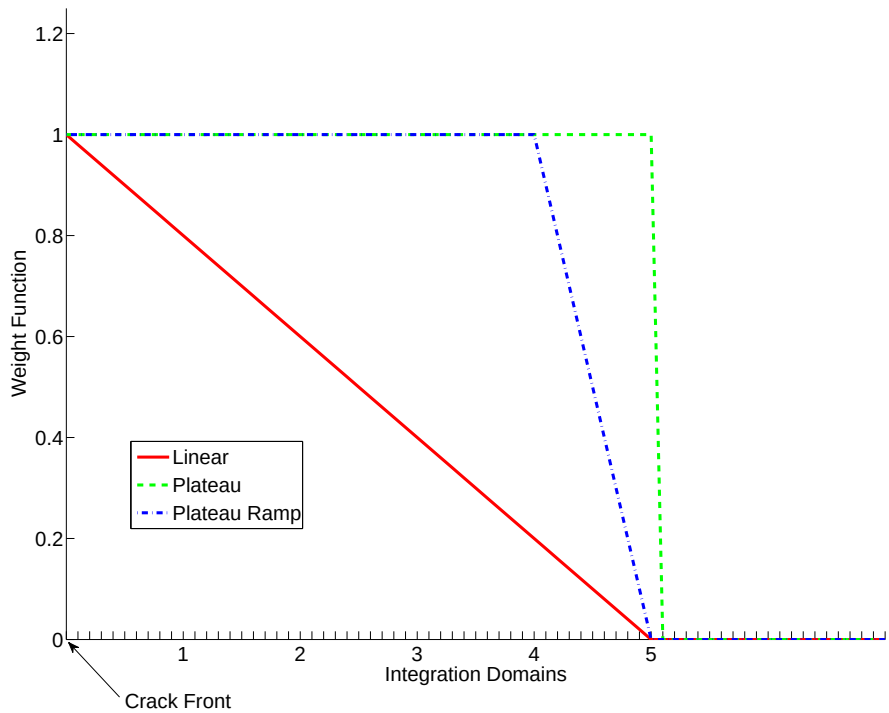

Figure 9.2: Example weight functions for a J-integral integration domain. Weight functions shown for domain 5.

tion 2.5 for more information about these command lines.

9.2.3 Output

A number of variables are generated for output when the computation of the J-integral is requested. The average value of J for each integration domain is available as a global variables, as described in Table 8.3. The pointwise value of J at nodes along the crack for each integration domain is available as a nodal variable, as shown in Table 8.8. Element variables such as the Eshelby energy-momentum tensor and fields defining the integration domains are also available, as listed in Table 8.18.

9.3 Peridynamics

Peridynamics is an extension of classical solid mechanics that allows for the modeling of bodies in which discontinuities occur spontaneously [8, 9, 10, 11, 12]. Unlike the classical continuum formulation, the peridynamic expression for the balance of linear momentum does not contain spatial derivatives and instead is based on an integral equation. For this reason, peridynamics is well suited for modeling phenomena involving spatial discontinuities such as cracking. This section presents

a basic overview of the peridynamics formulation implemented in Presto and suggested guidelines for setting up peridynamic analyses. For a comprehensive review of peridynamics theory, the reader is referred to [12]

9.3.1 Overview

Peridynamics is a nonlocal theory in which any point in the body $\mathbf{x}$ is acted on by forces due to the deformation of all points $\mathbf{x}'$ within a neighborhood of radius δ centered at $\mathbf{x}$. The radius δ is referred to as the horizon and the vector $\mathbf{x}' - \mathbf{x}$ is called a bond.

The peridynamic equation of motion is

$$\begin{aligned} \rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) &= \mathbf{L_u}(\mathbf{x},t) + \mathbf{b}(\mathbf{x},t) \qquad \forall\, \mathbf{x} \in \mathscr{B},\ \ t \geq 0, \\ \mathbf{L_u}(\mathbf{x},t) &= \int_{\mathscr{B}} \left\{ \underline{\mathbf{T}}[\mathbf{x},t]\,\langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{x}',t]\,\langle \mathbf{x} - \mathbf{x}' \rangle \right\} \mathrm{d}V_{\mathbf{x}'}. \end{aligned} \tag{9.7}$$

Here, $\mathscr{B}$ is the reference configuration of the body, ρ is the density in the reference configuration, $\mathbf{u}$ is the displacement, and $\mathbf{b}$ is the body force density.

The relationship between $\mathbf{x}$ and $\mathbf{x}'$ is expressed in terms of the *force state* at $\mathbf{x}$ at time t, $\underline{\mathbf{T}}[\mathbf{x},t]$. The force state is a function that associates with any bond $\mathbf{x}' - \mathbf{x}$ a force density per unit volume $\underline{\mathbf{T}}[\mathbf{x},t]\,\langle \mathbf{x}' - \mathbf{x} \rangle$ acting on $\mathbf{x}$. This force density per unit volume is referred to as a *pairwise force*.

The body $\mathscr{B}$ may be discretized in the reference configuration into a finite number of cells with each cell containing a single node at its center. The integral in Equation (9.7) may then be replaced by a summation,

$$\rho(\mathbf{x})\ddot{\mathbf{u}}_h(\mathbf{x},t) = \sum_{i=0}^{N} \left\{ \underline{\mathbf{T}}[\mathbf{x},t]\left\langle \mathbf{x}_i' - \mathbf{x} \right\rangle - \underline{\mathbf{T}}'[\mathbf{x}_i',t]\left\langle \mathbf{x} - \mathbf{x}_i' \right\rangle \right\} \Delta V_{\mathbf{x}_i'} + \mathbf{b}(\mathbf{x},t), \tag{9.8}$$

where N is the number of cells in the neighborhood of $\mathbf{x}$, $\mathbf{x}_i'$ is the position of the node centered in cell i, and $\Delta V_{\mathbf{x}_i'}$ is the volume of cell i. The length of the bond between two cells is determined as the distance between the nodes at the center of the cells.

Equation (9.8) requires evaluation of the pairwise forces $\underline{\mathbf{T}}[\mathbf{x},t]\left\langle \mathbf{x}_i' - \mathbf{x} \right\rangle$ and $\underline{\mathbf{T}}'[\mathbf{x}_i',t]\left\langle \mathbf{x} - \mathbf{x}_i' \right\rangle$, where the force states $\underline{\mathbf{T}}[\mathbf{x},t]$ and $\underline{\mathbf{T}}'[\mathbf{x}_i',t]$ are, in general, functions of the deformations of all cells within the neighborhoods of $\mathbf{x}$ and $\mathbf{x}_i'$, respectively. A constitutive model is required to compute the force state, $\underline{\mathbf{T}}[\mathbf{x},t]$, in terms of the deformation state in the neighborhood of $\mathbf{x}$ and possibly other variables as well.

The constitutive models available for peridynamics in Presto fall into two categories:

1. Constitutive models that are specific to peridynamics and make use of the complete deformation state when computing internal forces.

2. Classical constitutive models within the LAME library that have been made available from within peridynamics via a wrapper.

Constitutive models developed specifically for peridynamics are generally more robust than classical constitutive models that have been adapted for use within peridynamics, particularly in analyses involving extreme deformation and pervasive fracture. The *Linear Peridynamic Solid* material

model developed by Silling, et al. [10], described below, is the only model of the first type currently available in Presto. The peridynamics interface to classical material models offers a means for accessing the large number of material models within LAME. This interface is based on the computation of an approximate deformation gradient, $\bar{\mathbf{F}}$, described in Section 9.3.3.

9.3.2 Linear Peridynamic Solid Material Model

The linear peridynamic solid material model computes the pairwise force $\underline{\mathbf{T}}[\mathbf{x}, t]\left\langle \mathbf{x}_i' - \mathbf{x} \right\rangle$ acting on $\mathbf{x}$ based on the deformation of all cells $\mathbf{x}'$ within the neighborhood of $\mathbf{x}$,

$$\underline{\mathbf{T}}[\mathbf{x}, t]\left\langle \mathbf{x}_i' - \mathbf{x} \right\rangle = \underline{t}\ \underline{\mathbf{M}}[\mathbf{x}, t]\left\langle \mathbf{x}_i' - \mathbf{x} \right\rangle, \tag{9.9}$$

where $\underline{t}$ is the magnitude of the pairwise force and $\underline{\mathbf{M}}[\mathbf{x}, t]\left\langle \mathbf{x}_i' - \mathbf{x} \right\rangle$ is the unit vector pointing from the deformed position of $\mathbf{x}$ to the deformed position of $\mathbf{x}'$.

The magnitude of the pairwise force in a linear peridynamic solid is given by

$$\underline{t} = \frac{-3p}{m}\underline{\omega}\,\underline{x} + \frac{15\mu}{m}\underline{\omega}\,\underline{e}^d, \qquad p = -k\theta, \tag{9.10}$$

where the p is the peridynamic pressure, θ is the peridynamic dilatation, m is the weighted volume at $\mathbf{x}$, $\underline{\omega}$ is the value of the influence function between cells $\mathbf{x}$ and $\mathbf{x}'$, $\underline{x}$ is the length of the bond $\mathbf{x}' - \mathbf{x}$ in the undeformed configuration, $\underline{e}^d$ is the deviatoric part of the extension $\underline{e}$, and μ and k are material constants (the shear modulus and bulk modulus, respectively). For a complete description of the linear peridynamic solid material model, see [10].

9.3.3 Interface to Classical Material Models

A means for adapting classical material models for use with peridynamics has been developed by Silling, et al. [10]. The approach is based on the evaluation of an approximate deformation gradient, $\bar{\mathbf{F}}$, at $\mathbf{x}$,

$$\bar{\mathbf{F}} = \left(\sum_{i=0}^{N} \underline{\omega}_i\, \underline{\mathbf{Y}}_i \otimes \underline{\mathbf{X}}_i\, \Delta V_{\mathbf{x}_i} \right) \mathbf{K}^{-1}, \tag{9.11}$$

where $\mathbf{K}$ is the *shape tensor*, defined as

$$\mathbf{K} = \sum_{i=0}^{N} \underline{\omega}_i\, \underline{\mathbf{X}}_i \otimes \underline{\mathbf{X}}_i\, \Delta V_{\mathbf{x}_i}. \tag{9.12}$$

Here, $\mathbf{X}$ denotes a vector directed from $\mathbf{x}$ to $\mathbf{x}'$ in the reference configuration, and $\mathbf{Y}$ denotes a vector directed from $\mathbf{x}$ to $\mathbf{x}'$ in the deformed configuration. The operator $\otimes$ denotes dyadic product.

The approximate deformation gradient, as defined in Equation (9.11), allows for the computation of a strain measure or, alternatively, a strain increment, that can be passed to a classical material model. The classical material model is expected to return stress which is then transformed into a pairwise force as follows,

$$\underline{\mathbf{T}}\left\langle \mathbf{x}' - \mathbf{x} \right\rangle = \underline{\omega}\,\sigma\mathbf{K}^{-1}\left\langle \mathbf{x}' - \mathbf{x} \right\rangle, \tag{9.13}$$

where σ is the Piola stress.

The accuracy of the peridynamic interface to classical material models depends strongly on the calculation of the approximate deformation gradient, $\bar{\mathbf{F}}$. The approximate deformation gradient calculation may become unreliable in cases of extreme deformation, or in cases of pervasive material failure in which a large percentage of bonds at a given point are broken. This may result in nonphysical strain values being passed to the classical material model, and a subsequent nonphysical internal force calculation. In addition, the inversion of the shape tensor in Equation (9.13) will fail if the number of bonds for a given cell is less than three, or if all bonds for a given cell are coplanar. For these reasons, Presto will return zero stress for a peridynamic cell with more than 85% of its bonds broken, or for cells with less than three intact bonds that are not coplanar. Under these conditions, a cell will remain active in the simulation and may be acted on by other cells but will not contribute to the internal force. Cells for which all bonds have been broken will behave as mass particles.

Zero-energy modes are possible in the calculation of the approximate deformation gradient, $\bar{\mathbf{F}}$. Zero energy modes may result in nonphysical motion of cells within a simulation, typically manifesting as rapid oscillations. Presto provides a means for suppressing zero-energy modes through peridynamic hourglass control. Peridynamic hourglass control is based on the comparison of cell positions at the end of a timestep with the positions of those cells as predicted by direct application of the approximate deformation gradient computed at a cell $\mathbf{x}$. The suppression of zero-energy modes is achieved by applying a penalty force proportional to the difference between these values.

9.3.4 Modeling Fracture

Peridynamics includes a natural mechanism for modeling fracture through the breaking of peridynamic bonds. In an undamaged material, bonds connect a given cell $\mathbf{x}$ to each cell $\mathbf{x}'$ within its neighborhood in the reference configuration. A damage law dictates the conditions under which individual bonds are broken. Material discontinuities, such as cracks, form as a result of the accumulation of broken bonds.

The critical stretch damage model has been implemented in Presto to allow for the modeling of fracture within a peridynamics simulation. The critical stretch model assigns a damage value of zero (unbroken) or one (broken) as a function of the maximum stretch obtained by a bond and a critical stretch material parameter, s_{crit}. The damage value, ϕ, is given by the relation

$$\begin{aligned} \phi &= 0 \qquad s < s_{\text{crit}} \\ \phi &= 1 \qquad s \geq s_{\text{crit}}, \end{aligned} \tag{9.14}$$

where s is the stretch,

$$s = \frac{y_{\text{max}} - x}{x}. \tag{9.15}$$

Here, y_{max} is the maximum distance between the bonded cells $\mathbf{x}$ and $\mathbf{x}'$ achieved over the duration of the simulation, and x is the distances between $\mathbf{x}$ and $\mathbf{x}'$ in the reference configuration. The use of the maximum distance, y_{max}, ensures that the breaking of bonds is irreversible.

9.3.5 Usage Guidelines

This section provides basic usage guidelines for carrying out peridynamic analyses with Presto. Suggestions are provided for constructing input mesh files, applying boundary conditions, and selecting appropriate values for peridynamic parameters. For a description of the `PERIDYNAMICS SECTION` input syntax, see Section 5.2.13.

Model generation. A set of mesh generation tools is available for the construction of input meshes compatible with the peridynamics capabilities of Presto. The suggested workflow for creating a peridynamics-compatible input mesh is as follows:

1. Construct a hexahedral mesh containing the peridynamics mesh parts using Cubit.
2. Convert the elements in the resulting mesh file from hexahedron elements to sphere elements using the SEACAS tool `sphgen3d`.
3. Convert the Exodus I database produced by `sphgen3d` to the Exodus II format with the SEACAS tool `ex1ex2v2`.
4. In the case of analyses using both peridynamics and classical finite element analysis, or in the case where bond cutting blocks are used to control the creation of peridynamic bonds, combine an input mesh containing standard finite elements with an input mesh discretized with sphere elements using the SEACAS tool `gjoin`.

Warning: Nodesets defined on a hexahedral mesh are lost when the mesh is converted to sphere elements with `sphgen3d`. In addition to eliminating the nodesets defined in the original hexahedral mesh file, `sphgen3d` automatically creates a new nodeset corresponding to each mesh part in the model. Name conflicts will occur if the resulting sphere-element mesh is combined with a standard finite element mesh containing nodesets with names identical to those created automatically by `sphgen3d`.

Horizon. The horizon defines the region of nonlocality for a given cell $\mathbf{x}$ in a peridynamics analysis. Analysis results may be strongly dependent on the choice of the horizon. For example, the choice of horizon affects the localization of forces in the neighborhood of a discontinuity, as well as the dispersion of waves traveling through mesh parts modeled with peridynamics. In addition to affecting material behavior, the choice of horizon has a strong effect on the computational cost of a peridynamic analysis. In extreme cases, a large horizon may render an analysis intractable. A recommend value of the horizon is three times the mesh spacing. When using the `SCALE BY ELEMENT RADIUS` option, this corresponds to a horizon value of approximately five.

Boundary conditions. Boundary conditions for a nonlocal approach such as peridynamics differ fundamentally from boundary conditions in classical mechanics. To capture exactly the material response in the vicinity of a boundary condition, the boundary condition in a nonlocal model must be applied over a volume. For example, displacement boundary conditions applied at the surface of a mesh part should be applied to a volume that reaches into the body of the mesh part a distance

equal to the peridynamic horizon. This is not always practical (as with contact), and in many cases satisfactory results can be obtained by applying boundary conditions at the surface only. Users should be aware, however, that nonphysical edge effects will be present if boundary conditions are not applied in a way that is consistent with the nonlocal nature of peridynamics.

The application of boundary conditions for peridynamics analyses in Presto is also affected by the restrictions placed on nodeset definitions by `sphgen3d`. Nodesets defined on a hexahedral mesh are lost when the mesh is converted to sphere elements by `sphgen3d`. For this reason, boundary conditions must be applied on blocks. This requires careful construction of the initial hexahedral mesh to include blocks that correspond to regions over which boundary conditions will be applied.

Timestep. The timestep computed by peridynamic elements in Presto is an approximate value that may require modification to ensure a stable analysis. Peridynamic elements in Presto compute a stable time step under the assumptions of linear material behavior and the approximate equivalence of the bulk modulus in *state-based* peridynamics with the micromodulus in *bond-based* peridynamics. For details regarding the timestep computed by peridynamic elements in Presto, see [9]. Because the timestep computed by peridynamic elements is not guaranteed to be stable, it is recommended that the timestep be reduced using a scale factor of approximately 0.75. This can be achieved using the `TIME STEP SCALE FACTOR` command described in Chapter 3.

Hourglass stiffness. The use of classical material models with peridynamics in Presto may require the application of hourglass stiffness to reduce the effects of zero-energy modes in the computation of the approximate deformation gradient, $\bar{\mathbf{F}}$. Recommended values for hourglass stiffness are in the range 0.01 - 0.05. The value of hourglass stiffness is multiplied by a material's bulk modulus when computing the stiffening forces for peridynamics hourglass control. For a description of the corresponding input syntax, see Section 5.2.13.

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Chapter 10

User Subroutines

User-defined subroutines is a functionality shared by Adagio and Presto. This chapter discusses when and how to use user-defined subroutines. There are examples of user-defined subroutines in the latter part of this chapter. Some of the examples are code specific, i.e., they are applicable to Presto rather than Adagio or vice versa. All examples, regardless of their applicability, do provide important information about how to use the command options available for user-defined subroutines.

In the introductory part of Chapter 10, we first describe, in general, possible applications for the user subroutine functionality in Presto. Then, again in general, we describe the various pieces and steps that are required by the user to implement a user subroutine. Subsequently, we focus on various aspects of implementing the user subroutine functionality. Section 10.1 describes the details of the user subroutine. Section 10.2 describes the command lines associated with user subroutines that appear in the Presto input file. In Section 10.3, we explain how to build and use a version of Presto that incorporates your user subroutine. Finally, Section 10.4 provides examples of actual user subroutines, and Section 10.5 lists some subroutines that are now in the standard user library.

Applications. User subroutines are primarily intended as complex function evaluators that are to be used in conjunction with existing Presto capability (boundary conditions, element death, user output, etc.). For example, suppose we want to have a prescribed displacement boundary condition applied to a set of nodes, and we want the displacement at each node to vary with both time and spatial location of the node. The standard function option associated with the prescribed direction displacement boundary condition in Presto only allows for time variation; i.e., at any given time, the direction and the magnitude of the displacement at each node, regardless of the spatial location of the node, are the same. If we wanted to have a spatial variation of the displacement field in addition to the time variation, it would be necessary to implement a user subroutine for the prescribed direction displacement boundary condition. Other examples of possible uses of user subroutines are as follows:

- Element death is determined by a complex function based on a set of physical parameters and element stress.

- The user wants to compute the total contact force acting on a given surface.
- Element stress information must be transformed to a local coordinate system so that the stress values will be meaningful.
- An aerodynamic pressure based on velocity and surface normal is applied to a specified surface.

Some capability exists for using mesh connectivity. It is possible to compute an element quantity based on values at the element nodes.

Some difficulties might occur in parallel applications. If computations for element A depend on quantities in element B and elements A and B are on different processors, then the computations for A may not have access to quantities in element B. For most computations in user subroutines, however, this should not be a problem.

Implementing completely new capabilities, particularly if these capabilities involve parallel computing, may be difficult or impossible with user subroutines.

General Pieces and Steps. A number of pieces and steps are required to make use of user subroutines. Here, we present a brief description of the pieces and steps that a user will need for user subroutines without going into detail. The details are discussed in later parts of this chapter.

1. You must first determine whether your application fits in the user subroutine format. This can be done by considering the above requirements and examining the description of commands for functionality in Presto. For example, the basic kinematic boundary conditions and force conditions allow for the use of user subroutines. The description of these commands includes a discussion of how a user subroutine could be applied and what command line will invoke a user subroutine.

2. If you determine that your application can make use of the user subroutine functionality in Presto, you will then need to write the subroutine. The parts of the subroutine that interface to Presto have specified formats. The details of these interfaces are described in later sections. One part of the subroutine with a specified format is the call list. Other parts of the subroutine with a specified format are code that will do the following:

   - Read parameters from the Presto input file
   - Access a variety of information—field variables, analysis time, etc.—from Presto
   - Store computed quantities

   Parameters are values they may be passed from the Presto input file to the user subroutine. Suppose that the spatial variation for some quantity in the user subroutine uses some characteristic length and the user wishes to examine results generated by using several different values of the characteristic length. By setting up the characteristic length as a parameter, the value for the parameter in the user subroutine can easily be changed by changing the value for the parameter in the input file. This lets the user change the value for a variable inside the user subroutine without having to recompile the user subroutine.

The portion of your subroutine not built on the Presto specifications will reflect your specific application. The code to implement your application may include a loop over nodes that prescribes a displacement based on the current time for the analysis and the spatial location of the node.

3. After you write the user subroutine, you will need to have a command line in your input file that tells Presto you want to use the user subroutine you have written. For example, if your user subroutine is a specialized prescribed displacement boundary condition, then inside a `PRESCRIBED DISPLACEMENT` command block, you will have a command line of the form

   ```
   NODE SET SUBROUTINE = <string>subroutine_name
   ```

   that provides the name of your user subroutine.

4. Following the invocation of the user subroutine, there may be command lines for various parameters associated with the user subroutine. There may also be some additional command lines in other sections of the code required for your application. For example, you may have to add command lines in the region scope that will create an internal variable associated with a computed quantity so that the computed quantity can be written to the results file.

5. Once you have constructed the user subroutine, which is a FORTRAN file, and the Presto input file, you can build an executable version of Presto that will run your user subroutine. Your Presto run will then incorporate the functionality you have created in your user subroutine.

Figure 10.1 presents a very high-level overview of the various components that work together to implement the user subroutine functionality. The two main components needed for user subroutines, which are commands in the Presto input file and the actual user subroutine, are represented by the two columns in Figure 10.1.

Presto Input File Command Blocks and Command Lines

in domain scope
USER SUBROUTINE FILE
{This command line points to a user file.}

in region scope
NODE SET SUBROUTINE
SURFACE SUBROUTINE
ELEMENT BLOCK SUBROUTINE
{The above three command lines can point to a user subroutine.}
SUBROUTINE DEBUGGING OFF
SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER
SUBROUTINE INTEGER PARAMETER
SUBROUTINE STRING PARAMETER
{Parameter information in input file is transferred to subroutine, as indicated by arrow.}

in region scope – related commands
TIME STEP INITIALIZATION
USER VARIABLE
USER OUTPUT
RESULTS OUTPUT
HISTORY OUTPUT

File Containing One or More Subroutines

User-Defined Subroutine Interface

subroutine sub_name(call list)
{declaration of variables}
{retrieve parameters from Presto input file}
{query Presto for information}
{application specific code
.
.
}
{write computed values}
END

Query Functions
aupst_get_real_param
aupst_get_integer_param
aupst_get_string_param
aupst_evaluate_function
aupst_get_time
aupst_check_node_var, aupst_check_elem_var
aupst_get_node_var, aupst_get_elem_var
aupst_put_node_var, aupst_put_elem_var
aupst_check_global_var
aupst_get_global_var, aupst_put_global_var
aupst_local_put_global_var
aupst_get_elem_topology, aupst_get_elem_nodes
aupst_get_face_topology, aupts_get_face_nodes
aupst_get_one_elem_centroid
aupst_get_point
aupst_get_proc_num

Library Subroutines
aupst_cyl_transform
aupst_rec_transform

Figure 10.1: Overview of components required to implement user subroutine functionality, excluding compilation and execution commands.

10.1 User Subroutines: Programming

Currently, user subroutines are only supported in FORTRAN 77. Any subroutine that can be compiled with a FORTRAN 77 compiler on the target execution machine can be used. The user should be aware that some computers support different FORTRAN language extensions than others. (In the future, other languages such as FORTRAN 90, C, and C++ may be supported.)

User subroutine variable types must interface directly with the matching variable types used in the main Presto code. Thus, the FORTRAN 77 subroutines should use only integer, double precision, or character types for any data used in the interface or in any query function. Using the wrong data type may yield unpredictable results. The methods used to pass character types from Presto to FORTRAN user subroutines can be machine-dependent, but generally this functionality works quite well.

The basic structure for the user subroutine is as follows:

```
subroutine sub_name(call list)
{declaration of variables}
{retrieve parameters from Presto input file}
{query Presto for information}
{application-specific code
    .
    .
}
{write computed values}
END
```

In general, the user will begin the subroutine with variable declarations. After the variable declarations, the user can then query the Presto input file for parameters. Additional Presto information such as field variables or element topology can then be retrieved from Presto. Once the user has collected all the information for the application, the application-specific portion of the code can be written. After the application-specific code is complete, the user may store computed values.

Section 10.1.1 through Section 10.1.3 describe in detail the format for the interfaces to Presto that will allow the user to make the subroutine call, retrieve information from Presto, and write computed values. In these sections, mesh entities can be a node, an element face, or an element.

10.1.1 Subroutine Interface

The following interface is used for all user subroutines:

```
subroutine sub_name(int  num_objects,
           int  num_values,
           real evaluation_time,
           int  object_ids[],
           real output_values[],
           int  output_flags[],
           int  error_code)
```

The name of the user subroutine, `sub_name`, is selected by the user. Avoid names for the subroutine that are longer than 10 characters. This may cause build problems on some systems.

A detailed description of the input and output parameters is provided in Table 10.1 and Table 10.2.

Table 10.1: Subroutine Input Parameters

Input Parameter	**Data Type**	**Parameter Description**
num_objects	Integer	Number of input mesh entities. For example, if the subroutine is a node set subroutine, this would be the number of nodes on which the subroutine will operate.
num_values	Integer	Number of return values. This is the number of values per mesh entity.
evaluation_time	Real	Time at which the subroutine should be evaluated. This may vary slightly from the current analysis time. Velocities for example are evaluated one-half time step ahead.
object_ids (num_objects)	Integer	Array of mesh-entity identification numbers. The array has a length of num_objects. The input numbers are the global numbers of the input objects. The object identification numbers can be used to query information about a mesh entity.

10.1.2 Query Functions

Presto follows a design philosophy for user subroutines that a minimal amount of information should be passed through the call list. Additional information may be queried from within the subroutine. A user subroutine may query a wide variety of information from Presto.

Table 10.2: Subroutine Output Parameters

Output Parameter	**Data Type**	**Parameter Description**
output_values (num_values, num_objects)	Integer	Array of output values computed by the subroutine. The number of output values will be either the number of mesh entities or some multiple of the number of mesh entities. For example, if there were six nodes (num_objects equals 6) and one value was to be computed per node, the length of output_values would be 6. Similarly, if there were six nodes (num_objects equals 6) and three values were to be computed for each node (as for acceleration, which has X-, Y-, and Z-components), the length of output_values would be 18.
output_flags (num_objects)	Integer	Array of returned flags for each set of data values. When used, this array will generally have a length of num_objects. The usage of the flags depends on subroutine type; the flags are currently used only for element death and for kinematic boundary conditions. For the kinematic boundary conditions (displacement, velocity, acceleration) a flag of –1 means ignore the constraint, a flag of 0 means set the absolute constraint value, and a flag of 1 means set the constraint with direction and distance.
error_code	Integer	Error code returned by the user subroutine. A value of 0 indicates no errors. Any value other than zero is an error. If the return value is nonzero, Presto will report the error code and terminate the analysis.

10.1.2.1 Parameter Query

A number of user subroutine parameters may be set as described in Section 10.2.2.3. These subroutine parameters can be obtained from the Presto input file via the query functions listed below.

```
aupst_get_real_param(string var_name, real var_value,
                     int error_code)

aupst_get_integer_param(string var_name, int var_value,
                        int error_code)

aupst_get_string_param(string var_name, string var_value,
                     int error_code)
```

All three of these subroutine calls are tied to a corresponding "parameter" command line that will appear in the Presto input file. The parameter command lines are described in Section 10.2.2.3. These command lines are named based on the type of value they store, i.e., `SUBROUTINE REAL PARAMETER`, `SUBROUTINE INTEGER PARAMETER`, and `SUBROUTINE STRING PARAMETER`.

We will use the example of a real parameter to show how the subroutine call works in conjunction with the `SUBROUTINE REAL PARAMETER` command line. Suppose we have a real parameter radius that is set to a value of 2.75 on the `SUBROUTINE REAL PARAMETER` command line:

```
SUBROUTINE REAL PARAMETER: radius = 2.75
```

Also suppose we have a call to `aupst_get_real_parameter` in the user subroutine:

```
call aupst_get_real_parameter("radius",cyl_radius,error_code)
```

In the call to `aupst_get_real_parameter`, we have `var_name` set to `radius` and `var_value` defined as the real FORTRAN variable `cyl_radius`. The call to `aupst_get_real_parameter` will assign the value 2.75 to the FORTRAN variable `cyl_radius`. A similar pattern is followed for integer and string parameters.

The arguments for the parameter-related query functions are described in Table 10.3, Table 10.4, and Table 10.5. The function is repeated prior to each table for easy reference.

```
aupst_get_real_param(string var_name, real var_value,
                     int error_code)
```

Table 10.3: aupst_get_real_param Arguments

Parameter	**Usage**	**Data Type**	**Description**
var_name	Input	String	Name of a real-valued subroutine parameter, as defined in the Presto input file via the `SUBROUTINE REAL PARAMETER` command line.
var_value	Output	Real	Name of a real variable to be used in the FORTRAN subroutine. The FORTRAN variable var_value will be set to the value specified by the `SUBROUTINE REAL PARAMETER` command line.
error_code	Output	Integer	Error code indicating status of retrieving the parameter value from the input file. If the retrieval is successful, error_code is set to 0. If the parameter is not found or is the wrong type, error_code is set to a value other than 0.

```
aupst_get_integer_param(string var_name, int var_value,
                        int error_code)
```

Table 10.4: aupst_get_integer_param Arguments

Parameter	**Usage**	**Data Type**	**Description**
var_name	Input	String	Name of an integer-valued subroutine parameter, as defined in the Presto input file via the `SUBROUTINE INTEGER PARAMETER` command line.
var_value	Output	Integer	Name of an integer variable to be used in the FORTRAN subroutine. The FORTRAN variable var_value will be set to the value specified by the `SUBROUTINE INTEGER PARAMETER` command line.
error_code	Output	Integer	Error code indicating status of retrieving the parameter value from the input file. If the retrieval is successful, error_code is set to 0. If the parameter is not found or is the wrong type, error_code is set to a value other than 0.

```
aupst_get_string_param(string var_name, string var_value,
                       int error_code)
```

Table 10.5: aupst_get_string_param Arguments

Parameter	**Usage**	**Data Type**	**Description**
var_name	Input	String	Name of a string-valued subroutine parameter, as defined in the Presto input file via the `SUBROUTINE STRING PARAMETER` command line.
var_value	Output	String	Name of a string variable to be used in the FORTRAN subroutine. The FORTRAN variable var_value will be set to the value specified by the `SUBROUTINE STRING PARAMETER` command line.
error_code	Output	Integer	Error code indicating status of retrieving the parameter value from the input file. If the retrieval is successful, error_code is set to 0. If the parameter is not found or is the wrong type, error_code is set to a value other than 0.

10.1.2.2 Function Data Query

The function data query routine listed below may be used for extracting data from a function that is defined in a `DEFINITION FOR FUNCTION` command block in the Presto input file. This query allows the user to directly access information stored in a function defined in the Presto input file.

```
aupst_evaluate_function(string func_name, real input_times[],
                        int num_times, real output_data[])
```

The arguments for this function are described in Table 10.6.

Table 10.6: aupst_evaluate_function Arguments

Parameter	Usage	Data Type	Description
func_name	Input	String	Name of the function to look up.
input_times (num_times)	Input	Real	Array of times used to extract values of the function.
num_times	Input	Integer	Length of the array input_times.
output_data (num_times)	Output	Real	Array of output values of the named function at the specified times.

10.1.2.3 Time Query

The time query function can be used to determine the current analysis time. This is the time associated with the new time step. This time may not be equivalent to the `evaluation_time` argument passed into the subroutine (see Section 10.1.1, Table 10.1) as some boundary conditions need to be evaluated at different times than others. The parameter of the time query function listed below is given in Table 10.7.

```
aupst_get_time(real time)
```

Table 10.7: aupst_get_time Argument

Parameter	Usage	Data Type	Description
time	Output	Real	Current analysis time.

10.1.2.4 Field Variables

Field variables (displacements, stresses, etc.) may be defined on groups of mesh entities. A number of queries are available for getting and putting field variables. These queries involve passing in a set of mesh-entity identification numbers to receive field values on the mesh entities. There are

query functions to check for the existence and size of a field, functions to retrieve the field values, and functions to store new variables in a field. The field query functions listed below can be used to extract any nodal or element variable field.

```
aupst_check_node_var(int num_nodes, int num_components,
                     int node_ids[], string var_name,
                     int error_code)

aupst_check_elem_var(int num_elems, int num_components,
                     int elem_ids[], string var_name,
                     int error_code)

aupst_get_node_var(int num_nodes, int num_components,
                   int node_ids[], real return_data[],
                   string var_name, int error_code)

aupst_get_elem_var(int num_elems, int num_components,
                   int elem_ids[], real return_data[],
                   string var_name, int error_code)

aupst_get_elem_var_offset(int num_elems, int num_components,
                          int offset, int elem_ids[],
                          real return_data[], string var_name,
                          int error_code)

aupst_put_node_var(int num_nodes, int num_components,
                   int node_ids[], real new_data[],
                   string var_name, int error_code)

aupst_put_elem_var(int num_elems, int num_components,
                   int elem_ids[], real new_data[],
                   string var_name, int error_code)

aupst_put_elem_var_offset(int num_elems, int num_components,
                          int offset, int elem_ids[],
                          real new_data[], string var_name,
                          int error_code)
```

The arrays where data are stored are static arrays. These arrays of a set size will be declared at the beginning of a user subroutine. The query functions to check for the existence and size of a field can be used to ensure that the size of the array of information being returned from Presto does not exceed the size of the array allocated by the user.

The arguments to field query functions are defined in Table 10.8 through Table 10.15. The function is repeated before each table for easy reference.

```
aupst_check_node_var(int num_nodes, int num_components,
                     int node_ids[], string var_name,
                     int error_code)
```

Table 10.8: aupst_check_node_var Arguments

Parameter	**Usage**	**Data Type**	**Description**
num_nodes	Input	Integer	Number of nodes used to extract field information.
num_components	Output	Integer	Number of components in the field information. A displacement field at a node has three components, for example.
node_ids (num_nodes)	Input	Integer	Array of size num_nodes listing the node identification number for each node where field information will be retrieved.
var_name	Input	String	Name of the field variable. The field variable must be a defined Presto variable.
error_code	Output	Integer	Error code indicating status of retrieving the field. If the retrieval is successful, error_code is set to 0. If a nonzero value is returned for error_code, the field variable does not exist or is not defined on one or more of the input nodes.

```
aupst_check_elem_var(int num_elems, int num_components,
                     int elem_ids[], string var_name,
                     int error_code)
```

Table 10.9: aupst_check_elem_var Arguments

Parameter	**Usage**	**Data Type**	**Description**
num_elems	Input	Integer	Number of elements used to extract field information.
num_components	Output	Integer	Number of components in the field information. A stress field for a an eight-node hexahedron element has six components, for example.
elem_ids (num_elems)	Input	Integer	Array of size num_elems listing the element identification number for each element where field information will be retrieved.
var_name	Input	String	Name of the field variable. The field variable must be a defined Presto variable.
error_code	Output	Integer	Error code indicating status of retrieving the field. If the retrieval is successful, error_code is set to 0. If a nonzero value is returned for error_code, the field variable does not exist or is not defined on one or more of the input nodes.

```
aupst_get_node_var(int num_nodes, int num_components,
                   int node_ids[], real return_data[],
                   string var_name, int error_code)
```

Table 10.10: aupst_get_node_var Arguments

Parameter	**Usage**	**Data Type**	**Description**
num_nodes	Input	Integer	Number of nodes used to extract field information.
num_components	Input	Integer	Number of components in the field information. A displacement field at a node has three components, for example.
node_ids (num_nodes)	Input	Integer	Array of size num_nodes listing the node identification number for each node where field information will be retrieved.
return_data (num_components, num_nodes)	Output	Real	Array of size num_components × num_nodes containing the field data at each node.
var_name	Input	String	Name of the field variable. The field variable must be a defined Presto variable.
error_code	Output	Integer	Error code indicating status of retrieving the field. If the retrieval is successful, error_code is set to 0. If a nonzero value is returned for error_code, the field variable does not exist or is not defined on one or more of the input nodes.

```
aupst_get_elem_var(int num_elems, int num_components,
                   int elem_ids[], real return_data[],
                   string var_name, int error_code)
```

Table 10.11: aupst_get_elem_var Arguments

Parameter	**Usage**	**Data Type**	**Description**
num_elems	Input	Integer	Number of elements used to extract field information.
num_components	Input	Integer	Number of components in the field information. A stress field for a an eight-node hexahedron element has six components, for example.
elem_ids (num_elems)	Input	Integer	Array of size num_elems listing the element identification number for each element where field information will be retrieved.
return_data (num_components, num_elems)	Output	Real	Array of size num_components × num_elems containing the field data for each element.
var_name	Input	String	Name of the field variable. The field variable must be a defined Presto variable.
error_code	Output	Integer	Error code indicating status of retrieving the field. If the retrieval is successful, error_code is set to 0. If a nonzero value is returned for error_code, the field variable does not exist or is not defined on one or more of the input nodes.

```
aupst_get_elem_var_offset(int num_elems, int num_components,
                          int offset, int elem_ids[],
                          real return_data[], string var_name,
                          int error_code)
```

Table 10.12: aupst_get_elem_var_offset Arguments

Parameter	**Usage**	**Data Type**	**Description**
num_elems	Input	Integer	Number of elements used to extract field information.
num_components	Input	Integer	Number of components in the field information. A stress field for an eight-node hexahedron element has six components, for example.
offset	Input	Integer	Offset into var_name field variable at which to get data.
elem_ids (num_elems)	Input	Integer	Array of size num_elems listing the element identification number for each element where field information will be retrieved.
return_data (num_components, num_elems)	Output	Real	Array of size num_components × num_elems containing the field data for each element.
var_name	Input	String	Name of the field variable. The field variable must be a defined Presto variable.
error_code	Output	Integer	Error code indicating status of retrieving the field. If the retrieval is successful, error_code is set to 0. If a nonzero value is returned for error_code, the field variable does not exist or is not defined on one or more of the input nodes.

```
aupst_put_node_var(int num_nodes, int num_components,
                   int node_ids[], real new_data[],
                   string var_name, int error_code)
```

Table 10.13: aupst_put_node_var Arguments

Parameter	**Usage**	**Data Type**	**Description**
num_nodes	Input	Integer	Number of nodes for which the user will specify the field data.
num_components	Input	Integer	Number of components in the field information. A displacement field at a node has three components, for example.
node_ids (num_nodes)	Input	Integer	Array of size num_nodes listing the node identification number for each node where field information will be retrieved.
new_data (num_components, num_nodes)	Input	Real	Array of size num_components × num_nodes containing the new data for the field.
var_name	Input	String	Name of the field variable. The field variable must be a defined Presto variable.
error_code	Output	Integer	Error code indicating status of retrieving the field. If the retrieval is successful, error_code is set to 0. If a nonzero value is returned for error_code, the field variable does not exist or is not defined on one or more of the input nodes.

```
aupst_put_elem_var(int num_elems, int num_components,
                   int elem_ids[], real new_data[],
                   string var_name, int error_code)
```

Table 10.14: aupst_put_elem_var Arguments

Parameter	**Usage**	**Data Type**	**Description**
num_elems	Input	Integer	Number of elements for which the user will specify the field data.
num_components	Input	Integer	Number of components in the field information. A stress field for a an eight-node hexahedron element has six components, for example.
elem_ids (num_elems)	Input	Integer	Array of size num_elems listing the element identification number for each element where field information will be retrieved.
new_data (num_components, num_elems)	Input	Real	Array of size num_components × num_elems containing the new data for the field.
var_name	Input	String	Name of the field variable. The field variable must be a defined Presto variable.
error_code	Output	Integer	Error code indicating status of retrieving the field. If the retrieval is successful, error_code is set to 0. If a nonzero value is returned for error_code, the field variable does not exist or is not defined on one or more of the input nodes.

```
aupst_put_elem_var_offset(int num_elems, int num_components,
                          int offset, int elem_ids[],
                          real new_data[], string var_name,
                          int error_code)
```

Table 10.15: aupst_put_elem_var_offset Arguments

Parameter	Usage	Data Type	Description
num_elems	Input	Integer	Number of elements for which the user will specify the field data.
num_components	Input	Integer	Number of components in the field information. A stress field for an eight-node hexahedron element has six components, for example.
offset	Input	Integer	Offset into var_name field variable at which to put data.
elem_ids (num_elems)	Input	Integer	Array of size num_elems listing the element identification number for each element where field information will be retrieved.
new_data (num_components, num_elems)	Input	Real	Array of size num_components × num_elems containing the new data for the field.
var_name	Input	String	Name of the field variable. The field variable must be a defined Presto variable.
error_code	Output	Integer	Error code indicating status of retrieving the field. If the retrieval is successful, error_code is set to 0. If a nonzero value is returned for error_code, the field variable does not exist or is not defined on one or more of the input nodes.

10.1.2.5 Global Variables

Global variables may be extracted or set from user subroutines. A global variable has a single value for a given region.

Global variables have limited support for parallel operations. There are two subroutines to perform parallel modification of global variables: `aupst_put_global_var` and `aupst_local_put_global_var`.

- The subroutine `aupst_local_put_global_var` only modifies a temporary local copy of the global variable. The local copies on the various processors are reduced to create the true global value at the end of the time step. Global variables set with `aupst_local_put_global_var` do not have the single processor value available immediately. The true global variable will not be available through the `aupst_get_global_var` routine until the next time step.

- The subroutine `aupst_put_global_var` attempts to immediately modify and perform a parallel reduction of the value of a global variable. Care must be taken to call this routine on all processors at the same time with the same arguments. Failure to call the routine from all processors will result in the code hanging. For some types of subroutines this is not possible or reliable. For example, a boundary condition subroutine may not be called at all on a processor that contains no nodes in the set of nodes assigned to the boundary condition. It is recommended that `aupst_local_put_global_var` only be used in conjunction with a user subroutine referenced in a `USER OUTPUT` command block (Section 8.2.2).

Only user-defined global variables may be modified by the user subroutine (see Section 10.2.4). However, any global variable that exists on the region may be checked or extracted. The following subroutine calls pertain to global variables:

```
aupst_get_global_var(int num_comp, real return_data,
                     string var_name, int error_code)

aupst_put_global_var(int num_comp, real input_data,
                     string reduction_type,
                     string var_name, int error_code)

aupst_local_put_global_var(int num_comp, real input_data,
                     string var_name, string reduction_type,
                     int error_code)
```

The arguments for subroutine calls pertaining to global variables are defined in Table 10.16 through Table 10.19. The call is repeated before each table for easy reference.

```
aupst_check_global_var(int num_comp, string var_name
                       int error_code)
```

Table 10.16: aupst_check_global_var Arguments

Parameter	Usage	Data Type	Description
num_comp	Output	Integer	Number of components of the global variable.
var_name	Input	String	Name of the global variable.
error_code	Output	Integer	Error code indicating status of accessing the global variable. If there is no error in accessing this variable, error_code is set to 0. A nonzero value of error_code means the global variable does not exist or in some way cannot be accessed.

```
aupst_get_global_var(int num_comp, real return_data,
                     string var_name, int error_code)
```

Table 10.17: aupst_get_global_var Arguments

Parameter	Usage	Data Type	Description
num_comp	Input	Integer	Number of components of the global variable.
return_data	Output	Real	Value of the global variable.
var_name	Input	String	Name of the global variable.
error_code	Output	Integer	Error code indicating status of accessing the global variable. If there is no error in accessing this variable, error_code is set to 0. A nonzero value of error_code means the global variable does not exist or in some way cannot be accessed.

```
aupst_put_global_var(int num_comp, real input_data,
                     string reduction_type,
                     string var_name, int error_code)
```

Table 10.18: aupst_put_global_var Arguments

Parameter	**Usage**	**Data Type**	**Description**
num_comp	Input	Integer	Number of components of the global variable.
input_data	Input	Real	New value of the global variable.
reduction_type	Input	String	Type of parallel reduction to perform on the variable. Options are “sum”, “min”, “max”, and “none”.
var_name	Input	String	Name of the global variable.
error_code	Output	Integer	Error code indicating status of accessing the global variable. If there is no error in accessing this variable, error_code is set to 0. A nonzero value of error_code means the global variable does not exist, in some way cannot be accessed, or may not be overwritten.

```
aupst_local_put_global_var(int num_comp, real input_data,
                           string var_name,
                           string reduction_type,
                           int error_code)
```

Table 10.19: aupst_local_put_global_var Arguments

Parameter	Usage	Data Type	Description
num_comp	Input	Integer	Number of components of the global variable.
input_data	Input	Real	New value of the global variable.
reduction_type	Input	String	Type of parallel reduction to perform on the variable. Options are “sum”, “min”, and “max”. The operation type specified here must match the operation type given to the user-defined global variable when it is defined in the Presto input file.
var_name	Input	String	Name of the global variable.
error_code	Output	Integer	Error code indicating status of accessing the global variable. If there is no error in accessing this variable, error_code is set to 0. A nonzero value of error_code means the global variable does not exist, in some way cannot be accessed, or may not be overwritten.

10.1.2.6 Topology Extraction

The element and surface subroutines operate on groups of elements or faces. The elements and faces may have a variety of topologies. Topology queries can be used to get topological data about elements and faces. The topology of an object is represented by an integer. The integer is formed from a function of the number of dimensions, vertices, and nodes of an object. The topology of an object is given by:

```
topology = num_node + 100 * num_vert + 10000 * num_dim
```

In a FORTRAN routine, the number of nodes can easily be extracted with the mod function:

```
num_node = mod(topo,100)
num_vert = mod(topo / 100, 100)
num_dim  = mod(topo / 10000, 100)
```

Table 10.20: Topologies Used by Presto

Topology	Element / Face Type
00101	One-node particle
10202	Two-node beam, truss, or damper
20404	Four-node quadrilateral
20303	Three-node triangle
20304	Four-node triangle
20306	Six-node triangle
30404	Four-node tetrahedron
30408	Eight-node tetrahedron
30410	Ten-node tetrahedron
30808	Eight-node hexahedron

Table 10.20 lists the topologies currently in use by Presto.

The following topology query functions are available in Presto:

```
aupst_get_elem_topology(int num_elems, int elem_ids[],
                        int topology[], int error_code)

aupst_get_elem_nodes(int num_elems, int elem_ids[],
                     int elem_node_ids[], int error_code)

aupst_get_face_topology(int num_faces, int face_ids[],
                        int topology[], int error_code)

aupst_get_face_nodes(int num_faces, int face_ids[],
                     int face_node_ids[], int error_code)
```

The arguments for the topology extraction functions are defined in Table 10.21 through Table 10.24. The function is repeated before each table for easy reference.

```
aupst_get_elem_topology(int num_elems, int elem_ids[],
                        int topology[], int error_code)
```

Table 10.21: aupst_get_elem_topology Arguments

Parameter	**Usage**	**Data Type**	**Description**
num_elems	Input	Integer	Number of elements from which the topology will be extracted.
elem_ids (num_elems)	Input	Integer	Array of length num_elems listing the element identification for each element from which the topology will be extracted.
topology (num_elems)	Output	Integer	Array of length num_elems that has the topology for each element. See Table 8.18.
error_code	Output	Integer	Error code indicating status of retrieving the element identification numbers. If the retrieval is successful, error_code is set to 0. A nonzero value is returned for error_code if one of the element identification numbers is not valid.

```
aupst_get_elem_nodes(int num_elems, int elem_ids[],
                     int elem_node_ids[], int error_code)
```

Table 10.22: aupst_get_elem_nodes Arguments

Parameter	**Usage**	**Data Type**	**Description**
num_elems	Input	Integer	Number of elements from which the topology will be extracted.
elem_ids (num_elems)	Input	Integer	Array of length num_elems listing the element identification for each element from which the topology will be extracted.
elem_node_ids (number of nodes for element type × num_elems)	Output	Integer	Array containing the node identification numbers for each element requested. The length of the array is the total number of nodes contained in all elements. If the elements are eight-node hexahedra, then the number of nodes will be 8 × num_elems. The first set of eight entries in the array will be the eight nodes defining the first element. The second set of eight entries will be the eight nodes defining the second element, and so on.
error_code	Output	Integer	Error code indicating status of retrieving the element identification numbers. If the retrieval is successful, error_code is set to 0. A nonzero value is returned for error_code if one of the element identification numbers is not valid.

```
aupst_get_face_topology(int num_faces, int face_ids[],
                        int topology[], int error_code)
```

Table 10.23: aupst_get_face_topology Arguments

Parameter	**Usage**	**Data Type**	**Description**
num_faces	Input	Integer	Number of faces from which the topology will be extracted.
face_ids (num_faces)	Input	Integer	Array of length num_faces listing the face identification for each face from which the topology will be extracted.
topology (num_faces)	Output	Integer	Array of length num_faces containing the output topologies of each face.
error_code	Output	Integer	Error code indicating status of retrieving the face identification numbers. If the retrieval is successful, error_code is set to 0. A nonzero value is returned for error_code if one of the face identification numbers is not valid.

```
aupst_get_face_nodes(int num_faces, int face_ids[],
                     int face_node_ids[], int error_code)
```

Table 10.24: aupst_get_face_nodes Arguments

Parameter	**Usage**	**Data Type**	**Description**
num_faces	Input	Integer	Number of faces from which the topology will be extracted.
face_ids (num_faces)	Input	Integer	Array of length num_faces listing the face identification for each face from which the topology will be extracted.
face_node_ids (number of nodes for face type × num_faces)	Output	Integer	Array containing the node identification numbers for each face requested. The length of the array is the total number of nodes contained in all faces. If the faces are four-node quadrilaterals, then the number of nodes will be 4 × num_faces. The first set of four entries in the array will be the four nodes defining the first face. The second set of four entries will be the four nodes defining the second face, and so on.
error_code	Output	Integer	Error code indicating status of retrieving the face identification numbers. If the retrieval is successful, error_code is set to 0. A nonzero value is returned for error_code if one of the face identification numbers is not valid.

10.1.3 Miscellaneous Query Functions

A number of miscellaneous query functions are available for computing some commonly used quantities.

```
aupst_get_one_elem_centroid(int num_elems, int elem_ids[],
                      real centroids, int error_code)

aupst_get_point(string point_name, real point_coords,
                      int error_code)

aupst_get_proc_num(proc_num)
```

The arguments for the miscellaneous query functions are defined in Table 10.25 through Table 10.27. The function is repeated before each table for easy reference.

```
aupst_get_one_elem_centroid(int num_elems, int elem_ids[],
                      real centroids[], int error_code)
```

Table 10.25: aupst_get_one_elem_centroid Arguments

Parameter	**Usage**	**Data Type**	**Description**
num_elems	Input	Integer	Number of elements for which to extract the topology.
elem_ids (num_elems)	Input	Integer	Array of length num_elems listing the element identification for each element for which the centroid will be computed.
centroids (3, num_elems)	Output	Real	Array of length 3 × num_elems containing the centroid of each element.
error_code	Output	Integer	Error code indicating status of retrieving the element identification numbers. If the retrieval is successful, error_code is set to 0. A nonzero value is returned for error_code if one of the element identification numbers is not valid.

```
aupst_get_point(string point_name, real point_coords,
                     int error_code)
```

Table 10.26: aupst_get_point Arguments

Parameter	**Usage**	**Data Type**	**Description**
point_name	Input	String	SIERRA name for a given point.
point_coords (3)	Output	Real	Array of length 3 containing the x, y, and z coordinates of the point.
error_code	Output	Integer	Error code indicating status of retrieving the point. If the retrieval is successful, error_code is set to 0. A nonzero value is returned for error_code if the point cannot be found

```
aupst_get_proc_num(proc_num)
```

Table 10.27: aupst_get_proc_num Arguments

Parameter	**Usage**	**Data Type**	**Description**
proc_num	Output	Integer	Processor number of the calling process. This number can be used for informational purposes. A common example is that output could only be written by a single processor, e.g., processor 0, rather than by all processors.

10.2 User Subroutines: Command File

In addition to the actual user subroutine, you will need to add command lines to your input file to make use of your user subroutine. This section describes the command lines that are used in conjunction with user subroutines. This section also describes two additional command blocks, `TIME STEP INITIALIZATION` and `USER VARIABLE`. The `TIME STEP INITIALIZATION` command block lets you execute a user subroutine at the beginning of a time step as opposed to some later time. The `USER VARIABLE` command block can be used in conjunction with user subroutines or for user-defined output.

10.2.1 Subroutine Identification

As described in Section 2.1.4, there is one command line associated with the user subroutine functionality that must be provided in the SIERRA scope:

```
USER SUBROUTINE FILE = <string>file_name
```

The named file may contain one or more user subroutines. The file must have an extension of ".F", as in blast.F.

10.2.2 User Subroutine Command Lines

```
{begin command block}
  NODE SET SUBROUTINE = <string>subroutine name |
    SURFACE SUBROUTINE = <string>subroutine_name |
    ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
      = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
      = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
      = <string>param_value
{end command block}
```

A number of user subroutine command lines will appear in some Presto command block. User subroutine commands can appear in boundary condition, element death,user output, and state initialization command blocks. The possible command lines are shown above. The following sections describe the command lines related to user subroutines.

10.2.2.1 Type

User subroutines are currently available in three general types: node set, surface, and element.

Node set subroutines operate on groups of nodes. The command line for defining a node set subroutine is:

```
NODE SET SUBROUTINE = <string>subroutine_name
```

where `subroutine_name` is the name of the user subroutine. The name is case sensitive. A node set subroutine will operate on all nodes contained in an associated mechanics instance.

Surface subroutines work on groups of surfaces. A surface may be an external face of a solid element or the face of a shell element associated with either the positive or negative normal for the surface of the shell. The command line for defining a surface subroutine is:

```
SURFACE SUBROUTINE = <string>subroutine_name
```

Element block subroutines work on groups of elements. The command line for defining an element block subroutine is:

```
ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
```

An element may be a solid element such as a hexahedron or a two-dimensional element such as a shell.

Different Presto features may accept one or more types of user subroutines. Only one subroutine is allowed per command block.

10.2.2.2 Debugging

Subroutines may be run in a special debugging mode to help catch memory errors. For example, there is a potential for a user subroutine to write outside of its allotted data space by writing beyond the bounds of an input or output array. Generally, this causes Presto to crash, but it also has the potential to introduce other very hard-to-trace bugs into the Presto analysis. Subroutines run in debug mode require more memory and more processing time than subroutines not run in debug mode.

Subroutine debugging is on by default in debug executables. It can be turned off with the following command line:

```
SUBROUTINE DEBUGGING OFF
```

Subroutine debugging is off by default in optimized executables. It can be turned on with the following command line:

```
SUBROUTINE DEBUGGING ON
```

10.2.2.3 Parameters

All user subroutines have the ability to use parameters. Parameters are defined in the input file and are quickly accessible by the user subroutine during run time. Parameters are a way of making a single user subroutine much more versatile. For example, a user subroutine could be written to define a periodic loading on a structure. A parameter for the subroutine could be defined specifying the frequency of the function. In this way, the same subroutine can be used in different parts of

the model, and the subroutine behavior can be modified without recompiling the program. These command lines are placed within the scope of the command block in which the user subroutine is specified.

Real-valued parameters can be stored with the following command line:

```
SUBROUTINE REAL PARAMETER: <string>param_name
       = <real>param_value
```

Integer-valued parameters can be stored with the following command line:

```
SUBROUTINE INTEGER PARAMETER: <string>param_name
       = <integer>param_value
```

String-valued parameters can be stored with the following command line:

```
SUBROUTINE STRING PARAMETER: <string>param_name
       = <string>param_value
```

Any number of subroutine parameters may be defined. The subroutine parameters may be defined in any order within the command block. The user subroutine may request the values of the parameters but is not required to use them or even have any knowledge of their existence. An example of subroutine usage with parameters is as follows:

```
BEGIN PRESSURE
  SURFACE = surface_1
  SURFACE SUBROUTINE = blast_pressure
  SUBROUTINE REAL PARAMETER: blast_time = 1.2
  SUBROUTINE REAL PARAMETER: blast_power = 1.3e+07
  SUBROUTINE STRING PARAMETER: formulation = alpha
  SUBROUTINE INTEGER PARAMETER: decay_exponent = 2
  SUBROUTINE DEBUGGING ON
END PRESSURE
```

In the above example, four parameters are associated with the subroutine `blast_pressure`. Two of the parameters are real (`blast_time` and `blast_power`), one of the parameters is a string (`formulation`), and one of the parameters is an integer (`decay_exponent`). To access the parameters in the user subroutine, the user will need to include interface calls described in previous sections.

10.2.3 Time Step Initialization

```
BEGIN TIME STEP INITIALIZATION
  # mesh-entity set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list> surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name |
    SURFACE SUBROUTINE = <string>sub_name |
    ELEMENT BLOCK SUBROUTINE = <string>sub_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # additional command
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names

END TIME STEP INITIALIZATION
```

The `TIME STEP INITIALIZATION` command block, which appears in the region scope, is used to flag a user subroutine to run at the beginning of every time step. This subroutine can be used to compute quantities used by other command types. For example, if the traction on a surface was dependent on the area, the time step initialization subroutine could be used to calculate the area, and that area could be stored and later read when calculating the traction. The user initialization subroutine will pass the specified mesh objects to the subroutine for use in calculating some value.

The `TIME STEP INITIALIZATION` command block contains two groups of commands—mesh entity set and user subroutine. In addition to the command lines in the these command groups, there is an additional command line: `ACTIVE PERIODS` or `INACTIVE PERIODS`. Following are descriptions of the different command groups and the `ACTIVE PERIODS` or `INACTIVE PERIODS` command line.

10.2.3.1 Mesh-Entity Set Commands

The `mesh-entity set commands` portion of the `TIME STEP INITIALIZATION` command block specifies the nodes, element faces, or elements associated with the particular subroutine that

will be run at the beginning of the applicable time steps. This portion of the command block can include some combination of the following command lines:

```
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list> surface_names
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes, element faces, or elements. See Section 5.1 for more information about the use of these command lines for mesh entities. There must be at least one `NODE SET`, `SURFACE`, `BLOCK`, or `INCLUDE ALL BLOCKS` command line in the command block.

10.2.3.2 User Subroutine Commands

The following command lines are related to the user subroutine specification:

```
NODE SET SUBROUTINE = <string>subroutine_name |
  SURFACE SUBROUTINE = <string>subroutine_name |
  ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value
```

Only one of the first three command lines listed above can be specified in the command block. The particular command line selected depends on the mesh-entity type of the variable being initialized. For example, variables associated with nodes would be initialized if you are using the `NODE SET SUBROUTINE` command line, variables associated with faces if you are using the `SURFACE SUBROUTINE` command line, and variables associated with elements if you are using the `ELEMENT BLOCK SUBROUTINE` command line. The string `subroutine_name` is the name of a FORTRAN subroutine that is written by the user.

Following the selected subroutine command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 10.2.2 and consist of `SUBROUTINE DEBUGGING OFF`, `SUBROUTINE DEBUGGING ON`, `SUBROUTINE REAL PARAMETER`, `SUBROUTINE INTEGER PARAMETER`, and `SUBROUTINE STRING PARAMETER`. Examples of using these command lines are provided throughout Chapter 10.

10.2.3.3 Additional Command

The `ACTIVE PERIODS` or `INACTIVE PERIODS` command line can optionally appear in the `TIME STEP INITIALIZATION` command block:

```
ACTIVE PERIODS = <string list>period_names
INACTIVE PERIODS = <string list>period_names
```

The `ACTIVE PERIODS` or `INACTIVE PERIODS` command line is used to activate or deactivate the running of the user subroutine at the beginning of every time step for certain time periods. See Section 2.5 for more information about this optional command line.

10.2.4 User Variables

```
BEGIN USER VARIABLE <string>var_name
  TYPE = <string>NODE|ELEMENT|GLOBAL
    [<string>REAL|INTEGER LENGTH = <integer>length]|
    [<string>SYM_TENSOR|FULL_TENSOR|VECTOR]
  GLOBAL OPERATOR = <string>SUM|MIN|MAX
  INITIAL VALUE = <real list>values
  INITIAL VARIATION = <real list>values LINEAR DISTRIBUTION
  USE WITH RESTART
END [USER VARIABLE <string>var_name]
```

The `USER VARIABLE` command block is used to create a user-defined variable. This kind of variable may be used for scratch space in a user subroutine or for some user-defined output. A user-defined variable may be output to the results file or the history file just like any other defined variable; i.e., a user-defined variable once defined by the `USER VARIABLE` command block can be specified in a `USER OUTPUT` command block, a `RESULTS OUTPUT` command block, and a `HISTORY OUTPUT` command block.

User-defined variables are associated with mesh entities. For example, a node variable will exist at every node of the model. An element variable will exist on every element of the model. A global variable will have a single value for the entire model.

If the user-defined variable functionality is used in conjunction with restart, the `USE WITH RESTART` command line must be included.

Known Issue: User defined variables are not currently supported with heartbeat output (see Section 8.4).

The `USER VARIABLE` command block is placed within a Presto region. The command block begins with the input line:

```
BEGIN USER VARIABLE <string>var_name
```

and ends with the input line:

```
END [USER VARIABLE <string>var_name]
```

where `var_name` is a user-selected name for the variable.

In the above command block:

- A user-defined variable has an associated type that is specified by the `TYPE` command line, which itself contains several parameters. The `TYPE` command line is required.

  1. The variable must be a nodal quantity, an element quantity, or a global quantity. The options `NODE`, `ELEMENT`, and `GLOBAL` determine whether the variable will be a nodal, element, or global quantity. One of these options must appear on the `TYPE` command line.

2. The user-defined variable can be either an integer or a real, as specified by the INTEGER or REAL option.
3. The length of the variable must be set by using one of the options SYM_TENSOR, FULL_TENSOR, VECTOR, or LENGTH = <integer>length. If the LENGTH option is used, the user must specify whether the variable is an integer number or a real number by using the INTEGER or REAL option. If the SYM_TENSOR option is used, the variable has six real components. If the FULL_TENSOR is used, the variable has nine real components. If the VECTOR option is used, the variable has three real components. The three options SYM_TENSOR, FULL_TENSOR, and VECTOR all imply real numbers, and thus the REAL option need not be included in the command line when one of these three options is specified.

Some examples of the TYPE command line follow:

```
type = global real length = 1
type = element tensor
type = element real length = 3
type = node sym_tensor
type = node vector
```

- If you use the GLOBAL option on the TYPE command line, a global variable is created, and this global variable must be given an associated reduction type, which is specified by the GLOBAL OPERATOR command line. The reduction type tells Presto how to reduce the individual values stored on each processor to a mesh global value. Global reductions are performed at the end of each time step. Any modifications to a global variable made by an aupst_local_put_global_var call (see Section 10.1.2.5) will not be seen until the next time step after the user-defined global variables have been updated and reduced. The SUM operator sums all processor variable contributions. The MAX operator takes the maximum value of the aupst_local_put_global_var calls. The MIN operator takes the minimum value of the aupst_local_put_global_var calls.

- One or more initial values may be specified for the user-defined variable in the INITIAL VALUE command line. The number of initial values specified should be the same as the length of the variable, as specified in the TYPE command line either explicitly via the LENGTH option or implicitly via the SYM_TENSOR, FULL_TENSOR, or VECTOR option. The initial values will be copied to the variable space on every mesh object on which the variable is defined. Only real type variables may be given initial values at this time.

- The initial value of the user variable can be given some random distribution by use of the the INITIAL VARIATION command line. If the INITIAL VARIATION command is used the INITIAL VALUE command must also be used. In addition the number of values specified in the initial variation command must exactly match the number of values specified in the initial value command. When the initial variation command is used the initial values of the variable will be set as initial value plus or minus some random factor times the initial variation. Currently the only random distribution supported is the linear distribution. With

linear distribution the random values will be distributed evenly from initial value minus variation to initial value plus variation.

- All intrinsic type options such as `REAL`, `INTEGER`, `SYM_TENSOR`, `FULL_TENSOR`, `VECTOR` and the `LENGTH` option can be used with any of the mesh entity options (`NODE`, `ELEMENT`, `GLOBAL`).

- As indicated previously, if the user-defined variable functionality is used in conjunction with restart, the `USE WITH RESTART` command line must be included.

10.3 User Subroutines: Compilation and Execution

Running a code with user subroutines is a two-step process. First, you must create an executable version of Presto that recognizes the user subroutines. Next, you must use this version of Presto for an actual Presto run with an input file that incorporates the proper user subroutine command lines.

How the above two steps are carried out is site-specific. The actual process will depend on how Presto is set up at your installation. We will give an example that shows how the process is carried out on various systems at Sandia using SIERRA command lines. SIERRA is a general code framework and code management system at Sandia.

For the first step, you will need the user subroutine, in a FORTRAN file, and a Presto input file that makes use of the user subroutine. You will use a system command line of the general form shown below.

```
% sierra presto -i <string>input_file_name --make
```

Suppose that you have a subdirectory in your area called `test` and you wish to incorporate a user subroutine called `blast_load`. The actual user subroutine will be in a file called `blast_load.F`, and the associated input file will be called `blast_load_1.i`. Both of these files will be in the directory `test`. In the input file, you will have the following command line in the SIERRA scope:

```
USER SUBROUTINE FILE = blast_load.F
```

You will also have some subset of the command lines described in the previous section in your Presto input file. The specific form of the system command line to execute the first step of the user subroutine process is shown below.

`% sierra presto -i blast_load_1.i --make` The above command will create a local version of Presto in a local directory named `UserSubsProject`. The system command line to run the local version of Presto is shown below.

```
% sierra presto -i <string>input_file_name
        -x UserSubsProject
```

The specific form of the system command line you will execute in the subdirectory test is shown below.

```
% sierra presto -i blast_load_1.i -x UserSubsProject
```

The second command line runs Presto using `blast_load_1.i` as an input file and utilizes the user subroutines in the process. Again, all of this is a site-specific example. You must determine how Presto is set up at your installation to determine what system command lines are necessary to build Presto with user subroutines and then use this version of Presto.

10.4 User Subroutines: Examples

10.4.1 Pressure as a Function of Space and Time

(The following example provides functionality—a blast load on a surface—more applicable to Presto than Adagio. It is included in both manuals as it is instructive in the general use of a user-defined subroutine.)

The following code is an example of a user subroutine to compute blast pressures on a group of faces. The blast pressure simulates a blast occurring at a specified position and time. The blast wave radiates out from the center of the blast and dissipates over time. This subroutine is included in the input file as follows:

```
#In the SIERRA scope:
user subroutine file = blast_load.F

#In the region scope:
begin pressure
  surface = surface_1
  surface subroutine = blast_load
  subroutine real parameter: pos_x = 5.0
  subroutine real parameter: pos_y = 5.0
  subroutine real parameter: pos_z = 1.6
  subroutine real parameter: wave_speed = 1.5e+02
  subroutine real parameter: blast_time = 0.0
  subroutine real parameter: blast_energy = 1.0e+09
  subroutine real parameter: blast_wave_width = 0.75
end pressure
```

The FORTRAN 77 subroutine listing follows. Note that it would be possible to increase the speed of this subroutine by calling the topology functions (see Section 10.1.2.6) on groups of elements, though this would increase subroutine complexity.

```
c
c  Subroutine to simulate a blast load on a surface
c
      subroutine blast_load(num_faces, num_vals,
     &  eval_time, faceID, pressure, flags, err_code)

      implicit none
c
c  Subroutine input arguments
c
      integer num_faces
      double precision eval_time
      integer faceID(num_faces)
```

```
      integer num_vals
c
c  Subroutine output arguments
c
      double precision pressure(num_vals, num_faces)
      integer flags(num_faces)
      integer err_code
c
c  Variables to hold the subroutine parameters
c
      double precision pos_x, pos_y, pos_z, wave_speed,
     &                 blast_time, blast_energy,
     &                 blast_wave_width
c
c  Local variables
c
      integer iface, inode
      integer cur_face_id, face_topo, num_nodes
      integer num_comp_check
      double precision dist, blast_o_rad, blast_i_rad
      double precision blast_volume, blast_pressure
      integer query_error
      double precision face_center(3)
c
c  Create some static variables to hold queried
c  information.  Assume no face has more than 10
c  nodes
c
      double precision face_nodes(10)
      double precision face_coords(3, 10)
c
c  Extract the subroutine parameters
c
      call aupst_get_real_param("pos_x",pos_x,query_error)
      call aupst_get_real_param("pos_y",pos_y,query_error)
      call aupst_get_real_param("pos_z",pos_z,query_error)
      call aupst_get_real_param("wave_speed",wave_speed,
     &                          query_error)
      call aupst_get_real_param("blast_energy",
     &                          blast_energy,query_error)
      call aupst_get_real_param("blast_time",
     &                          blast_time,query_error)
      call aupst_get_real_param("blast_wave_width",
     &                  blast_wave_width, query_error)
c
c  Determine the outer radius of the blast wave
```

```
c
      blast_o_rad = (eval_time - blast_time) * wave_speed
      if(blast_o_rad .le. 0.0) return;
c
c  Determine the inner radius of the blast wave
c
      blast_i_rad = blast_o_rad - blast_wave_width
      if(blast_i_rad .le. 0.0) blast_i_rad = 0.0
c
c  Determine the total volume the blast wave occupies
c
      blast_volume = 3.1415 * (4.0/3.0) *
     &               (blast_o_rad**2 - blast_i_rad**2)
c
c  Determine the total pressure on faces inside the
c  blast wave
c
      blast_pressure = blast_energy / blast_volume
c
c  Loop over all faces in the set
c
      do iface = 1, num_faces
c
c  Extract the topology of the current face
c
        cur_face_id = faceID(iface)
        call aupst_get_face_topology(1, cur_face_id,
     &                           face_topo, query_error)
c
c  Determine the number of nodes of the current face
c
        num_nodes = mod(face_topo,100)
c
c  Extract the node ids for nodes contained in the current
c  face
c
        call aupst_get_face_nodes(1, cur_face_id,
     &                            face_nodes, query_error)
c
c  Extract the nodal coordinates of the face nodes
c
        call aupst_get_node_var(num_nodes, 3, face_nodes,
     &          face_coords, "coordinates", query_error)
c
c  Compute the centroid of the face
c
        face_center(1) = 0.0
```

```
        face_center(2) = 0.0
        face_center(3) = 0.0
        do inode = 1, num_nodes
          face_center(1) = face_center(1) +
     &                     face_coords(1,inode)
          face_center(2) = face_center(2) +
     &                     face_coords(2,inode)
          face_center(3) = face_center(3) +
     &                     face_coords(3,inode)
        enddo
        face_center(1) = face_center(1)/num_nodes
        face_center(2) = face_center(2)/num_nodes
        face_center(3) = face_center(3)/num_nodes
c
c  Determine the distance from the current face
c  to the blast center
c
        dist = sqrt((face_center(1) - pos_x)**2 +
     &              (face_center(2) - pos_y)**2 +
     &              (face_center(3) - pos_z)**2)
c
c  Apply pressure to the current face if it falls within
c  the blast wave
c
        if(dist .ge. blast_i_rad .and.
     &     dist .le. blast_o_rad) then
          pressure(1,iface) = blast_pressure
        else
          pressure(1,iface) = 0.0
        endif
      enddo
      err_code = 0
      end
```

10.4.2 Error Between a Computed and an Analytic Solution

The following code is a user subroutine to compute the error between Presto-computed results and results from an analytic manufactured solution. This subroutine is called by a `USER OUTPUT` command block immediately prior to producing an output Exodus file. The error for the mesh is computed by taking the squared difference between the computed and analytic displacements at every node. Finally, a global sum of the error is produced along with the square root norm of the error.

This user subroutine requires a user variable, which is defined in the Presto input file. The command block for the user variable specified in this user subroutine is as follows:

```
begin user variable conv_error
```

```
 type = global real length = 1
  global operator = sum
  initial value = 0.0
end user variable conv_error
```

The subroutine is called in the Presto input file as follows:

```
begin user output
  node set = nodelist_10
  node set subroutine = conv0_error
  subroutine real parameter: char_length = 1.0
  subroutine real parameter: char_time   = 1.0e-3
  subroutine real parameter: x_offset    = 0.0
  subroutine real parameter: y_offset    = 0.0
  subroutine real parameter: z_offset    = 0.0
  subroutine real parameter: t_offset    = 0.0
  subroutine real parameter: u0          = 0.01
  subroutine real parameter: v0          = 0.02
  subroutine real parameter: w0          = 0.03
  subroutine real parameter: alpha       = 1.0
  subroutine real parameter: youngs_modulus = 10.0e6
  subroutine real parameter: poissons_ratio = 0.3
  subroutine real parameter: density        = 0.0002588
  subroutine real parameter: num_nodes      = 125.0
end user output
```

The FORTRAN listing for the subroutine is as follows:

```
      subroutine conv0_error(num_nodes, num_vals,
     &  eval_time, nodeID, values, flags, ierror)
      implicit none

      integer num_nodes
      integer num_vals
      double precision eval_time
      integer nodeID(num_nodes)
      double precision values(1)
      integer flags(1)
      integer ierror
c
c     Local vars
c
      integer inode
      integer error_code
      double precision clength, ctime, xoff, yoff, zoff, toff
      double precision zero, one, two, three, four, nine
```

```
      double precision mod_coords(3,3000)
      double precision cdispl(3,3000)
      integer num_comp_check
      double precision expat
      double precision x, y, z, t
      double precision u0, v0, w0, alpha
      double precision pi
      double precision half
      double precision mdisplx, mdisply, mdisplz
      double precision xdiff, ydiff, zdiff
      double precision conv_error
      double precision numnod

      pi    = 3.141592654
      half  = 0.5
      zero  = 0.0
      one   = 1.0
      two   = 2.0
      three = 3.0
      four  = 4.0
      nine  = 9.0
c
c  Check that the nodal coordinates will fit into the
c  statically allocated array
c
      if(num_nodes .gt. 3000) then
        write(6,*) ŠERROR in sphere disp, Ś,
     &  num_nodes exceeds static array sizeŠ
        ierror = 1
        return
      endif
c
c  Extract the model coordinates for all nodes
c
      call aupst_check_node_var(num_nodes, num_comp_check,
     &                          nodeID, "model_coordinates",
     &                          ierror)
      if(ierror .ne. 0) return
      if(num_comp_check .ne. 3) return
      call aupst_get_node_var(num_nodes, num_comp_check,
     &       nodeID, mod_coords, "model_coordinates",
     &       ierror)
c
c  Extract the computed displacements for all nodes
c
      call aupst_check_node_var(num_nodes, num_comp_check,
     &                          nodeID, "displacement",
```

```
     &                           ierror)
      if(ierror .ne. 0) return
      if(num_comp_check .ne. 3) return
      call aupst_get_node_var(num_nodes, num_comp_check,
     &       nodeID, cdispl, "displacement",
     &       ierror)
c
c  Extract the subroutine parameters.
c
      call aupst_get_real_param("char_length",
     &                           clength,error_code)
      call aupst_get_real_param("char_time",
     &                           ctime,error_code)
      call aupst_get_real_param("x_offset",xoff,error_code)
      call aupst_get_real_param("y_offset",yoff,error_code)
      call aupst_get_real_param("z_offset",zoff,error_code)
      call aupst_get_real_param("t_offset",toff,error_code)
      call aupst_get_real_param("u0",u0,error_code)
      call aupst_get_real_param("v0",v0,error_code)
      call aupst_get_real_param("w0",w0,error_code)
      call aupst_get_real_param("alpha",alpha,error_code)
      call aupst_get_real_param("num_nodes",
     &                           numnod,error_code)
c
c  Calculate a solution scaling factor
c
      expat = half * ( one - cos( pi * eval_time / ctime ) )
c
c  Compute the expected solution at each node and do a
c  sum of the differences from the analytic solution
c
      conv_error = zero
      do inode = 1, num_nodes
c
c  Set the displacement value from the manufactured solution
c
        x = ( mod_coords(1,inode) - xoff ) / clength
        y = ( mod_coords(2,inode) - yoff ) / clength
        z = ( mod_coords(3,inode) - zoff ) / clength
c
        mdisplx = u0 * sin(x) * cos(two*y) * cos(three*z)
     *              * expat
        mdisply = v0 * cos(three*x) * sin(y) * cos(two*z)
     *              * expat
        mdisplz = w0 * cos(two*x) * cos(three*y) * sin(z)
     *              * expat
c
```

```
        xdiff = mdisplx - cdispl(1,inode)
        ydiff = mdisply - cdispl(2,inode)
        zdiff = mdisplz - cdispl(3,inode)
        conv_error = conv_error + xdiff*xdiff
     *                          + ydiff*ydiff
     *                          + zdiff*zdiff
c
      enddo
c
      ierror = 0
c
c  Do a parallel sum of the squared errors and extract
c  the total summed value on all processors
c
      call aupst_put_global_var(1,conv_error,
     &                          "conv_error","sum",ierror)
      call aupst_get_global_var(1,conv_error,
     &                          "conv_error",ierror)
c
c  Take the square root of the errors and store that as
c  the net error norm
c
      conv_error = sqrt(conv_error) / sqrt(numnod)
      call aupst_put_global_var(1,conv_error,
     &                          "conv_error","none",ierror)
c
      return
      end
```

10.4.3 Transform Output Stresses to a Cylindrical Coordinate System

The following code is a user subroutine to transform element stresses in global x, y, and z coordinates to a global cylindrical coordinate system. This subroutine could be used to transform the relatively meaningless shell stress in x, y, and z coordinates to more meaningful tangential, hoop, and radial stresses. The subroutine is called from a `USER OUTPUT` command block. It reads in the old stresses, transforms them, and writes them back out to a user-created scratch variable, defined via a `USER VARIABLE` command block, for output.

```
begin user variable cyl_stress
  type = element sym_tensor length = 1
  initial value = 0.0 0.0 0.0 0.0 0.0 0.0
end user variable

begin user output
  block = block_1
  element block subroutine = aupst_cyl_transform
```

```
  subroutine string parameter: origin_point = Point_O
  subroutine string parameter: z_point      = Point_Z
  subroutine string parameter: xz_point     = Point_XZ
  subroutine string parameter: input_stress = memb_stress
  subroutine string parameter: output_stress = cyl_stress
end user output
```

The FORTRAN listing for the subroutine is as follows:

```
      subroutine aupst_cyl_transform(num_elems, num_vals,
     *  eval_time, elemID, values, flags, ierror)
      implicit none
#include<framewk/Fmwk_type_sizes_decl.par>
#include<framewk/Fmwk_type_sizes.par>
c
c  Subroutine Arguments
c
c  num_elems: Input: Number of elements to calculate on
c  num_vals : Input: Ignored
c  eval_time: Input: Time at which to evaluate the stress.
c  elemID   : Input: Global sierra IDs of the input elements
c  values   : I/O  : Ignored, stress will be stored manually
c  flags    : I/O  : Ignored
c  ierror   :Output: Returns non-zero if an error occurs
c
      integer num_elems
      integer num_vals
      double precision eval_time
      integer elemID(num_elems)
      double precision values(1)
      integer flags(1)
      integer ierror
c
c  Fortran cannot dynamically allocate memory, thus worksets
c  will be iterated over by  chucks each of size chunk_size.
c
      integer chunk_size
      parameter (chunk_size = 100)
      integer chunk_ids(chunk_size)
c
c  Subroutine parameter data
c
      character*80     origin_point_name
      double precision origin_point(3)
      character*80     z_point_name
      double precision z_point(3)
      character*80     xz_point_name
```

```
      double precision xz_point(3)
      character*80     input_stress_name
      character*80     output_stress_name
c
c  Local element data for centroids and rotation vectors
c
      double precision cent(3)
      double precision centerline_pos(3)
      double precision dot_prod
      double precision z_vec(3)
      double precision r_vec(3)
      double precision theta_vec(3)
      double precision rotation_tensor(9)
c
c  Chunk data storage
c
      double precision elem_centroid(3, chunk_size)
      double precision input_stress_val(6, chunk_size)
      double precision output_stress_val(6, chunk_size)
c
c  Simple iteration variables
c
      integer error_code
      integer ichunk, ielem
      integer zero_elem, nel
c
c  Extract the current subroutine parameters.  origin_point
c  is the origin of the coordinate system
c  z_point is a point on the z axis of the coordinate system
c  xz_point is a point on the xz plane
c
      call aupst_get_string_param("origin_point",
     &                            origin_point_name,
     &                            error_code)
      call aupst_get_string_param("z_point",
     &                            z_point_name,
     &                            error_code)
      call aupst_get_string_param("xz_point",
     &                            xz_point_name,
     &                            error_code)
      call aupst_get_string_param("input_stress",
     &                            input_stress_name,
     &                            error_code)
      call aupst_get_string_param("output_stress",
     &                            output_stress_name,
     &                            error_code)
c
```

```
c  Use the point names to look up the coordinates of each
c  relevant point
c
      call aupst_get_point(origin_point_name, origin_point,
     &                     error_code)
      call aupst_get_point(z_point_name, z_point,
     &                     error_code)
      call aupst_get_point(xz_point_name, xz_point,
     &                     error_code)
c
c  Compute the z axis vector
c
      z_vec(1) = z_point(1) - origin_point(1)
      z_vec(2) = z_point(2) - origin_point(2)
      z_vec(3) = z_point(3) - origin_point(3)
c
c  Transform z_vec into a unit vector, abort if it is invalid
c
      call aupst_unitize_vector(z_vec, ierror)
      if(ierror .ne. 0) return
c
c  Loop over chunks of the data arrays
c
      do ichunk = 1, (num_elems/chunk_size + 1)
c
c  Determine the first and last element number for the
c  current chunk of elements
c
       zero_elem = (ichunk-1) * chunk_size
       if((zero_elem + chunk_size) .gt. num_elems) then
        nel = num_elems - zero_elem
       else
        nel = chunk_size
       endif
c
c  Copy the elemIDs for all elems in the current chunk to a
c  temporary array
c
       do ielem = 1, nel
       chunk_ids(ielem) = elemID(zero_elem + ielem)
       enddo
c
c  Extract the element centroids and stresses
c
       call aupst_get_elem_centroid(nel, chunk_ids,
     &                              elem_centroid,
     &                              ierror)
```

```
      call aupst_get_elem_var(nel, 6, chunk_ids,
     &                        input_stress_val,
     &                        input_stress_name, ierror)
c
c  Loop over each element in the current chunk
c
      do ielem = 1, nel
c
c  Find the closest point on the cylinder centerline axis
c  to the element centroid
c
        cent(1) = elem_centroid(1, ielem) - origin_point(1)
        cent(2) = elem_centroid(2, ielem) - origin_point(2)
        cent(3) = elem_centroid(3, ielem) - origin_point(3)
        dot_prod = cent(1) * z_vec(1) +
     &             cent(2) * z_vec(2) +
     &             cent(3) * z_vec(3)
        centerline_pos(1) = z_vec(1) * dot_prod
        centerline_pos(2) = z_vec(2) * dot_prod
        centerline_pos(3) = z_vec(3) * dot_prod
c
c  Compute the current normal radial vector
c
        r_vec(1) = cent(1) - centerline_pos(1)
        r_vec(2) = cent(2) - centerline_pos(2)
        r_vec(3) = cent(3) - centerline_pos(3)
        call aupst_unitize_vector(r_vec, ierror)
        if(ierror .ne. 0) return
c
c  Compute the current hoop vector
c
        theta_vec(1) = z_vec(2)*r_vec(3) - r_vec(2)*z_vec(3)
        theta_vec(2) = z_vec(3)*r_vec(1) - r_vec(3)*z_vec(1)
        theta_vec(3) = z_vec(1)*r_vec(2) - r_vec(1)*z_vec(2)
c
c  The r, theta, and z vectors describe the new stress
c  coordinate system, Transform the input stress tensor
c  in x,y,z coords to the output stress tensor in r, theta,
c  and z coords use the unit vectors to create a rotation
c  tensor
c
        rotation_tensor(k_f36xx) = r_vec(1)
        rotation_tensor(k_f36yx) = r_vec(2)
        rotation_tensor(k_f36zx) = r_vec(3)
        rotation_tensor(k_f36xy) = theta_vec(1)
        rotation_tensor(k_f36yy) = theta_vec(2)
        rotation_tensor(k_f36zy) = theta_vec(3)
```

```
        rotation_tensor(k_f36xz) = z_vec(1)
        rotation_tensor(k_f36yz) = z_vec(2)
        rotation_tensor(k_f36zz) = z_vec(3)
c
c  Rotate the current stress tensor to the new configuration
c
        call fmth_rotate_symten33(1, 1, 0, rotation_tensor,
     &                            input_stress_val(1,ielem),
     &                           output_stress_val(1,ielem))
       enddo
c
c  Store the new stress
c
        call aupst_put_elem_var(nel, 6, chunk_ids,
     &                           output_stress_val,
     &                           output_stress_name, ierror)
      enddo
      ierror = 0
      end
```

10.5 User Subroutines: Library

A number of user subroutines are used commonly and have been permanently incorporated into the code. These subroutines are used just like any other subroutines, but they do not need to be compiled into the code. (The user need be concerned only about the Presto command lines.) This section describes the usage of each of these subroutines.

10.5.1 aupst_cyl_transform

Author: Nathan Crane

Purpose:

The purpose of this subroutine is to transform element stresses from a global rectangular coordinate system to a local cylindrical coordinate system. This subroutine is generally called by a `USER OUTPUT` command block. For example:

```
begin user output
  block = block_1
  element block subroutine = aupst_cyl_transform
  subroutine string parameter: origin_point = Point_O
  subroutine string parameter: z_point      = Point_Z
  subroutine string parameter: xz_point     = Point_XZ
  subroutine string parameter: input_stress = memb_stress
  subroutine string parameter: output_stress = cyl_stress
end user output
```

Requirements:

This subroutine requires a tensor variable to store the cylindrical stress into a variable for each element. The variable is created by the following command block in the Presto region:

```
begin user variable cyl_stress
   type = element sym_tensor length = 1
   initial value = 0.0 0.0 0.0 0.0 0.0 0.0
end user variable
```

Parameters:

Parameter Name	Usage	Description
origin_point	String	Name of the point at the cylinder origin.
z_point	String	Point on the cylinder axis.
xz_point	String	Point on the line that passes through theta = 0 on the cylinder.
input_stress	String	Name of the Presto internal input stress tensor variable.
output_stress	String	Name of the Presto internal output stress tensor variable.

10.5.2 aupst_rec_transform

Author: Daniel Hammerand

Purpose:

The purpose of this subroutine is to transform element stresses from a global rectangular coordinate system to a different local rectangular coordinate system. This subroutine is generally called by a `USER OUTPUT` command block. For example:

```
begin user output
  block = block_1
  element block subroutine = aupst_rec_transform
  subroutine string parameter: origin_point = Point_O
  subroutine string parameter: z_point      = Point_Z
  subroutine string parameter: xz_point     = Point_XZ
  subroutine string parameter: input_stress = memb_stress
  subroutine string parameter: output_stress = new_stress
end user output
```

Requirements:

This subroutine requires a tensor variable to store the new stress into a variable for each element. The variable is created by the following command block in the Presto region:

```
begin user variable new_stress
  type = element sym_tensor length = 1
  initial value = 0.0 0.0 0.0 0.0 0.0 0.0
end user variable
```

Parameters:

Parameter Name	Usage	Description
origin_point	String	Name of the point at the cylinder origin.
z_point	String	Point on the cylinder axis.
xz_point	String	Point on the line that passes through theta = 0 on the cylinder.
input_stress	String	Name of the Presto internal input stress tensor variable.
output_stress	String	Name of the Presto internal output stress tensor variable.

10.5.3 copy_data

Author: Jason Hales

Purpose:

The purpose of this subroutine is to copy data from one variable to another with offsets given for both variables. This subroutine is generally called by a `USER OUTPUT` command block. For example:

```
begin user output
  block = block_1
  element block subroutine = copy_data
  subroutine integer parameter: source_offset = 4
  subroutine string parameter:  source_name = stress
  subroutine integer parameter: destination_offset = 1
  subroutine string parameter:  destination_name = uservarxy
end user output
```

Requirements:

This subroutine requires that the source and destination fields exist and have lengths at least as great as the values supplied as offsets. The fields used may be defined by the user as variables. In this example, the variable is created by the following command block in the Presto region:

```
begin user variable uservarxy
  type = element real length = 1
  initial value = 0.0
end user variable
```

Parameters:

Parameter Name	Usage	Description
source_offset	Integer	The offset into the source variable.
source_name	String	The name of the source variable.
destination_offset	Integer	The offset into the destination variable.
destination_name	String	The name of the destination variable.

10.5.4 trace

Author: Jason Hales

Purpose:

The purpose of this subroutine is to compute the trace of a tensor. This subroutine is generally called by a `USER OUTPUT` command block. For example:

```
begin user output
  block = block_1
  element block subroutine = trace
  subroutine string parameter:  source_name = log_strain
  subroutine string parameter:  destination_name = uvarbulkstrain
end user output
```

Requirements:

This subroutine requires that the source and destination fields exist. The source field should have a length of six. The destination field should have a length of one. The destination field will typically be defined by the user as a variable. In this example, the variable is created by the following command block in the Presto region:

```
begin user variable uvarbulkstrain
  type = element real length = 1
  initial value = 0.0
end user variable
```

Parameters:

Parameter Name	Usage	Description
source_name	String	The name of the source variable.
destination_name	String	The name of the destination variable.

Chapter 11

Transfers

It is sometimes desirable to chain two or more analyses (procedures) together. A common example of this is the need to preload an assembly quasistatically and then subject that assembly to a loading environment best suited to an explicit transient dynamics analysis. The displacements and stresses produced by the quasistatic preload are initial conditions for the transient dynamics event. These displacements and stresses must be transferred from the initial analysis to the subsequent one.

This chapter reviews the concept of transfers in SIERRA and outlines the syntax required to perform a transfer of information between procedures.

11.1 SIERRA Transfers

Applications built on the SIERRA computational framework share underlying data structures. This makes it convenient to couple applications together using transfers.

The coupling available through SIERRA is of two types. The first is what is called intra-procedural coupling. In this case, multiple regions within a single procedure share data. This enables multi-physics analysis such as thermal-mechanical coupling. The details of this type of coupling, along with the syntax to support it, will not be covered here. Coupled codes such as Calagio and Arpeggio use this type of coupling.

The second type of coupling is inter-procedural coupling. Here, the result from one procedure is handed to the next procedure. This is the type of coupling used when moving from one analysis stage to another in Adagio and Presto. When using this type of coupling, the two procedures generally have only one region each.

11.2 Inter-procedural Transfers

The inter-procedural transfers used by Adagio and Presto can transfer data from one or all blocks of the preceding or sending procedure to the subsequent or receiving procedure. The commands to control the transfers should appear at the procedure scope in the second procedure.

When using the inter-procedural transfers, all of the appropriate element data will be transferred from the sending to the receiving elements. Nodal data will be transferred based on the type of analysis done in the two procedures. For example, if the first procedure is a quasistatic analysis and the second is an explicit transient dynamics analysis, the displacements of the nodes will be transferred but not their velocities.

Warning: Transfer of data for node-based tetrahedra is currently not fully supported. A coupled analysis with node-based tetrahedra will only be correct if the tet elements are not deformed in the first (sending) procedure, in which case initialization in the second (receiving) procedure is appropriate.

The set of available commands are below.

```
BEGIN PROCEDURAL TRANSFER <string>name

  BLOCK = <string list>block_name
  INCLUDE ALL BLOCKS
  REMOVE BLOCK = <string list>block_name

  BEGIN INTERPOLATION TRANSFER <string>name

    BLOCK BY BLOCK
    NEAREST ELEMENT COPY
```

```
    SEND BLOCKS = <string list>block_name
    SEND COORDINATES = ORIGINAL|CURRENT

    RECEIVE BLOCKS = <string list>block_name
    RECEIVE COORDINATES = original|current

    TRANSFORMATION TYPE = NONE|RIGIDBODY

  END [INTERPOLATION TRANSFER <string>name]
END [PROCEDURAL TRANSFER <string>name]
```

The inter-procedural transfers can be invoked in one of two ways. If the sending and receiving regions use the same finite element model, data can be copied from the sending to the receiving region. In this case, the first three lines of syntax in the transfer block can be used to copy data for all blocks except those that are rigid bodies.

If different finite element models are used by the sending and receiving meshes, or if it is desired to copy data for rigid bodies, the `INTERPOLATION TRANSFER` block must be used, and the first three lines in the `PROCEDURAL TRANSFER` block should not be used. If the lines appropriate for the copy of data are used when they do not apply, their behavior is undefined.

11.2.1 Copying Data with Inter-procedural Transfers

To copy data from one or more blocks in a sending region to the matching blocks in the receiving region, use these line commands:

```
  BLOCK = <string list>block_name
  INCLUDE ALL BLOCKS
  REMOVE BLOCK = <string list>block_name
```

The first of these, the `BLOCK` line command, is used to list blocks that should be copied. If it is desired to copy data for all blocks, use the `INCLUDE ALL BLOCKS` line command. Finally, one or more blocks may be removed from the set of all blocks with the `REMOVE BLOCK` line command. Either the `BLOCK` or `INCLUDE ALL BLOCKS` line command must appear.

11.2.2 Interpolating Data with Interpolation Transfers

When different finite element models are used by the sending and receiving regions, or when it is desired to transfer data for rigid bodies, the `INTERPOLATION TRANSFER` must be used.

If data for a rigid body is to be transferred, use the `TRANSFORMATION TYPE = RIGIDBODY` line command along with the `SEND BLOCKS` and `RECEIVE BLOCKS` line commands. Transfers of rigid

body information should be entered for each rigid body separately, which is done simply by listing only one block on each of the `SEND BLOCKS` and `RECEIVE BLOCKS` lines.

When transferring data for non-rigid body blocks, the only required line commands are the `SEND BLOCKS` and `RECEIVE BLOCKS` line commands. These each list one or more blocks to be included in the transfer.

The interpolation transfers move data from sending to receiving meshes by performing searches and interpolating using shape functions. For nodal data, a node in the receiving mesh is located in the sending mesh. The node will be found in (or near) an element in the sending mesh. The parametric coordinates of the point associated with the receiving node will be calculated based on the sending element, and those parametric coordinates will be used in conjunction with the shape functions and the data on the nodes of the sending element to calculate values for the receiving node.

For the transfer of element data, the location of the center of the receiving element will be located in the sending mesh. This point will appear in (or near) an element in the sending mesh. A patch of elements in the sending mesh will be created centered around the element that contains the point associated with the receiving element. The data in the patch of sending elements will be interpolated using a least squares approach to the point associated with the receiving element, and the result will be given to the receiving element.

The interpolation transfer will give the best results when the sending and receiving meshes are very similar. If the meshes do not represent the same volumes in space, for example, the interpolated values will be suspect at best.

On rare occasions, it may be desired to use the current coordinates instead of the original coordinates in performing the search used by the transfers. Use the `SEND COORDINATES = CURRENT` and/or `RECEIVE COORDINATES = CURRENT` line commands for this purpose.

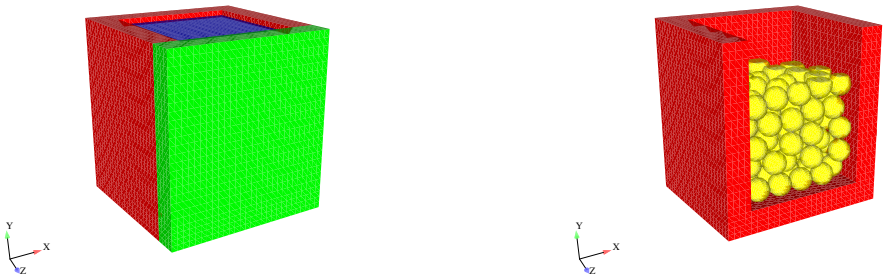
In some instances, the sending and receiving meshes are very similar such that there is a one-to-one correspondence between the list of sending blocks and the list of receiving blocks. In other words, it may be desired to send data from a given block to a corresponding block, from another block to its pair, and so forth. If this is the case, use of the `BLOCK BY BLOCK` line command will cause a separate transfer to be created for each pair of sending and receiving blocks. This is useful to ensure that data from a single block will be sent to one and only one receiving block. This could also be accomplished by listing multiple transfer blocks in the input file.

The `NEAREST ELEMENT COPY` line command changes the behavior of the transfer of element variables. Instead of a least squares approach, the use of this line command will cause data to be sent directly from the nearest sending element to the receiving element.

Appendix A

Example Problem

This chapter provides an example problem to illustrate the construction of an input file for an analysis. The example problem consists of 124 spheres made of lead enclosed in a steel box. The steel box has an open top into which a steel plate is placed (see Figure A.1). A prescribed velocity is then applied on the steel plate, pushing it into the box and crushing the spheres contained within using frictionless contact. This problem is a severe test for the contact algorithms as the spheres crush into a nearly solid block. See Figure A.2 for results of this problem.



(a) Undeformed Mesh (b) Initial Crush of Spheres

Figure A.1: Mesh for example problem: (a) box (red and green surfaces) with plate in top (blue surface) and (b) mesh with blue and green surfaces removed to show internal spheres (yellow) with initial crush.

The input file is described below, with comments to explain every few lines. Following the description, the full input file is listed again. Most of the key words in this example are all lowercase, which is different from the convention we have used to describe the command lines in this document. However, all the lowercase usage in the following example is an acceptable format in Presto.

The input file starts with a begin sierra statement (i.e., the first line of the `SIERRA` command block), as is required for all input files:

```
begin sierra crush_124_spheres
```

(a) Additional Crush of Spheres (b) Final Deformed Configuration

Figure A.2: Mesh with blue and green surfaces removed to show internal spheres (yellow) after initial crush shown in Figure A.1 (b).

We now need to define the functions used with this problem. The boundary conditions require a function for the initial velocity, as follows:

```
begin definition for function constant_velocity
  type is piecewise linear
  ordinate is velocity
  abscissa is time
  begin values
    0.0 30.0
    1.0 30.0
  end values
end definition for function constant_velocity
```

To define the boundary conditions, we need to define the direction for the initial velocity—this is in the y-direction. We could also choose to simply specify the Y component for the initial condition, but this input file uses directions.

```
define direction y_axis with vector 0.0 1.0 0.0
```

Next we define the material models that will be used for this analysis. There are two materials in this problem: steel for the box, and lead for the spheres. Both materials use the elastic-plastic material model (denoted as `elastic_plastic`).

```
begin property specification for material steel
  density = 7871.966988

  begin parameters for model elastic_plastic
    youngs modulus = 1.999479615e+11
    poissons ratio = 0.33333
    yield stress = 275790291.7
    hardening modulus = 275790291.7
```

```
    beta = 1.0
  end parameters for model elastic_plastic

end property specification for material steel

begin property specification for material lead
  density = 11253.30062

  begin parameters for model elastic_plastic
    youngs modulus = 1.378951459e+10
    poissons ratio = 0.44
    yield stress = 13789514.59
    hardening modulus = 0.0
    beta = 1.0
  end parameters for model elastic_plastic

end property specification for material lead
```

Now we define the finite element mesh. This includes specification of the file that contains the mesh, as well as a list of all the element blocks we will use from the mesh and the material associated with each block. The name of the file is `crush_124_spheres.g`. The specification of the database type is optional—ExodusII is the default. Currently, each element block must be defined individually. For this particular problem, all the spheres are the same element block. Each sphere is a distinct geometry entity, but all spheres constitute one element block in the Exodus II database. Note that the three element blocks that make up the box and lid all reference the same material description. The material description is *not* repeated three times. The material description for steel appears once and is then referenced three times.

```
begin finite element model mesh1
  Database Name = crush_124_spheres.g
  Database Type = exodusII

  begin parameters for block block_1
    material linear_elastic_steel
    solid mechanics use model elastic_plastic
  end parameters for block block_1

  begin parameters for block block_2
    material linear_elastic_steel
    solid mechanics use model elastic_plastic
  end parameters for block block_2

  begin parameters for block block_3
    material linear_elastic_steel
    solid mechanics use model elastic_plastic
  end parameters for block block_3
```

```
  begin parameters for block block_4
    material linear_elastic_lead
    solid mechanics use model elastic_plastic
  end parameters for block block_4

end finite element model mesh1
```

As an alternative to referencing the material description for steel three times as done above, you could define multiple element blocks simultaneously on the same command line. Thus, the three element block specifications with the material `linear_elastic_steel` could be consolidated into one, as follows:

```
 begin parameters for block block_1 block 2 block 3
   material linear_elastic_steel
   solid mechanics use model elastic_plastic
 end parameters for block block_1 block 2 block 3
```

At this point we have finished specifying physics-independent quantities. We now want to set up the Presto procedure and region, along with the `time control` command block. We start by defining the beginning of the procedure scope, the `time control` command block, and the beginning of the region scope. Only one `time stepping block` command block is needed for this analysis. The termination time is set to 7×10^{-4}.

```
begin presto procedure Apst_Procedure

begin time control
  begin time stepping block p1
    start time = 0.0
    begin parameters for presto region presto
      time step scale factor = 1.0
      time step increase factor = 2.0
      step interval = 25
    end parameters for presto region presto
  end time stepping block p1

  termination time = 7.0e-4
end time control

  begin presto region presto
```

Next we associate the finite element model we defined above (mesh1) with this presto region.

```
    use finite element model mesh1
```

Now we define the boundary conditions on the problem. We prescribe the velocity on the top surface of the box (`nodelist_100`) to crush the spheres, and we confine the bottom surface of the box (`nodelist_200`) not to move. Note that although we use node sets to define these boundary conditions, we could have used the corresponding side sets.

```
begin prescribed velocity
  node set = nodelist_100
  direction = y_axis
  function = constant_velocity
  scale factor = -1.0
end

begin fixed displacement
  node set = nodelist_200
  components = Y
end
```

Now we define the contact for this problem. For this problem, we want all four element blocks to be able to contact each other, with a normal tolerance of 0.0001 and a tangential tolerance of 0.0005. In this case, we simply define the same contact characteristics for all interactions. However, we could also specify tolerances and kinematic partition factors for individual interactions. Since no friction model is defined in the block below, the contact defaults to frictionless contact. (There are numerous options you can use to control the contact algorithm. The options you choose will affect contact algorithm efficiency and solution accuracy. See Chapter 7 to determine how to set input for the `CONTACT DEFINITION` command block to obtain the best level of efficiency and accuracy for your particular problem.)

```
begin contact definition
  skin all blocks = on
  begin search options
    normal tolerance = 0.0001
    tangential tolerance = 0.00005
  end
  begin interaction defaults
    general contact = on
    self contact = on
  end
end
```

Now we define what variables we want in the results file, as well as how often we want this file to be written. Here we request files written every 7×10^{-6} sec of analysis time. This will result in results output at one hundred time steps (plus the zero time step) since the termination time is set to 7×10^{-4} sec. The output file will be called `crush_124_spheres.e`, and it will be an Exodus II file (the database type command is optional; it defaults to ExodusII). The variables we are requesting are the displacements and external forces at the nodes, the rotated stresses for the elements, the time-step increment, and the kinetic energy.

```
      begin Results Output output_presto
        Database Name = crush_124_spheres.e
        Database Type = exodusII
        At Time 0.0, Increment = 7.0e-6
        nodal displacement as displ
        nodal force_external as fext
        element stress as stress
        global KineticEnergy as KE
        global timestep
      end
```

Now we end the presto region, presto procedure, and sierra blocks to complete the input file.

```
    end presto region presto
  end presto procedure Apst_Procedure
end sierra crush_124_spheres
```

Here is the resulting full input file for this problem:

```
begin sierra crush_124_spheres
  begin definition for function constant_velocity
    type is piecewise linear
    ordinate is velocity
    abscissa is time
    begin values
      0.0 30.0
      1.0 30.0
    end values
  end definition for function constant_velocity
  define direction y_axis with vector 0.0 1.0 0.0

  begin property specification for material steel
    density = 7871.966988

    begin parameters for model elastic_plastic
      youngs modulus = 1.999479615e+11
      poissons ratio = 0.33333
      yield stress = 275790291.7
      hardening modulus = 275790291.7
      beta = 1.0
    end parameters for model elastic_plastic

  end property specification for material steel

  begin property specification for material lead
    density = 11253.30062

    begin parameters for model elastic_plastic
      youngs modulus = 1.378951459e+10
      poissons ratio = 0.44
      yield stress = 13789514.59
      hardening modulus = 0.0
      beta = 1.0
    end parameters for model elastic_plastic

  end property specification for material lead

  begin finite element model mesh1
    Database Name = crush_124_spheres.g
    Database Type = exodusII

    begin parameters for block block_1
      material linear_elastic_steel
      solid mechanics use model elastic_plastic
    end parameters for block block_1
```

```
  begin parameters for block block_2
    material linear_elastic_steel
    solid mechanics use model elastic_plastic
  end parameters for block block_2

  begin parameters for block block_3
    material linear_elastic_steel
    solid mechanics use model elastic_plastic
  end parameters for block block_3

  begin parameters for block block_4
    material linear_elastic_lead
    solid mechanics use model elastic_plastic
  end parameters for block block_4

end finite element model mesh1

begin presto procedure Apst_Procedure

  begin time control
    begin time stepping block p1
      start time = 0.0
      begin parameters for presto region presto
        time step scale factor = 1.0
        time step increase factor = 2.0
        step interval = 25
      end parameters for presto region presto
    end time stepping block p1

    termination time = 7.0e-4
  end time control

  begin presto region presto

    use finite element model mesh1

    begin prescribed velocity
      node set = nodelist_100
      direction = y_axis
      function = constant_velocity
      scale factor = -1.0
    end prescribed velocity

    begin fixed displacement
      node set = nodelist_200
      components = Y
    end fixed displacement
```

```
      begin contact definition
        skin all blocks = on
         begin search options
           normal tolerance = 0.0001
           tangential tolerance = 0.00005
         end
         begin interaction defaults
           general contact = on
           self contact = on
         end
       end

       begin Results Output output_presto
         Database Name = crush_124_spheres.e
         Database Type = exodusII
         At Time 0.0, Increment = 7.0e-6
         nodal displacement as displ
         nodal force_external as fext
         element stress as stress
         global KineticEnergy as KE
         global timestep
       end results output output_presto

    end presto region presto
  end presto procedure Apst_Procedure
end sierra crush_124_spheres
```

Appendix B

Command Summary

This appendix gives all of the Presto commands in the proper scope.

```
# SIERRA scope specification
BEGIN SIERRA <string>name

  # Title

    TITLE = <string list>title

  # Restart time

    RESTART TIME = <real>restart_time
    RESTART = AUTOMATIC

  # User subroutine file

  USER SUBROUTINE FILE = <string>file name

  # Function definition

  BEGIN DEFINITION FOR FUNCTION <string>function_name
    TYPE = <string>CONSTANT|PIECEWISE LINEAR|PIECEWISE CONSTANT|
      ANALYTIC
    ABSCISSA = <string>abscissa_label
      [scale = <real>abscissa_scale(1.0)]
      [offset = <real>abscissa_offset(0.0)]
    ORDINATE = <string>ordinate_label
      [scale = <real>ordinate_scale(1.0)]
      [offset = <real>ordinate_offset(0.0)]
    X SCALE = <real>x_scale(1.0)
    X OFFSET = <real>x_offset(0.0)
    Y SCALE = <real>y_scale(1.0)
    Y OFFSET = <real>y_offset(0.0)
```

```
  BEGIN VALUES
    <real>x_1   <real>y_1
    <real>x_2   <real>y_2
    ...
    <real>x_n   <real>y_n
  END [VALUES]
  AT DISCONTINUITY EVALUATE TO <string>LEFT|RIGHT(LEFT)
  EVALUATE EXPRESSION = <string>analytic_expression1;
    analytic_expression2;...
  DEBUG = ON|OFF(OFF)
END [DEFINITION FOR FUNCTION <string>function_name]

# Definitions

DEFINE POINT <string>point_name WITH COORDINATES
  <real>value_1 <real>value_2 <real>value_3

DEFINE DIRECTION <string>direction_name WITH VECTOR
  <real>value_1 <real>value_2 <real>value_3

DEFINE AXIS <string>axis_name WITH POINT
  <string>point_1 POINT <string>point_2

DEFINE AXIS <string>axis_name WITH POINT
  <string>point_name DIRECTION <string>direction

# Local coordinate system

BEGIN ORIENTATION <string>orientation_name
  SYSTEM = <string>RECTANGULAR|Z RECTANGULAR|CYLINDRICAL|
    SPHERICAL(RECTANGULAR)
  #
  POINT A = <real>global_ax <real>global_ay <real>global_az
  POINT B = <real>global_bx <real>global_by <real>global_bz
  #
  ROTATION ABOUT <integer> 1|2|3(1) = <real>theta(0.0)
END [ORIENTATION <string>orientation_name]

# Rigid bodies

BEGIN RIGID BODY <string>rb_name
  MASS = <real>mass
  POINT MASS = <real>mass [AT <real>X <real>Y <real>Z]
  REFERENCE LOCATION = <real>X <real>Y <real>Z
  INERTIA = <real>Ixx <real>Iyy <real>Izz <real>Ixy
    <real>Iyz <real>Izx
  POINT INERTIA = <real>Ixx <real>Iyy <real>Izz <real>Ixy
```

```
    <real>Iyz <real>Izx
  MAGNITUDE = <real>magnitude_of_velocity
  DIRECTION = <string>direction_definition
  ANGULAR VELOCITY = <real>omega
  CYLINDRICAL AXIS = <string>axis_definition
  INCLUDE NODES IN <string>surface_name
    [if <string>field_name <|<=|=|>=|> <real>value]
END [RIGID BODY <string>rb_name]

# Elastic material

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL ELASTIC
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
  END [PARAMETERS FOR MODEL ELASTIC]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Thermoelastic material

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
```

```
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL THERMOELASTIC
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    YOUNGS MODULUS FUNCTION = <string>ym_function_name
    POISSONS RATIO FUNCTION = <string>pr_function_name
  END [PARAMETERS FOR MODEL THERMOELASTIC]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# neo-Hookean material

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL NEO_HOOKEAN
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
  END [PARAMETERS FOR MODEL NEO_HOOKEAN]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Elastic fracture material

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
```

```
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL ELASTIC_FRACTURE
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    MAX STRESS = <real>max_stress
    CRITICAL CRACK OPENING STRAIN = <real>critical_strain
  END [PARAMETERS FOR MODEL ELASTIC_FRACTURE]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Elastic-plastic material

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL ELASTIC_PLASTIC
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    YIELD STRESS = <real>yield_stress
    HARDENING MODULUS = <real>hardening_modulus
    BETA = <real>beta_parameter(1.0)
  END [PARAMETERS FOR MODEL ELASTIC_PLASTIC]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

```
# Elastic-plastic power-law hardening

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL EP_POWER_HARD
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    YIELD STRESS = <real>yield_stress
    HARDENING CONSTANT = <real>hardening_constant
    HARDENING EXPONENT = <real>hardening_exponent
    LUDERS STRAIN = <real>luders_strain
  END [PARAMETERS FOR MODEL EP_POWER_HARD]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Elastic plastic power-law hardening with failure

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL DUCTILE_FRACTURE
    YOUNGS MODULUS = <real>youngs_modulus
```

```
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    YIELD STRESS = <real>yield_stress
    HARDENING CONSTANT = <real>hardening_constant
    HARDENING EXPONENT = <real>hardening_exponent
    LUDERS STRAIN <real>luders_strain
    CRITICAL TEARING PARAMETER = <real>crit_tearing
    CRITICAL CRACK OPENING STRAIN = <real>critical_strain
  END [PARAMETERS FOR MODEL DUCTILE_FRACTURE]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Multilinear elastic plastic

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL MULTILINEAR_EP
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    YIELD STRESS = <real>yield_stress
    BETA = <real>beta_parameter(1.0)
    HARDENING FUNCTION = <string>hardening_function_name
    YOUNGS MODULUS FUNCTION = <string>ym_function_name
    POISSONS RATIO FUNCTION = <string>pr_function_name
    YIELD STRESS FUNCTION =
      <string>yield_stress_function_name
  END [PARAMETERS FOR MODEL MULTILINEAR_EP]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Multilinear elastic plastic with failure
```

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL ML_EP_FAIL
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    YIELD STRESS = <real>yield_stress
    BETA = <real>beta_parameter(1.0)
    HARDENING FUNCTION = <string>hardening_function_name
    YOUNGS MODULUS FUNCTION = <string>ym_function_name
    POISSONS RATIO FUNCTION = <string>pr_function_name
    YIELD STRESS FUNCTION =
      <string>yield_stress_function_name
    CRITICAL TEARING PARAMETER = <real>crit_tearing
    CRITICAL CRACK OPENING STRAIN = <real>critical_strain
  END [PARAMETERS FOR MODEL ML_EP_FAIL]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# BCJ plasticity

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
```

```
  #
  BEGIN PARAMETERS FOR MODEL BCJ
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    C1 = <real>c1
    C2 = <real>c2
    C3 = <real>c3
    C4 = <real>c4
    C5 = <real>c5
    C6 = <real>c6
    C7 = <real>c7
    C8 = <real>c8
    C9 = <real>c9
    C10 = <real>c10
    C11 = <real>c11
    C12 = <real>c12
    C13 = <real>c13
    C14 = <real>c14
    C15 = <real>c15
    C16 = <real>c16
    C17 = <real>c17
    C18 = <real>c18
    C19 = <real>c19
    C20 = <real>c20
    DAMAGE EXPONENT = <real>damage_exponent
    INITIAL ALPHA_XX = <real>alpha_xx
    INITIAL ALPHA_YY = <real>alpha_yy
    INITIAL ALPHA_ZZ = <real>alpha_zz
    INITIAL ALPHA_XY = <real>alpha_xy
    INITIAL ALPHA_YZ = <real>alpha_yz
    INITIAL ALPHA_XZ = <real>alpha_xz
    INITIAL KAPPA = <real>initial_kappa
    INITIAL DAMAGE = <real>initial_damage
    YOUNGS MODULUS FUNCTION = <string>ym_function_name
    POISSONS RATIO FUNCTION = <string>pr_function_name
    SPECIFIC HEAT = <real>specific_heat
    THETA OPT = <integer>theta_opt
    FACTOR = <real>factor
    RHO = <real>rho
    TEMP0 = <real>temp0
  END [PARAMETERS FOR MODEL BCJ]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Power law creep
```

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL POWER_LAW_CREEP
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    CREEP CONSTANT = <real>creep_constant
    CREEP EXPONENT = <real>creep_exponent
    THERMAL CONSTANT = <real>thermal_constant
  END [PARAMETERS FOR MODEL POWER_LAW_CREEP]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Soil and crushable foam

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL SOIL_FOAM
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
```

```
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    A0 = <real>const_coeff_yieldsurf
    A1 = <real>lin_coeff_yieldsurf
    A2 = <real>quad_coeff_yieldsurf
    PRESSURE CUTOFF = <real>pressure_cutoff
    PRESSURE FUNCTION = <string>function_press_volstrain
  END [PARAMETERS FOR MODEL SOIL_FOAM]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name

# Foam plasticity

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL FOAM_PLASTICITY
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    PHI = <real>phi
    SHEAR STRENGTH  = <real>shear_strength
    SHEAR HARDENING = <real>shear_hardening
    SHEAR EXPONENT  = <real>shear_exponent
    HYDRO STRENGTH  = <real>hydro_strength
    HYDRO HARDENING = <real>hydro_hardening
    HYDRO EXPONENT  = <real>hydro_exponent
    BETA = <real>beta
  END [PARAMETERS FOR MODEL FOAM_PLASTICITY]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Low density foam

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
```

```
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL LOW_DENSITY_FOAM
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    A = <real>A
    B = <real>B
    C = <real>C
    NAIR  = <real>NAir
    P0  = <real>P0
    PHI = <real>Phi
  END [PARAMETERS FOR MODEL LOW_DENSITY_FOAM]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Elastic three-dimensional orthotropic

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  BEGIN PARAMETERS FOR MODEL ELASTIC_3D_ORTHOTROPIC
    # general parameters (any two are required)
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    # required parameters
    YOUNGS MODULUS AA = <real>Eaa_value
    YOUNGS MODULUS BB = <real>Ebb_value
    YOUNGS MODULUS CC = <real>Ecc_value
    POISSONS RATIO AB = <real>NUab_value
    POISSONS RATIO BC = <real>NUbc_value
    POISSONS RATIO CA = <real>NUca_value
    SHEAR MODULUS AB = <real>Gab_value
```

```
    SHEAR MODULUS BC = <real>Gbc_value
    SHEAR MODULUS CA = <real>Gca_value
    COORDINATE SYSTEM = <string>coordinate_system_name
    DIRECTION FOR ROTATION = <real>1|2|3
    ALPHA = <real>alpha_in_degrees
    SECOND DIRECTION FOR ROTATION = <real>1|2|3
    SECOND ALPHA = <real>second_alpha_in_degrees
    THERMAL STRAIN AA FUNCTION = <string>ethaa_function_name
    THERMAL STRAIN BB FUNCTION = <string>ethbb_function_name
    THERMAL STRAIN CC FUNCTION = <string>ethcc_function_name
  END [PARAMETERS FOR MODEL ELASTIC_3D_ORTHOTROPIC]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Wire mesh

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL WIRE_MESH
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    YIELD FUNCTION = <string>yield_function
    TENSION = <real>tensile_strength
  END [PARAMETERS FOR MODEL WIRE_MESH]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Orthotropic crush

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
```

```
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL ORTHOTROPIC_CRUSH
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    YIELD STRESS = <real>yield_stress
    EX  = <real>modulus_x
    EY  = <real>modulus_y
    EZ  = <real>modulus_z
    GXY = <real>shear_modulus_xy
    GYZ = <real>shear_modulus_yz
    GZX = <real>shear_modulus_zx
    VMIN = <real>min_crush_volume
    CRUSH XX = <string>stress_volume_xx_function_name
    CRUSH YY = <string>stress_volume_yy_function_name
    CRUSH ZZ = <string>stress_volume_zz_function_name
    CRUSH XY =
      <string>shear_stress_volume_xy_function_name
    CRUSH YZ =
      <string>shear_stress_volume_yz_function_name
    CRUSH ZX =
      <string>shear_stress_volume_zx_function_name
  END [PARAMETERS FOR MODEL ORTHOTROPIC_CRUSH]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Orthotropic rate

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
```

```
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL ORTHOTROPIC_RATE
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    YIELD STRESS = <real>yield_stress
    MODULUS TTTT = <real>modulus_tttt
    MODULUS TTLL = <real>modulus_ttll
    MODULUS TTWW = <real>modulus_ttww
    MODULUS LLLL = <real>modulus_llll
    MODULUS LLWW = <real>modulus_llww
    MODULUS WWWW = <real>modulus_wwww
    MODULUS TLTL = <real>modulus_tltl
    MODULUS LWLW = <real>modulus_lwlw
    MODULUS WTWT = <real>modulus_wtwt
    TX = <real>tx
    TY = <real>ty
    TZ = <real>tz
    LX = <real>lx
    LY = <real>ly
    LZ = <real>lz
    MODULUS FUNCTION = <string>modulus_function_name
    RATE FUNCTION = <string>rate_function_name
    T FUNCTION = <string>t_function_name
    L FUNCTION = <string>l_function_name
    W FUNCTION = <string>w_function_name
    TL FUNCTION = <string>tl_function_name
    LW FUNCTION = <string>lw_function_name
    WT FUNCTION = <string>wt_function_name
  END [PARAMETERS FOR MODEL ORTHOTROPIC_RATE]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Elastic laminate

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BEGIN PARAMETERS FOR MODEL ELASTIC_LAMINATE
    A11 = <real>a11_value
    A12 = <real>a12_value
    A16 = <real>a16_value
    A22 = <real>a22_value
    A26 = <real>a26_value
```

```
    A66 = <real>a66_value
    A44 = <real>a44_value
    A45 = <real>a45_value
    A55 = <real>a55_value
    B11 = <real>b11_value
    B12 = <real>b12_value
    B16 = <real>b16_value
    B22 = <real>b22_value
    B26 = <real>b26_value
    B66 = <real>b66_value
    D11 = <real>d11_value
    D12 = <real>d12_value
    D16 = <real>d16_value
    D22 = <real>d22_value
    D26 = <real>d26_value
    D66 = <real>d66_value
    COORDINATE SYSTEM = <string>coord_sys_name
    DIRECTION FOR ROTATION = 1|2|3
    ALPHA = <real>alpha_value_in_degrees
    THETA = <real>theta_value_in_degrees
    NTH11 FUNCTION = <string>nth11_function_name
    NTH22 FUNCTION = <string>nth22_function_name
    NTH12 FUNCTION = <string>nth12_function_name
    MTH11 FUNCTION = <string>mth11_function_name
    MTH22 FUNCTION = <string>mth22_function_name
    MTH12 FUNCTION = <string>mth12_function_name
  END [PARAMETERS FOR MODEL ELASTIC_LAMINATE]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Fiber membrane

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL FIBER_MEMBRANE
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
```

```
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    CORD DENSITY = <real>cord_density
    CORD DIAMETER = <real>cord_diameter
    MATRIX DENSITY = <real>matrix_density
    TENSILE TEST FUNCTION = <string>test_function_name
    PERCENT CONTINUUM = <real>percent_continuum
    EPL = <real>epl
    AXIS X = <real>axis_x
    AXIS Y = <real>axis_y
    AXIS Z = <real>axis_z
    MODEL = <string>RECTANGULAR
    STIFFNESS SCALE = <real>stiffness_scale
    REFERENCE STRAIN = <real>reference_strain
  END [PARAMETERS FOR MODEL FIBER_MEMBRANE]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Incompressible solid

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL INCOMPRESSIBLE_SOLID
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    BULK MODULUS = <real>bulk_modulus
    SHEAR MODULUS = <real>shear_modulus
    LAMBDA = <real>lambda
    K SCALING = <real>k_scaling
    2G SCALING = <real>2g_scaling
    TARGET E = <real>target_e
    MAX POISSONS RATIO = <real>max_poissons_ratio
    REFERENCE STRAIN = <real>reference_strain
    SCALING FUNCTION = <string>scaling_function_name
  END [PARAMETERS FOR MODEL INCOMPRESSIBLE_SOLID]
```

```
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Mooney Rivlin

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  BEGIN PARAMETERS FOR MODEL MOONEY_RIVLIN
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    BULK MODULUS = <real>bulk_modulus
    SHEAR MODULUS = <real>shear_modulus
    LAMBDA = <real>lambda
    C10 = <real>c10
    C01 = <real>c01
    C10 FUNCTION = <string>c10_function_name
    C01 FUNCTION = <string>c01_function_name
    BULK FUNCTION = <string>bulk_function_name
    THERMAL EXPANSION FUNCTION = <string>eth_function_name
    TARGET E = <real>target_e
    TARGET E FUNCTION = <string>etar_function_name
    MAX POISSONS RATIO = <real>max_poissons_ratio
    REFERENCE STRAIN = <real>reference_strain
  END [PARAMETERS FOR MODEL MOONEY_RIVLIN]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# NVLE 3D Orthotropic

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  BEGIN PARAMETERS FOR MODEL NLVE_3D_ORTHOTROPIC
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    COORDINATE SYSTEM = <string>coordinate_system_name
    DIRECTION FOR ROTATION = <real>1|2|3
    ALPHA = <real>alpha_in_degrees
    SECOND DIRECTION FOR ROTATION = <real>1|2|3
    SECOND ALPHA = <real>second_alpha_in_degrees
    FICTITIOUS LOGA FUNCTION = <string>fict_loga_function_name
    FICTITIOUS LOGA SCALE FACTOR = <real>fict_loga_scale_factor
    # In each of the five ``PRONY'' command lines and in
```

```
# the RELAX TIME command line, the value of i can be from
# 1 through 30
1PSI PRONY <integer>i = <real>psi1_i
2PSI PRONY <integer>i = <real>psi2_i
3PSI PRONY <integer>i = <real>psi3_i
4PSI PRONY <integer>i = <real>psi4_i
5PSI PRONY <integer>i = <real>psi5_i
RELAX TIME <integer>i = <real>tau_i
REFERENCE TEMP = <real>tref
REFERENCE DENSITY = <real>rhoref
WLF C1 = <real>wlf_c1
WLF C2 = <real>wlf_c2
B SHIFT CONSTANT = <real>b_shift
SHIFT REF VALUE = <real>shift_ref
WWBETA 1PSI = <real>wwb_1psi
WWTAU 1PSI = <real>wwt_1psi
WWBETA 2PSI = <real>wwb_2psi
WWTAU 2PSI = <real>wwt_2psi
WWBETA 3PSI = <real>wwb_3psi
WWTAU 3PSI = <real>wwt_3psi
WWBETA 4PSI = <real>wwb_4psi
WWTAU 4PSI = <real>wwt_4psi
WWBETA 5PSI = <real>wwb_5psi
WWTAU 5PSI = <real>wwt_5psi
DOUBLE INTEG FACTOR = <real>dble_int_fac
REF RUBBERY HCAPACITY = <real>hcapr
REF GLASSY HCAPACITY = <real>hcapg
GLASS TRANSITION TEM = <real>tg
REF GLASSY C11 = <real>c11g
REF RUBBERY C11 = <real>c11r
REF GLASSY C22 = <real>c22g
REF RUBBERY C22 = <real>c22r
REF GLASSY C33 = <real>c33g
REF RUBBERY C33 = <real>c33r
REF GLASSY C12 = <real>c12g
REF RUBBERY C12 = <real>c12r
REF GLASSY C13 = <real>c13g
REF RUBBERY C13 = <real>c13r
REF GLASSY C23 = <real>c23g
REF RUBBERY C23 = <real>c23r
REF GLASSY C44 = <real>c44g
REF RUBBERY C44 = <real>c44r
REF GLASSY C55 = <real>c55g
REF RUBBERY C55 = <real>c55r
REF GLASSY C66 = <real>c66g
REF RUBBERY C66 = <real>c66r
REF GLASSY CTE1 = <real>cte1g
```

```
REF RUBBERY CTE1 = <real>cte1r
REF GLASSY CTE2 = <real>cte2g
REF RUBBERY CTE2 = <real>cte2r
REF GLASSY CTE3 = <real>cte3g
REF RUBBERY CTE3 = <real>cte3r
LINEAR VISCO TEST = <real>lvt
T DERIV GLASSY C11 = <real>dc11gdT
T DERIV RUBBERY C11 = <real>dc11rdT
T DERIV GLASSY C22 = <real>dc22gdT
T DERIV RUBBERY C22 = <real>dc22rdT
T DERIV GLASSY C33 = <real>dc33gdT
T DERIV RUBBERY C33 = <real>dc33rdT
T DERIV GLASSY C12 = <real>dc12gdT
T DERIV RUBBERY C12 = <real>dc12rdT
T DERIV GLASSY C13 = <real>dc13gdT
T DERIV RUBBERY C13 = <real>dc13rdT
T DERIV GLASSY C23 = <real>dc23gdT
T DERIV RUBBERY C23 = <real>dc23rdT
T DERIV GLASSY C44 = <real>dc44gdT
T DERIV RUBBERY C44 = <real>dc44rdT
T DERIV GLASSY C55 = <real>dc55gdT
T DERIV RUBBERY C55 = <real>dc55rdT
T DERIV GLASSY C66 = <real>dc66gdT
T DERIV RUBBERY C66 = <real>dc66rdT
T DERIV GLASSY CTE1 = <real>dcte1gdT
T DERIV RUBBERY CTE1 = <real>dcte1rdT
T DERIV GLASSY CTE2 = <real>dcte2gdT
T DERIV RUBBERY CTE2 = <real>dcte2rdT
T DERIV GLASSY CTE3 = <real>dcte3gdT
T DERIV RUBBERY CTE3 = <real>dcte3rdT
T DERIV GLASSY HCAPACITY = <real>dhcapgdT
T DERIV RUBBERY HCAPACITY = <real>dhcaprdT
REF PSIC = <real>psic_ref
T DERIV PSIC = <real>dpsicdT
T 2DERIV PSIC = <real>d2psicdT2
PSI EQ 2T = <real>psitt
PSI EQ 3T = <real>psittt
PSI EQ 4T = <real>psitttt
PSI EQ XX 11 = <real>psiXX11
PSI EQ XX 22 = <real>psiXX22
PSI EQ XX 33 = <real>psiXX33
PSI EQ XX 12 = <real>psiXX12
PSI EQ XX 13 = <real>psiXX13
PSI EQ XX 23 = <real>psiXX23
PSI EQ XX 44 = <real>psiXX44
PSI EQ XX 55 = <real>psiXX55
PSI EQ XX 66 = <real>psiXX66
```

```
PSI EQ XXT 11 = <real>psiXXT11
PSI EQ XXT 22 = <real>psiXXT22
PSI EQ XXT 33 = <real>psiXXT33
PSI EQ XXT 12 = <real>psiXXT12
PSI EQ XXT 13 = <real>psiXXT13
PSI EQ XXT 23 = <real>psiXXT23
PSI EQ XXT 44 = <real>psiXXT44
PSI EQ XXT 55 = <real>psiXXT55
PSI EQ XXT 66 = <real>psiXXT66
PSI EQ XT 1 = <real>psiXT1
PSI EQ XT 2 = <real>psiXT2
PSI EQ XT 3 = <real>psiXT3
PSI EQ XTT 1 = <real>psiXTT1
PSI EQ XTT 2 = <real>psiXTT2
PSI EQ XTT 3 = <real>psiXTT3
REF PSIA 11 = <real>psiA11
REF PSIA 22 = <real>psiA22
REF PSIA 33 = <real>psiA33
REF PSIA 12 = <real>psiA12
REF PSIA 13 = <real>psiA13
REF PSIA 23 = <real>psiA23
REF PSIA 44 = <real>psiA44
REF PSIA 55 = <real>psiA55
REF PSIA 66 = <real>psiA66
T DERIV PSIA 11 = <real>dpsiA11dT
T DERIV PSIA 22 = <real>dpsiA22dT
T DERIV PSIA 33 = <real>dpsiA33dT
T DERIV PSIA 12 = <real>dpsiA12dT
T DERIV PSIA 13 = <real>dpsiA13dT
T DERIV PSIA 23 = <real>dpsiA23dT
T DERIV PSIA 44 = <real>dpsiA44dT
T DERIV PSIA 55 = <real>dpsiA55dT
T DERIV PSIA 66 = <real>dpsiA66dT
REF PSIB 1 = <real>psiB1
REF PSIB 2 = <real>psiB2
REF PSIB 3 = <real>psiB3
T DERIV PSIB 1 = <real>dpsiB1dT
T DERIV PSIB 2 = <real>dpsiB2dT
T DERIV PSIB 3 = <real>dpsiB3dT
PSI POT TT = <real>psipotTT
PSI POT TTT = <real>psipotTTT
PSI POT TTTT = <real>psipotTTTT
PSI POT XT 1 = <real>psipotXT1
PSI POT XT 2 = <real>psipotXT2
PSI POT XT 3 = <real>psipotXT3
PSI POT XTT 1 = <real>psipotXTT1
PSI POT XTT 2 = <real>psipotXTT2
```

```
    PSI POT XTT 3 = <real>psipotXTT3
    PSI POT XXT 11 = <real>psipotXXT11
    PSI POT XXT 22 = <real>psipotXXT22
    PSI POT XXT 33 = <real>psipotXXT33
    PSI POT XXT 12 = <real>psipotXXT12
    PSI POT XXT 13 = <real>psipotXXT13
    PSI POT XXT 23 = <real>psipotXXT23
    PSI POT XXT 44 = <real>psipotXXT44
    PSI POT XXT 55 = <real>psipotXXT55
    PSI POT XXT 66 = <real>psipotXXT66
  END [PARAMETERS FOR MODEL NLVE_3D_ORTHOTROPIC]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Stiff elastic

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  # thermal strain option
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL STIFF_ELASTIC
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    BULK MODULUS = <real>bulk_modulus
    SHEAR MODULUS = <real>shear_modulus
    LAMBDA = <real>lambda
    SCALE FACTOR = <real>scale_factor
    REFERENCE STRAIN = <real>reference_strain
  END [PARAMETERS FOR MODEL STIFF_ELASTIC]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Swanson

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  BEGIN PARAMETERS FOR MODEL SWANSON
```

```
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    BULK MODULUS = <real>bulk_modulus
    SHEAR MODULUS = <real>shear_modulus
    LAMBDA = <real>lambda
    A1 = <real>a1
    P1 = <real>p1
    B1 = <real>b1
    Q1 = <real>q1
    C1 = <real>c1
    R1 = <real>r1
    CUT OFF STRAIN = <real>ecut
    THERMAL EXPANSION FUNCTION = <string>eth_function_name
    TARGET E = <real>target_e
    TARGET E FUNCTION = <string>etar_function_name
    MAX POISSONS RATIO = <real>max_poissons_ratio
    REFERENCE STRAIN = <real>reference_strain
  END [PARAMETERS FOR MODEL SWANSON]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Viscoelastic Swanson
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  BIOTS COEFFICIENT = <real>biots_value
  #
  BEGIN PARAMETERS FOR MODEL VISCOELASTIC_SWANSON
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    BULK MODULUS = <real>bulk_modulus
    SHEAR MODULUS = <real>shear_modulus
    LAMBDA = <real>lambda
    A1 = <real>a1
    P1 = <real>p1
    B1 = <real>b1
    Q1 = <real>q1
    C1 = <real>c1
    R1 = <real>r1
    CUT OFF STRAIN = <real>ecut
    THERMAL EXPANSION FUNCTION = <string>eth_function_name
    PRONY SHEAR INFINITY = <real>ginf
    PRONY SHEAR 1 = <real>g1
    PRONY SHEAR 2 = <real>g2
    PRONY SHEAR 3 = <real>g3
    PRONY SHEAR 4 = <real>g4
    PRONY SHEAR 5 = <real>g5
    PRONY SHEAR 6 = <real>g6
    PRONY SHEAR 7 = <real>g7
```

```
    PRONY SHEAR 8 = <real>g8
    PRONY SHEAR 9 = <real>g9
    PRONY SHEAR 10 = <real>g10
    SHEAR RELAX TIME 1 = <real>tau1
    SHEAR RELAX TIME 2 = <real>tau2
    SHEAR RELAX TIME 3 = <real>tau3
    SHEAR RELAX TIME 4 = <real>tau4
    SHEAR RELAX TIME 5 = <real>tau5
    SHEAR RELAX TIME 6 = <real>tau6
    SHEAR RELAX TIME 7 = <real>tau7
    SHEAR RELAX TIME 8 = <real>tau8
    SHEAR RELAX TIME 9 = <real>tau9
    SHEAR RELAX TIME 10 = <real>tau10
    WLF COEF C1 = <real>wlf_c1
    WLF COEF C2 = <real>wlf_c2
    WLF TREF = <real>wlf_tref
    NUMERICAL SHIFT FUNCTION = <string>ns_function_name
    TARGET E = <real>target_e
    TARGET E FUNCTION = <string>etar_function_name
    MAX POISSONS RATIO = <real>max_poissons_ratio
    REFERENCE STRAIN = <real>reference_strain
  END [PARAMETERS FOR MODEL VISCOELASTIC_SWANSON]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Traction Decay

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  #
  BEGIN PARAMETERS FOR MODEL TRACTION_DECAY
    NORMAL DECAY LENGTH = <real>
    TANGENTIAL DECAY LENGTH = <real>
  END [PARAMETERS FOR MODEL TRACTION_DECAY]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Tvergaard Hutchinson

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  #
  BEGIN PARAMETERS FOR MODEL TVERGAARD_HUTCHINSON
    INIT TRACTION METHOD = IGNORE|ADD (IGNORE)
    LAMBDA_1 = <real>
    LAMBDA_2 = <real>
    NORMAL LENGTH SCALE = <real>
    TANGENTIAL LENGTH SCALE = <real>
    PEAK TRACTION = <real>
```

```
    PENETRATION STIFFNESS MULTIPLIER = <real>
    NORMAL INITIAL TRACTION DECAY LENGTH = <real>
    TANGENTIAL INITIAL TRACTION DECAY LENGTH = <real>
    USE ELASTIC UNLOADING = NO|YES (YES)
  END [PARAMETERS FOR MODEL TVERGAARD_HUTCHINSON]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Thouless Parmigiani

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  #
  BEGIN PARAMETERS FOR MODEL THOULESS_PARMIGIANI
    INIT TRACTION METHOD = IGNORE|ADD (IGNORE)
    LAMBDA_1_N = <real>
    LAMBDA_2_N = <real>
    LAMBDA_1_T = <real>
    LAMBDA_2_T = <real>
    NORMAL LENGTH SCALE = <real>
    TANGENTIAL LENGTH SCALE = <real>
    PEAK NORMAL TRACTION = <real>
    PEAK TANGENTIAL TRACTION = <real>
    PENETRATION STIFFNESS MULTIPLIER = <real>
    USE ELASTIC UNLOADING = NO|YES (YES)
  END [PARAMETERS FOR MODEL THOULESS_PARMIGIANI]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# RVE

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  #
  BEGIN PARAMETERS FOR MODEL RVE
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
  END [PARAMETERS FOR MODEL RVE]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Define mesh

BEGIN FINITE ELEMENT MODEL <string>mesh_descriptor
  DATABASE NAME = <string>mesh_file_name
  DATABASE TYPE = <string>database_type(exodusII)
  ALIAS <string>mesh_identifier AS <string>user_name
  OMIT BLOCK <string>block_list
  COMPONENT SEPARATOR CHARACTER = <string>separator
  BEGIN PARAMETERS FOR BLOCK [<string list>block_names]
```

```
    MATERIAL <string>material_name
    SOLID MECHANICS USE MODEL <string>model_name
    INCLUDE ALL BLOCKS
    REMOVE BLOCK = <string list>block_names
    SECTION = <string>section_id
    LINEAR BULK VISCOSITY =
      <real>linear_bulk_viscosity_value(0.06)
    QUADRATIC BULK VISCOSITY =
      <real>quad_bulk_viscosity_value(1.20)
    HOURGLASS STIFFNESS =
      <real>hour_glass_stiff_value(solid = 0.05,
      shell/membrane = 0.0)
    HOURGLASS VISCOSITY =
      <real>hour_glass_visc_value(solid = 0.0,
      shell/membrane = 0.0)
    MEMBRANE HOURGLASS STIFFNESS =
      <real>memb_hour_glass_stiff_value(0.0)
    MEMBRANE HOURGLASS VISCOSITY =
      <real>memb_hour_glass_visc_value(0.0)
    BENDING HOURGLASS STIFFNESS =
      <real>bend_hour_glass_stiff_value(0.0)
    BENDING HOURGLASS VISCOSITY =
      <real>bend_hour_glass_visc_value(0.0)
    TRANSVERSE SHEAR HOURGLASS STIFFNESS =
      <real>tshr_hour_glass_stiff_value(0.0)
    TRANSVERSE SHEAR HOURGLASS VISCOSITY =
      <real>tshr_hour_glass_visc_value(0.0)
    EFFECTIVE MODULI MODEL = <string>PRESTO|PRONTO|
      CURRENT|ELASTIC(PRONTO)
    ELEMENT NUMERICAL FORMULATION = <string>OLD|NEW(OLD)
    ACTIVE FOR PROCEDURE <string>proc_name DURING PERIODS
      <string list>period_names
    INACTIVE FOR PROCEDURE <string>proc_name DURING PERIODS
      <string list>period_names
  END [PARAMETERS FOR BLOCK <string list>block_names]
END [FINITE ELEMENT MODEL <string>mesh_descriptor]

# Element sections

BEGIN SOLID SECTION <string>solid_section_name
  COORDINATE SYSTEM = <string>Coordinate_system_name
  FORMULATION = <string>MEAN_QUADRATURE|
    SELECTIVE_DEVIATORIC|VOID(MEAN_QUADRATURE)
  DEVIATORIC PARAMETER = <real>deviatoric_param
  STRAIN INCREMENTATION = <string>MIDPOINT_INCREMENT|
    STRONGLY_OBJECTIVE|NODE_BASED(MIDPOINT_INCREMENT)
  NODE BASED ALPHA FACTOR = <real>bulk_stress_weight(0.01)
```

```
  NODE BASED BETA FACTOR = <real>shear stress_weight(0.35)
  HOURGLASS FORMULATION = <string>TOTAL|INCREMENTAL(INCREMENTAL)
  HOURGLASS INCREMENT = <string>ENDSTEP|MIDSTEP (ENDSTEP)
  HOURGLASS ROTATION = <string> APPROXIMATE|SCALED (APPROXIMATE)
  RIGID BODY = <string>rigid_body_name
  RIGID BODIES FROM ATTRIBUTES = <integer>first_id
    TO <integer>last_id
  USE LAME|STRUMENTO(LAME)
END [SOLID SECTION <string>solid_section_name]

BEGIN COHESIVE SECTION <string>cohesive_section_name
  NUMBER OF INTEGRATION POINTS = <integer>num_int_points(1)
END [COHESIVE SECTION <string>cohesive_section_name]

BEGIN SHELL SECTION <string>shell_section_name
  THICKNESS = <real>shell_thickness
  THICKNESS MESH VARIABLE =
    <string>THICKNESS|<string>var_name
  THICKNESS TIME STEP = <real>time_value
  THICKNESS SCALE FACTOR = <real>thick_scale_factor(1.0)
  INTEGRATION RULE = TRAPEZOID|GAUSS|LOBATTO|SIMPSONS|
    USER(TRAPEZOID)
  NUMBER OF INTEGRATION POINTS = <integer>num_int_points(5)
  FORMULATION = MEAN_QUADRATURE|NQUAD (MEAN_QUADRATURE)
  BEGIN USER INTEGRATION RULE
    <real>location_1 <real>weight_1
    <real>location_2 <real>weight_2
    .
    .
    <real>location_n <real>weight_n
  END [USER INTEGRATION RULE]
  LOFTING FACTOR = <real>lofting_factor(0.5)
  OFFSET MESH VARIABLE = <string>var_name
  ORIENTATION = <string>orientation_name
  DRILLING STIFFNESS FACTOR = <real>stiffness_factor(0.0)
  RIGID BODY = <string>rigid_body_name
  RIGID BODIES FROM ATTRIBUTES = <integer>first_id
    TO <integer>last_id
  USE LAME|STRUMENTO(LAME)
END [SHELL SECTION <string>shell_section_name]

BEGIN MEMBRANE SECTION <string>membrane_section_name
  THICKNESS = <real>mem_thickness
  THICKNESS MESH VARIABLE =
    <string>THICKNESS|<string>var_name
  THICKNESS TIME STEP = <real>time_value
  THICKNESS SCALE FACTOR = <real>thick_scale_factor(1.0)
```

```
  FORMULATION = <string>MEAN_QUADRATURE|
    SELECTIVE_DEVIATORIC(MEAN QUADRATURE)
  DEVIATORIC PARAMETER = <real>deviatoric_param
  LOFTING FACTOR = <real>lofting_factor(0.5)
  RIGID BODY = <string>rigid_body_name
  RIGID BODIES FROM ATTRIBUTES = <integer>first_id
    TO <integer>last_id
END [MEMBRANE SECTION <string>membrane_section_name]

BEGIN BEAM SECTION <string>beam_section_name
  SECTION = <string>ROD|TUBE|BAR|BOX|I
  WIDTH = <real>section_width
  WIDTH VARIABLE = <string>width_var
  HEIGHT = <real>section_width
  HEIGHT VARIABLE= <string>height_var
  WALL THICKNESS = <real>wall_thickness
  WALL THICKNESS VARIABLE = <string>wall_thickness_var
  FLANGE THICKNESS = <real>flange_thickness
  FLANGE THICKNESS VARIABLE = <string>flange_thickness_var
  T AXIS = <real>tx <real>ty <real>tz
  T AXIS VARIABLE = <string>t_axis_var
  REFERENCE AXIS = <string>CENTER|RIGHT|
    TOP|LEFT|BOTTOM(CENTER)
  AXIS OFFSET = <real>s_offset <real>t_offset
  AXIS OFFSET GLOBAL = <real>x_offset <real>y_offset <real>z_offset
  AXIS OFFSET VARIABLE = <string>axis_offset_var
  RIGID BODY = <string>rigid_body_name
  RIGID BODIES FROM ATTRIBUTES = <integer>first_id
    TO <integer>last_id
  USE LAME|STRUMENTO(LAME)
END [BEAM SECTION <string>beam_section_name]

BEGIN TRUSS SECTION <string>truss_section_name
  AREA = <real>cross_sectional_area
  INITIAL LOAD = <real>initial_load
  PERIOD = <real>period
  RIGID BODY = <string>rigid_body_name
  RIGID BODIES FROM ATTRIBUTES = <integer>first_id
    TO <integer>last_id
  USE LAME|STRUMENTO(LAME)
END [TRUSS SECTION <string>truss_section_name]

BEGIN DAMPER SECTION <string>damper_section_name
  AREA = <real>damper_cross_sectional_area
END [DAMPER SECTION <string>damper_section_name]

BEGIN POINT MASS SECTION <string>pointmass_section_name
```

```
  VOLUME = <real>volume
  MASS = <real>mass
  IXX = <real>Ixx
  IYY = <real>Iyy
  IZZ = <real>Izz
  IXY = <real>Ixy
  IXZ = <real>Ixz
  IYZ = <real>Iyz
  RIGID BODY = <string>rigid_body_name
  RIGID BODIES FROM ATTRIBUTES = <integer>first_id
    TO <integer>last_id
  MASS VARIABLE = <string>mass_variable_name
  INERTIA VARIABLE = <string>inertia_variable_name
  OFFSET VARIABLE = <string>offset_variable_name
  ATTRIBUTES VARIABLE NAME = <string>attrib_variable_name
END [POINT MASS SECTION <string>pointmass_section_name]

BEGIN PARTICLE SECTION <string>sph_section_name
  RADIUS MESH VARIABLE =
    <string>var_name|<string>attribute|SPHERE INITIAL
    RADIUS = <real>rad
  RADIUS MESH VARIABLE TIME STEP = <string>time
  PROBLEM DIMENSION = <integer>1|2|3(3)
  CONSTANT SPHERE RADIUS
  FINAL RADIUS MULTIPLICATION FACTOR = <real>factor(1.0)
  FORMULATION = <string>GPA|MASS_PARTICLE|SPH(SPH)
  MONAGHAN EPSILON = <real>monaghan_epsilon(0.0)
  MONAGHAN N = <real>monaghan_n(0.0)
  SPH ALPHAQ PARAMETER = <real>alpha(1.0)
  SPH BETAQ PARAMETER = <real>beta(2.0)
  DENSITY FORMULATION = <string>MATERIAL|KERNEL(MATERIAL)
  USE LAME|STRUMENTO(LAME)
END [PARTICLE SECTION <string>sph_section_name]


BEGIN SUPERELEMENT SECTION <string>section_name
  BEGIN MAP
    <integer>node_index_1 <integer>component_index_1
    <integer>node_index_2 <integer>component_index_2
    ...
    <integer>node_index_n <integer>component_index_n
  END
  BEGIN STIFFNESS MATRIX
    <real>k_1_1 <real>k_1_2 ...  <real>k_1_n
    <real>k_2_1 <real>k_2_2 ...  <real>k_2_n
    ...         ...         ...  ...
    <real>k_n_1 <real>k_n_2 ...  <real>k_n_n
```

```
  END
  BEGIN DAMPING MATRIX
    <real>c_1_1 <real>c_1_2 ...  <real>c_1_n
    <real>c_2_1 <real>c_2_2 ...  <real>c_2_n
    ...         ...         ...  ...
    <real>c_n_1 <real>c_n_2 ...  <real>c_n_n
  END
  BEGIN MASS MATRIX
    <real>m_1_1 <real>m_1_2 ...  <real>m_1_n
    <real>m_2_1 <real>m_2_2 ...  <real>m_2_n
    ...          ...        ...  ...
    <real>m_n_1 <real>m_n_2 ...  <real>m_n_n
  END
  FILE = <string>netcdf_file_name
END [SUPERELEMENT SECTION <string>section_name]

 BEGIN PERIDYNAMICS SECTION <string>section_name
   MATERIAL MODEL FORMULATION = <string>CLASSICAL|PERIDYNAMICS
   HORIZON = <real>horizon [SCALE BY ELEMENT RADIUS]
   BOND DAMAGE MODEL = <string>CRITICAL_STRETCH|NONE(NONE)
      [<real>critical_stretch]
   HOURGLASS STIFFNESS = <real>stiffness(0.0)
   BOND CUTTING BLOCK = <string list>block_names
   BOND VISUALIZATION = <string>OFF|ON(OFF)
 END [PERIDYNAMICS SECTION <string>section_name]

# Zoltan parameters
BEGIN ZOLTAN PARAMETERS <string>parameter_name
  LOAD BALANCING METHOD  = <string>recursive coordinate
    bisection|recursive inertial bisection|hilbert space
    filling curve|octree
  DETERMINISTIC DECOMPOSITION = <string>false|true
  IMBALANCE TOLERANCE = <real>imb_tol
  OVER ALLOCATE MEMORY = <real>over_all_mem
  REUSE CUTS = <string>false|true
  ALGORITHM DEBUG LEVEL = <integer>alg_level
    #  0<=(alg_level)<=3
  CHECK GEOMETRY = <string>false|true
  KEEP CUTS = <string>false|true
  LOCK RCB DIRECTIONS = <string>false|true
  SET RCB DIRECTIONS = <string>do not order cuts|xyz|xzy|
    yzx|yxz|zxy|zyx
  RECTILINEAR RCB BLOCKS = <string>false|true
  RENUMBER PARTITIONS = <string>false|true
  OCTREE DIMENSION = <integer>oct_dimension
  OCTREE METHOD = <string>morton indexing|grey code|hilbert
  OCTREE MIN OBJECTS = <integer>min_obj  #  1<=(min_obj)
```

```
  OCTREE MAX OBJECTS = <integer>max_obj  #  1<=(max_obj)
  ZOLTAN DEBUG LEVEL = <integer>zoltan_level
    #  0<=(zoltan_level)<=10
  DEBUG PROCESSOR NUMBER = <integer>proc  #  1<=proc
  TIMER = <string>wall|cpu
  DEBUG MEMORY = <integer>dbg_mem  #  0<=(dbg_mem)<=3
END [ZOLTAN PARAMETERS <string>parameter_name]

# Output scheduler

BEGIN OUTPUT SCHEDULER <string>scheduler_name
  START TIME = <real>output_start_time
  TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
  AT TIME <real>time_begin INCREMENT =
    <real>time_increment_dt
  ADDITIONAL TIMES = <real>output_time1
    <real>output_time2 ...
  AT STEP <integer>step_begin INCREMENT =
    <integer>step_increment
  ADDITIONAL STEPS = <integer>output_step1
    <integer>output_step2 ...
  TERMINATION TIME = <real>termination_time_value
 END [OUTPUT SCHEDULER <string>scheduler_name]

# Begin Procedure scope
BEGIN PRESTO PROCEDURE <string>presto_procedure_name

  PRINT BANNER INTERVAL = <integer>print_banner_interval(MAX_INT)

  BEGIN PROCEDURAL TRANSFER <string>name

    BLOCK = <string list>block_name
    INCLUDE ALL BLOCKS
    REMOVE BLOCK = <string list>block_name

    BEGIN INTERPOLATION TRANSFER <string>name

      BLOCK BY BLOCK
      NEAREST ELEMENT COPY

      SEND BLOCKS = <string list>block_name
      SEND COORDINATES = ORIGINAL|CURRENT

      RECEIVE BLOCKS = <string list>block_name
      RECEIVE COORDINATES = ORIGINAL|CURRENT

      TRANSFORMATION TYPE = NONE|RIGIDBODY
```

```
  END [INTERPOLATION TRANSFER <string>name]
END [PROCEDURAL TRANSFER <string>name]

# Time block
BEGIN TIME CONTROL
  BEGIN TIME STEPPING BLOCK <string>time_block_name
    START TIME = <real>start_time_value
    BEGIN PARAMETERS FOR PRESTO REGION
      <string>region_name
      INITIAL TIME STEP = <real>initial_time_step_value
      TIME STEP SCALE FACTOR =
        <real>time_step_scale_factor(1.0)
      TIME STEP INCREASE FACTOR =
        <real>time_step_increase_factor(1.1)
      STEP INTERVAL = <integer>nsteps(100)
      USER TIME STEP = <real>time_step
    END [PARAMETERS FOR PRESTO REGION
      <string>region_name]
  END [TIME STEPPING BLOCK <string>time_block_name]
  TERMINATION TIME = <real>termination_time
END TIME CONTROL

# Begin Region scope

BEGIN PRESTO REGION <string>presto_region_name

  USE FINITE ELEMENT MODEL <string>model_name
  GLOBAL ENERGY REPORTING = EXACT|APPROXIMATE|OFF (EXACT)
  EXTENSIVE RIGID BODY VARS OUTPUT = OFF|HISTORY|RESULTS|ALL (ALL)


  # Time step control using Lanczos

  BEGIN LANCZOS PARAMETERS <string>lanczos_name
    NUMBER EIGENVALUES = <integer>num_eig(20)
    STARTING VECTOR = <string>STRETCH_X|STRETCH_Y|STRETCH_Z
      (STRETCH_X)
    VECTOR SCALE = <real>vec_scale(1.0e-5)
    TIME SCALE = <real>time_scale(0.9)
    STEP INTERVAL = <integer>step_int(1)
    INCREMENT INTERVAL = <integer>incr_int(5)
    TIME STEP LIMIT = <real>step_lim(0.10)
  END [LANCZOS PARAMETERS <string>lanczos_name]

  # Time step control using nodes
```

```
BEGIN NODE BASED TIME STEP PARAMETERS <string>nbased_name
  INCREMENT INTERVAL = <integer>incr_int(5)
  STEP INTERVAL = <integer>step_int(500)
  TIME STEP LIMIT = <real>step_lim(0.10)
END [NODE BASED TIME STEP PARAMETERS <string>nbased_name]

# Mass scaling

BEGIN MASS SCALING
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  TARGET TIME STEP = <real>target_time_step
  ALLOWABLE MASS INCREASE RATIO
    = <real>mass_increase_ratio
  #
  # additional command
  ACTIVE PERIODS = <string list>periods
  INACTIVE PERIODS = <string list>periods
END MASS SCALING

# Torsional spring

BEGIN TORSIONAL SPRING MECHANISM <string>spring_name
  NODE SETS = <string>nodelist_int1
    <string>nodelist_int2
    <string>nodelist_int3 <string>nodelist_int4
  TORSIONAL STIFFNESS = <real>stiffness
  INITIAL TORQUE = <real>init_load
  PERIOD = <real>time_period
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [TORSIONAL SPRING MECHANISM <string>spring_name]

# Mass property calculations

BEGIN MASS PROPERTIES
  #
  # block set commands
  BLOCK = <string list>block_names
```

```
  INCLUDE ALL BLOCKS
  REMOVE BLOCK = <string list>block_names
  #
  # structure command
  STRUCTURE NAME = <string>structure_name
END [MASS PROPERTIES]

# SPH utility commands

BEGIN SPH OPTIONS
  SPH SYMMETRY PLANE <string>+X|+Y|+Z|-X|-Y|-Z
    <real>position_on_axis(0.0)
  SPH DECOUPLE STRAINS: <string>material1 <string>material2
END [SPH OPTIONS]

# Element death

BEGIN ELEMENT DEATH <string>death_name
  #
  # block set commands
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE BLOCK = <string list>block_names
  #
  # criterion commands
  CRITERION IS AVG|MAX|MIN NODAL VALUE OF
    <string>var_name <|<=|=|>=|> <real>tolerance
  CRITERION IS ELEMENT VALUE OF
    <string>var_name <|<=|=|>=|> <real>tolerance [KILL WHEN
    <integer>num_intg INTEGRATION POINTS REMAIN]
  CRITERION IS GLOBAL VALUE OF
    <string>var_name <|<=|=|>=|> <real>tolerance
  ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  MATERIAL CRITERION
    = <string list>material_model_names [KILL WHEN
    <integer>num_intg INTEGRATION POINTS REMAIN]
  #
  # evaluation commands
  CHECK STEP INTERVAL = <integer>num_steps
  CHECK TIME INTERVAL = <real>delta_t
```

```
  DEATH START TIME = <real>time
  #
  # miscellaneous option commands
  SUMMARY OUTPUT STEP INTERVAL = <integer>output_step_interval
  SUMMARY OUTPUT TIME INTERVAL = <real>output_time_interval
  DEATH ON INVERSION = OFF|ON(OFF)
  DEATH STEPS = <integer>death_steps(1)
  FORCE VALID ACME CONNECTIVITY
  AGGRESSIVE CONTACT CLEANUP = <string>OFF|ON(OFF)
  #
  # particle conversion commands
  BEGIN PARTICLE CONVERSION
    PARTICLE SECTION = <string>section_name
    NEW MATERIAL = <string>material_name
      MODEL = <string>model_name
    TRANSFER = <string>NONE|STRESS_ONLY|ALL
    MAX NUM PARTICLES = <integer>num
    MIN PARTICLE CONVERSION VOLUME = <real>vol
  END [PARTICLE CONVERSION]
  DEATH METHOD = <string>DEACTIVATE ELEMENT|
  DEACTIVATE NODAL MPCS|DISCONNECT ELEMENT|
  INSERT COHESIVE ZONES(DEACTIVATE ELEMENT)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
  #
  # cohesive zone setup commands
  COHESIVE SECTION = <string>sect_name
  COHESIVE MATERIAL = <string>mat_name
  COHESIVE MODEL = <string>model_name
  COHESIVE ZONE INITIALIZATION METHOD = <string>NONE|
    ELEMENT STRESS AVG(NONE)
END [ELEMENT DEATH <string>death_name]

# Derived output

BEGIN DERIVED OUTPUT
  COMPUTE AND STORE VARIABLE =
    <string>derived_quantity_name
END DERIVED OUTPUT

# Mesh rebalance

BEGIN REBALANCE
  ELEMENT GROUPING TYPE = SPLIT SPH AND STANDARD ELEMENTS|
    UNIFORM UNIFIED(SPLIT SPH AND STANDARD ELEMENTS)
  INITIAL REBALANCE = ON|OFF(OFF)
  PERIODIC REBALANCE = ON|OFF|AUTO(OFF)
```

```
  REBALANCE STEP INTERVAL = <integer>stepInterval
  LOAD RATIO THRESHOLD = <real>loadRatio
  COMMUNICATION RATIO THRESHOLD = <real>communicationRatio
  ZOLTAN PARAMETERS = <string>parameterName
END [REBALANCE]

# Remeshing
BEGIN REMESH
  MAX REMESH STEP INTERVAL = <integer>stepInterval (Infinity)
  MAX REMESH TIME INTERVAL = <real>timeInterval (Infinity)
  NEW MESH MAX EDGE LENGTH RATIO = <real>newMaxRatio (1.25)
  NEW MESH MIN EDGE LENGTH RATIO = <real>newMinRatio (0.25)
  NEW MESH MIN SHAPE = <real>newMinShape (0.125)
  REMESH AT MAX EDGE LENGTH RATIO = <real>maxCutoffRatio
    (newMaxEdgeLengthRatio*1.75)
  REMESH AT MIN EDGE LENGTH RATIO = <real>minCutoffRatio
    (newMinEdgeLengthRatio*0.25)
  REMESH AT SHAPE = <real>cutoffShape (0.025)
  CONTACT CLEANUP = AUTO|OFF|ON (AUTO)
  DEBUG OUTPUT LEVEL = <integer>level (0)
  MAX REMESH REBALANCE METRIC = <integer>rebalanceMetric (1.25)
  MIN SHAPE IMPROVEMENT = <real>minShapeImprovement(0.001)
  MAX NUM PATCH RECREATIONS = <integer>maxNumPatchRecreations(5)
  POISON CRITICAL VALUE = <integer>poisonCriticalValue(4)
  POISON SUBTRACTION INTERVAL =
    <integer>poisonSubtractionInterval(10)
  MAX ITERATIONS = <integer>maxIterations(5)

  BEGIN REMESH BLOCK SET
    BLOCK = <string list>blockNames
    REMOVE BLOCK = <string list>blockNames
    INCLUDE ALL BLOCKS
  END [REMESH BLOCK SET]

  BEGIN ADAPTIVE REFINEMENT
    #
    # adaptive refinement control commands
    ADAPT TYPE = NODE_PROXIMITY|POINT_PROXIMITY|
      SHARP_EDGE_PROXIMITY
    RADIUS = <real>radius
    ADAPT SHARP ANGLE = <real>angle (45)
    ADAPT SMOOTH ANGLE = <real>angle (10)
    GEOMETRIC POINT COORDINATES = <real>x <real>y <real>z
    ADAPT SIZE RATIO = <real>ratio (2.0)
    #
    # tool mesh entity commands
    NODE SET = <string list>nodelist_names
```

```
    REMOVE NODE SET = <string list>nodelist_names
    SURFACE = <string list>surface_names
    REMOVE SURFACE = <string list>surface_names
    BLOCK = <string list>block_names
    REMOVE BLOCK = <string list>block_names
    INCLUDE ALL BLOCKS
    #
    # activation commands
    ACTIVE PERIODS = <string>period_names
    INACTIVE PERIODS = <string>period_names
  END [ADAPTIVE REFINEMENT]
END [REMESH]

# Initial condition

BEGIN INITIAL CONDITION
  #
  # mesh-entity set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # variable identification commands
  INITIALIZE VARIABLE NAME = <string>var_name
  VARIABLE TYPE = [NODE|EDGE|FACE|ELEMENT|GLOBAL]
  #
  # specification command
  MAGNITUDE = <real list>initial_values
  #
  # probability distribution commands
  DISTRIBUTION = WEIBULL PARAMETERS = <real list>dist_values
    SEED = <integer>dist_seed
  DISTRIBUTION REFERENCE = NODE|EDGE|FACE|ELEMENT|GLOBAL
    <string>size_var_name VALUE = <real>size_ref_val
  #
  # input mesh commands
  READ VARIABLE = <string>var_name
  COPY VARIABLE = <string>var_name
    [FROM MODEL <string>model_name]
  TIME = <real>time
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name |
```

```
    SURFACE SUBROUTINE = <string>subroutine_name |
    ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # additional command
  SCALE FACTOR = <real>scale_factor(1.0)
END [INITIAL CONDITION]

# Boundary conditions

BEGIN FIXED DISPLACEMENT
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # component commands
  COMPONENT = <string>X/Y/Z | COMPONENTS =
    <string>X/Y/Z
  #
  # additional command
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [FIXED DISPLACEMENT]

BEGIN PRESCRIBED DISPLACEMENT
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
```

```
  # function commands
  DIRECTION = <string>defined_direction |
    COMPONENT = <string>X|Y|Z |
    CYLINDRICAL AXIS = <string>defined_axis |
    RADIAL AXIS = <string>defined_axis
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # external database commands
  READ VARIABLE = <string>var_name
  COPY VARIABLE = <string>var_name
    [FROM MODEL <string>model_name]
  TIME = <real>time
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [PRESCRIBED DISPLACEMENT]

BEGIN PRESCRIBED VELOCITY
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # function commands
  DIRECTION = <string>defined_direction |
    COMPONENT = <string>X|Y|Z |
    CYLINDRICAL AXIS = <string>defined_axis |
    RADIAL AXIS = <string>defined_axis
  FUNCTION = <string>function_name
  #
```

```
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # external database commands
  READ VARIABLE = <string>var_name
  COPY VARIABLE = <string>var_name
    [FROM MODEL <string>model_name]
  TIME = <real>time
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [PRESCRIBED VELOCITY]

BEGIN PRESCRIBED ACCELERATION
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # function commands
  DIRECTION = <string>defined_direction |
    COMPONENT = <string>X|Y|Z
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
```

```
  #
  # external database commands
  READ VARIABLE = <string>var_name
  COPY VARIABLE = <string>var_name
    [FROM MODEL <string>model_name]
  TIME = <real>time
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [PRESCRIBED ACCELERATION]

BEGIN FIXED ROTATION
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # component commands
  COMPONENT = <string>X/Y/Z | COMPONENTS =
    <string>X/Y/Z
  #
  # additional command
  ACTIVE PERIODS = <string list>periods_names
  INACTIVE PERIODS = <string list>periods_names
END [FIXED ROTATION]

BEGIN PRESCRIBED ROTATION
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # function commands
  DIRECTION = <string>defined_direction |
    COMPONENT = <string>X|Y|Z
```

```
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # external database commands
  READ VARIABLE = <string>var_name
  COPY VARIABLE = <string>var_name
    [FROM MODEL <string>model_name]
  TIME = <real>time
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [PRESCRIBED ROTATION]

BEGIN PRESCRIBED ROTATIONAL VELOCITY
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # function commands
  DIRECTION = <string>defined_direction |
    COMPONENT = <string>X|Y|Z
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
```

```
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # external database commands
  READ VARIABLE = <string>var_name
  COPY VARIABLE = <string>var_name
    [FROM MODEL <string>model_name]
  TIME = <real>time
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [PRESCRIBED ROTATIONAL VELOCITY]

BEGIN REFERENCE AXIS ROTATION
  #
  # block command
  BLOCK = <string list>block_names
  #
  # specification commands
  REFERENCE AXIS X FUNCTION = <string>function_name
  REFERENCE AXIS Y FUNCTION = <string>function_name
  REFERENCE AXIS Z FUNCTION = <string>function_name
  #
  # rotation commands
  ROTATION = <string>function_name
  ROTATIONAL VELOCITY = <string>function_name
  #
  # torque command
  TORQUE = <string>function_name
  #
  # additional command
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [REFERENCE AXIS ROTATION]

BEGIN INITIAL VELOCITY
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
```

```
  REMOVE BLOCK = <string list>block_names
  #
  # direction commands
  COMPONENT = <string>X|Y|Z |
    DIRECTION = <string>defined_direction
  MAGNITUDE = <real>magnitude_of_velocity
  #
  # angular velocity commands
  CYLINDRICAL AXIS = <string>defined_axis
  ANGULAR VELOCITY = <real>angular_velocity
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
END [INITIAL VELOCITY]

BEGIN PRESSURE
  #
  # surface set commands
  SURFACE = <string list>surface_names
  REMOVE SURFACE = <string list>surface_names
  #
  # function command
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  SURFACE SUBROUTINE = <string>subroutine_name |
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # external pressure sources
  READ VARIABLE = <string>variable_name
  OBJECT TYPE = <string>NODE|FACE(NODE)
  TIME = <real>time
  FIELD VARIABLE = <string>field_variable
```

```
  #
  # output external forces from pressure
  EXTERNAL FORCE CONTRIBUTION OUTPUT NAME
    = <string>variable_name
  #
  # additional commands
  USE DEATH = <string>death_name
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [PRESSURE]

BEGIN TRACTION
  #
  # surface set commands
  SURFACE = <string list>surface_names
  REMOVE SURFACE = <string list>surface_names
  #
  # function commands
  DIRECTION = <string>direction_name
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [TRACTION]

BEGIN PRESCRIBED FORCE
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
```

```
  REMOVE BLOCK = <string list>block_names
  #
  # function commands
  DIRECTION = <string>defined_direction |
    COMPONENT = <string>X|Y|Z
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [PRESCRIBED FORCE]

BEGIN PRESCRIBED MOMENT
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # function commands
  DIRECTION = <string>defined_direction |
    COMPONENT = <string>X|Y|Z
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
```

```
    = <string>param_value
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [PRESCRIBED MOMENT]

BEGIN GRAVITY
  #
  # node set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  DIRECTION = <string>defined_direction
  FUNCTION = <string>function_name
  GRAVITATIONAL CONSTANT = <real>g_constant
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [GRAVITY]

BEGIN PRESCRIBED TEMPERATURE
  #
  # block set commands
  BLOCK = <string_list>block_names
  INCLUDE ALL BLOCKS
  REMOVE BLOCK
  #
  # function command
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
```

```
  # read variable commands
  READ VARIABLE = <string>mesh_var_name
  COPY VARIABLE = <string>var_name
    [FROM MODEL <string>model_name]
  TIME = <real>time
  TEMPERATURE TYPE = SOLID_ELEMENT|SHELL_ELEMENT(SOLID_ELEMENT)
  #
  # coupled analysis commands
  RECEIVE FROM TRANSFER [FIELD TYPE = NODE|ELEMENT(NODE)]
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [PRESCRIBED TEMPERATURE]

BEGIN PORE PRESSURE
  #
  # block set commands
  BLOCK = <string_list>block_names
  INCLUDE ALL BLOCKS
  REMOVE BLOCK
  #
  # function command
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # read variable commands
  READ VARIABLE = <string>mesh_var_name
  COPY VARIABLE = <string>var_name
    [FROM MODEL <string>model_name]
  TIME = <real>time
  #
  # coupled analysis commands
  RECEIVE FROM TRANSFER [FIELD TYPE = NODE|ELEMENT(NODE)]
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
```

```
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [PORE PRESSURE]

BEGIN FLUID PRESSURE
  #
  # surface set commands
  SURFACE = <string list>surface_names
  #
  # specification commands
  DENSITY = <real>fluid_density
  DENSITY FUNCTION = <string>density_function_name
  GRAVITATIONAL CONSTANT = <real>gravitational_acceleration
  FLUID SURFACE NORMAL = <string>global_component_names
  DEPTH = <real>fluid_depth
  DEPTH FUNCTION = <string>depth_function_name
  #
  # additional commands
  REFERENCE POINT = <string>reference_point_name
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [FLUID PRESSURE]

# Specialized boundary conditions

BEGIN CAVITY EXPANSION
  EXPANSION RADIUS = <string>SPHERICAL|CYLINDRICAL
    (spherical)
  SURFACE = <string list>surface_ids
  REMOVE SURFACE = <string list>surface_ids
  FREE SURFACE = <real>top_surface_zcoord
    <real>bottom_surface_zcoord
  NODE SETS TO DEFINE BODY AXIS =
    <string>nodelist_1 <string>nodelist_id2
  TIP RADIUS = <real>tip_radius
  BEGIN LAYER <string>layer_name
    LAYER SURFACE = <real>top_layer_zcoord
      <real>bottom_layer_zcoord
    PRESSURE COEFFICIENTS = <real>c0 <real>c1
      <real>c2
    SURFACE EFFECT = <string>NONE|SIMPLE_ON_OFF(NONE)
    FREE SURFACE EFFECT COEFFICIENTS = <real>coeff1
      <real>coeff2
  END [LAYER <string>layer_name]
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [CAVITY EXPANSION]
```

```
BEGIN BLAST PRESSURE
  SURFACE = <string list>surface_ids
  REMOVE SURFACE = <string list>surface_ids
  BURST TYPE = <string>SURFACE|AIR
  TNT MASS IN LBS = <real>tnt_mass_lbs
  BLAST TIME = <real>blast_time
  BLAST LOCATION = <real>loc_x <real>loc_y <real>loc_z
  ATMOSPHERIC PRESSURE IN PSI = <real>atmospheric_press
  AMBIENT TEMPERATURE IN FAHRENHEIT = <real>temperature
  FEET PER MODEL UNITS = <real>feet
  MILLISECONDS PER MODEL UNITS = <real>milliseconds
  PSI PER MODEL UNITS = <real>psi
  PRESSURE SCALE FACTOR = <real>pressure_scale(1.0)
  IMPULSE SCALE FACTOR = <real>impulse_scale(1.0)
  POSITIVE DURATION SCALE FACTOR = <real>duration_scale(1.0)
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [BLAST PRESSURE]

BEGIN SILENT BOUNDARY
  SURFACE = <string list>surface_names
  REMOVE SURFACE = <string list>surface_names
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [SILENT BOUNDARY]

BEGIN SPOT WELD
  NODE SET = <string list>nodelist_ids
  REMOVE NODE SET = <string list>nodelist_ids
  SURFACE = <string list>surface_ids
  REMOVE SURFACE = <string list>surfac_ids
  SECOND SURFACE = <string>surface_id
  NORMAL DISPLACEMENT FUNCTION =
    <string>function_nor_disp
  NORMAL DISPLACEMENT SCALE FACTOR =
    <real>scale_nor_disp(1.0)
  TANGENTIAL DISPLACEMENT FUNCTION =
    <string>function_tang_disp
  TANGENTIAL DISPLACEMENT SCALE FACTOR =
    <real>scale_tang_disp(1.0)
  FAILURE ENVELOPE EXPONENT = <real>exponent
  FAILURE FUNCTION = <string>fail_func_name
  FAILURE DECAY CYCLES = <integer>number_decay_cycles(10)
  SEARCH TOLERANCE = <real>search_tolerance
  IGNORE INITIAL OFFSET = NO|YES(NO)
  ACTIVE PERIODS = <string list>period_names
```

```
  INACTIVE PERIODS = <string list>period_names
END [SPOT WELD]

BEGIN LINE WELD
  SURFACE = <string list> surface_names
  REMOVE SURFACE = <string list> surface_names
  BLOCK = <string list> block_names
  REMOVE BLOCK = <string list>block_names
  SEARCH TOLERANCE = <real>search_tolerance
  R DISPLACEMENT FUNCTION =
    <string>r_disp_fucntion_name
  R DISPLACEMENT SCALE FACTOR = <real>r_disp_scale
  S DISPLACEMENT FUNCTION =
    <string>s_disp_function_name
  S DISPLACEMENT SCALE FACTOR = <real>s_disp_scale
  T DISPLACEMENT FUNCTION =
    <string>t_disp_function_name
  T DISPLACEMENT SCALE FACTOR = <real>t_disp_scale
  R ROTATION FUNCTION =
    <string>r_rotation_function_name
  R ROTATION SCALE FACTOR = <real>r_rotation_scale
  S ROTATION FUNCTION =
    <string>s_rotation_function_name
  S ROTATION SCALE FACTOR = <real>s_rotation_scale
  T ROTATION FUNCTION =
    <string>t_rotation_function_name
  T ROTATION SCALE FACTOR = <real>t_rotation_scale
  FAILURE ENVELOPE EXPONENT = <real>k
  FAILURE DECAY CYCLES = <integer>number_decay_cycles
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
END [LINE WELD]

BEGIN VISCOUS DAMPING <string>damp_name
  #
  # block set commands
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE BLOCK = <string list>block_names
  #
  MASS DAMPING COEFFICIENT = <real>mass_damping
  STIFFNESS DAMPING COEFFICIENT = <real>stiff_damping
  #
  # additional command
  ACTIVE PERIODS = <string list>period names
  INACTIVE PERIODS = <string list>period_names
END [VISCOUS DAMPING <string>damp_name]
```

```
BEGIN VOLUME REPULSION OLD <string>repulsion
  FRICTION COEFFICIENT = <real>fric_coeff
  SCALE FACTOR = <real>scale_factor
  OVERLAP TYPE = [NODAL|VOLUMETRIC]

  BEGIN BLOCK SET <string>set
    BLOCK = <string list>block_names
    INCLUDE ALL BLOCKS
    REMOVE BLOCK = <string list>block_names
    #
    SURFACE = <string list>surface_names
    REMOVE SURFACE = <string list>surface_names
    #
    ACTIVE PERIODS = <string list>period names
    INACTIVE PERIODS = <string list>period names
    #
    LINE CYLINDER RADIUS = <real>cylinder_radius
    ELEMENT REPRESENTATION = [BEAM_ELEMENT_CYLINDERS|
      TRUE_SOLID_VOLUME|NODES]
  END [BLOCK SET <string>set]
END [VOLUME REPULSION OLD <string>repulsion]


BEGIN MPC
  #
  # Master/Slave MPC commands
  MASTER NODE SET = <string list>master_nset
  MASTER NODES = <integer list>master_nodes
  MASTER SURFACE = <string list>master_surf
  MASTER BLOCK = <string list>master_block
  SLAVE NODE SET = <string list>slave_nset
  SLAVE NODES = <integer list>slave_nodes
  SLAVE SURFACE = <string list>slave_surf
  SLAVE BLOCK = <string list>slave_block
  #
  # Tied contact search command
  SEARCH TOLERANCE = <real>tolerance
  VOLUMETRIC SEARCH TOLERANCE = <real>vtolerance
  #
  # Tied MPC commands
  TIED NODES = <integer list>tied_nodes
  TIED NODE SET = <string list>tied_nset
END [MPC]

RESOLVE MULTIPLE MPCS = ERROR|FIRST WINS|LAST WINS(ERROR)
```

```
BEGIN SUBMODEL
  #
  EMBEDDED BLOCKS = <string list>embedded_block
  ENCLOSING BLOCKS = <string list>enclosing_block
END [SUBMODEL]

# Contact

BEGIN CONTACT DEFINITION <string>name
  #
  CONTACT SURFACE <string>name
    CONTAINS <string list>surface_names
  #
  SKIN ALL BLOCKS = <string>ON|OFF(OFF)
    [EXCLUDE <string list> block_names]
  #
  BEGIN CONTACT SURFACE <string>name
    BLOCK = <string list>block_names
    SURFACE = <string list>surface_names
    NODE SET = <string list>node_set_names
    REMOVE BLOCK = <string list>block_names
    REMOVE SURFACE = <string list>surface_names
    REMOVE NODE SET = <string list>nodelist_names
  END [CONTACT SURFACE <string>name]
  #
  CONTACT NODE SET <string>surface_name
    CONTAINS <string>nodelist_names
  #
  CONTACT FORMULATION TYPE = <string>ACME|DASH(ACME)
  #
  BEGIN ANALYTIC PLANE <string>name
    NORMAL = <string>defined_direction
    POINT = <string>defined_point
    REFERENCE RIGID BODY = <string>rb_name
  END [ANALYTIC PLANE <string>name]
  #
  BEGIN ANALYTIC CYLINDER <string>name
    CENTER = <string>defined_point
    AXIAL DIRECTION = <string>defined_axis
    RADIUS = <real>cylinder_radius
    LENGTH = <real>cylinder_length
    CONTACT NORMAL = <string>OUTSIDE|INSIDE
  END [ANALYTIC CYLINDER <string>name]
  #
  BEGIN ANALYTIC SPHERE <string>name
    CENTER = <string>defined_point
    RADIUS = <real>sphere_radius
```

```
END [ANALYTIC SPHERE <string>name]
#
UPDATE ALL SURFACES FOR ELEMENT DEATH = <string>ON|OFF(ON)
#
BEGIN REMOVE INITIAL OVERLAP
  OVERLAP NORMAL TOLERANCE = <real>over_norm_tol
  OVERLAP TANGENTIAL TOLERANCE = <real>over_tang_tol
  SHELL OVERLAP ITERATIONS = <integer>max_iter(10)
  SHELL OVERLAP TOLERANCE = <real>shell_over_tol(0.0)
END [REMOVE INITIAL OVERLAP]
#
MULTIPLE INTERACTIONS = <string>ON|OFF(ON)
MULTIPLE INTERACTIONS WITH ANGLE = <real>angle_in_deg(60.0)
#
BEGIN SURFACE NORMAL SMOOTHING
  ANGLE = <real>angle_in_deg
  DISTANCE = <real>distance
  RESOLUTION = <string>NODE|EDGE
END [SURFACE NORMAL SMOOTHING]
#
ERODED FACE TREATMENT = <string>NONE|ALL(ALL)
#
BEGIN SHELL LOFTING
  SURFACE = <string_list>surface_names
  REMOVE SURFACE = <string_list>removed_surface_names
  LOFTING ALGORITHM = <string>ON|OFF(ON)
  COINCIDENT SHELL TREATMENT = <string>DISALLOW|IGNORE|
    SIMPLE(DISALLOW)
  COINCIDENT SHELL HEX TREATMENT = <string>DISALLOW|
    IGNORE|TAPERED|EMBEDDED(DISALLOW)
  CONTACT SHELL THICKNESS =
    ACTUAL_THICKNESS|LET_CONTACT_CHOOSE(ACTUAL_THICKNESS)
  ALLOWABLE SHELL THICKNESS TO ELEMENT SIZE RATIOS =
    <real>lower_bound(0.1) TO <real>upper_bound(1.0)
END [SHELL LOFTING]
#
BEGIN FRICTIONLESS MODEL <string>name
END [FRICTIONLESS MODEL <string>name]
#
BEGIN CONSTANT FRICTION MODEL <string>name
  FRICTION COEFFICIENT = <real>coeff
END [CONSTANT FRICTION MODEL <string>name]
#
BEGIN TIED MODEL <string>name
END [TIED MODEL <string>name]
#
BEGIN GLUED MODEL <string>name
```

```
END [GLUED MODEL <string>name]
#
BEGIN SPRING WELD MODEL <string>name
  NORMAL DISPLACEMENT FUNCTION = <string>func_name
  NORMAL DISPLACEMENT SCALE FACTOR =
    <real>scale_factor(1.0)
  TANGENTIAL DISPLACEMENT FUNCTION = <string>func_name
  TANGENTIAL DISPLACEMENT SCALE FACTOR =
    <real>scale_factor(1.0)
  FAILURE ENVELOPE EXPONENT = <real>exponent(2.0)
  FAILURE DECAY CYCLES = <integer>num_cycles(1)
  FAILED MODEL = <string>failed_model_name|FRICTIONLESS
    (FRICTIONLESS)
END [SPRING WELD MODEL <string>name]
#
BEGIN SURFACE WELD MODEL <string>name
  NORMAL CAPACITY = <real>normal_cap
  TANGENTIAL CAPACITY = <real>tangential_cap
  FAILURE DECAY CYCLES = <integer>num_cycles(1)
  FAILED MODEL = <string>failed_model_name|FRICTIONLESS
    (FRICTIONLESS)
END [SURFACE WELD MODEL <string>name]
#
BEGIN AREA WELD MODEL <string>name
  NORMAL CAPACITY = <real>normal_cap
  TANGENTIAL CAPACITY = <real>tangential_cap
  FAILURE DECAY CYCLES = <integer>num_cycles(1)
  FAILED MODEL = <string>failed_model_name|FRICTIONLESS
    (FRICTIONLESS)
END [AREA WELD MODEL <string>name]
#
BEGIN ADHESION MODEL <string>name
  ADHESION FUNCTION = <string>func_name
  ADHESION SCALE FACTOR = <real>scale_factor(1.0)
END [ADHESION MODEL <string>name]
#
BEGIN COMPLIANT JOINT MODEL <string>name
  NORMAL MODULUS = <real>norm_mod
  SHEAR MODULUS = <real>shear_mod
  APERTURE = <real>aperture
  APERTURE LIMIT = <real>aperture_limit
  FRICTION COEFFICIENT = <real>fric_coef
  COHESION = <real>cohesion
END [COMPLIANT JOINT MODEL <string>name]
#
BEGIN COHESIVE ZONE MODEL <string>name
  TRACTION DISPLACEMENT FUNCTION = <string>func_name
```

```
  TRACTION DISPLACEMENT SCALE FACTOR = <real>scale_factor(1.0)
  CRITICAL NORMAL GAP = <real>crit_norm_gap
  CRITICAL TANGENTIAL GAP = <real>crit_tangential_gap
END [COHESIVE ZONE MODEL <string>name]
#
BEGIN JUNCTION MODEL <string>name
  NORMAL TRACTION FUNCTION = <string>func_name
  NORMAL TRACTION SCALE FACTOR = <real>scale_factor(1.0)
  TANGENTIAL TRACTION FUNCTION = <string>func_name
  TANGENTIAL TRACTION SCALE FACTOR = <real>scale_factor(1.0)
  NORMAL CUTOFF DISTANCE FOR TANGENTIAL TRACTION =
    <real>distance
END [JUNCTION MODEL <string>name]
#
BEGIN THREADED MODEL <string>name
  NORMAL TRACTION FUNCTION = <string>func_name
  NORMAL TRACTION SCALE FACTOR = <real>scale_factor(1.0)
  TANGENTIAL TRACTION FUNCTION = <string>func_name
  TANGENTIAL TRACTION SCALE FACTOR =
    <real>scale_factor(1.0)
  TANGENTIAL TRACTION GAP FUNCTION = <string>func_name
  TANGENTIAL TRACTION GAP SCALE FACTOR =
    <real>scale_factor(1.0)
  NORMAL CAPACITY = <real>normal_cap
  TANGENTIAL CAPACITY = <real>tangential_cap
  FAILURE ENVELOPE EXPONENT = <real>exponent(2.0)
  FAILURE DECAY CYCLES = <integer>num_cycles(1)
  FAILED MODEL = <string>failed_model_name|FRICTIONLESS
    (FRICTIONLESS)
END [THREADED MODEL <string>name]
#
BEGIN PV_DEPENDENT MODEL <string>name
  STATIC COEFFICIENT = <real>stat_coeff
  DYNAMIC COEFFICIENT = <real>dyn_coeff
  VELOCITY DECAY = <real>vel_decay
  REFERENCE PRESSURE = <real>p_ref
  OFFSET PRESSURE = <real>p_off
  PRESSURE EXPONENT = <real>p_exp
END [PV_DEPENDENT MODEL <string>name]
#
BEGIN TIME VARIANT MODEL <string>name
  MODEL = <string>model
    DURING PERIODS <string_list>time_periods
END [TIME VARIANT MODEL]
#
BEGIN USER SUBROUTINE MODEL <string>name
  INITIALIZE MODEL SUBROUTINE = <string>init_model_name
```

```
  INITIALIZE TIME STEP SUBROUTINE = <string>init_ts_name
  INITIALIZE NODE STATE DATA SUBROUTINE =
    <string>init_node_data_name
  LIMIT FORCE SUBROUTINE = <string>limit_force_name
  ACTIVE SUBROUTINE = <string>active_name
  INTERACTION TYPE SUBROUTINE = <string>interaction_name
END [USER SUBROUTINE MODEL <string>name]
#
BEGIN SEARCH OPTIONS [<string>name]
  GLOBAL SEARCH INCREMENT = <integer>num_steps(1)
  GLOBAL SEARCH ONCE = <string>ON|OFF(OFF)
  SEARCH TOLERANCE = <string>AUTOMATIC|USER_DEFINED(AUTOMATIC)
  NORMAL TOLERANCE = <real>norm_tol
  TANGENTIAL TOLERANCE = <real>tang_tol
  FACE MULTIPLIER = <real>face_multiplier(0.1)
  SECONDARY DECOMPOSITION = <string>ON|OFF(OFF)
END [SEARCH OPTIONS <string>name]
#
BEGIN USER SEARCH BOX <string>name
  CENTER = <string>center_point
  X DISPLACEMENT FUNCTION = <string>x_disp_function_name
  Y DISPLACEMENT FUNCTION = <string>y_disp_function_name
  Z DISPLACEMENT FUNCTION = <string>z_disp_function_name
  X DISPLACEMENT SCALE FACTOR = <real>x_disp_scale_factor
  Y DISPLACEMENT SCALE FACTOR = <real>y_disp_scale_factor
  Z DISPLACEMENT SCALE FACTOR = <real>z_disp_scale_factor
END [SEARCH OPTIONS <string>name]
#
BEGIN ENFORCEMENT OPTIONS [<string>name]
  MOMENTUM BALANCE ITERATIONS = <integer>num_iter(5)
  NUM GEOMETRY UPDATE ITERATIONS = <integer>num_iter(5)
END [ENFORCEMENT OPTIONS <string>name]
#
BEGIN INTERACTION DEFAULTS [<string>name]
  CONTACT SURFACES = <string list>surface_names
  SELF CONTACT = <string>ON|OFF(OFF)
  GENERAL CONTACT = <string>ON|OFF(OFF)
  AUTOMATIC KINEMATIC PARTITION = <string>ON|OFF(OFF)
  INTERACTION BEHAVIOR = <string>SLIDING|
    INFINITESIMAL_SLIDING|NO_INTERACTION(SLIDING)
  FRICTION MODEL = <string>friction_model_name|
    FRICTIONLESS(FRICTIONLESS)
  CONSTRAINT FORMULATION = <string>NODE_FACE|FACE_FACE
END [INTERACTION DEFAULTS <string>name]
#
BEGIN INTERACTION [<string>name]
  SURFACES = <string>surface1 <string>surface2
```

```
    MASTER = <string>surface
    SLAVE = <string>surface
    KINEMATIC PARTITION = <real>kin_part
    NORMAL TOLERANCE = <real>norm_tol
    TANGENTIAL TOLERANCE = <real>tang_tol
    FACE MULTIPLIER = <real>face_multiplier(0.1)
    OVERLAP NORMAL TOLERANCE = <real>over_norm_tol
    OVERLAP TANGENTIAL TOLERANCE = <real>over_tang_tol
    FRICTION MODEL = <string>friction_model_name|
      FRICTIONLESS(FRICTIONLESS)
    AUTOMATIC KINEMATIC PARTITION
    INTERACTION BEHAVIOR = <string>SLIDING|
      INFINITESIMAL_SLIDING|NO_INTERACTION(SLIDING)
    CONSTRAINT FORMULATION = <string>NODE_FACE|FACE_FACE
  END [INTERACTION <string>name]
  #
  BEGIN DASH OPTIONS
    SCALE FACTOR = <real>factor(1.0)
    ENFORCEMENT CONVERGENCE TOLERANCE = <real>1.0e-05
    HIDDEN SELF CONTACT = <string>TRUE|FALSE(TRUE)
    LOFTED SPHERE REPRESENTATION =
      TETRAHEDRON|OCTAHEDRON|CUBE|ICOSAHEDRON(ICOSAHEDRON)
  END
  #
END [CONTACT DEFINITION <string>name]

# Results specification

BEGIN RESULTS OUTPUT <string>results_name
  DATABASE NAME = <string>results_file_name
  DATABASE TYPE =
    <string>database_type(exodusII)
  OVERWRITE = <string>OFF|ON|TRUE|FALSE|YES|NO
    (ON|TRUE|YES)
  TITLE <string>user_title
  NODE <string>variable_name
    [AS <string>dbase_variable_name] ...
    <string>variable_name [AS
    <string>dbase_variable_name]
    | NODAL <string>variable_name
        [AS <string>dbase_variable_name] ...
        <string>variable_name [AS
        <string>dbase_variable_name]
  NODESET <string>variable_name
    [AS <string>dbase_variable_name] ...
    <string>variable_name [AS
    <string>dbase_variable_name]
```

```
  | NODESET <string>variable_name
      [AS <string>dbase_variable_name]
      INCLUDE|ON|EXCLUDE <string list>nodelist_names
      ... <string>variable_name
      [AS <string>dbase_variable_name] INCLUDE|ON|EXCLUDE
      <string list>nodelist_names
FACE <string>variable_name
  [AS <string>dbase_variable_name] ...
  <string>variable_name [AS
  <string>dbase_variable_name]
  | FACE <string>variable_name
      [AS <string>dbase_variable_name]
      INCLUDE|ON|EXCLUDE <string list>surface_names
      ...  <string>variable_name
      [AS <string>dbase_variable_name] INCLUDE|ON|EXCLUDE
      <string list>surface_names
ELEMENT <string>variable_name
  [AS <string>dbase_variable_name] ...
  <string>variable_name [AS
  <string>dbase_variable_name]
  | ELEMENT <string>variable_name
      [AS <string>dbase_variable_name]
      INCLUDE|ON|EXCLUDE <string list>block_names
      ... <string>variable_name
      [AS dbase_variable_name] INCLUDE|ON|EXCLUDE
      <string list>block_names
GLOBAL <string>variable_name
  [AS <string>dbase_variable_name] ...
  <string>variable_name [AS
  <string>dbase_variable_name]
INCLUDE = <string>list_of_included_element_blocks
EXCLUDE = <string>list_of_excluded_element_blocks
OUTPUT MESH = EXPOSED_SURFACE|BLOCK_SURFACE
COMPONENT SEPARATOR CHARACTER = <string>character|NONE
START TIME = <real>output_start_time
TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
AT TIME <real>time_begin INCREMENT =
  <real>time_increment_dt
ADDITIONAL TIMES = <real>output_time1
  <real>output_time2 ...
AT STEP <integer>step_begin INCREMENT =
  <integer>step_increment
ADDITIONAL STEPS = <integer>output_step1
  <integer>output_step2 ...
TERMINATION TIME = <real>termination_time_value
SYNCHRONIZE OUTPUT
USE OUTPUT SCHEDULER <string>scheduler name
```

```
  OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|SIGHUP|SIGINT|
    SIGPIPE|SIGQUIT|SIGTERM|SIGUSR1|SIGUSR2|SIGABRT|
    SIGKILL|SIGILL|SIGSEGV
END [RESULTS OUTPUT <string>results_name]

# User output

BEGIN FILTER <string>filter_name
  ACOEFF = <real_list>a_coeff
  BCOEFF = <real_list>b_coeff
  INTERPOLATION TIME STEP = <real>ts
END [FILTER]

BEGIN USER OUTPUT
  #
  # mesh-entity set commands
  NODE SET = <string_list>nodelist_names
  SURFACE = <string_list>surface_names
  BLOCK = <string_list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list> surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # compute result commands
  COMPUTE GLOBAL <string>result_var_name AS
    <string>SUM | AVERAGE | MAX | MIN OF <string>NODAL |
    ELEMENT <string>value_var_name [(<integer>component_num)]
  COMPUTE NODAL <string>result_var_name AS
    <string>MAX OVER TIME|MIN OVER TIME|ABSOLUTE VALUE MAX
    OVER TIME OF NODAL <string>value_var_name
    [(<integer>component_num)]
  COMPUTE ELEMENT <string>result_var_name AS
    <string>MAX OVER TIME|MIN OVER TIME|ABSOLUTE VALUE MAX
    OVER TIME OF ELEMENT <string>value_var_name
    [(<integer>component_num)]
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name |
    SURFACE SUBROUTINE = <string>subroutine_name |
    ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
```

```
    = <string>param_value
  #
  # copy command
  COPY ELEMENT VARIABLE <string>ev_name TO NODAL
    VARIABLE <string>nv_name
  #
  # variable transformation
  TRANSFORM NODAL|ELEMENT VARIABLE <string>source_variable
     TO COORDINATE SYSTEM <string>coord_sys_name AS target_name
  #
  # compute for element death
  COMPUTE AT EVERY TIME STEP
  #
  # additional command
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names

END [USER OUTPUT]

# Time step initialization

BEGIN TIME STEP INITIALIZATION
  #
  # mesh-entity set commands
  NODE SET = <string_list>nodelist_names
  SURFACE = <string_list>surface_names
  BLOCK = <string_list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list> surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name |
    SURFACE SUBROUTINE = <string>sub_name |
    ELEMENT BLOCK SUBROUTINE = <string>sub_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # additional command
  ACTIVE PERIODS = <string list>period_names
  INACTIVE PERIODS = <string list>period_names
```

```
END TIME STEP INITIALIZATION

# User variable

BEGIN USER VARIABLE <string>var_name
  TYPE = <string>NODE|ELEMENT|GLOBAL
    [<string>REAL|INTEGER LENGTH = <integer>length]|
    [<string>SYM_TENSOR|FULL_TENSOR|VECTOR]
  GLOBAL OPERATOR = <string>SUM|MIN|MAX
  INITIAL VALUE = <real list>values
  INITIAL VARIATION = <real list>values LINEAR DISTRIBUTION
  USE WITH RESTART
END [USER VARIABLE <string>var_name]

# History specification

BEGIN HISTORY OUTPUT <string>history_name
  DATABASE NAME = <string>history_file_name
  DATABASE TYPE =
    <string>database_type(exodusII)
  OVERWRITE = <string>OFF|ON|TRUE|FALSE|YES|NO
   (ON|TRUE|YES)
  TITLE <string>user_title
  GLOBAL <string>variable_name
    [AS <string>history_variable_name]
  NODE|NODAL|EDGE|FACE|ELEMENT <string>variable_name
    AT NODE|NODAL|EDGE|FACE|ELEMENT <integer>entity_id
    [AS <string>history_variable_name]
  NODE|NODAL|EDGE|FACE|ELEMENT <string>variable_name
    NEAREST LOCATION <real>global_x,
      <real>global_y>, <real>global_z
    [AS <string>history_variable_name]
  START TIME = <real>output_start_time
  TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
  AT TIME <real>time_begin INCREMENT =
    <real>time_increment_dt
  ADDITIONAL TIMES = <real>output_time1
    <real>output_time2 ...
  AT STEP <integer>step_begin INCREMENT =
    <integer>step_increment
  ADDITIONAL STEPS = <integer>output_step1
    <integer>output_step2 ...
  TERMINATION TIME = <real>termination_time_value
  SYNCHRONIZE OUTPUT
  USE OUTPUT SCHEDULER <string>scheduler_name
  OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|
```

```
    SIGHUP|SIGINT|SIGPIPE|SIGQUIT|SIGTERM|
    SIGUSR1|SIGUSR2|SIGABRT|
    SIGKILL|SIGILL|SIGSEGV
END [HISTORY OUTPUT <string>history_name]

# Heartbeat specification

BEGIN HEARTBEAT OUTPUT <string>heartbeat_name
  STREAM NAME = <string>heartbeat_file_name
  FORMAT = SPYHIS|DEFAULT
  GLOBAL <string>variable_name
    [AS <string>heartbeat_variable_name]
  NODE|NODAL|EDGE|FACE|ELEMENT <string>variable_name
    AT NODE|NODAL|EDGE|FACE|ELEMENT <integer>entity_id
    [AS <string>heartbeat_variable_name]
  NODE|NODAL|EDGE|FACE|ELEMENT <string>variable_name
    NEAREST LOCATION <real>global_x,
      <real>global_y>, <real>global_z
    [AS <string>heartbeat_variable_name]
  START TIME = <real>output_start_time
  TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
  AT TIME <real>time_begin INCREMENT =
    <real>time_increment_dt
  ADDITIONAL TIMES = <real>output_time1
    <real>output_time2 ...
  AT STEP <integer>step_begin INCREMENT =
    <integer>step_increment
  ADDITIONAL STEPS = <integer>output_step1
    <integer>output_step2 ...
  TERMINATION TIME = <real>termination_time_value
  SYNCHRONIZE OUTPUT
  USE OUTPUT SCHEDULER <string>scheduler_name
  OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|SIGHUP|SIGINT|
    SIGPIPE|SIGQUIT|SIGTERM|SIGUSR1|SIGUSR2|SIGABRT|
    SIGKILL|SIGILL|SIGSEGV
  PRECISION = <integer>precision
  LABELS = <string>OFF|ON
  LEGEND = <string>OFF|ON
  TIMESTAMP FORMAT <string>timestamp_format
  MONITOR = <string>RESULTS|RESTART|HISTORY
END [HEARTBEAT OUTPUT <string>heartbeat_name]

# Restart specification

BEGIN RESTART DATA <string>restart_name
  DATABASE NAME = <string>restart_file_name
  INPUT DATABASE NAME = <string>restart_input_file
```

```
    OUTPUT DATABASE NAME =
      <string>restart_output_file
    DATABASE TYPE =
      <string>database_type(exodusII)
    OVERWRITE = <string>OFF|ON|TRUE|FALSE|YES|NO
      (ON|TRUE|YES)
    START TIME = <real>restart_start_time
    TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
    AT TIME <real>time_begin INCREMENT =
      <real>time_increment_dt
    ADDITIONAL TIMES = <real>output_time1
      <real>output_time2 ...
    AT STEP <integer>step_begin INCREMENT =
      <integer>step_increment
    ADDITIONAL STEPS = <integer>output_step1
      <integer>output_step2 ...
    TERMINATION TIME = <real>termination_time_value
    OVERLAY COUNT = <integer>overlay_count
    CYCLE COUNT = <integer>cycle_count
    SYNCHRONIZE OUTPUT
    USE OUTPUT SCHEDULER <string>scheduler_name
    OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|SIGHUP|SIGINT|
      SIGPIPE|SIGQUIT|SIGTERM|SIGUSR1|SIGUSR2|SIGABRT|
      SIGKILL|SIGILL|SIGSEGV
    OPTIONAL
  END [RESTART DATA <string>restart_name]

  # J-Integral

  BEGIN J INTEGRAL <jint_name>
    #
    # integral parameter specification commands
    CRACK DIRECTION = <real>dir_x <real>dir_y <real>dir_z
    CRACK PLANE SIDE SET = <string list>side_sets
    CRACK TIP NODE SET = <string list>node_sets
    INTEGRATION RADIUS = <real>int_radius
    NUMBER OF DOMAINSS = <integer>num_domains
    FUNCTION = PLATEAU|PLATEAU_RAMP|LINEAR(PLATEAU)
    SYMMETRY = OFF|ON(OFF)
    #
    # time period selection commands
    ACTIVE PERIODS = <string list>period_names
    INACTIVE PERIODS = <string list>period_names
  END J INTEGRAL <jint_name>

END [PRESTO REGION <string>presto_region_name]
```

```
# Control modes region

BEGIN CONTROL MODES REGION
  #
  # model setup
  USE FINITE ELEMENT MODEL <string>model_name
  CONTROL BLOCKS [WITH <string>coarse_block] =
    <string list>control_blocks
  #
  # time step control
  TIME STEP RATIO SCALING = <real>cm_time_scale(1.0)
  TIME STEP RATIO FUNCTION = <string>cm_time_func
  LANCZOS TIME STEP INTERVAL = <integer>lanczos_interval
  POWER METHOD TIME STEP INTERVAL = <integer>pm_interval
  #
  # mass scaling
  HIGH FREQUENCY MASS SCALING = <real>cm_mass_scale(1.0)
  #
  # stiffness damping
  HIGH FREQUENCY STIFFNESS DAMPING COEFFICIENT =
    <real>cm_stiff_damp(0.0)
  #
  # kinematic boundary condition commands
  BEGIN FIXED DISPLACEMENT
    #
    #  Parameters for fixed displacement
    #
  END [FIXED DISPLACEMENT]
  #
  # output commands
  BEGIN RESULTS OUTPUT <string> results_name
    #
    # Parameters for results output
    #
  END RESULTS OUTPUT <string> results_name
END [CONTROL MODES REGION]

# RVE Region

BEGIN RVE REGION <string>rve_region_name
  #
  # Definition of RVEs
  ELEMENTS <integer>elem_i:<integer>elem_j
    BLOCKS <integer>blk_i:<integer>blk_j
    SURFACE|NODESET <integer>start_id INCREMENT <integer>incr
  #
  # ADAGIO REGION commands valid here with the exceptions
```

```
      # discussed in Section 9.1.  These include but are
      # not limited to:
      #
      # Boundary Conditions
      #
      # Results Output Definition
      #
      # Solver Definition
      #
    END [RVE REGION <string>rve_region_name]

  END [PRESTO PROCEDURE <string>presto_procedure_name]

END [SIERRA <string>name]
```

Appendix C

Consistent Units

This appendix describes common consistent sets of units. In using Presto, it is crucial to maintain a consistent set of units when entering material properties and interpreting results. The only variables that have intrinsic units are rotations, which are in radians. All other variables depend on the consistent set of units that the user uses in inputting the material properties and dimensioning the geometry.

A consistent set of units is made by picking the base units, which when using SI unit systems are length, mass, and time. If English unit systems are used, these base units are length, force, and time. All other units are then derived from these base units. Table C.1 provides several examples of commonly used consistent sets of units. In general, the names of the unit systems in this table are taken from the names of the base units. For example, CGS stands for (centimeters, grams, seconds) and IPS stands for (inches, pounds, seconds).

One of the most common mistakes related to consistent units comes in when entering density. For example, in the IPS system, a common error is to enter the density of stainless steel as 0.289 lb/in^3, when it should be entered as 7.48e-4 $lb \cdot s^2/in$. The weight per unit volume should be divided by the gravitational constant (386.4 in/s^2 in this case) to obtain a mass per unit volume.

Table C.1: Consistent Unit Sets

Unit	Unit System				
	SI	CGS	IPS	FPS	MMTS
Mass	kg	g	$\frac{lb \cdot s^2}{in}$	$slug$	$tonne$
Length	m	cm	in	ft	mm
Time	s	s	s	s	s
Density	$\frac{kg}{m^3}$	$\frac{g}{cm^3}$	$\frac{lb \cdot s^2}{in^4}$	$\frac{slug}{ft^3}$	$\frac{tonne}{mm^3}$
Force	N	$dyne$	lb	lb	N
Pressure	Pa	$\frac{dyne}{cm^2}$	psi	psf	MPa
Moment	$N \cdot m$	$dyne \cdot cm$	$in \cdot lb$	$ft \cdot lb$	$N \cdot mm$
Temperature	K	K	$^\circ R$	$^\circ R$	K
Energy	J	erg	$lb \cdot in$	$lb \cdot ft$	mJ
Velocity	$\frac{m}{s}$	$\frac{cm}{s}$	$\frac{in}{s}$	$\frac{ft}{s}$	$\frac{mm}{s}$
Acceleration	$\frac{m}{s^2}$	$\frac{cm}{s^2}$	$\frac{in}{s^2}$	$\frac{ft}{s^2}$	$\frac{mm}{s^2}$

Appendix D

Constraint Enforcement Hierarchy

When a node has multiple constraints, they are enforced in a specific order. Table D.1 shows the order of enforcement of the various types of constraints.

Table D.1: Constraint Enforcement Order

1	Contact
2	Kinematic
3	MPC
4	Rigid Body

If any of the constraints are in conflict, the last constraint enforced will override previously enforced constraints. For example, if a kinematic boundary condition and a MPC are both active on a node and conflict with each other, the kinematic boundary condition will be enforced first, followed by the MPC. As a result, the MPC will be enforced and will override the kinematic boundary condition.

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