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Emphasis/Nevada STDEM User's Guide Version 1.0

Rebecca S. Coats, Michael. F. Pasik, David B. Seidel

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

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Rebecca S. Coats, Michael F. Pasik, David B. Seidel
Electromagnetics and Plasma Physics Analysis Department
Sandia National Laboratories
P.O. Box 5800
Albuquerque, NM 87185-1152

Abstract

STDEM is the structured mesh time-domain electromagnetic and plasma physics component of Emphasis/Nevada. This report provides a guide on using STDEM.

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Introduction

Emphasis, the electromagnetic physics analysis system, is a suite of codes for the simulation of electromagnetic and plasma physics phenomena. The time-dependent components of Emphasis have been implemented using the Nevada framework [1]. The notation Emphasis/Nevada is used to highlight this relationship and/or distinguish the time-dependent components of Emphasis. In theory the underlying framework should have little influence on the user's interaction with the application. In practice the framework tends to be more invasive as it provides key services such as input parsing and defines fundamental concepts and terminology. While the framework offers many technological advancements from a software development point of view, from a user's perspective the key benefits of the underlying framework are the common interface for all framework physics modules as well as the ability to perform coupled physics simulations.

STDEM is the structured time-domain electromagnetic and plasma physics component of Emphasis/Nevada. STDEM provides for the full-wave solution to Maxwell's equations on multi-block three-dimensional structured grids using finite-difference time-domain (FDTD) algorithms. Additionally STDEM provides for the fully relativistic, self-consistent simulation of charged particles using particle-in-cell (PIC) algorithms.

Note for QUICKSILVER Users

STDEM represents the implementation of the QUICKSILVER technology within the Nevada framework. A path has been provided to ease the transition from QUICKSILVER to STDEM. Sections containing information for QUICKSILVER users will be explicitly marked like this paragraph.

NOTE

At the present time, STDEM incorporates much of the basic physics and diagnostics capabilities needed to perform practical simulations. However, not all the production capabilities users have come to expect have been fully incorporated into STDEM. Capabilities are being added rapidly as facilitated by the framework. The incorporation of capabilities is being prioritized based on program and application input. Refer to the [Additional Emphasis Resources](#) chapter on how to provide your input.

This manual assumes familiarity with setting up three-dimensional electromagnetic or plasma physics simulations. The purpose of this manual is to assist a knowledgeable user with the specifics of setting-up and performing simulations using STDEM.

1.1 Features

This section highlights the features of STDEM.

1.1.1 Overall

- Time-domain

- Three dimensional, Cartesian coordinate system
- Multiple region (or block)
- Serial and parallel execution

1.1.2 Field Solvers

- Conditionally stable, explicit finite difference, time-biased finite difference [\[2\]](#)

1.1.3 Material Support

- Perfect dielectrics
- Volumetric and infinitesimally thin perfect conductors

1.1.4 Boundary Conditions

- Perfect Electric Conductor (PEC)
- Perfect Magnetic Conductor (PMC or mirror)
- First-order absorbing (outlet)
- Periodic

1.1.5 Sources

- Electric current source
- Beam emission source

1.1.6 Diagnostics

- Field histories at a point as a function of time
- Particle counts for created, killed, and surviving particles as a function of time
- Volume snapshots of field components at instances of time

1.1.7 Mesh Generation Tools/Formats

- MERCURY/PFF [\[3\]](#)

1.1.8 Post-Processing Tools

- PFIDL [\[4\]](#)
- EnSight [\[5\]](#)

1.1.9 File Formats

- Portable File Format (PFF) [\[6\]](#) structured mesh descriptions
- HISPLT [\[7\]](#) time history files

- Sets and Fields (SAF) [\[8\]](#) structured field snapshots

2 Tutorial

2.1 Introduction

This chapter provides a hands-on introduction to STDEM by leading the reader through setting up and running a simulation of a rectangular cavity.

NOTE

This tutorial uses the MERCURY preprocessor for creating the mesh description. In order to repeat the steps of this tutorial the QUICKSILVER environment must have been properly configured.

2.2 Overview

The problem of interest is a $2 \times 3 \times 1.5$ cm rectangular cavity driven by an electric current line source. The line source is centered in the cavity and spans the entire extent of the cavity in the z direction.

This tutorial guides the reader through the key steps required to perform an STDEM simulation

- Creating a mesh description
- Creating a simulation description
- Running Emphasis

2.3 Creating the Mesh Description

The first step in setting up a simulation involves defining the problem domain. For the tutorial problem the simulation domain is defined to be the interior of the cavity.

```
sh$ merk
> system cartesian
> block 0 0 0 0.02 0.03 0.015
```

The next step involves discretizing the simulation domain. We will use a mesh consisting of $10 \times 20 \times 15$ cells.

```
> uniform i 0 0.02
Enter 'DX NC or QUIT?' &> nc 10
```

```

> uniform j 0 0.03
Enter 'DX NC or QUIT?' &> nc 20
> uniform k 0 0.015
Enter 'DX NC or QUIT?' &> nc 15

```

Next we need to describe the geometry. In this case the geometry consists of the six perfectly conducting cavity walls.

```

> pec 0 0 0 0 0.03 0.015 wall
> pec 0.02 0 0 0.02 0.03 0.015 wall
> pec 0 0 0 0.02 0.0 0.015 wall
> pec 0 0.03 0 0.02 0.03 0.015 wall
> pec 0 0 0 0.02 0.03 0 wall
> pec 0 0 0.015 0.02 0.03 0.015 wall

```

This completes the creation of the mesh description. We will need two pieces of information related to the mesh in order to complete the simulation description in the following section. In general, to select a stable simulation time step we need information about the smallest cell size and the material properties. MERCURY makes selecting a simulation time step easy by providing an upper limit based on the Courant condition.

```

> courant
-----
Timestep Limits      limit (sec)
-----
Courant Stability    2.563E-12
Particle Transit     3.336E-12
-----

```

The other piece of information we need in order to complete a simulation description is what material numbers have been assigned to cells. In MERCURY this information is summarized when the mesh is exported to Emphasis.

```

> write emphasis cavity

index  material
  1    wall
  2    vacuum

```

For additional information on the MERCURY commands used in this section the user should refer to the available online help.

```

> help

```

2.4 Creating the Simulation Description

We now need to specify general simulation execution parameters, STDEM physics-specific model parameters, and material model parameters. Collectively these three categories of information are referred to as the simulation description and are stored in the simulation

input file. STDEM uses a free-format, case-insensitive, text file containing keywords or keyword groups to describe a simulation. Categories can appear in any order but they cannot be intermixed.

Note for QUICKSILVER Users

MERCURY supports a translation option that allows the QUICKSILVER command syntax you are familiar with to be used to create a simulation description. For the purposes of this tutorial, however, the STDEM command syntax will be used directly.

NOTE

The complete simulation description is shown in [Figure 4.1](#).

We will begin by entering the general simulation execution parameters, including a title, the duration of the simulation and the frequency of output. In a text editor create the file “cavity.inp” and add the following lines to the file.

```
TITLE
  Simple cavity

TERMINATION CYCLE = 250

EMIT HISPLT, CYCLE INTERVAL = 1
EMIT PLOT, CYCLE INTERVAL = 50
EMIT SCEEN, CYCLE INTERVAL = 25
```

NOTE

Keywords can contain spaces, so in the lines above we have used commas and equal signs to separate adjacent keywords and parameters. For the tutorial we will adopt the convention of using upper case for keywords and lower case for parameters.

Next we need to specify that we would like to use the STDEM physics models. Add an STDEM keyword group to the input file by adding the following lines to the tutorial input file.

```
STRUCTURED TD ELECTROMAGNETICS
END
```

NOTE

A keyword group is a sequence of keywords and numeric values bounded by a main keyword and the keyword END. Keywords within a keyword group may appear in any order.

Similarly, to specify the use of Particle-in-Cell STDEM physics models, we would use the STDEM PIC keyword group by instead adding the following lines:

```
STRUCTURED TD ELECTROMAGNETIC PIC
END
```

Within this keyword group we need to specify STDEM physics related parameters. Specify the previously exported mesh description by adding the following lines between the lines STRUCTURED TD ELECTROMAGNETICS and END.

```
MESH, PFF  
  FILE = "cavity.pff"  
END
```

A time step for the STDEM field solver is based on the mesh/material properties as discussed earlier. Add the following line inside the STDEM keyword group.

```
CONSTANT TIME STEP = 2.5e-12
```

Even though we have yet to address material descriptions, we are going to tell the STDEM field solver that the cavity is filled with vacuum (in order to improve performance) by adding the following line to the STDEM keyword group.

```
DIELECTRIC ALGORITHM, CONSTANT=1.0
```

In order to have STDEM treat the cavity walls as perfect conductors, we will make the conductivity of the wall material higher than the threshold used by STDEM. Add the following line to the STDEM keyword group to explicitly set the threshold value.

```
ELECTRICAL CONDUCTIVITY THRESHOLD = 1.0e6
```

Next we need to specify the location and spatial/temporal variation of the source. The coordinates of the starting point and ending point of the grid segment parameter specify the location of the source. All the edges between the two points in the specified component direction will be driven. For this problem we will use a line source oriented in the z direction and spanning the entire extent of the cavity, so the ordinates will be degenerate in two of the dimensions. To the STDEM keyword group add the following lines of text.

```
CURRENT SOURCE, SEGMENT=0.01 0.015 0.0 0.01 0.015 0.015  
  COMPONENT=k, TEMPORAL=FUNCTION 102
```

NOTE

Input lines are limited to 160 characters but long commands can be placed on multiple input lines since a newline is a keyword delimiter.

Because we have not specified any spatial distribution the current will be constant. We will need to define the function indicated in the above command giving the temporal dependence of the source. To the STDEM keyword group add the following lines to define a linear ramp.

```
FUNCTION 102  
  0.0 0.0  
  30e-9 1.0  
  1.0 1.0  
END
```

NOTE

When specifying a floating point number be sure to include the decimal point (e.g., use either 0. or 0.0 not 0).

Next we must describe the material models to be used in the simulation. Recall when we created the mesh description we had the materials “wall” and “vacuum” numbered 1 and 2 respectively. For this simulation we will use the simple electrical material model, which models a material with a constant permittivity, permeability and electrical conductivity. Because the two materials will have different parameters we will need two models. After the STDEM keyword group add the following lines.

```
MATERIAL 1 wall
  MODEL = 101
END
```

```
MATERIAL 2 vacuum
  MODEL = 102
END
```

NOTE

In the material command, the numbered ID following the MATERIAL keyword must match the material numbers assigned to the cells. We have chosen to include an optional label that happens to match the names we used in the mesh generation software.

Next we need to specify the material parameters for each model specified in the material commands. Recall that in order for the walls to be treated as perfect conductors, the specified conductivity must be larger than the threshold value we entered in the STDEM keyword group. Add the following lines defining the material parameters.

```
MODEL 101 simple electrical
  EPS = 1.0
  MU = 1.0
  SIGMA = 1e7
END
```

```
MODEL 102 simple electrical
  EPS = 1.0
  MU = 1.0
  SIGMA = 0.0
END
```

NOTE

The simple electrical material model takes the *relative* permittivity, *relative* permeability and electrical conductivity as input parameters.

We have entered all the necessary parameters for the three categories (simulation execution, STDEM physics, and material models). Complete the simulation description by adding the following line to the end of the file.

```
EXIT
```

Save the file contents to the file name “cavity.inp”.

2.5 Running Emphasis

In order to run Emphasis the Nevada environment must be properly configured (see the [Executing Emphasis](#) chapter). To run the tutorial problem with Emphasis use the following command.

```
Alegra cavity
```

2.6 Conclusion

Congratulations, you have completed your first STDEM simulation. The following chapters provide a reference guide to the material covered in this tutorial. Try using the reference guide to modify the tutorial problem. For example, try running the tutorial problem in parallel (hint: use the MERCURY commands “processors” and “decompose” and the Alegra --nprocs command line option).

3 Mesh Description

The mesh description must be created using an STDEM-compatible mesh generation software package. The following key information from the mesh will be needed when specifying the physics models.

- Smallest cell size and material properties. This information is needed to determine the simulation time step for STDEM’s conditionally stable algorithms.
- Material numbers assignments to cells. Material models in the simulation description are associated with the material numbers assigned to cells.

NOTE

STDEM mesh descriptions are assumed to use length units of meters.

Note for QUICKSILVER Users

The MERCURY preprocessor can be used to describe the simulation domain, define a mesh, specify geometry, and decompose the mesh for parallel execution with STDEM. To convert a MERCURY simulation and mesh description for use with STDEM use the MERCURY command “write emphasis”. The MERCURY command “courant” can be used to determine an appropriate time step. Material names and numbers are summarized when MERCURY exports the mesh.

4 Simulation Description

There are two approaches for describing the simulation parameters. The first approach uses the command syntax accepted by QUICKSILVER and relies on the preprocessor MERCURY to translate the commands to the appropriate STDEM syntax. The second approach is to enter the simulation description directly using the STDEM command syntax. Most experienced users will relate that difficulties with setting up simulations involve the creation of the geometry/mesh. The description of the simulation parameters is typically the least time-consuming part of setting up a simulation. Both approaches offer different advantages that are summarized below. Users are encouraged to experiment with both approaches, especially given the availability of automatic translation.

Direct

- Compatible with other Nevada framework applications (UTDEM, CABANA, etc.).
- Uses position-independent keyword syntax.
- Compatible with the APREPRO [\[9\]](#) symbolic preprocessor.
- Does not require MERCURY to make simple changes to simulation parameters.

Translation approach

- Provides a transition path from QUICKSILVER
- Simulations can be run with either STDEM or QUICKSILVER
- The MERCURY preprocessor [\[3\]](#) can be used which supports command archiving, syntax checking, etc.
- Compatible with the PREMEREK [\[10\]](#) symbolic preprocessor

Note for QUICKSILVER Users

Use the MERCURY translation option to become familiar with the STDEM syntax.

STDEM uses a free format, case insensitive, text file containing keywords or keyword groups to describe a simulation. With few exceptions, keywords or keyword groups may be in any order the user finds convenient.

NOTE

STDEM simulation descriptions are assumed to use the SI (System International) unit system.

4.1.1 Input Lines

An input line is limited to 160 characters. Placing more characters on a line can lead to platform-dependent results. A long command can be spread across multiple input lines since a newline acts as a keyword delimiter.

4.1.2 Comments

Comments begin with a dollar sign or asterisk symbol. All text that follows a comment character on an input line is ignored.

4.1.3 Keywords

A keyword is a short sequence of English words denoting some action or quantity. For example, the following are three examples of keywords.

```
TITLE
CURRENT SOURCE
ELECTRICAL CONDUCTIVITY THRESHOLD
```

Keyword processing is case insensitive and only enough characters of each word of a keyword need be entered to uniquely identify it. The number of words per keyword is significant and varies according to the specific keyword or keyword group. Keywords may or may not require additional grammatical construct to follow them.

NOTE

When floating-point values are required they must include a decimal point.

NOTE

A comma, colon, semicolon, equals sign, or newline must separate adjacent keywords. A blank is sufficient only to separate a keyword from a numeric field, not one keyword from another.

The user may optionally separate keywords and numeric fields using blanks, commas, semicolons, colons, newlines, or equal signs.

4.1.4 Keyword Groups

A keyword group is a sequence of keywords and numeric values bounded by a main keyword and the keyword END. For example

```
MODEL 4 SIMPLE ELECTRICAL
  SIGMA = 0.0
  EPS = 1.0
  MU = 1.0
END
```

Keywords within a keyword group may appear in any order.

4.1.5 Categories

STDEM input is divided into three general categories: execution control, physics related, and material modeling. Categories can appear in any order but they cannot be intermixed. For example, the complete input file from the tutorial is shown in [Figure 4.1](#).

```
TITLE
  simple cavity

TERMINATION CYCLE = 250

EMIT HISPLT, CYCLE INTERVAL = 1
EMIT PLOT, CYCLE INTERVAL = 50
EMIT SCEEN, CYCLE INTERVAL = 25
```

```

$ ----- STDEM physics -----
STRUCTURED TD ELECTROMAGNETICS

MESH, PFF
  FILE = "cavity.pff"
END

CONSTANT TIME STEP = 2.5e-12

DIELECTRIC ALGORITHM, CONSTANT=1.0

ELECTRICAL CONDUCTIVITY THRESHOLD = 1.0e6

CURRENT SOURCE, SEGMENT=0.01 0.015 0.0 0.01 0.015 0.015
  COMPONENT=k, TEMPORAL=FUNCTION 102

FUNCTION 102
  0.0 0.0
  30e-9 1.0
  1.0 1.0
END

END

$ ----- material models -----

MATERIAL 1 wall
  MODEL = 101
END

MATERIAL 2 vacuum
  MODEL = 102
END

MODEL 101 simple electrical
  EPS = 1.0
  MU = 1.0
  SIGMA = 1e7
END

MODEL 102 simple electrical
  EPS = 1.0
  MU = 1.0
  SIGMA = 0.0
END

EXIT

```

Figure 4.1. Complete Simulation Description of the Tutorial Problem

5 Keyword Descriptions

This chapter describes the keywords that can be used in STDEM simulation descriptions. First, common constructs used by multiple keywords are described. Next, the five categories of keywords (STDEM physics, STDEM PIC physics, output diagnostics, execution control, and material modeling) are described. Keywords are organized alphabetically within each section.

The following conventions have been observed when describing keywords. Keywords are shown in upper case. Keyword parameters are shown in lower case. Simple numeric and character parameters are indicated by their type (`int`, `real`, or `string`). Optional keywords, constructs, or parameters are enclosed in square brackets. Alternative choices for a keyword are enclosed in curly braces and separated by a “|”, as in `{ABC | DEF}`, meaning ABC or DEF.

5.1 Common Constructs

There are a number of common grammatical constructs that are used by more than one keyword. If a construct directly follows a keyword, an appropriate delimiter (e.g., a comma or equals sign) must separate them.

5.1.1 function-set

```
FUNCTION int [SCALE real] [SHIFT real]
```

The function-set construct specifies a user-defined function table with an optional scaling factor and shift. If a keyword requires a function-set but only a constant value is needed, the function-set construct may take the form of a single real value. The scale option may be applied to this value. Not all Emphasis commands support the SCALE and SHIFT options. The function referenced by a keyword need not appear before the keyword, but must appear somewhere in the simulation description.

5.1.2 grid-segment

```
SEGMENT real real real real real real
```

The grid segment construct specifies the coordinates of two points on the grid that define a segment. The first three numbers specify the coordinates of the starting point and the last three numbers specify the coordinates of the ending point of the grid segment. Depending on the number of degenerate coordinate values a segment may define a point, line, plane, or volume.

5.1.3 time-or-cycle-interval

```
TIME [INTERVAL] real
```

or

```
CYCLE [INTERVAL] int
```

The time-or-cycle-interval construct specifies an interval of time or interval of cycles used by the keyword. Time intervals are specified as floating point values and cycle intervals are specified as integer values. The extra word `INTERVAL` is optional and may be included for readability.

5.1.4 time-range

```
FROM [TIME] real TO real
```

5.1.5 vector-function-set

```
X, function-set [Y, function-set [Z, function-set]]
```

The vector-function-set construct specifies a 1-, 2- or 3-dimensional vector function. Each component of the vector function is a separate function-set specification.

5.2 STDEM Physics

5.2.1 CONSTANT TIME STEP

```
CONSTANT TIME STEP real
```

This keyword specifies the simulation time step. The real parameter must satisfy the solver's stability condition.

NOTE

No checking is performed to ensure the supplied time step meets the solver's stability condition.

5.2.2 CURRENT SOURCE

```
CURRENT SOURCE, grid-segment COMPONENT={i|j|k}, [TYPE =  
{electric|magnetic}] [AMPLITUDE real] [TEMPORAL function-set]  
[SPATIAL vector-function-set]
```

This keyword defines a current source. The grid segment parameter specifies the extent of the source and may define a line, plane, or volume. The component parameter specifies the direction of the current. The optional type parameter specifies the type of source (default is electric). An optional amplitude parameter may be provided to scale the amplitude of the current (the default value is one). Optional temporal and/or spatial variations may be specified using functions (by default the current is constant). Use the predefined unity function (`FUNCTION 0`) in the vector-function-set to specify constant spatial dependence in invariant directions.

NOTE

Only the electric type is presently supported. The temporal function-set and spatial vector-function-set parameters presently do not support the optional shift and scale parameters.

5.2.3 DIELECTRIC ALGORITHM

DIELECTRIC ALGORITHM, CONSTANT real

This keyword enables an optimized field solver in a region containing a homogeneous dielectric. The constant parameter specifies the relative permittivity for the entire region. This keyword should only be used when there is a homogenous dielectric present.

NOTE

Results are undefined when this keyword is used when multiple dielectric materials are present.

5.2.4 ELECTRICAL CONDUCTIVITY THRESHOLD

ELECTRICAL CONDUCTIVITY THRESHOLD real

This keyword is used to specify which conductors will be treated as perfect conductors. Conductors whose electrical conductivity exceeds the specified threshold value will be treated as perfect (tangential and internal electric fields vanish).

NOTE

Only perfect conductors are presently supported.

5.2.5 FIELD SOLVER

FIELD SOLVER, EXPLICIT

or

FIELD SOLVER, TIME BIASED, ALPHA real real real
[ITERATIONS int] [TAU real real...]

or

FIELD SOLVER, PML, BLOCKS int... PROFILE vector-function-set

The FIELD SOLVER command keyword allows the user to specify which finite-difference algorithm to use for the electromagnetic field solution as well as provide any needed parameters for the particular algorithm chosen. Presently, multiple algorithms are supported: EXPLICIT, TIME BIASED, and PML. If the FIELD SOLVER command keyword is not provided, the EXPLICIT algorithm will be used.

The TIME BIASED algorithm [\[2\]](#) has three parameter keywords, one of which is required (ALPHA). The ALPHA keyword provides three real values, α_1 , α_2 , and α_3 , which represent the magnetic flux density weighting factors for the current timestep, the previous timestep,

and the twice-previous timestep, respectively. The values supplied for this keyword are subject to the following three constraints:

$$\begin{aligned}\alpha_1 + \alpha_2 + \alpha_3 &= 1, \\ \alpha_1 &> \alpha_3, \text{ and} \\ \alpha_2^2 - 4\alpha_1\alpha_3 &> 0.\end{aligned}$$

The ITERATION keyword specifies the number of iterations, N_{iter} , to be used by the algorithm, and should equal the number of real values supplied by the TAU keyword. The TAU keyword is used to specify monotonically decreasing relaxation coefficients, $\{\tau_i\}$, for each iteration i of the algorithm. N_{iter} and $\{\tau_i\}$ are subject to the following constraints:

$$\begin{aligned}N_{iter} &> \frac{\pi}{2} \sqrt{\frac{\alpha_1}{\alpha_2^2 - 4\alpha_1\alpha_3}} + \frac{1}{2}, \\ \tau_1 &= 1, \text{ and} \\ 0 < \tau_i < 1, & \text{ for } i = 2, \dots, N_{iter}.\end{aligned}$$

If neither of these optional keywords is specified, then N_{iter} is set to the minimum integer that satisfies the constraint above and the values of $\{\tau_i\}$ are optimized by an algorithm based on the zeros of Chebyshev polynomials (see [2]). If just the ITERATION keyword is supplied, the values of $\{\tau_i\}$ are optimized as described previously. Finally, if the TAU keyword is supplied without the ITERATION keyword, N_{iter} is set to the number of values supplied with the TAU keyword. Finally, note that if any of the aforementioned constraints are not satisfied, the simulation will stop without running any timesteps.

The Perfectly Matched Layer (PML) algorithm [12], [13] takes two parameters. By proper orientation and parameter selection the PML blocks can be used to truncate the computational domain in a manner mimicking an anechoic chamber. The BLOCKS parameter specifies the user block numbers of the PML blocks. Each PML block should be terminated with a PEC, PMC or INLET boundary condition. The PROFILE parameter specifies the functions that describe the σ/ε profile in each coordinate direction. The σ/ε profile must be zero across the first cell of the PML block in the direction normal to the interface plane between PML and non-PML blocks. Over the remainder of the PML block, the σ/ε profile is typically chosen to vary parabolically from zero to $\frac{\sigma_{\max}}{\varepsilon}$. In most cases the following rule-of-thumb offers reasonable performance

$$\sigma_{\max} = \frac{1}{150\pi\Delta}$$

where Δ is the cell size along the direction of attenuation. Care should be observed when selecting σ/ε profiles because choosing an abrupt or rapidly increasing profile may actually degrade performance by increasing the size of the numerical reflections from the PML interface. The APREPRO [9] preprocessor can be useful in generating profile function tables.

In most cases, PML blocks are typically eight or more cells thick in the direction of attenuation.

NOTE

Conductor and dielectric material(s) in non-PML blocks should be extended into adjacent PML block(s).

NOTE

To insure stability in parallel, each PML block connection must consist of either full or partial block faces (i.e., edge only connections are not supported).

5.2.6 FUNCTION

```
FUNCTION int
  real real
  [real real]
...
END
```

This keyword group defines a function in terms of a table of x-y real pairs. The function, identified by the integer field after the FUNCTION keyword can be referenced by other keywords. Linear interpolation is used between table points. FUNCTION 0 is predefined to be unity.

5.2.7 INLET

```
INLET, grid-segment NORMAL={+1|-1} POISSON int TEMPORAL
function-set [BETA real]
```

This keyword defines an inlet port boundary condition. The inlet port boundary condition excites a transverse electromagnetic mode (TEM) using an externally provided two-dimensional static field distribution. A first-order absorbing boundary condition is applied to the reflected fields. The grid segment parameter must define a plane on the boundary or interior to a region. The normal parameter specifies the direction of the inward normal relative to the coordinate system. The simulation geometry should not vary in the normal direction for a minimum of one cell to minimize reflections. The Poisson parameter identifies the externally provided static TEM field distribution. The temporal keyword identifies the function specifying the time variation of the source. Because the time variation is evaluated at retarded time to separate the incident and reflected fields, the specified variation must result in a causal source (i.e., the function must evaluate to zero before the start of the simulation). The optional beta parameter specifies the outgoing wave velocity relative to the speed of light in vacuum (default is -1.0 which indicates to compute a wave velocity on a cell-by-cell basis).

NOTE

The temporal function-set parameters presently do not support the optional shift and scale parameters.

5.2.8 OUTLET

OUTLET, grid-segment NORMAL={+1|-1} [BETA real]

This keyword group defines a first-order absorbing boundary condition. The grid segment parameter must define a plane on the boundary or internal to a region. The normal parameter specifies the direction of the inward normal relative to the coordinate system. The optional beta parameter specifies the outgoing wave velocity relative to the speed of light in vacuum (default is -1.0 which indicates to compute a wave velocity on a cell-by-cell basis).

5.2.9 PEC

PEC, grid-segment

This keyword defines an infinitesimally thin perfect electric conductor (tangential electric field vanishes). The grid segment must define a plane but may be located internally or on the boundary of a region.

5.2.10 PERIODIC LIMITS

PERIODIC LIMITS, COORDINATE = {i|j|k}, LIMITS real real

This keyword defines a periodic boundary condition. The coordinate parameter indicates the coordinate in which the periodicity occurs. The limits parameters define the location of the planes of periodicity.

5.2.11 PMC

PMC, grid-segment

This keyword defines a perfect magnetic conductor (tangential magnetic field vanishes) or mirror boundary condition. The grid segment parameter must define a plane on the boundary of the simulation.

5.2.12 POISSON

POISSON, FILENAME = "file"

This keyword makes externally computed Poisson solutions available to a simulation for boundary conditions and initial values. The filename parameter specifies the file containing the Poisson solutions.

NOTE

At the present time only two-dimensional Poisson solutions written by MERCURY are supported by this keyword.

5.2.13 SURFACE FIELD CHECK

SURFACE FIELD CHECK, [FIELDS=string]

The SURFACE FIELD CHECK command keyword provides a mechanism to instruct EMPHASIS to check for discrepancies between field values shared by adjoining blocks. The parameter keyword FIELDS is used to specify which fields to check. Its value is a string of concatenated single characters, each representing a particular field type. In STDEM physics, two fields can be checked, the electric field and the magnetic flux density, indicated by the characters E and B, respectively.

5.3 STDEM PIC Physics

The STRUCTURED TD ELECTROMAGNETIC PIC keyword group is used to request the use of the structured-grid, time-domain, electromagnetic PIC (STDEM PIC) physics. Note that this physics package is a superset of STDEM physics, and consequently all command keywords that are legal in the STRUCTURED TD ELECTROMAGNETICS keyword group are also legal in this keyword group. This section describes the additional command keywords provided by this keyword group.

5.3.1 BEAM EMISSION

```
BEAM EMISSION, grid-segment NORMAL int SPECIES=string
[CYCLE INTERVAL int] [N1 int] [N2 int] [EMIT PROBABILITY real]
ENERGY DISTRIBUTION=
CONSTANT real|RANDOM real [real]|MAXWELLIAN real
[THETA DISTRIBUTION=CONSTANT [real]|RANDOM [real real]|COSINE]
[PHI DISTRIBUTION=CONSTANT [real]|RANDOM [real real]]
[AMPLITUDE real] [TEMPORAL function-set]
```

This command keyword defines a beam emission source. The beam emission source describes a planar surface over which particles are emitted into the simulation region. The particle species, emission characteristics, and amplitude are provided by the several available parameter options. The grid-segment construct describes the planar emission surface and the NORMAL parameter specifies the direction emitted particles move from the surface (a negative value denotes emission opposite the positive normal coordinate direction, otherwise the emission is in the same direction). The SPECIES keyword is used to provide the name of the particle species to be emitted and must match the name of a species that has been defined using the DEFINE SPECIES command keyword. The CYCLE INTERVAL parameter specifies the emission frequency in timesteps, with a default value of 1. N1 and N2 specify the number of emitted particles in the two tangential coordinate directions local to the emission surface, t_1 and t_2 , respectively, with default values of 1. The coordinates $(\hat{t}_1, \hat{t}_2, \hat{n})$ form a local right-handed coordinate system $(\hat{t}_1 \times \hat{t}_2 = \hat{n})$, where \hat{n} is the outward normal of the emission surface. By convention, \hat{t}_1 is defined to be in the positive direction of the next cyclic coordinate of the global right-handed coordinate system $(\hat{i}, \hat{j}, \hat{k})$, e.g., if $\hat{n} = \pm \hat{j}$, then $\hat{t}_1 = +\hat{k}$. Because $(\hat{t}_1, \hat{t}_2, \hat{n})$ is a right-handed system, \hat{t}_2 is constrained to be in the next cyclic coordinate, with the same sign as the normal. From the previous example in which $\hat{n} = \pm \hat{j}$, we have that $\hat{t}_2 = \pm \hat{i}$. [Table 5.1](#) shows the values of \hat{t}_1 and \hat{t}_2 for all possible values of \hat{n} .

The EMIT PROBABILITY parameter allows the specification of the probability, between 0 and 1, that any particle will actually be inserted into the system. It defaults to 1.0.

Table 5.1. Definition of local emission surface coordinate system for allowed values of outward emission surface normal.

Outward Surface Normal (\hat{n})	\hat{i}	$-\hat{i}$	\hat{j}	$-\hat{j}$	\hat{k}	$-\hat{k}$
First Tangential Surface Coordinate (\hat{t}_1)	\hat{j}	\hat{j}	\hat{k}	\hat{k}	\hat{i}	\hat{i}
Second Tangential Surface Coordinate (\hat{t}_2)	\hat{k}	$-\hat{k}$	\hat{i}	$-\hat{i}$	\hat{j}	$-\hat{j}$

The ENERGY DISTRIBUTION keyword describes the energy distribution of the emitted beam particles. Three options are available: CONSTANT, RANDOM, and MAXWELLIAN. The CONSTANT option has a single value that gives the beam energy in electron Volts (eV). The RANDOM option has two values that give the minimum and maximum energies (in eV) for a uniform distribution of beam energy. If only one value is specified, it is assumed to be the maximum energy of the distribution, and the minimum energy is assumed to be zero. The Maxwellian option has one value that gives the mean energy of the distribution in eV. For this option, the energies of the emitted particles will be distributed using $dN/dE = (1/kT) \exp(-E/kT)$, where kT is the supplied mean energy of the distribution.

The THETA DISTRIBUTION keyword describes the direction of emission with respect to the polar angle (θ) from the surface. Three options are available: CONSTANT, RANDOM, and COSINE. The CONSTANT option has a single value that gives the θ of the emitted beam particles in degrees ($^\circ$). If this value is not supplied, it defaults to zero (i.e., particle velocity is normal to the emission surface). The RANDOM option has two values that give the minimum and maximum θ (in $^\circ$) for a uniform distribution over θ . If these values are not specified, default values of 0° and 90° will be used. The COSINE option will use a cosine distribution (i.e., $dN/d\theta = \cos \theta$) over the range from 0° to 90° . Note that if the THETA DISTRIBUTION keyword is not explicitly specified, it will default to CONSTANT with value zero, unless ENERGY DISTRIBUTION is specified to be MAXWELLIAN, in which case THETA DISTRIBUTION defaults to COSINE, or unless PHI DISTRIBUTION is specified to be RANDOM, in which case THETA DISTRIBUTION defaults to RANDOM.

Similarly, the PHI DISTRIBUTION keyword describes the direction of emission with respect to the azimuth angle (ϕ) defined as the angle from the positive t_1 axis toward the positive t_2 axis (see [Table 5.1](#)). Two options are available: CONSTANT and RANDOM. The CONSTANT option has a single value that gives the ϕ of the emitted beam particles in degrees ($^\circ$). If this value is not supplied, it defaults to zero. The RANDOM option has two values that give the minimum and maximum ϕ (in $^\circ$) for a uniform distribution over ϕ . If these values are not specified, default values of 0° and 360° will be used. Note that if the PHI DISTRIBUTION keyword is not explicitly specified, it will default to CONSTANT with value zero, unless ENERGY DISTRIBUTION is set to MAXWELLIAN or

THETA_DISTRIBUTION is *not* set to CONSTANT, in which case PHI DISTRIBUTION defaults to RANDOM.

Finally, the BEAM_EMISSION command keyword has the following two keyword options that provide a means to specify the amplitude of the beam current. The AMPLITUDE keyword provides a scalar multiplier for the beam amplitude, in amperes, with a default value of 1.0. The TEMPORAL keyword provides a means to specify non-constant time dependence for the beam amplitude. If specified, the amplitude at any instant in time is the product of the scalar multiplier provided by the AMPLITUDE keyword and the value of the function-set specified by TEMPORAL evaluated at the current simulation time. If TEMPORAL is not specified, the beam current is just the value supplied for the AMPLITUDE keyword independent of simulation time. Presently, the beam current is assumed to be distributed uniformly over the entire emission segment, i.e., the current density is constant.

5.3.2 DEFINE SPECIES

```
DEFINE SPECIES
  string, MASS=real CHARGE STATE int
  ...
END
```

The DEFINE SPECIES command keyword group provides a means of defining charged-particle species to be used with the various particle source and diagnostic commands (currently only BEAM_EMISSION and PARTICLE HISTORY). One or more particle species may be defined in one DEFINE SPECIES keyword group. Each species is specified by three required parameters. The first parameter is a string that provides a user-specified name for the species. This name is used to reference the defined species in the all other input commands that require the use of a particle species in their specification. The two remaining parameters for specifying a species are the MASS and CHARGE STATE, which describe the particle species mass (in AMU), and charge state, respectively. The charge state is a signed integer that gives the particle's charge relative to that of a proton. For example, an electron's charge state would be -1 and triply ionized carbon would be $+3$.

5.3.3 PARTICLE_HISTORY

```
PARTICLE_HISTORY
  string, SPECIES=string, STATUS=string
  ...
END
```

The PARTICLE HISTORY command keyword group provides a means of requesting output history diagnostics for various types of aggregate particle information. One or more such requests may be made in one PARTICLE HISTORY keyword group. Each request is specified by an initial keyword string that gives the type of the request. Currently the only supported keyword is COUNT, which gives the number of particles of the specified species and status. The SPECIES keyword allows the specification of a single particle species as defined by the DEFINE SPECIES command keyword group, or the special value ALL,

which combines the information for all particle species in the simulation. If not explicitly specified, SPECIES defaults to ALL. The STATUS keyword filters the aggregated information based upon the present status of the particles. Legal values for this keyword are CREATED, KILLED, and SURVIVING, which request the cumulative number of particles created during the simulation, the cumulative number of particles killed during the simulation, and the number of particles that currently survive in the simulation, respectively.

5.3.4 SURFACE CORRECTOR

SURFACE CORRECTOR, [STATUS = ON|OFF]

The SURFACE CORRECTOR command keyword allows the user to control whether or not current density values on the surfaces of structured blocks are corrected to avoid the introduction of single-bit discrepancies between field values shared by adjoining blocks. Such discrepancies can lead to unstable behavior in the field solution. If this command is not specified, or if the STATUS keyword is not provided, the default value of STATUS is ON. This value should be set to OFF only by an experienced user who understands the nature of the instability that results from not performing this correction, or if for some reason the user desires to observe or verify the existence of the instability for his particular simulation configuration.

5.3.5 SURFACE FIELD CHECK

SURFACE FIELD CHECK, [FIELDS=string]

The SURFACE FIELD CHECK command keyword provides a mechanism to instruct EMPHASIS to check for discrepancies between field values shared by adjoining blocks. The parameter keyword FIELDS is used to specify which fields to check. Its value is a string of concatenated single characters, each representing a particular field type. In STDEM_PIC physics, three fields can be checked, the electric field, the magnetic flux density, and the current density, indicated by the characters E, B, and J, respectively.

5.4 Output Diagnostics

5.4.1 SAF Field Snapshots

```
PLOT, SAF
  FILE=string
  SAF VARIABLE, string, [AS=string] [FIRST int] [LAST int]
  [SKIP int]
  ...
END
```

The PLOT, SAF command keyword group provides a method of specifying periodic dumps of registered scalar structured field variables to a specified SAF-format output file. Two command keywords are recognized within this keyword group, FILE and SAF VARIABLE. The FILE keyword is used to specify the name to be used for the created output file. Note

that if the file name has any lowercase characters, the string must be delimited by quotation marks (“”). The SAF VARIABLE command keyword’s first parameter is a string containing the registered name of the structured field. Currently, only the following STDEM-registered fields are supported: ELECTRIC_FIELD_I, ELECTRIC_FIELD_J, ELECTRIC_FIELD_K, MAGNETIC_FLUX_DENSITY_I, MAGNETIC_FLUX_DENSITY_J, and MAGNETIC_FLUX_DENSITY_K. The AS keyword allows the user to provide an alias string that will be used to label the field in the SAF file. If not supplied, the name of the registered variable is used. Note again that if any of the supplied string values contain lowercase characters, they must be delimited by quotation marks. By default, the frequency of output of the requested fields to the SAF file is controlled by Nevada’s EMIT PLOT command. An optional mechanism is provided to further filter the output frequency of each individual field output request by the use of the FIRST, LAST, and SKIP keywords. Output will occur only if the number of current timestep (k) is greater than or equal to the value of the FIRST keyword (k_b), less than or equal to the value of the LAST keyword (k_e), and the difference between k and k_b is integrally divisible by the value of the SKIP keyword (k_s), i.e., $(k - k_b)/k_s$ is an integer. For the special case that k_e is zero, the constraint $k \leq k_e$ will not be enforced. Finally, note that for a field to be written to the output file, *both* the constraints provided by the EMIT PLOT command *and* those provided by FIRST, LAST, and SKIP must be simultaneously satisfied.

5.5 Execution Control

5.5.1 CRT

CRT, {on|off}

This keyword is used to enable or disable the interactive menu. When enabled, the user can enter the word STOP to stop the calculation at the end of the next cycle or enter the word HELLO to access an interactive menu system offering several different runtime options. This capability needs to be disabled when running in background.

5.5.2 EMIT HISPLT

EMIT HISPLT, time-or-cycle-interval [time-range]

This keyword defines the interval at which time history values are output. An optional time range parameter can limit the window of output.

5.5.3 EMIT RESTART

EMIT RESTART, time-or-cycle interval [time-range]

This keyword defines the interval at which restart dumps are written. An optional time range parameter can limit the window of output.

5.5.4 EMIT SCREEN

EMIT SCREEN, time-or-cycle-interval [time-range]

This keyword defines the interval at which a brief simulation summary is displayed to the standard output. An optional time range parameter can limit the window of output. The output summarizes the current cycle number, current time, current time step, the cell limiting the current time step (always -1 for STDEM), the CPU time/timestep/cell with and without I/O, and the number of nodes remeshed (always 0 for STDEM). For example,

```
(250) t=5.7500e-08 dt=2.3000e-10 (-1) [2.5847e-07,9.8039e-08]
{0}
```

5.5.5 EXIT

EXIT

This keyword indicates the end of the simulation description. It is required and should appear at the end of input to be processed.

5.5.6 READ RESTART

READ RESTART TIME real

or

READ RESTART DUMP int

This keyword specifies that a simulation should be restarted from a previously written restart dump generated by an EMIT RESTART keyword. The first form restarts the simulation at the point closest to the specified time. The second form restarts the simulation using the specified restart dump number (not simulation time cycle). The restart dump number of -1 can be used to restart using the latest available restart dump or started as new if no dumps are available.

NOTE

Because a restart dump only contains the state of a simulation, the original simulation description with only *minor* changes should be used to restart simulations.

Note for QUICKSILVER Users

When restarting Emphasis you must include the original simulation description, not just the appropriate restart read keyword and new simulation termination time.

5.5.7 RESTART DUMPS

RESTART DUMPS int

This keyword uses an integer parameter to specify the maximum number of restart dumps to retain. By default, if this keyword does not appear in a simulation description only two dumps are retained.

5.5.8 TERMINATION CYCLE

```
TERMINATION CYCLE int
```

This keyword specifies the duration of the simulation. The parameter specifies the last cycle or time step number to simulate.

5.5.9 TERMINATION TIME

```
TERMINATION TIME real
```

This keyword specifies the duration of the simulation. The parameter specifies the last time value to simulate.

5.5.10 TITLE

```
TITLE  
string
```

This keyword can be used to associate a title with a simulation.

NOTE

Only the first 80 characters of the title are recorded.

5.6 Material Modeling

5.6.1 MATERIAL

```
MATERIAL int [string]  
    MODEL int  
    [MODEL int]  
...  
END
```

This keyword defines a material and associates material models with the material. The material is identified by the integer parameter. An optional string may be specified to tag the material. Material models are specified within the material keyword group. The models are applied in the order they appear within the keyword group.

5.6.2 MODEL

```
MODEL int string  
    parameter [{int | real}]  
    parameter [{int | real}]  
...
```

END

This keyword defines a material model. The model is identified by the integer parameter. The type of material model is specified by the string parameter. Optional material model parameters (specific to the material model) are specified within the model keyword group.

5.6.3 SIMPLE ELECTRICAL

The simple electrical material model represents a material with a constant relative permittivity, relative permeability and electrical conductivity.

Table 5.2. Input Parameters for Simple Electrical

Parameter Name	Type	Description
EPS	Real	Relative permittivity
MU	Real	Relative permeability
SIGMA	Real	Electrical conductivity

6 Executing Emphasis

6.1 User Environment

The Nevada framework primarily supports POSIX-compliant, UNIX-based operating systems. In order to use Emphasis the following Nevada environmental variables need to be properly set.

- The environmental variable `ALEGRA_ROOT` needs to be set the root directory of the Nevada installation.
- The environmental variable `ALEGRA_ARCH` needs to be set to the appropriate architecture (`linux-gcc`, `solaris-7.0`, `irix64-6.5`, `xtflop`, `icc`, `cplant-ross`).
- The environmental variable `ALEGRA_EXE` needs to be set to the complete path of the Emphasis or Alegra/Nevada team 3D executable.
- The environmental variable `ALEGRA_MP` needs to be set to `mp_none` for serial execution or `mp_mpi` (default) for parallel execution.
- The environmental variable `MPIHOME` (or `LAMHOME`) needs to be set to the location of the MPI [\[11\]](#) environment Nevada has been configured to use.

- The environmental variable `ACCESS` needs to be set if preprocessing of input files with APREPRO [9] is desired.

Additionally the directories `$ALEGRA_ROOT/$ALEGRA_ARCH/bin` and `$ALEGRA_ROOT/etc` should be added to the user's path.

6.2 Command Syntax

To execute Nevada based applications use the Alegra command. The Alegra command includes support for the options shown in [Table 6.1](#).

Table 6.1. Supported Nevada Command Line Options.

Option	Description
<code>-a</code>	Preprocess the input file with APREPRO
<code>-c</code>	Disable the CRT mode (required for running in background)
<code>-h</code>	Display help on all supported options
<code>--nprocs <i>n</i></code>	Run in parallel on <i>n</i> processors
<i>runid</i>	Identifies the simulation and used for generating filenames.

To run Emphasis in background the following command (POSIX shell) is suggested

```
nohup Alegra -c runid >stdout 2>stderr </dev/null &
```

6.3 File Descriptions

[Table 6.2](#) indicates how the `runid` option is used to specify Nevada filenames.

Table 6.2. Nevada File Descriptions

Filename	Type	Description
<code>runid.inp</code>	input	The textual simulation description.
<code>*.pff</code>	input	The binary mesh description. The actual filename is specified in the simulation description. For compatibility with other applications the recommended convention is to use the <code>.pff</code> extension.

runid.ech	output	An echo of the simulation description. Any errors in the syntax of the simulation description will be indicated in this file.
runid.out	output	A detail textual summary of the simulation settings.
runid.his	output	A binary file containing the simulation time history signals.
*.saf	output	A binary file containing snapshots of structured fields. The actual filename is specified in the simulation description. For compatibility with other applications the recommended convention is to use the .saf extension.
runid.dpl	output	A textual list of the restart dumps that have been written.
runid.dmp.*	output	A binary restart dump of the state of a simulation. In serial, the filename ends with the dump number. In parallel, each processor produces one file. The filename ends with three integer values, indicating the total number of processors, which processor the dump belongs to, and the dump number.

Restarted simulations append an `_n` where `n` is an integer number to the `.out` and `.his` extensions in order to prevent these files from being overwritten.

7 Additional Emphasis Resources

In most cases users of STDEM should have been provided with a point of contact, a knowledgeable analyst/developer to assist with using STDEM. He/she should be your primary resource for using STDEM. All users are also encouraged to interact with other users and developers through the majordomo mailing list emphasis-users@sandia.gov. For information on how to use the mailing list send a message with a body consisting of the line "help" to majordomo@sandia.gov. Internal users may access the Emphasis web site at <http://emphasis.sandia.gov>. Internal users can also access portions of the Emphasis SourceForge website <https://sourceforge.sandia.gov/projects/emphasis>. At the SourceForge website users can browse, search, and submit feature requests and bug reports; download documentation; and browse or search mailing list archives.

External users should contact their Sandia point-of-contact regarding access to these resources.

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