SANDIA REPORT

SAND2012-8592
Unlimited Release
Printed September 2012

A VU Governance Process Applied to a Bison Fuel Rod Validation Exercise

Patrick M. Knupp

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

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Approved for public release; further dissemination unlimited.

Sandia National Laboratories

Issued by Sandia National Laboratories, operated for the United States Department of Energy by Sandia Corporation.

NOTICE: This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government, nor any agency thereof, nor any of their employees, nor any of their contractors, subcontractors, or their employees, make any warranty, express or implied, or assume any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represent that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government, any agency thereof, or any of their contractors or subcontractors. The views and opinions expressed herein do not necessarily state or reflect those of the United States Government, any agency thereof, or any of their contractors.

Printed in the United States of America. This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from
U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831

Telephone: (865) 576-8401
Facsimile: (865) 576-5728
E-Mail: reports@adonis.osti.gov
Online ordering: http://www.osti.gov/bridge

Available to the public from
U.S. Department of Commerce
National Technical Information Service
5285 Port Royal Rd
Springfield, VA 22161

Telephone: (800) 553-6847
Facsimile: (703) 605-6900
E-Mail: orders@ntis.fedworld.gov
Online ordering: http://www.ntis.gov/help/ordermethods.asp?loc=7-4-0#online

SAND2012-8592
Unlimited Release
Printed September 2012

A VU Governance Process Applied to a Bison Fuel Rod Validation Exercise

Patrick Knupp
Uncertainty Quantification Dept. 1441
Sandia National Laboratories
P.O. Box 5800
Albuquerque, New Mexico 87185-1318

Abstract

A VU governance process, known as Discovery, Accumulation, and Assessment, was applied to a NEAMS Bison Fuel Rod Validation Exercise. The main outcomes were a VU plan for the Bison Validation effort and an improved DAA process. This document provides a sketch of the DAA process and its implementation in the Synopsis software. The application to Bison showed a tendency to skip important parts of the governance process. This points out the need for mechanisms such as Synopsis to improve VU governance. An appendix shows the data and information collected during the process, as it pertains to the Bison Validation effort.

Acknowledgment

This document was written with the support of the NEAMS VU management team, specifically Jim Stewart and Laura Swiler. We also wish to thank members of the Bison team, especially Jason Hales and Rich Williamson, for engaging in the DAA process.

Contents

1 Introduction **7**

Brief Description of the DAA Process 8

The Discovery Phase 9

The Accumulation and Assessment Phase 11

The Synopsis Software 12

2 Application of the DAA/VA governance process to a Bison Validation Effort **15**

Discovery: Customizing the abstract VUH 15

Discovery: Customizing the abstract VU Data Descriptors 17

Accumulation: Filling the concrete VU Data Descriptors 18

Assessment: Applying the DAA Status Metric 19

3 Conclusion **21**

References **22**

Appendix

A Preliminary Bison Hierarchical Entities and Placeholders **25**

List of Figures

1.1 Abstract Integrated Simulation Software Hierarchy (ISSH) 10

1.2 The Abstract VU Hierarchy (VUH) 11

1.3 A Screen Shot of Synopsis Showing the Bison VU Hierarchy 14

2.1 The Bison VU Hierarchy for the Fuel Rod Validation Exercise 17

2.2 DAA Status Metric applied to the Bison VUH on 6-10-12 19

Chapter 1

Introduction

BISON is a new multidimensional finite element computer code being developed at Idaho National Laboratory under the Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program to simulate the behavior of nuclear fuels [1]. An important application of the code is to simulate Light Water Reactor (LWR) fuel rods. In 2012, the BISON team embarked on an effort to validate some of its fuel rod sub-models using experimental data from the HALDEN IFA-432 Rod 1 experiment [2]. The VU cross-cut team within NEAMS, whose mission includes providing support to the Fuels and Reactors IPSC's in the form of verification, validation, and uncertainty quantification (VU) technology, engaged the Bison team in support of the on-going fuel rod validation exercise. As part of the support provided by the VU cross-cut team to the BISON validation effort, a new state-of-the-art VU governance technology, known as the Discovery, Accumulation, and Assessment (DAA) process was deployed. This report describes preliminary results of the deployment.

VU is commonly understood to consist of a collection of *practices* by which computational simulation capabilities are developed and used in a scientific (or rigorous) manner. Major practices within VU include code and solution verification, validation to experimental data, and characterization & quantification of sources of uncertainty. The pursuit of the collection of VU practices with respect to a particular application requires, in addition to the practices themselves, a well-defined set of *processes* to coordinate, plan, apply, organize, record, and communicate the work. The set of such processes constitutes a VU *governance* process.

While a lot has been written about VU practices (see, for example, [4], [5], [6], [7]), relatively little has been written to date, about VU processes. As a result, a significant fraction of the VU work that is pursued within the computational simulation community, in relation to particular applications, currently takes place without an explicit governance process in place. This is a particularly serious omission in the case of large application projects with many team members. Lacking a governance process, VU practices are often pursued in isolation of other practices (e.g., validation without verification) and a relatively small portion of the full picture gets communicated effectively. A number of other undesirable consequences can also occur. To ameliorate this situation somewhat, a particular VU governance process known as DAA was developed in 2011-12. A brief overview of DAA is given next, but the reader should bear in mind that many details are left out in order to not distract from the focus of this report, which is to discuss the results of applying the DAA process to the BISON validation exercise. Details of the process can be found in [3] and elsewhere.

Brief Description of the DAA Process

The DAA process requires a person who is knowledgeable about VU and who is independent of the simulation capability development and analyst teams to serve as the DAA *process master*. The job of the process master is to assist the development and analyst teams in proper execution of the DAA process through its various phases and stages.

A distinguishing feature of DAA is the use of pre-defined hierarchies that incorporate important concepts from the VU community and which are customized to the application during the DAA process in order to create a VU plan which is consistent with best practices within VU. The process master uses the pre-defined templates to guide the DAA process and to facilitate assessment. Three types of templates are provided by DAA:

1. a hierarchy which generically describes a simulation capability development and analysis sequence known as the abstract Integrated Simulation Software Hierarchy (ISSH),
2. a set of hierarchies which generically describe VU practice sequences known as abstract VU Hierarchies (VUH's), and
3. a set of generic placeholders within each of the nodes of the hierarchies known as VU data descriptors (VUDD's).

Given a concrete Application (such as Bison), the process master, with the help of team developers and analysts, facilitates the following activities (known as stages) within the DAA process:

1. Discovery Phase
   (a) Customize the abstract Integrated Software Simulation Hierarchy (ISSH) to the Application in order to create a concrete ISSH.
   (b) Review and Approve the concrete ISSH.
   (c) For each node in the concrete ISSH, create a concrete VU Hierarchy (VUH) by customizing the abstract VUH to the Application.
   (d) Review and Approve each of the concrete VUH's.
   (e) For each node in each concrete VUH, create concrete placeholders for VU data by customizing the abstract placeholders provided by DAA.
   (f) Review and Approve each of the concrete placeholders.
2. Accumulation and Assessment Phase
   (a) Perform VU practices according to the VU Plan created during Discovery (the plan is defined by the concrete ISSH and VUH hierarchies and their VUDD's) to generate candidate VU data.

(b) Review and approve the candidate VU data.

(c) Fill the concrete placeholders with approved VU data.

(d) Monitor progress of the accumulation stage using the VU status metric.

(e) Use the Predictive Capability Maturity Method (PCMM) and Predictive Maturity Index (PMI) methodologies to assess the Application from a VU perspective.

(f) Perform formal reviews by panels of experts.

Some of these activities are described in more detail below.

The Discovery Phase

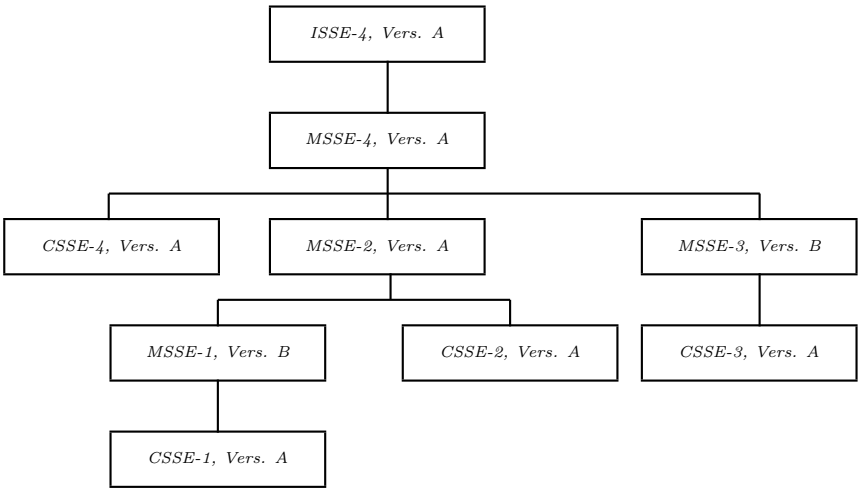
Ideally, the first step in VU governance is to collect relevant information concerning the application and to plan the work involved in the VU practices accordingly.[1] Within the DAA process, this step is called the *Discovery* phase; it's purpose is to create a VU plan for the application. To facilitate the collection of application information that is relevant to VU, the Discovery process makes use of an abstract hierarchy, called the Integrated Simulation Software Hierarchy (ISSH), that is somewhat similar to the better-known Validation Hierarchy [4]. As Figure 1.1 shows, the abstract hierarchy contains nodes which represent both simulation capabilities as they existed at the start of the project (CSSE's), at intermediate evolutionary stages (MSSE's), and at the final stage (ISSE) when the software product (and its uses) are to be delivered to the customer. The different nodes are distinguished by the introduction of capabilities which have VU significance (e.g. a new physics model has been added to a simulation code).

The job of the process master in the first stage (1a) is to assist the development/analysis team in customizing the abstract hierarchy into a concrete representation of the project's planned simulation products. Part of this process is to assign for each node of the concrete hierarchy a VU objective (the event of VU significance). Common VU objectives defined in DAA include (1) import and assessment of existing capabilities from outside the project, (2) verification of software, (3) validation to experiment, and (4) product end-use. The abstract ISSH hierarchy in DAA was designed specifically for use within the pursuit of VU governance; thus, when this hierarchy is tailored to become a description of a specific application project, the result should be a VU-centric description of the application that can be used effectively to govern the VU work. Once a concrete ISSH hierarchy has been completed, it is reviewed by the team to ensure completeness and correctness (stage 1b). If the review is positive, one proceeds to (1c), the next stage in the Discovery Process.

Stage 1c in the Discovery Process is to plan the VU work in terms of VU practices associated with the development and use of each node of the ISSH hierarchy. To facilitate this step, DAA provides several abstract hierarchies (one for each VU objective type) known as VU hierarchies (VUH's), which are to be customized to the application in stage 1c. As Figure 1.2

[1] In DAA, this can be done even when the some of the work has already commenced.

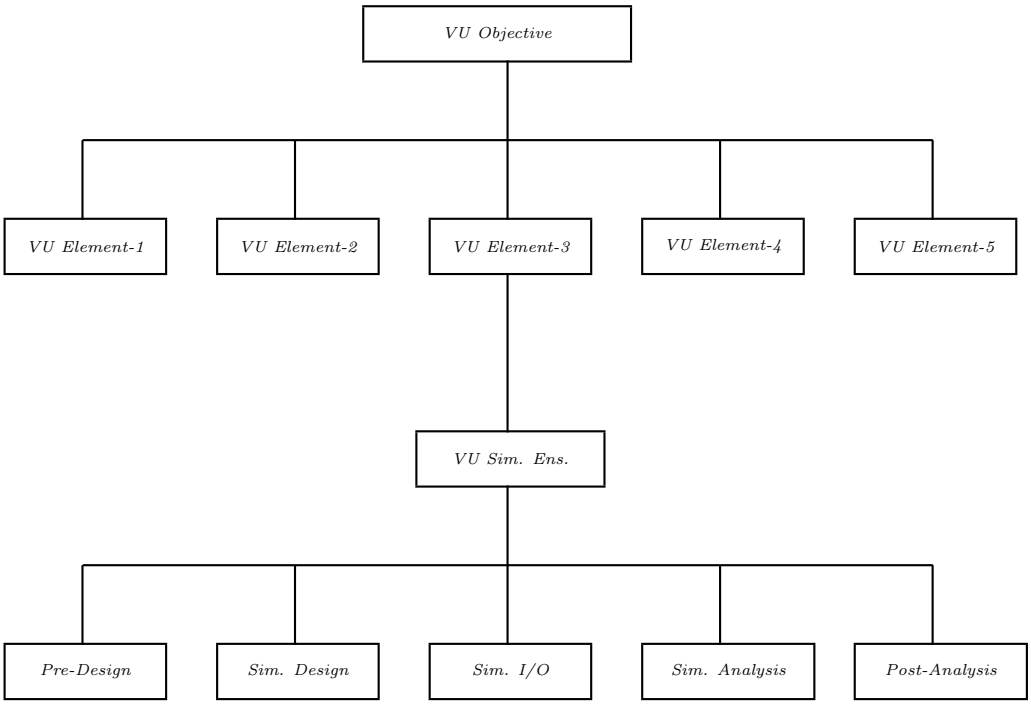
Figure 1.1. Abstract Integrated Simulation Software Hierarchy (ISSH)



shows, the top level of every abstract VUH consists of a VU objective. On the next level below are VU practices adapted from the Predictive Capability Maturity Model (PCMM). Below each of these practices are numerical experiments (simulation ensembles) which contain the computations or tests involved within each VU practice. The abstract VU hierarchies within DAA were designed so-as to guide the teams' planning process in order to produce a plan that aligns with or accounts for best VU practices, as defined by the VU community. For every node in the ISSH hierarchy, the team (assisted by the process master) must create a concrete VU hierarchy by tailoring the provided abstract VUH to accurately represent and organize the planned VU work. Each of these hierarchies must be reviewed and approved by the team to ensure that a faithful representation of the VU plan (at this level of detail) has been created (stage 1d).

Stage 1e in the Discovery phase is to flesh out the VU plan in more detail and, in so doing, provide a mechanism by which data pertaining to the VU work can be collected, saved, and disseminated. DAA facilitates this stage by providing, for each node of the ISSH and its VUH's, a set of default placeholders (or VU Data Descriptors). The set of descriptors depends upon the type of node within the VUH. For example, a code verification node will contain descriptors which ask for information concerning code verification activities in relation to a specific simulation capability within the ISSH. A math model development node will contain descriptors which ask for information in relation to a specific model within a simulation capability that is to be validated. Once the default (or abstract) VUDD's are customized, they are reviewed and approved by the team (stage 1f). This ends the Discovery phase. The result is a customized description of the capability development and analysis team's plans

Figure 1.2. The Abstract VU Hierarchy (VUH)



in VU terminology and which describes specific data which is to be collected and stored. In essence, the output of the Discovery phase is a VU plan for the project.

The Accumulation and Assessment Phase

In this phase of DAA, the team engages in VU practices that are defined by the VU plan developed in the Discovery phase. Starting with a single concrete VUH, the goal is to fill as many of the customized placeholders within the VUH as possible. For example, there is a set of placeholders having to do with the practice of identifying and quantifying sources of uncertainty within the Experiment node of a Validation-to-Experiment VUH. As the team engages in this practice, they will generate and accumulate information and numbers which can be used to fill the associated set of placeholders. This information/data is called *candidate* VU data. The accumulation of candidate VU data is the primary activity in stage 2a of the DAA process. In stage 2b, the candidate data is reviewed by the process master to ensure that it matches the scope and intent of the specific placeholder(s) to be filled. If the candidate data is approved, the process master fills the placeholder by storing the data in the appropriate location (stage 2c). Stages 2b and 2c can take place continuously as data

is generated and need not wait for everything to be accumulated.

Assessment takes place concurrently with Accumulation so that feedback can be incorporated into the work and so that progess towards achieving predictivity can be measured. The simplest assessment metric in DAA is called the Accumulation Status Metric and is computed by dividing the number of filled placeholders by the total number of (filled and unfilled) placeholders. This can be done in a fine grained manner, by computing the metric for each node within each VUH, or at more coarse-grained levels such as computing one value of the metric for an entire VUH. This metric is useful because the information and data which fills the placeholders has under-gone quality control processes in stages 1f and 2c. The values of the status metric are stored so that progress over time can be monitored (stage 2d). Assessment may also be based on the Predictive Capability Maturity Model (stage 2e). In that case, target PCMM levels 0, 1, 2, 3 are assigned to nodes within the VUH's during the Discovery process. The target levels then help determine the other placeholders which appear in VUH because each set of placeholders is associated with a certain level of rigor. Within DAA, PCMM-based assessment is equivalent to ensuring that certain placeholders are filled. Assessment based on the Predictive Maturity Index can also be performed in a similar manner. Finally, Assessment can be based on reviews by panels of experts. In this case, the experts can use the evidence provided by DAA as part of their assessment (stage 2f).

When the DAA process is completed, one has a VU plan, an assessment, and supporting evidence (in the form of filled placeholders). Moreover, all this information is organized in such a way that these items can be communicated to any stake-holder. Subsequent development of the simulation capability on a different project can retrieve the collected evidence and make use of it. If multiple projects use DAA to perform VU governance, then VU work and reporting becomes standardized, making it easier to assess results across unrelated projects.

The Synopsis Software

The DAA process is greatly facilitated by the use of software that emulates the stages in the process and manages the flow of information and data. To this end, prototype software called Synopsis was developed during FY12 to serve as an implementation of the DAA/VU governance process. The front-end is a graphical user interface built on top of Matlab. All appropriate team members are given access to Synopsis and can enter data or view current project status. The process master has the highest levels of permission and can perform certain functions that other team members can't (e.g., only the process master can promote the DAA process from one stage to the next). Synopsis writes data to disk or to a repository that provides configuration control and sychronization amongst team members. Users can check out the latest version of the process and check in changes.

The abstract ISSH, VUH's, and VU data descriptors are stored in Synopsis' memory and

can be viewed on-screen. In stage 1a, the team customizes the abstract ISSH by creating concrete nodes in the hierarchy. Each node is defined by entering a name, a node type, a VU objective, it's parent and children nodes, and other so-called Entity Data Descriptors. The concrete hierarchy is created on-screen via the GUI and, in stage 1a, can be edited and re-drawn (see Figure 1.3). All team members can load the concrete hierarchy into Synopsis, view it, print it, and comment on it. When the hierarchy appears complete, the process master promotes the project to stage 1b in which team members review and approve the concrete ISSH that has been created.[2] In later stages, Synopsis enables the team to customize the set of VU hierarchies, the VU Data Descriptors, and finally, to perform accumulation and assessment.

Synopsis functionalities include the ability to:

1. customize abstract hierarchies to create concrete hierarchies, which can be viewed, stored, printed, annotated,
2. synchronize activities and disseminate information amongst team members,
3. create project status reports at various levels of detail,
4. archive and retrieve data and information (organized in directories defined by the hierarchies),
5. perform PCMM and other assessments. Measure progress over time,
6. initiate and perform quality control processes,
7. fill, re-fill, un-fill, waive, customize, create new, and annotate VU Data Descriptors,
8. include conditional Data Descriptors,
9. query a DAA terminology dictionary, and
10. customize the DAA/Synopsis process itself according to project preferences.

Early versions of the software were valuable in terms of being able to demonstrate aspects of the DAA process to various internal audiences. Not all of the Synopsis functionalities listed above were completed in FY12. This prevented us from fully applying Synopsis to the Bison project.

[2]The concrete ISSH can continue to evolve as the project evolves, but that introduces another level of complexity in the description of the process so we omit it here.

Bison Fuel Rod Validation with Discovery, Accumulation, & Assessment Process

Migration of Bison/DAA to Synopsis Software

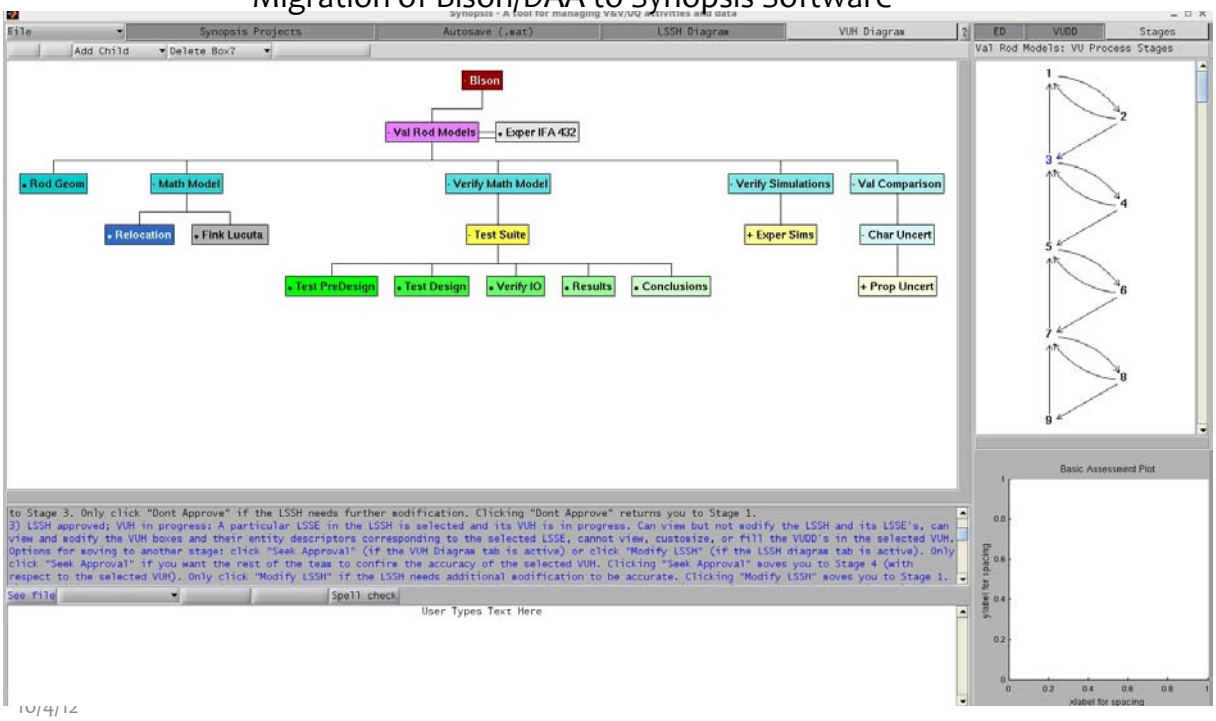


Figure 1.3. A Screen Shot of Synopsis Showing the Bison VU Hierarchy

Chapter 2

Application of the DAA/VA governance process to a Bison Validation Effort

There were two goals in applying DAA to the on-going Bison Fuel Rod Validation effort. First, we wanted to help the Bison team with their VU governance processes as they attempted to validate their fuel rod models. Second, we wanted to test the DAA process against a NEAMS project in order to improve the DAA process itself. By necessity, P. Knupp served as the DAA process master.

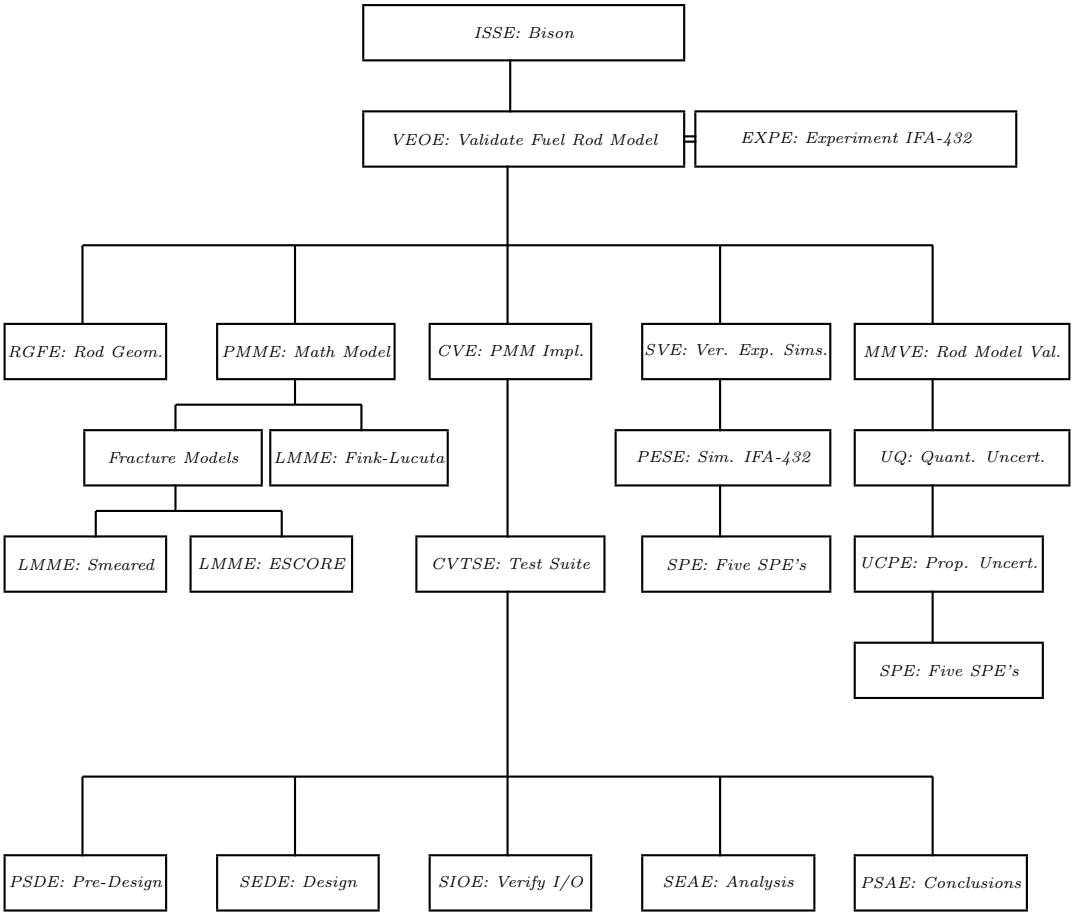
In applying DAA to Bison, many of the process stages, and even whole phases were not strictly followed. For example, Stages 1a and 1b were skipped because the Bison team, being new to DAA, and being focused on their validation deliverable for FY12, did not wish to devote time to describing the complete plan for Bison capability development and use within the DAA context. It was agreed that, for the time being, there would be only one node in the ISSH hierarchy, called Bison. In accordance with DAA, a VU objective of the type 'Validation to Experiment' was assigned to this node. With that assignment, the team was ready to engage in Discovery stage 1c. Details on that are reported in Section 2 below. The team also did not strictly engage in the Accumulation and Assessment phase of DAA, partly because the validation effort was not mature enough (i.e., not enough VU data had been generated), and partly for reasons which will be explained later. The team did engage in activities related to Stages 2c and 2d (Sections 2 and 2). In our opinion, had the Synopsis software been available (i.e, mature enough), the team would have had to follow the DAA process more strictly.

Discovery: Customizing the abstract VUH

The customization of the VUH to the Bison Fuel Rod Validation effort was performed by the process master, primarily by referring to [1] and to [3]. The customized hierarchy is shown in Figure 2.1. At the top of the hierarchy we show the single node in the ISSH called Bison. Below it is the assigned VU objective, of type 'Validation to Experiment', which was named *Validate Fuel Rod Model*. Validation requires experimental data generated by one or more experiments. In this case, there was one experiment from the Haldane series called

IFA-432 which was being used in the validation effort. The concrete hierarchy thus has a node of type Experiment Entity as a sibling of the VU objective node. Data and information pertaining to the experiment (and to related VU activities) in the form of filled VU data descriptors reside within this node. The next level of the concrete VU hierarchy consist of five VU practices: Representation and Geometric Fidelity (RGF), Math Model Development (MMD or PMM), Code Verification (CV), Solution Verification (SV), and Math Model Validation (MMV). These nodes were named Fuel Rod Geometry, Particular Math Models, PMM Implementation, Verify Experiment Simulations, and Fuel Rod Model Validation, respectively. These five practices should ideally be performed temporally from left to right and variations from that order can be detected by Synopsis. Use of the abstract VUH to create the concrete hierarchy means that the VU plan does not consist of Validation only (even though that is the stated VU objective), but includes necessary preliminary activities such as code and solution verification. This is one primary purpose of the abstract hierarchies: to ensure that the VU practices associated with a given VU objective are properly identified. The hierarchies also provide context and relationships, as well as serve to organize the data. Underneath the Math Model node are three specific math models within Bison that are the focus of the Validation exercise. They include the Fink-Lucuta model of temperature-dependent thermal conductivity, and two fracture models (referred to here as 'smeared' and 'ESCORE'). Underneath the code verification node there is a node called code verification test suite in which details concerning the suite of tests used to verify the particular math model are given. This node is an example of what DAA calls a 'simulation ensemble'. Simulation ensembles can appear underneath RGF, math models, SV, and MMV, as well as code verification and can have different purposes. For example, under the Solution Verification node there is a simulation ensemble called 'verify the experiment simulations' in which the specific numerical solutions produced in simulating the experiments are verified. There is another simulation ensemble under math model validation in which experimental and numerical uncertainties are quantified and propagated. Finally, every simulation ensemble requires underneath five nodes pertaining to the execution of a simulation ensemble: initialization, design of simulations, verification of inputs and outputs, analysis of outputs, and derivation of conclusions from the analysis. These five node types also must appear under the solution verification and UQ simulation ensembles but, due to lack of space, are not shown in Figure 2.1. With the concrete VU hierarchy in place, Discovery stage 1c is complete. The concrete hierarchy was tacitly approved by the Bison team since they did not question it. This was not too surprising since the hierarchy, for the most part, follows widely understood VU practices. The true value of this process arises in the fact that information and data, called out by the VU data descriptors, will be contained within the nodes once the accumulation phase is initiated. Use of Synopsis ensures that data is stored properly and that missing data can be brought to the teams' attention. Stage 1c and 1d were completed in about one week.

Figure 2.1. The Bison VU Hierarchy for the Fuel Rod Validation Exercise



Discovery: Customizing the abstract VU Data Descriptors

In Stage 1e, the list of abstract VU Data Descriptors provided by DAA was customized to the application by the process master. Currently, DAA does not have a fully-developed set of abstract VU data descriptors for every node within its hierarchies, but a preliminary list of abstract descriptors can be found in the appendix to [3]. These were used as the basis for customizing descriptors within each node of the concrete VU hierarchy. The purpose of having a list of abstract descriptors is to help the team think about and plan the inputs and outputs to the VU practices in which they will engage. Customizing VU data descriptors requires considerable experience with VU and can be a rather time-consuming process. It would take even longer if there were not a list of abstract placeholders to refer to and many important placeholders could be overlooked. The abstract descriptors are stored within Synopsis and the list will evolve over time as the software is applied to more and more projects. The customized descriptors serve as placeholders for VU data that the project

needs to create in order to complete work called out by the VU plan. Appendix I of this report shows the customized VU data descriptors for each node-type in the concrete ISSH and VUH for the Bison validation effort. Descriptors have two basic types called (a) Entity Descriptors and (b) VU data descriptors. Entity descriptors are pre-defined and cannot be customized. They are used to define the nodes (entities) within the hierarchies, asking for things like the name of the node, its version number, and the names of the nodes' parent and children. Entity descriptors are filled during stages 1a and 1c of the Discovery process and the act of filling them is part of the overall process of creating a VU plan. VU data descriptors, on the other hand, can only be filled during Accumulation (stage 2c). In stage 1e, one is concerned with identifying (customizing) the VU data descriptors in order to create a VU plan for the Application. Stage 1e, in this application to Bison, took about a month to complete. *In completing this stage, we succeeded in creating a VU plan for the Bison Validation effort.*

Accumulation: Filling the concrete VU Data Descriptors

Accumulation begins with stage 2a, in which candidate VU data is generated. Some of the VU data called out by the Bison VU Plan developed under DAA pertains to existing software or to existing experimental data. For example, the Physical Experiment Entity has a descriptor that asks the team to provide (or upload) the report on the results of the Haldane experiment. In the Integrated Simulation Software Entity, a descriptor asks for any papers related to the Bison software. These types of VUDDs are usually easy to fill because the information already exists and is accessible. As a result, these kinds of descriptors generally get filled prior to undertaking any activities that require a lot of work to generate the data to fill the corresponding VUDD. An example would be the performance of mesh refinement studies to fill a VUDD asking for the observed order-of-accuracy of a code verification test. Since both the Bison Validation effort and the application of DAA to it were just getting underway in FY12, the VUDDs that were actually filled were mostly of the former type. See the Appendix for the data and information provided by the Bison Team in order to fill some of the VUDDs. Note that in some cases, the VUDDs have been annotated in order to ask for clarification or provide additional information. Stage 2b, in which the candidate data is reviewed and approved, was skipped. Had the DAA process been run from within Synopsis, this review would have taken place automatically each time a member of the team attempted to fill a data descriptor. Synopsis will also provide the capability to upload the requested documents and allow users to view those documents. Stage 2c took approximately two months before the Status Metric described in the next section was applied. Stage 2c was not completed during this year nor was it expected to be since it takes a great deal of work.

Assessment: Applying the DAA Status Metric

Assessment can and should take place periodically while Accumulation is taking place. After the VU data reported in the Appendix was supplied, the process master applied the DAA Status Metric to assess the state of the work. Recall that the DAA status metric is simply the ratio of filled VU data descriptors to the total number of VU data descriptors within some hierarchical unit. The process master selected the Entities within the concrete VUH as the hierarchical unit, i.e., a status metric was computed for each node in the VUH shown in Figure 2.1. The resulting status metric values are shown in Figure 2.2. The figure shows that some of the hierarchical nodes have a high percentage of their VUDD's filled, while others have not been filled at all. This reflects the fact that the project was in its early stages and that entities were being addressed in the proper order. Synopsis would store these kinds of figures as the metric is applied over time to create a sequence of figures showing progress in filling the VUDD's. The status metric needs to be supplemented by an assessment based on PCMM, however, we were not in a position to do so this year.

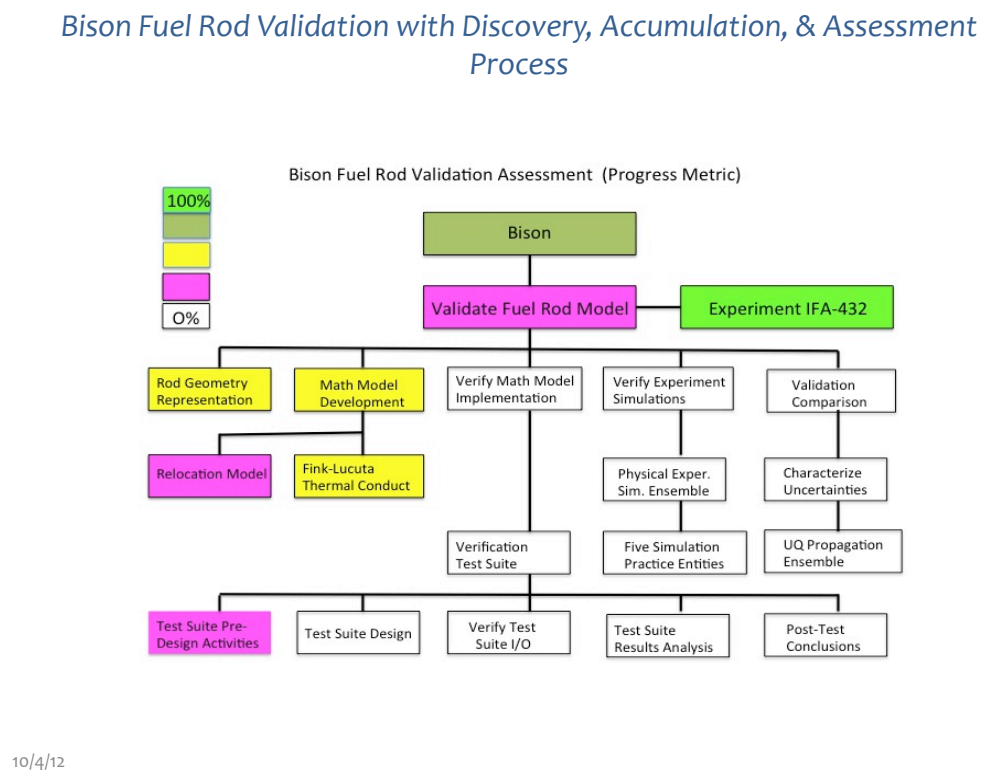


Figure 2.2. DAA Status Metric applied to the Bison VUH on 6-10-12

Chapter 3

Conclusion

This report briefly described a VU governance process called Discovery, Accumulation, and Assessment (DAA). The process consists of multiple stages which are intended to address many VU governance issues including planning, the practices of VU, and assessment. The DAA process was partially implemented in prototype software called Synopsis. At the same time as the software was being developed, the DAA process was applied to on-going efforts by the Bison team to validate fuel rod models against experimental data from the Haldane experiments. The goal in applying DAA to the Bison validation effort was to support the Bison team by introducing VU governance processes in concert with their validation work and, secondarily, to improve the DAA governance process itself via lessons learned from the attempt. In applying the DAA process to Bison, a number of stages were skipped and the process ended the year in stage 2c (the filling of placeholders with VU data). Many of the stages that were skipped would not have been skipped if we had had the Synopsis software available in time. Moreover, the information and data collected during this application of DAA would have been stored electronically, rather than only existing in the form of this report. Completing this software is essential to the success of DAA. We were, however, able to create a VU Plan for the Bison validation effort, in the form of a customized VU hierarchy complete with customized VU data descriptors which serve as placeholders for the planned work. We were also able to compute the Accumulation Status Metric showing the status of the effort at the end of the second quarter. Overall, we were pleased that the abstract hierarchies and descriptors provided by DAA proved useful during the customization process. Our long-term vision is to apply DAA (through Synopsis) to a computational simulation project from start to finish so that the DAA process can be fully demonstrated and improved, and so that its full impact can be appreciated.

References

[1] R. Williamson, J. Hales, S. Novascone, M. Tonks, D. Gaston, C. Permann, D. Andrs, R. Martineau, *Multidimensional Multiphysics Simulation of Nuclear Fuel Behavior*, preprint, 2012.

[2] E. Bradley, M. Cunningham, D. Lanning, Final data report for the instrumented fuel rod assembly (IFA)-432. Technical Report NUREG/CR-2567, PNNL-4220, 1982.

[3] P. Knupp and A. Urbina, *A Design for a V&V and UQ Discovery Process*, SAND20011-6677, Sandia National Laboratories, 2011.

[4] W. Oberkampf and C. Roy, *Verification and Validation in Scientific Computing*, Cambridge University Press, 2010.

[5] P. .J. Roache, *Fundamentals of Verification and Validation*, Hermosa Pub., Socorro NM, 2009.

[6] R. Nelson, C. Unal, J. Stewart, B. Williams, *Using Error and Uncertainty Quantification to Verify and Validate Modeling and Simulation*, Los Alamos National Laboratory, LA-UR-10-06125, 2010.

[7] V&V 20 Committee, *Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer*, ASME V&V 20-2009, ASME, 2009.

Appendix A

Preliminary Bison Hierarchical Entities and Placeholders

Integrated Simulation Software Entity (ISSE) Descriptors

Entity Descriptors:

* The particular name of this entity:

  Answer: Bison ISSE

* The version number of this entity:

  Answer: Version 1.0

* The location of this entity within the DA&A Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 2-1-2012

* The particular name of this ISSE's child Mid-Sequence or Cornerstone Simulation Software Entites.

  Answer: None.

Recursive Descriptors:

⊗ The VU Objective Type assigned to this Entity:

  Answer: VE (Validation to Experiment)

Integrated Simulation Software Entity (ISSE) Descriptors (continued)

VU Data Descriptors - I

** Software Name, Version, Date.

Answer: BISON, Version of the Day

** Names of included libraries, versions, dates.

Answer: PETSc (2.3.3); libmesh (version tied to version of the day); hypre (2.4.0b)

** Location of the Simulation Software.

Answer: ?

Note: [What is meant here?] PK- This would be the Bison Repository and/or the precise version that is used to perform the simulations within the VU Hierarchy that is being addressed. In principle, the simulation ensembles under the VU hierarchy should be reproducible as Bison changes over time.

** Explanation as to why this is an Integrated Simulation Software Entity.

Answer: Because this entity uses version of the day, the Landmark Simulation Capability Development Sequence is collapsed into a single entity. By definition, every Landmark Simulation Software Hierarchy must contain an Integrated Simulation Software Entity.

** Explanation of the role of this entity within the Landmark Simulation Software Hierarchy.

Answer: This entity represents the Bison software in terms of version of the day. This means that any input/output files within simulation ensembles saved within the DA&A process must work with the version of the day. Any statements about the code must be true for VOTD.

** General Description of ISSE.

Answer: BISON is a code for nuclear reactor fuel performance simulations. The code solves a system of PDE's in 3D for transient heat conduction, oxygen diffusion, and nonlinear inelastic solid mechanics. Empirical closure models relate temperature, density, and oxygen concentration. Code uses a Jacobian-free Newton-Krylov solver with physics-based pre-conditioner.

Integrated Simulation Software Entity (ISSE) Descriptors (continued)

VU Data Descriptors - II

** Upload any papers related to this ISEE.

Answer: R.L. Williamson, J.D. Hales, S.R. Novascone, et. al., Multidimensional Multiphysics Simulation of Nuclear Fuel Behavior, Journal of Nuclear Materials, Vol. 423, Issues 1-3, April 2012, pages 149-163.

Note: PK - The project should ensure that any document that fills a VU Data Descriptor be available upon request. In Synopsis, users will be able to upload such documents to the Synopsis/DAA repository.

** Upload any PIRT or GAP Analysis reports that pertain to this ISSE.

Answer: ?

** Upload Users-Guide.

Answer: ?

** Upload Theory Manual.

Answer: ?

** Upload other Supplemental Descriptive Materials.

Answer: See https://hpcsc.inl.gov/data/trac/FPCP/wiki/BISON

Note: PK - I tried this link, but it didn't load, perhaps because it's a secure site?

** Does this Software have a working Regression Test Suite?

Answer: Yes

** Characterize the kinds of tests within the Regression Test Suite.

Answer: Comparisons of numerical solutions to analytic solutions. Tests that check that incorrect inputs are caught and reported.

VE Objective Entity (VEOE) Descriptors

Entity Descriptors:

* The particular name of this entity. *Answer:* Validate LWR Fuel Rod Models

* The version number of this entity. *Answer*: 1.0

* The location of this entity within the Repository. *Answer*: N/A

* The date this entity was created or last updated. *Answer*: 3-26-2012

* The particular name of this entity's associated concrete Landmark Simulation Software Entity. *Answer*: Bison ISSE

* The particular name of this entity's child Geometric Fidelity Entity

  Answer: Simulated Rod Geometry

* The particular name of this entity's child Particular Math Model Entity.

  Answer: Particular Equations for Fuel Rod Experiment Simulations

* The particular name of this entity's child Code Verification Entity.

  Answer: PMM Implementation

* The particular name of this entity's child Solution Verification Entity.

  Answer: Verify Experiment Simulations

* The particular name of this entity's child Math Model Validation Entity.

  Answer: LWR Fuel Rod Model Validation Comparison

* The particular name(s) of the Physical Experiment Entities contained within this VE Objective Entity.

  Answer: Experiment IFA-432 Rod 1 BOL (Beginning of Life)

VE Objective Entity (VEOE) Descriptors

VU Data Descriptors

** Why was this Objective assigned to its corresponding Landmark Simulation Software Entity?

Answer: We want to assess (validate) Bison models by comparing to Experimental Data.

** Describe any known requirements on the Goodness-of-Fit. *Answer*: ?

** VU Data related to PMI-based Assessment: *Answer*: ?

** The value of the complexity and robustness factor. *Answer*: ?

** The volume of the extrapolation space. *Answer*: ?

** The volume of the application space. *Answer*: ?

** The value of the Discrepancy metric. *Answer*: ?

** The value of the PMI. *Answer*: ?

** The local models assessed by the Index. *Answer*: ?

** Provide a credible claim regarding the results of completing this Objective. *Answer*: BISON performs well compared to experimental data on the IFA-432 Rod 1 BOL test.

** How do the individual claims for each of the VU Elements in this entities' Element Chain contribute to the above claim?

Answer: ?

** How does the above claim meaningfully contribute to the claims made for the other VU Objectives within the Landmark Simulation Software Hierarchy?

Answer: ?

Physical Experiment Entity (EXPE) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: Experiment IFA-432 Rod 1 BOL

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 3-26-2012

* The particular name of this entity's containing VE Objective Entity.

  Answer: Validate LWR Fuel Rod Models

Physical Experiment Entity (EXPE) Descriptors

VU Data Descriptors - I

** Provide or cite experiment test plan document. *Answer*: ?

** Provide or cite the experimental results report.

Answer: E.R. Bradley, M.E. Cunningham, and D.D. Lanning, Final data report for the instrumented fuel assembly (IFA)-432. Technical Report NUREG/CR-2567, PNNL-4240, 1982.

** Provide or cite location of the experimental data. *Answer:* D.D. Lanning, C.E. Beyer, G.A. Berna, FRAPCON-3: Integral Assessment. Technical Report NUREG/CR-6534, PNNL-11513, 1997.

** What physical quantities were measured?

Answer: Fuel centerline temperature histories.

** What was the measurement device?

Answer: Thermocouples

** Where were the measurement devices located?

Answer: Top and bottom end of fuel rod column

** If only some of the data was used in the validation exercise, indicate the part that was used.

Answer: BOL data only

** Explanation of the relevance of this data to the Particular Math Model which is being validated.

Answer: Centerline temperature is dependent on thermal conductivity of the fuel, gap response, and fission gas release, among other models.

** How relevant is the experimental data within this context: (i) very relevant because the experimental data is close to the application space, (ii) mildly relevant because some extrapolation to the application space is needed, (iii) not relevant (data is far from the application space).

Answer: Very relevant

Notes: RK – It is very relevant because ?

Physical Experiment Entity (EXPE) Descriptors

VU Data Descriptors - II

** What is the source of the experimental data: (i) historical data, (ii) expert opinion, (iii) extrapolated from other experimental data, (iv) other (explain).

Answer: Historical data

** Characterize the sources of uncertainty in the experimental data.

Answer: ?

** Have the uncertainties in the experimental data been quantified?

Answer: Unknown

** The method used to quantify the experiment uncertainties was (i) measurement errors, measurement techniques, and post-processing, (ii) unit-to-unit variability, (iii) test-to-test variability, (iv) boundary conditions and inputs, (v) experimental biases, (vi) test environment vs. actual environment.

Answer: ?

** Describe the experiment geometry.

Answer: See FRAPCON-3: Integral Assessment.

Notes: PK - pages numbers would be nice here. Synopsis will ask for these.

** Characterize the critical experiment materials.

Answer: UO_2 fuel (95% TD), Zircaloy-2 cladding, Helium fill gas

** Describe experiment 'boundary conditions'.

Answer: See FRAPCON-3: Integral Assessment for power history, pressure, fast flux, etc.

Notes: PK - pages numbers would be nice here.

RGF Entity (RGFE) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: Simulated Rod Geometry

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 2-2-2012

* The particular name of this entity's concrete parent VU Objective Entity

  Answer: Validate LWR Fuel Rod Models

* The particular name(s) of this entity's concrete child Simulation Ensemble Entities

  Answer: ?

RGF Entity (RGFE) Descriptors

VU Data Descriptors

** Describe the simulated geometry.

Answer: 2D axisymmetric, single cylinder, with a hole along the symmetry axis to accommodate the thermocouples. The clad was modeled as a simple cylindrical tube with end caps and an upper plenum.

** How does the mathematical and computer representation of the physical geometry differ from the physical geometry?

Answer: An actual fuel rod has more details (such as a spring), but these details are of secondary importance.

** Characterize the impact of these differences on the conclusions reached in the parent VU Objective.

Answer: Minor if any.

Notes: PK - Is this statement an expert opinion or is there any other basis for making it?

** Was a Geometric Model Sensitivity Study Performed?

Answer: ?

** If not, why not?

Answer: ?

** Provide a credible claim regarding the results of completing this Element.

Answer: ?

** How do the individual claims for each of the Simulation Ensemble Entities within this entity contribute to the above claim?

Answer: ?

** How does the above claim meaningfully contribute to the claims made within the other VU elements under the concrete VU Objective?

Answer: ?

Particular (Global) Math Model Entity (PMME) Descriptors

Entity Descriptors

* The particular name of this entity.

  Answer: Particular Equations for Fuel Rod Experiment Simulations

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 3-8-2012

* The particular name(s) of the Local Math Model Entities that belong to the Particular Math Model (include all local models, whether or not they are validated).

  Answer:

  1. Fink-Lucuta Thermal Conductivity,
  2. Relocation Model,
  3. Forsberg-Massih fission gas release model,
  4. Fill-gas dependent gap conductance,
  5. Irradiation-induced creep cladding model,
  6. Irradiation growth cladding model,
  7. Creep UO_2 model

     Notes: PK - what combinations of these models will be used in the experiment simulations? Does each combination refer to the same experimental dataset noted in the EXPE? (If not, you may need to add another VE objective). What happened to the fracture models described below? Should those entity boxes be deleted?

Particular (Global) Math Model Entity (PMME) Descriptors

VU Data Descriptors:

** What is the specific thing that this set of particular equations pertains to?

Answer: The simulations of Experiment IAF-432.

Notes: PK- Rod 1 BOL data only?

** Give the equations in this Particular (global) Math Model. Include interior equations, boundary conditions, physical domain, temporal domain, initial conditions.

Answer: Static equilibrium (stress divergence); heat equation.

** Known limitations of the Particular (global) Math Model with respect to its use within this context.

Answer: ?

** The name of the Particular (Global) Math Model Data.

Answer: ?

** Description of the Particular (Global) Math Model Data including its source or pedigree.

Answer: ?

** The Particular (Global) Math Model Data.

Answer: ?

** Known limitations of the Particular (global) Model Data with respect to its use within this context.

Answer: ?

Local Math Model Entity (LMME) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: Fink-Lucuta Temperature-dependent Thermal Conductivity

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 3-8-2012

* The particular name of this entity's parent Particular (global) Math Model Entity.

  Answer: Particular Equations for Fuel Rod Experiment Simulations

* The name of any accessory sub-continuum software entity.

  Answer: None.

Local Math Model Entity (LMME) Descriptors

VU Data Descriptors -I:

** What is the physical phenomena modeled by this LMM?

Answer: Temperature and burnup-dependent thermal conductivity of UO_2

** Description of this Local Math Model (include equations as necessary).

Answer: ?

** Source or Pedigree for this Local Math Model.

Answer: J.K. Fink, *Thermophysical properties of uranium dioxide, J. Nucl. Materials*, 279(1):1-18, 2000.

P.G. Lucuta, H.J. Matzke, I.J. Hastings, *A pragmatic approach to modeling thermal conductivity of irradiated UO_2 fuel: review and recommendations*, J. Nucl. Materials, 232:166-180, 1996.

** Why was this model used instead of another?

Answer: Because we want to validate it.

** Is this Local Math Model to be Validated within this context?

Answer: Yes, in conjunction with one of the two fracture models included in the list of local math models.

* If not, then why not? *Answer:* N/A

** Is the local math model (1) developed from first principles, (2) developed from data, or (3) other?

Answer: ?

** Is the science basis for this model well established? *Answer:* ?

Local Math Model Entity (LMME) Descriptors

VU Data Descriptors -II:

** What are the limits of applicability of this model?

Answer: Temperatures between 500 and 3000 degrees Kelvin.

** Is this model appropriate relative to its intended use in this context?

Answer: Yes

** Is this model based on curve fits to data?

Answer: ?

** How were the curve fits obtained?

Answer: ?

** Why was this model form used instead of another?

Answer: ?

** Has this local model been assessed for accuracy?

Answer: ?

** For this math model, how were the parameters determined: (i) using handbooks, (ii) using expert opinion, (iii) from calibration to available experimental data, (iv) the model is phenomenological and thus the parameters are developed from data, (v) other (explain).

Answer: ?

** The name of this entity's Local Math Model Data.

Answer: ?

** Description of the Local Math Model Data, including source or pedigree.

Answer: ?

** The Local Math Model Data

Answer: ?

Local Math Model Entity (LMME) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: Smeared Fracture Model

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 3-8-2012

* The particular name of this entity's parent Particular (global) Math Model Entity.

  Answer: Particular Equations for Fuel Rod Experiment Simulations

* The name of any accessory sub-continuum software entity.

  Answer: ?

Local Math Model Entity (LMME) Descriptors

VU Data Descriptors -I:

** What is the physical phenomena modeled by this LMM?

Answer: Fracturing of sintered UO_2

** Description of this Local Math Model (include equations as necessary).

Answer: Only radial cracking permitted, based on a constant fracture strength.

** Source or Pedigree for this Local Math Model.

Answer: ?

** Why was this model used instead of another?

Answer: ?

** Is this Local Math Model to be Validated within this context?

Answer: Yes, in conjunction with the Fink-Lucuta Thermal Conductivity Model,

* If not, then why not?

Answer: N/A

** Is the local math model (1) developed from first principles, (2) developed from data, or (3) other?

Answer: ?

** Is the science basis for this model well established?

Answer: ?

** What are the limits of applicability of this model?

Answer: ?

** Is this model appropriate relative to its intended use in this context?

Answer: ?

Local Math Model Entity (LMME) Descriptors

VU Data Descriptors -II:

** Is this model based on curve fits to data?

Answer: No.

** How were the curve fits obtained?

Answer: N/A

** Why was this model form used instead of another?

Answer: ?

** Has this local model been assessed for accuracy?

Answer: ?

** For this math model, how were the parameters determined: (i) using handbooks, (ii) using expert opinion, (iii) from calibration to available experimental data, (iv) the model is phenomenological and thus the parameters are developed from data, (v) other (explain).

Answer: ?

** The name of this entity's Local Math Model Data.

Answer: UO_2 fracture strength.

** Description of this Local Math Model Data, including source or pedigree.

Answer: ?

** The Local Math Model Data

Answer: Fracture strength of 130 MPa.

Local Math Model Entity (LMME) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: ESCORE Fracture Relocation Model

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 3-8-2012

* The particular name of this entity's parent Particular (global) Math Model Entity.

  Answer: Particular Equations for Fuel Rod Experiment Simulations

* The name of any accessory sub-continuum software entity.

  Answer: ?

Local Math Model Entity (LMME) Descriptors

VU Data Descriptors -I:

** What is the physical phenomena modeled by this LMM?

Answer: ?

** Description of this Local Math Model (include equations as necessary).

Answer: ?

** Source or Pedigree for this Local Math Model.

Answer: Y. Rashid, R. Dunham, R. Montgomery, *Fuel analysis and licensing code: FALCON MOD01*, Technical report EPRI 1011308. Electric Power Research Institute. December 2004.

** Why was this model used instead of another?

Answer: ?

** Is this Local Math Model to be Validated within this context?

Answer: Yes, in conjunction with the Fink-Lucuta Thermal Conductivity Model.

* If not, then why not?

Answer: N/A

** Is the local math model (1) developed from first principles, (2) developed from data, or (3) other?

Answer: ?

** Is the science basis for this model well established?

Answer: ?

** What are the limits of applicability of this model?

Answer: ?

** Is this model appropriate relative to its intended use in this context?

Answer: ?

Local Math Model Entity (LMME) Descriptors

VU Data Descriptors -II:

** Is this model based on curve fits to data?

Answer: ?

** How were the curve fits obtained?

Answer: ?

** Why was this model form used instead of another?

Answer: ?

** Has this local model been assessed for accuracy?

Answer: ?

** For this math model, how were the parameters determined: (i) using handbooks, (ii) using expert opinion, (iii) from calibration to available experimental data, (iv) the model is phenomenological and thus the parameters are developed from data, (v) other (explain).

Answer: ?

** The name of this entity's Local Math Model Data.

Answer: ?

** Description of this Local Math Model Data, including source or pedigree.

Answer: ?

** The Local Math Model Data

Answer: ?

Local Math Model Entity (LMME) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: Forsberg-Massih fission gas release model

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 4-6-2012

* The particular name of this entity's parent Particular (global) Math Model Entity.

  Answer: Particular Equations for Fuel Rod Experiment Simulations

* The name of any accessory sub-continuum software entity.

  Answer: ?

Local Math Model Entity (LMME) Descriptors

VU Data Descriptors -I:

** What is the physical phenomena modeled by this LMM?

Answer: ?

** Description of this Local Math Model (include equations as necessary).

Answer: ?

** Source or Pedigree for this Local Math Model.

Answer: ?

** Why was this model used instead of another?

Answer: ?

** Is this Local Math Model to be Validated within this context?

Answer: ?

* If not, then why not? *Answer:* ?

** Is the local math model (1) developed from first principles, (2) developed from data, or (3) other?

Answer: ?

** Is the science basis for this model well established? *Answer:* ?

Local Math Model Entity (LMME) Descriptors

VU Data Descriptors -II:

** What are the limits of applicability of this model?

Answer: ?

** Is this model appropriate relative to its intended use in this context?

Answer: ?

** Is this model based on curve fits to data?

Answer: ?

** How were the curve fits obtained?

Answer: ?

** Why was this model form used instead of another?

Answer: ?

** Has this local model been assessed for accuracy?

Answer: ?

** For this math model, how were the parameters determined: (i) using handbooks, (ii) using expert opinion, (iii) from calibration to available experimental data, (iv) the model is phenomenological and thus the parameters are developed from data, (v) other (explain).

Answer: ?

** The name of this entity's Local Math Model Data.

Answer: ?

** Description of the Local Math Model Data, including source or pedigree.

Answer: ?

** The Local Math Model Data

Answer: ?

Local Math Model Entity (LMME) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: Fill-gas dependent gap conductance

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 4-6-2012

* The particular name of this entity's parent Particular (global) Math Model Entity.

  Answer: Particular Equations for Fuel Rod Experiment Simulations

* The name of any accessory sub-continuum software entity.

  Answer: ?

Local Math Model Entity (LMME) Descriptors

VU Data Descriptors -I:

** What is the physical phenomena modeled by this LMM?

Answer: ?

** Description of this Local Math Model (include equations as necessary).

Answer: ?

** Source or Pedigree for this Local Math Model.

Answer: ?

** Why was this model used instead of another?

Answer: ?

** Is this Local Math Model to be Validated within this context?

Answer: ?

* If not, then why not? *Answer:* ?

** Is the local math model (1) developed from first principles, (2) developed from data, or (3) other?

Answer: ?

** Is the science basis for this model well established? *Answer:* ?

Local Math Model Entity (LMME) Descriptors

VU Data Descriptors -II:

** What are the limits of applicability of this model?

Answer: ?

** Is this model appropriate relative to its intended use in this context?

Answer: ?

** Is this model based on curve fits to data?

Answer: ?

** How were the curve fits obtained?

Answer: ?

** Why was this model form used instead of another?

Answer: ?

** Has this local model been assessed for accuracy?

Answer: ?

** For this math model, how were the parameters determined: (i) using handbooks, (ii) using expert opinion, (iii) from calibration to available experimental data, (iv) the model is phenomenological and thus the parameters are developed from data, (v) other (explain).

Answer: ?

** The name of this entity's Local Math Model Data.

Answer: ?

** Description of the Local Math Model Data, including source or pedigree.

Answer: ?

** The Local Math Model Data

Answer: ?

Local Math Model Entity (LMME) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: Irradiation-induced creep cladding model

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 4-6-2012

* The particular name of this entity's parent Particular (global) Math Model Entity.

  Answer: Particular Equations for Fuel Rod Experiment Simulations

* The name of any accessory sub-continuum software entity.

  Answer: ?

Local Math Model Entity (LMME) Descriptors

VU Data Descriptors -I:

** What is the physical phenomena modeled by this LMM?

Answer: ?

** Description of this Local Math Model (include equations as necessary).

Answer: ?

** Source or Pedigree for this Local Math Model.

Answer: ?

** Why was this model used instead of another?

Answer: ?

** Is this Local Math Model to be Validated within this context?

Answer: ?

* If not, then why not? *Answer:* ?

** Is the local math model (1) developed from first principles, (2) developed from data, or (3) other?

Answer: ?

** Is the science basis for this model well established? *Answer:* ?

Local Math Model Entity (LMME) Descriptors

VU Data Descriptors -II:

** What are the limits of applicability of this model?

Answer: ?

** Is this model appropriate relative to its intended use in this context?

Answer: ?

** Is this model based on curve fits to data?

Answer: ?

** How were the curve fits obtained?

Answer: ?

** Why was this model form used instead of another?

Answer: ?

** Has this local model been assessed for accuracy?

Answer: ?

** For this math model, how were the parameters determined: (i) using handbooks, (ii) using expert opinion, (iii) from calibration to available experimental data, (iv) the model is phenomenological and thus the parameters are developed from data, (v) other (explain).

Answer: ?

** The name of this entity's Local Math Model Data.

Answer: ?

** Description of the Local Math Model Data, including source or pedigree.

Answer: ?

** The Local Math Model Data

Answer: ?

Local Math Model Entity (LMME) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: Irradiation growth cladding model

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 4-6-2012

* The particular name of this entity's parent Particular (global) Math Model Entity.

  Answer: Particular Equations for Fuel Rod Experiment Simulations

* The name of any accessory sub-continuum software entity.

  Answer: ?

Local Math Model Entity (LMME) Descriptors

VU Data Descriptors -I:

** What is the physical phenomena modeled by this LMM?

Answer: ?

** Description of this Local Math Model (include equations as necessary).

Answer: ?

** Source or Pedigree for this Local Math Model.

Answer: ?

** Why was this model used instead of another?

Answer: ?

** Is this Local Math Model to be Validated within this context?

Answer: ?

* If not, then why not? *Answer:* ?

** Is the local math model (1) developed from first principles, (2) developed from data, or (3) other?

Answer: ?

** Is the science basis for this model well established? *Answer:* ?

Local Math Model Entity (LMME) Descriptors

VU Data Descriptors -II:

** What are the limits of applicability of this model?

Answer: ?

** Is this model appropriate relative to its intended use in this context?

Answer: ?

** Is this model based on curve fits to data?

Answer: ?

** How were the curve fits obtained?

Answer: ?

** Why was this model form used instead of another?

Answer: ?

** Has this local model been assessed for accuracy?

Answer: ?

** For this math model, how were the parameters determined: (i) using handbooks, (ii) using expert opinion, (iii) from calibration to available experimental data, (iv) the model is phenomenological and thus the parameters are developed from data, (v) other (explain).

Answer: ?

** The name of this entity's Local Math Model Data.

Answer: ?

** Description of the Local Math Model Data, including source or pedigree.

Answer: ?

** The Local Math Model Data

Answer: ?

Local Math Model Entity (LMME) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: Creep UO_2 model

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 4-6-2012

* The particular name of this entity's parent Particular (global) Math Model Entity.

  Answer: Particular Equations for Fuel Rod Experiment Simulations

* The name of any accessory sub-continuum software entity.

  Answer: ?

Local Math Model Entity (LMME) Descriptors

VU Data Descriptors -I:

** What is the physical phenomena modeled by this LMM?

Answer: ?

** Description of this Local Math Model (include equations as necessary).

Answer: ?

** Source or Pedigree for this Local Math Model.

Answer: ?

** Why was this model used instead of another?

Answer: ?

** Is this Local Math Model to be Validated within this context?

Answer: ?

* If not, then why not? *Answer:* ?

** Is the local math model (1) developed from first principles, (2) developed from data, or (3) other?

Answer: ?

** Is the science basis for this model well established? *Answer:* ?

Local Math Model Entity (LMME) Descriptors

VU Data Descriptors -II:

** What are the limits of applicability of this model?

Answer: ?

** Is this model appropriate relative to its intended use in this context?

Answer: ?

** Is this model based on curve fits to data?

Answer: ?

** How were the curve fits obtained?

Answer: ?

** Why was this model form used instead of another?

Answer: ?

** Has this local model been assessed for accuracy?

Answer: ?

** For this math model, how were the parameters determined: (i) using handbooks, (ii) using expert opinion, (iii) from calibration to available experimental data, (iv) the model is phenomenological and thus the parameters are developed from data, (v) other (explain).

Answer: ?

** The name of this entity's Local Math Model Data.

Answer: ?

** Description of the Local Math Model Data, including source or pedigree.

Answer: ?

** The Local Math Model Data

Answer: ?

CV Entity (CVE) Descriptors[a]

Entity Descriptors:

* The particular name of this entity.

  Answer: Verification of the Particular Math Model Implementation

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 3-9-2012

* The particular name of this entity's concrete parent VU Objective Entity.

  Answer: Validate LWR Fuel Rod Models

* The particular name of this entity's Code Verification Test Suite (CVTS).

  Answer: CVTS for Fuel Rod PMM

* The name of any Comparison Software Entity.

  Answer: ?

[a]The goal in this verification element is to demonstrate that the Particular (global and local) Math Model, as discretized and implemented in software, is solved correctly. The demonstration usually requires a collection of dynamic tests (known here as the CVTS) of the software, in which some or all of the output is compared to a mathematical or computational fiducial.

CV Entity (CVE) Descriptors

VU Data Descriptors

** How well does the Test Suite cover the implementation of the PMM discretization and solution algorithms?

Answer: ?

** Were appropriate verification methods employed in the Test Suite?

Answer: ?

** Were appropriate Acceptance Criteria employed in analyzing the test results?

Answer: ?

** Was the implementation of the PMM discretization and numerical algorithms verified by the Test Suite?

Answer: ?

** List the evidence that supports this claim.

Answer: ?

** Provide a credible claim regarding the results of completing this CV Element.

Answer: ?

** How does the above claim meaningfully contribute to the claims made within the other VU elements under the concrete VU Objective?

Answer: ?

Code Verification Test Suite Entity (CVTSE) Descriptors[a]

Entity Descriptors:

* The particular name of this entity.

  Answer: CVTS for Fuel Rod PMM

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 3-9-2012

* The particular name of this entity's concrete parent VU Element Entity.

  Answer: Verification of the PMM Implementation

* The particular names of this entity's concrete child Simulation Practice Entities.

  Answer: Pre-Design, Test Suite Design, Verify I/O, Test Results Analysis, Conclusions

[a] A CVTS is not the same as an RTS (Regression Test Suite). Many codes have a regression test suite that is run regularly (e.g. nightly) to ensure that all tests in the suite produce the same results as with the previous instance of the code. Regression test suites tend to be very broad in that they test many things, among them, that important demonstrations of code capability continue to work. In contrast, the tests pertaining to a CVTS are focused more narrowly because they primarily test the parts of the code which are involved in solving the PMM correctly. In addition, the CVTS contains documentation which explains the purpose of the test, relates the parts of the code that are tested to the PMM, gives the derivation of the fiducial, and explains the results of the test and how they demonstrate that the PMM is correctly solved. Every test in the CVTS should be placed within the RTS once it is passed.

Code Verification Test Suite Entity (CVTSE) Descriptors

VU Data Descriptors

** The computer which ran these simulations.

Answer: ?

** Name and version of the simulation software.

Answer: ?

** Location of this simulation ensemble in the Repository.

Answer: ?

** The name(s) of the input files in this ensemble.

Answer: ?

** The name(s) of the corresponding raw output files.

Answer: ?

** The names of the corresponding post-processed output files.

Answer: ?

Pre-Simulation Design Entity (PSDE) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: CV Test Suite Pre-Design Activities

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 3-9-2012

* The particular name of this entity's concrete parent Simulation Ensemble Entity

  Answer: CVTS for Fuel Rod PMM

* Name of Accessory Comparison Software Entities, if any.

  Answer: ?

VU Data Descriptors

** Check the method(s) of Code Verification that will be employed in the test suite:

  - Code-to-code comparison
  - Comparison to another numerical solution
  - Comparison to an exact solution on a single mesh
  - Comparison to an exact solution on multiple meshes (confirm convergence)
  - Order-verification (confirm theoretical rate-of-convergence)
  - Other

** Provide a justification for the choice(s) of methods made.

  Answer: ?

Simulation Ensemble Design Entity (SEDE) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: Code Verification Test Suite Design

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 3-9-2012

* The particular name of this entity's concrete parent Simulation Ensemble Entity

  Answer: CVTS for Fuel Rod PMM

Simulation Ensemble Design Entity (SEDE) Descriptors

VU Data Descriptors-I

** List of the Tests in this Test Suite

Answer: ?

** For each test, identify the part(s) of the PMM that it tests in terms of the following:

- Term(s) in the interior equations.
- Coefficients in the interior equations
- Boundary Condition
- Initial Condition
- A Coupling Term
- A Local Math Model
- Numerical Algorithm
- Solution Functionals

** For each item, state which terms, which coefficients, which boundary conditions, etc., are tested.

Answer: ?

** For each test, state the method of verification, the fiducial, and the acceptance criterion, and give its derivation or justification.

Answer: ?

** For each test, state (in terms of code options) the numerical algorithm to be used/tested. This includes the linear solver, mesh and element type, numerical damping terms, etc.

Answer: ?

** For each test, how does it help establish the correctness of the implementation?

Answer: ?

Simulation Ensemble Design Entity (SEDE) Descriptors

VU Data Descriptors-II

** List any parts of the PMM that are not tested by these tests.

Answer: ?

** Does the collection of tests cover all of the dependent variables in the PMM?

Answer: ?

** Does the collection of tests cover all of the associated solution functionals?

Answer: ?

** Provide a Test Suite Design Document, if any.

Answer: ?

Simulation I/O Data Entity (SIOE) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: CV - Verify I/O

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 3-9-2012

* The particular name of this entity's concrete parent Simulation Ensemble Entity

  Answer: CVTS for Fuel Rod PMM

* Name of Post-Pocssing Software Entity, if any

  Answer: ?

Simulation I/O Data Entity (SIOE) Descriptors

VU Data Descriptors

** The data in the input files was verified by:

  - The person(s) who created the file,
  - A team peer,
  - Someone external to the team,
  - Other (describe)

** The data in the input files was verified by:

  - Visual inspection,
  - Independent reproduction,
  - Other (describe)

Simulation Ensemble Analysis Entity (SEAE) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: Code Verification Test Results Analysis

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 3-9-2012

* The particular name of this entity's concrete parent Simulation Ensemble Entity

  Answer: CVTS for Fuel Rod PMM

VU Data Descriptors

** Note any changes to the Test Suite Design (the fiducial, acceptance criterion, etc.) that were made after the design was completed.

  Answer: ?

** For each test (or group of tests), show a comparison between the simulation output and the fiducial.

  Answer: ?

** For each test, is the acceptance criterion met?

  Answer: ?

** For each test, was the acceptance criterion reasonable?

  Answer: ?

** Provide a Verification Test Results Document, if any.

  Answer: ?

Post-Simulation Ensemble Analysis Entity (PSAE) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: Code Verification Conclusions

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 3-9-2012

* The particular name of this entity's concrete parent Simulation Ensemble Entity

  Answer: CVTS for Fuel Rod PMM

Post-Simulation Ensemble Analysis Entity (PSAE) Descriptors

VU Data Descriptors

** Were any coding mistakes or algorithmic deficiencies discovered during the course of this verification? If so, describe the mistakes and what was done to correct them.

Answer: ?

** Have the tests in the CVTS that were passed (i.e., met their acceptance criterion) been added to the Regression Test Suite?

Answer: ?

** Check the following PMM items if their implementation was verified by one or more of the tests in the CVTS:

1. Term(s) in the interior equations.
2. Coefficients in the interior equations
3. Boundary Conditions
4. Initial Condition
5. A Coupling Term
6. A Local Math Model
7. Numerical Algorithm
8. Solution Functionals

** Identify any parts of the PMM which are not completely verified in terms of correctness.

Answer: ?

SV Entity (SVE) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: Verify Experiment Simulations

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: ?

* The date this entity was created or last updated.

  Answer: 3-14-12

* The particular name of this entity's concrete parent VU Objective Entity

  Answer: Validate Fuel Rod Model

* The particular name(s) of this entity's concrete child Simulation Ensemble Entities

  Answer: Simulation of Fuel Rod Experiments (IFA-432).

SV Entity (SVE) Descriptors

VU Data Descriptors

** Was the software verified with respect to the PMM before the calculations under this Element were performed?

Answer: ?

** How well were the numerical solutions to the experiment simulations verified? Explain.

Answer: ?

** Were appropriate solution verification methods employed? Explain.

Answer: ?

** How well was the experiment setup captured in the simulations? Explain.

Answer: ?

** Is the particular math model solved in the experiment simulations the same as that described by the PMM entity? Explain.

Answer: ?

** Provide a credible claim regarding the results of completing this SV Element.

Answer: ?

** How does the above claim meaningfully contribute to the claims made within the other VU elements under the concrete VU Objective?

Answer: ?

Physical Experiment Simulation Entity (PESE) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: Simulation of Fuel Rod Experiments (IFA-432)

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: ?

* The date this entity was created or last updated.

  Answer: 3-14-2012

* The particular name of this entity's concrete parent VU Element Entity

  Answer: Verify Experiment Simulations

* The particular names of this entity's concrete child Simulation Practice Entities

  Answer: Experiment Simulation/SV Pre-Design Activities; Experiment Simulation Design with Solution Verification; Verify Experiment Simulation I/O; Experiment Simulation/Solution Verification Results Analysis; Solution Verification Conclusions

Physical Experiment Simulation Entity (PESE) Descriptors

VU Data Descriptors

** The computer which ran these simulations.

Answer: ?

** Name and version of the simulation software.

Answer: ?

** Location of this simulation ensemble in the Repository.

Answer: ?

** The name(s) of the input files in this ensemble.

Answer: ?

** The name(s) of the corresponding raw output files.

Answer: ?

** The names of the corresponding post-processed output files.

Answer: ?

Pre-Simulation Design Entity (PSDE) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: Experiment Simulation/SV Pre-Design Activities

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 3-14-2012

* The particular name of this entity's concrete parent Simulation Ensemble Entity

  Answer: Simulate Fuel Rod Experiments (IFA-432)

Pre-Simulation Design Entity (PSDE) Descriptors

VU Data Descriptors

** What are the specific aspects of the PMM that you are most interested in validating?

Answer: (1) Fink-Lucuta with Smeared Fracture Model and (2) Fink-Lucuta with ESCORE Fracture Model

** Aside from the above, how well does the PMM reflect the physical conditions of the experiment set up with regard to

- Domain Geometry
- the Boundary Conditions
- the Initial Conditions
- Other

** Check the practices within Solution Verification that will be employed in this simulation ensemble:

- None
- Mesh Refinement to Establish if in Asymptotic Regime
- Time-step refinement to Establish if in Asymptotic Regime
- Solution-adaptive mesh
- Sensitivity of Solution to Numerical Parameter Input
- Error Estimation
- Error Bar Estimation
- Other

** For each practice marked above, identify the particular method within the practice that will be employed. (e.g., error estimation - ZZ on the pressure).

Answer: ?

** Provide a justification for the choice(s) of methods made and not made.

Answer: ?

Simulation Ensemble Design Entity (SEDE) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: Experiment Simulation Design with Solution Verification

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: ?

* The date this entity was created or last updated.

  Answer: 3-14-2012

* The particular name of this entity's concrete parent Simulation Ensemble Entity

  Answer: Simulate Fuel Rod Experiments (IFA-432)

Simulation Ensemble Design Entity (SEDE) Descriptors

VU Data Descriptors

** List the simulation output quantities of interest.

Answer: ?

** The simulation output quantities of interest will be compared to the physical measurements by

- direct comparison
- post-processing the simulation output quantities
- post-processing the physical measurements
- post-processing both

** Explain your answer to the previous.

Answer: ?

** What will be the physical input parameters to the simulations?

Answer: ?

** For each physical parameter, explain how its value was or will be determined.

Answer: ?

** Describe the options that will be used with respect to the numerical solution algorithm (e.g., linear solver option, mesh and element type, numerical damping terms, etc.).

Answer: ?

** Will the solution verification methods identified in the PSDE be applied to (1) each of the experiment simulations, (2) only to some, or (3) only to one.

Answer: ?

** How will the solution verification methods be incorporated into the experiment simulation design?

Answer: ?

** Provide a Experiment Simulation Design Document, if any.

Answer: ?

Simulation I/O Data Entity (SIOE) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: Verify Experiment Simulation I/O

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: ?

* The date this entity was created or last updated.

  Answer: 3-14-2012

* The particular name of this entity's concrete parent Simulation Ensemble Entity

  Answer: Simulate Fuel Rod Experiments (IFA-432)

* Name of Post-Processing Software Entity, if any

  Answer: ?

Simulation I/O Data Entity (SIOE) Descriptors

VU Data Descriptors

** The data in the input files was verified by:

- The person(s) who created the file,
- A team peer,
- Someone external to the team,
- Other (describe)

** The data in the input files was verified by:

- Visual inspection,
- Independent reproduction,
- Other (describe)

** The data in the output files was verified by:

- The person(s) who created the file,
- A team peer,
- Someone external to the team,
- Other (describe)

** The data in the output files was verified by:

- Visual inspection of plotted results,
- Other (describe)

Simulation Ensemble Analysis Entity (SEAE) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: Experiment Simulation/Solution Verification Results Analysis

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 3-14-2012

* The particular name of this entity's concrete parent Simulation Ensemble Entity

  Answer: Simulate Fuel Rod Experiments (IFA-432)

Simulation Ensemble Analysis Entity (SEAE) Descriptors

VU Data Descriptors

** Note any changes to the Experiment Simulation Design that were made after the design was completed.

Answer: ?

** If mesh refinement studies were performed, show and/or quantify the sensitivity of the solution to the mesh size.

Answer: ?

** If time-step refinement studies were performed, show and/or quantify the sensitivity of the solution to the time-step size.

Answer: ?

** Show and/or quantify the sensitivity of the solution to numerical algorithm tolerances.

Answer: ?

** If error estimation techniques were employed, show and/or quantify the error in the simulation output quantities of interest.

Answer: ?

** If error bar calculations were performed, show and/or quantify the error bars in the simulation output quantities of interest.

Answer: ?

** If solution adaptive meshes were used, show the adapted meshes and solutions.

Answer: ?

** Provide a Experiment Simulation/Solution Verification Results Document, if any.

Answer: ?

Post-Simulation Ensemble Analysis Entity (PSAE) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: Solution Verification Conclusions

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 3-14-2012

* The particular name of this entity's concrete parent Simulation Ensemble Entity

  Answer: Simulate Fuel Rod Experiments (IFA-432)

Post-Simulation Ensemble Analysis Entity (PSAE) Descriptors

VU Data Descriptors

** Do the computed numerical solutions appear to be in the asymptotic range for both space and time? Explain.

Answer: ?

** Was an appropriate value for the numerical tolerances and termination criteria determined? Explain.

Answer: ?

** If the mesh was adapted, what is the evidence that the adaptation was effective?

Answer: ?

** If the error was estimated, what was the maximum relative and absolute error? For what output quantities was the error estimated?

Answer: ?

** If error bars were calculated, what conclusion can you draw from them? Explain.

Answer: ?

MMV Entity (MMVE) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: LWR Fuel Rod Model Validation Comparison

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 3-20-2012

* The particular name of this entity's concrete parent VE Objective Entity

  Answer: Validate Fuel Rod Model

* The particular name(s) of this entity's concrete child Simulation Ensemble Entities

  Answer: ?

MMV Entity (MMVE) Descriptors

VU Data Descriptors - I

** What are the quantities of interest that will be compared between the experiment and the simulations?

Answer: ?

** How will the comparison between the experiment data and simulation output be conducted in the face of uncertainties in both?

- by plotting the simulation output and experimental data on the same plot,
- by comparing the amount of error between experimental and simulation data,
- by doing probabilstic comparisons,
- by performing statistical tests of hypotheses,
- other (describe).

** What validation metrics will be used?

Answer: ?

** In terms of appropriateness, justify the decision to use these metrics as opposed to other possibilities.

Answer: ?

** Has a criterion, based on the chosen validation metric, been established to assess whether the model is valid or not? If so, what is it?

Answer: ?

MMV Entity (MMVE) Descriptors

VU Data Descriptors - II

** Was the previous criterion satisfied in the comparisons?

Answer: ?

** Was the numerical solution verified prior to making the comparison to experiment?

Answer: ?

** Was model accuracy assessed?

Answer: ?

** Having performed this validation exercise, state the range of physical input parameters for which you believe it is valid to use this model.

Answer: ?

** What limitations of the model were identified as a result of this validation?

Answer:

** Provide a document showing and discussing these comparisons.

Answer: ?

** Provide a credible claim regarding the results of completing this MMV Element.

Answer: ?

UQ Entity (UQE) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: Characterize, Propagate, and Quantify Uncertainty in the Experiment Simulations

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 4-6-2012

* The particular name of this entity's concrete parent VU Objective Entity

  Answer: Validate LWR Fuel Rod Model Validation Comparison

* The particular name(s) of this entity's concrete child Simulation Ensemble Entities

  Answer: Characterize and Propagate Uncertainties through the Experiment Simulations for the purpose of Validation Comparison

UQ Entity (UQE) Descriptors

VU Data Descriptors

** Has a framework been established to characterize, incorporate, propagate, and quantify sources of aleatoric and epistemic uncertainty with respect to this Validation comparison?

Answer:

** If yes, then please describe.

Answer:

** How was the uncertainty in the simulation input characterized?

Answer:

** Was a sensitivity analysis performed in order to establish the sensitivity of the prediction to the input parameters in the experiment simulation?

Answer:

** How was the uncertainty in the input propagated?

Answer:

** How was the uncertainty in the prediction quantified?

Answer:

** Provide a credible claim regarding the results of completing this Element.

Answer: ?

Uncertainty Characterization and Propagation Ensemble Entity (UCPE) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: Characterize and Propagate Uncertainties through the Experiment Simulations for the purpose of Validation Comparison

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: ?

* The date this entity was created or last updated.

  Answer: 4-4-2012

* The particular name of this entity's concrete parent VU Element Entity

  Answer: LWR Fuel Rod Model Validation Comparison

* The particular names of this entity's concrete child Simulation Practice Entities

  Answer: UCP Pre-Design Activities; UCP Simulation Design; Verify UCP Simulation I/O; UCP Simulation Results Analysis; UCP Simulation Conclusions

Uncertainty Characterization and Propagation Ensemble Entity (UCPE) Descriptors

VU Data Descriptors

** The computer which ran these simulations.

Answer: ?

** Name and version of the simulation software.

Answer: ?

** Location of this simulation ensemble in the Repository.

Answer: ?

** The name(s) of the input files in this ensemble.

Answer: ?

** The name(s) of the corresponding raw output files.

Answer: ?

** The names of the corresponding post-processed output files.

Answer: ?

**

**

Pre-Simulation Design Entity (PSDE) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: UCP Pre-Design Activities

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 4-6-2012

* The particular name of this entity's concrete parent Simulation Ensemble Entity

  Answer: Characterize and Propagate Uncertainties through the Experiment Simulations for the purpose of Validation Comparison

Pre-Simulation Design Entity (PSDE) Descriptors

VU Data Descriptors

**

Simulation Ensemble Design Entity (SEDE) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: UCP Simulation Design

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: ?

* The date this entity was created or last updated.

  Answer: 4-6-2012

* The particular name of this entity's concrete parent Simulation Ensemble Entity

  Answer: Characterize and Propagate Uncertainties through the Experiment Simulations for the purpose of Validation Comparison

Simulation Ensemble Design Entity (SEDE) Descriptors

VU Data Descriptors

**

Simulation I/O Data Entity (SIOE) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: Verify UCP Simulation I/O

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: ?

* The date this entity was created or last updated.

  Answer: 4-6-2012

* The particular name of this entity's concrete parent Simulation Ensemble Entity

  Answer: Characterize and Propagate Uncertainties through the Experiment Simulations for the purpose of Validation Comparison

* Name of Post-Processing Software Entity, if any

  Answer: ?

Simulation I/O Data Entity (SIOE) Descriptors

VU Data Descriptors

** The data in the input files was verified by:

- The person(s) who created the file,
- A team peer,
- Someone external to the team,
- Other (describe)

** The data in the input files was verified by:

- Visual inspection,
- Independent reproduction,
- Other (describe)

** The data in the output files was verified by:

- The person(s) who created the file,
- A team peer,
- Someone external to the team,
- Other (describe)

** The data in the output files was verified by:

- Visual inspection of plotted results,
- Other (describe)

Simulation Ensemble Analysis Entity (SEAE) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: UCP Simulation Results Analysis

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 4-6-2012

* The particular name of this entity's concrete parent Simulation Ensemble Entity

  Answer: Characterize and Propagate Uncertainties through the Experiment Simulations for the purpose of Validation Comparison

Simulation Ensemble Analysis Entity (SEAE) Descriptors

VU Data Descriptors

**

Post-Simulation Ensemble Analysis Entity (PSAE) Descriptors

Entity Descriptors:

* The particular name of this entity.

  Answer: UCP Simulation Conclusions

* The version number of this entity.

  Answer: 1.0

* The location of this entity within the Repository.

  Answer: N/A

* The date this entity was created or last updated.

  Answer: 4-6-2012

* The particular name of this entity's concrete parent Simulation Ensemble Entity

  Answer: Characterize and Propagate Uncertainties through the Experiment Simulations for the purpose of Validation Comparison

Post-Simulation Ensemble Analysis Entity (PSAE) Descriptors

VU Data Descriptors

**

DISTRIBUTION:

	MS	,
		,
1	MS 0899	Technical Library, 9536 (electronic copy)

Sandia National Laboratories