NUCLEAR ENERGY ADVANCED MODELING AND SIMULATION (NEAMS)

Software Verification and Validation Plan Requirements
Version 0

NEAMS
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

U.S. DEPARTMENT OF ENERGY
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Prepared by: Date 7/25/2013

Robert M. Versluis

NEAMS Program Quality Representative

Concurred by: Date 7/25/2013

Darrell Huff

NE QA Manager

Approved by: Date 7/31/2013

Trevor L. Cook

Acting Director, Advanced Modeling and Simulation

Office of Nuclear Energy

Approved by: Date 8/20/2013

R. Shane Johnson

DAS, Science and Technology Innovation

Office of Nuclear Energy

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Revision History

REV.	EFFECTIVE DATE	REVISION DESCRIPTION
0	Date of Approval on Page 1	Initial issuance by the Office of Advanced Modeling and Simulation, NE-41

List of Acronyms

AIAA	American Institute of Aeronautics and Astronautics
ANSI	American National Standard Institute
ASME	American Society of Mechanical Engineers
DoD	Department of Defense
DOE	U.S. Department of Energy
FCRD	Fuel Cycle Research and Development
FCT	Fuel Cycle Technology
NEAMS	Nuclear Energy Advanced Modeling and Simulation
HQ	Headquarters
NE	DOE Office of Nuclear Energy
NEPA	National Environmental Policy Act
NEUP	Nuclear Energy Universities Program
NQA-1	ASME Document, Quality Assurance Requirements for Nuclear Facility Applications
NRC	Nuclear Regulatory Commission
NTD	National Technical Director
PDE	Partial Differential Equation
QA	Quality Assurance
QAP	Quality Assurance Program
QAPD	Quality Assurance Program Document
QRL	Quality Rigor Level
R&D	Research and Development

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1. INTRODUCTION

1.1 NEAMS

Since the appearance of digital computers in the middle of the 20th century, scientific computing has changed the way technology is developed. Where once a research and development (R&D) team was limited by what could be observed or tested in a laboratory, today that same team can gain insight about performance, safety, and reliability of systems by studying them in a "virtual test environment" provided by modern scientific computing.

The Office of Nuclear Energy's Nuclear Energy Advanced Modeling and Simulation (NEAMS) program produces new modeling and simulation capabilities to be used by researchers, designers, and analysts. It does not do the modeling and simulation for them, but rather it provides them with improved and advanced tools to conduct more powerful modeling and simulation activities. These advanced capabilities are delivered in the form of the ***NEAMS ToolKit***, which:

- comprises a suite of computational modules that rely on fundamental, mechanistic descriptions of the laws of physics governing the performance and safety of reactor systems and their associated fuels.
- is contained within a framework that enables tight and full coupling when required, to afford the ability to predict the outcome of complex, often competing phenomena in operating reactor systems.

NEAMS tools are beginning to take hold in NE's programs, academia, industry, and the international community. Within the NE R&D programs alone, nearly every mission can benefit from the application of NEAMS tools including: increasing power plant efficiency, enhancing nuclear safety, reducing capital costs of new reactors, developing new classes of reactors, and closing the fuel cycle.

1.2 End-Use of Computational Models

A collection of NEAMS ToolKit modules capable of simulating the behavior of a phenomenon or system will be referred to as a "***computational model***." Computational models may be used for different purposes such as scoping analysis, design, and safety analysis. Each purpose has an outcome that dictates the level of verification and validation (V&V) that is appropriate. Necessarily, there is a relation between end use and software quality standards that apply to the computational model. This document addresses categories of end-uses using the same three Quality Rigor Levels (QRLs) introduced by the NE Fuel Cycle Technology (FCT) QAPD[1] and defines the V&V requirements for each QRL.

1.3 Purpose

The purpose of the NEAMS Software V&V Plan is to define what the NEAMS program expects in terms of V&V for the computational models that are developed under NEAMS auspices, recognizing that the NEAMS software developers are subject to the requirements of the QA and SQA Plans of their institution and any additional QA requirements imposed by the NE organization, such as the NE QAP and the FCT QAPD.

2. VERIFICATION AND VALIDATION

The NEAMS program has adopted a definition of V&V for modeling and simulation that follows closely the definitions used by the Department of Defense (DoD)[2], the American Institute of Aeronautics and Astronautics (AIAA)[3] and the American Society of Mechanical Engineers (ASME)[4].

Verification: The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model.
Validation: The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.

To give more meaning to these definitions, the NEAMS program borrows from the language and concepts used by the authors of the Predictive Capability Maturity Model (PCMM)[5], which is a structured method for assessing the level of maturity of modeling and simulation software. The six modeling and simulation elements used to assess maturity in this model are (1) representation and geometric fidelity, (2) physics and material model fidelity, (3) code verification, (4) solution verification, (5) model validation, and (6) uncertainty quantification and sensitivity analysis. These six elements are important in judging the trustworthiness and credibility of a modeling and simulation effort that deals primarily with the numerical solution of PDEs describing the engineering system of interest.

2.1 Representation and geometric fidelity

Representation and geometric fidelity is directed toward the level of detailed characterization of the system being analyzed or specification of the geometrical features of that system.

2.2 Physics and material model fidelity

Physics and material model fidelity deals primarily with (1) the degree to which models are physics based, (2) the degree to which the models are calibrated, (3) the degree to which the models are being extrapolated from the validation and calibration database to the conditions of the application of interest, and (4) the quality and degree of coupling of multiphysics effects that exist in the application of interest.

2.3 Code verification

Code verification focuses on (1) correctness and fidelity of the numerical algorithms used in the code relative to the mathematical model (the PDE model); (2) correctness of the source code; and (3) configuration management, control, and testing of software through software quality engineering practices.

2.4 Solution verification

Solution verification deals with (1) assessment of numerical solution errors in the computed results and (2) assessment of confidence in the computational results as the results may be affected by human errors.

2.5 Model validation

Model validation concentrates on (1) thoroughness and precision of the accuracy assessment of the computational results relative to the experimental measurements; (2) completeness and precision of the characterization of the experimental conditions and measurements; and (3) relevancy of the experimental conditions, physical hardware, and measurements in the validation experiments compared to the application of interest.

2.6 Uncertainty quantification and sensitivity analysis

Uncertainty quantification and sensitivity analysis focuses on (1) thoroughness and soundness of the uncertainty quantification effort, including the identification and characterization of all plausible sources of uncertainty; (2) accuracy and correctness of propagating uncertainties through a computational model and interpreting uncertainties in the system response quantities of interest; and (3) thoroughness and precision of a sensitivity analysis to determine the most important contributors to uncertainty in system responses.

3. QUALITY RIGOR LEVELS AND ASSOCIATED V&V REQUIREMENTS

The FCT QAPD states the QA requirements applicable work conducted under the auspices of the FCT organization. These same FCT QAPD requirements are adopted for work conducted under the auspices of NEAMS program. They are additional requirements, which apply to software development activities carried out under NEAMS auspices, and they do not replace the laboratory's own QA program.

The FCT QAPD requirements are specified at three Quality Rigor Levels (QRLs) based on the intended or potential end use of the results of the work being performed. This section describes how the QRLs are used to define V&V requirements for NEAMS-developed software at different levels of end use.

3.1 Quality Rigor Level 1 V&V Requirements

Quality Rigor Level 1 is generally applied to those computational models which support nuclear energy system design and licensing activities under NRC regulations for potential future facilities. The following table provides examples of these activities and identifies the corresponding V&V requirements.

NOTE: The NEAMS program will assign lead responsibility for conducting QRL-1 activities only to laboratories having an established NQA-1-2000 (or later version) program. Other laboratories supporting such work are not required to have in place or establish an NQA-1-compliant program in order to meet the requirements of this document.

Table 1: Quality Rigor Level 1 V&V Requirements

Quality Rigor Level 1	
Examples of Types of Activities	**Quality Rigor Level 1 Requirements**
System Design and Development: Computational models are used to support design and testing of reactor systems, sub-systems, and components; safety analyses and definition of operational and safety limits; optimization of performance within safety limits; severe accidents. **Licensing**: Computational models are used to support licensing; simulation support to confirmatory experiments. **Consequences of Failure:** Suboptimal design from economic and/or safety perspective; excessive safety and operational margins; energy cost penalties; accidents and plant damage; accidents and public at risk	**Computational Model Verification** Daily regression testing; automated error tracking; configuration management including documentation. **Computational Model Validation** Complete-system validation; sensitivity studies, uncertainty quantification. **Documentation** For each computational model, provide an annually updated V&V Plan that describes how regression testing, error tracking, and configuration management are implemented; and that defines a detailed validation matrix that addresses • available data collections with their quality pedigree; • applicable and available benchmarks; • data gaps; Indicate desirable experimental campaigns that would provide the needed data collections. Discuss uncertainty quantification and model calibration with respect to quantities of interest.

3.2 Quality Rigor Level 2 V&V Requirements

Quality Rigor Level 2 is generally applied to research and development activities which need a higher level of confidence in the results relative to that required for Quality Rigor Level 3 activities. The computational models support activities such as viability R&D and performance R&D of advanced reactor concepts. Quality Rigor Level 2 is also applied to activities that provide direct input to program decisions and are either more controversial or would receive wide distribution outside the NEAMS or represent such a high level of resource investment that, in the judgment of those making the Quality Rigor Level Designation, the work should be designated at a higher Quality Rigor Level.

The following table provides examples of these activities and identifies the corresponding quality assurance requirements.

Table 2: Quality Rigor Level 2 V&V Requirements

Quality Rigor Level 2	
Examples of Types of Activities	**Quality Rigor Level 2 Requirements**
Concept Viability R&D: Computational models are used to support system concepts, perform scoping studies, trade studies, etc; Computational models are used to support experimentalist in designing and conducting fuels, materials, and flow tests to demonstrate viability of concept and subsystems. **Consequences of Failure:** Prepare samples that fail; miss potentially successful samples; flawed test campaign; unsafe test equipment, accidents in the laboratory. **Concept Performance R&D:** Computational models are used to support system concept designer to perform studies to optimize design; support experimentalist to design and conduct confirmatory tests of subsystems and concept. **Consequences of Failure:** Design suboptimal components; miss potentially successful designs; flawed test campaign; unsafe test equipment; accidents in the laboratory or test facility.	**Computational Model Verification** Regular regression testing; error tracking; configuration management including documentation. **Computational Model Validation** Benchmark validation; subsystem validation; sensitivity studies. **Documentation** For each computational model, provide an annually updated V&V Plan that describes how regression testing, error tracking, and configuration management are implemented; and that defines a preliminary validation matrix that addresses • available data collections with their quality pedigree; • applicable and available benchmarks; • data gaps; Indicate desirable experimental campaigns that would provide the needed data collections. Discuss uncertainty quantification and model calibration with respect to quantities of interest.

3.3 Quality Rigor Level 3 V&V Requirements

Quality Rigor Level 3 is generally applied to research and development activities that are exploratory, preliminary, or investigative in nature. The following table provides examples of these activities and identifies the corresponding V&V requirements.

Table 3: Quality Rigor Level 3 V&V Requirements

Quality Rigor Level 3	
Examples of Types of Activities	**Quality Rigor Level 3 Requirements**
Software architecture development Development of computational infrastructure and methods **Consequences of Failure:** Cannot simulate physics on the scale and fidelity desired.	**Computational Model Verification**: Regular regression testing; error tracking; configuration management including documentation. **Computational Model Validation**: Unit test validation; sensitivity studies.
Basic research Research and modeling of phenomena. Design and conduct of experiments to measure unit problems, benchmarking. **Consequences of Failure:** Converges to wrong solution, wrong physics predictions.	Conduct technical review of work products.

4. DEFINITIONS

Activity: A planned effort that spans duration of time in order to accomplish a specific scope of work or milestone/deliverable.

Assessment: An observation or monitoring to provide confidence that ongoing activities are adequately and effectively performed. Often used interchangeably with surveillance or review.

Audit: A planned and documented activity performed to determine by investigation, examination, or evaluation of objective evidence, the adequacy of and compliance with established procedures, instructions, drawings, and other applicable documents, and the effectiveness of implementation.

Deliverable: A document or product identified in a work package with a due date and work scope.

Milestone: A document, product or deliverable identified in a work package with a due date and work scope.

Participant: Any individual or organization performing work for the NEAMS Program.

Review: An observation or monitoring to provide confidence that ongoing activities are adequately and effectively performed. Often used interchangeably with surveillance or assessment.

Surveillance: An assessment technique that uses observation or monitoring to provide confidence that ongoing activities are adequately and effectively performed. Often used interchangeably with review or assessment.

Technical Review: A review to verify compliance to work package requirements, and technical adequacy of the work. Additionally, a review performed in accordance with the requirements specified in FCT QAPD Appendix B.

For other definitions refer to the latest version of DOE Order 414.1 "Quality Assurance" and NQA-1-2000 (or later version) "Quality Assurance Requirements for Nuclear Facility Applications.

5. REFERENCES

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[1] Fuel Cycle Technologies Quality Assurance Program Document, Rev 2, 2010

[2] DoD Instruction 5000.61: Modeling and Simulation (M&S) Verification, Validation, and Accreditation (VV&A). 1996, Defense Modeling and Simulation Office,Office of the Director of Defense Research and Engineering.

[3] AIAA: Guide for the Verification and Validation of Computational Fluid Dynamics Simulations. 1998, American Institute of Aeronautics and Astronautics, AIAA-G-077,1998.

[4] ASME: Guide for Verification and Validation in Computational Solid Mechanics. 2006, American Society of Mechanical Engineers, ASME V&V 10-2006.

[5] PCMM: W.L. Oberkampf, M. Pilch, and T.G. Trucano. (2007) Predictive Capability Maturity Model for Computational Modeling and Simulation. SAND2007-5948. Albuquerque, NM: Sandia National Laboratories.