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Vision Document for the AMP Nuclear Fuel Performance Code

February 2011

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1 INTRODUCTION

The Advanced Modeling and Simulation Office (AMSO) with the United States (U.S.) Department of Energy (DOE) Office of Nuclear Energy (DOE/NE) oversees the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program and the Consortium for Advanced LWR Simulation (CASL), an Energy Innovation Hub. NEAMS is a program to develop advanced modeling and simulation capabilities for state-of-the-art and next generation nuclear energy applications and is composed of four Integrated Performance and Safety Code (IPSC) elements and four Cross-Cutting elements.

The vision for the Fuels IPSC is to deliver an assessed (verified and validated) simulation capability to the fuel design and research community that is capable of predicting the behavior of nuclear fuel, cladding, and structural materials during nominal operation and anticipated operational transients that are beyond the well validated empirical basis that has historically required many integral experiments and operational experience for even moderate changes to fuel designs. Within the Fuels IPSC, the AMP(Advanced MultiPhysics) Nuclear Fuel Performance code (AMP) is targeted for the design and evaluation of Integral Effects Experiments, prediction and evaluation of in-reactor operation, and sensitivity/uncertainty evaluations that will be used to guide the development of lower-length-scale (LLS) research [1]. There is also substantial work in progress to understand the lower-length-scale physics (grain-scale and below) of nuclear fuel, cladding, and structural materials within the Fuels IPSC, as well as the Fundamental Methods and Models (FMM) Cross-Cutting program element.

2 POSITIONING

2.1 Problem Statement

The lack of a modern engineering-scale nuclear fuel performance and safety code affects:

- the nuclear fuel research community,
  - because there is no vehicle for efficiently evaluating the performance and safety benefits of novel designs and materials,
- the nuclear fuel industry,
  - by constraining their ability to understand, and correct, the primary phenomena that lead to fuel failures, which has a significant financial impact,
- the lower-length-scale (LLS) simulation researchers,
  - because there is no vehicle for efficiently evaluating the affects of their innovations on the integral performance and safety of the fuel, and
- the LLS research program managers,

– because there is no consistent means, for a wide variety of fuel/reactor configurations, of evaluating the sensitivity of integral fuel performance to individual fundamental (separate) effects, which is needed to effectively utilize limited resources.

A successful solution would be the development of an assessed (verified and validated), easy-to-use, multi-dimensional, parallel, extensible fuel performance and safety code, at the continuum- and (limited) grain- scales, that is general enough to model a tremendous variety of fuel/reactor configurations with a simple mechanism for incorporating additional material models and a comprehensive approach to sensitivity analysis that incorporates all forms of uncertainties.

2.2 Product Position Statement

The AMP Nuclear Fuel Performance code is clearly described as unique with the position statement in Table 1.

Table 1: Position Statement

The AMP Nuclear Fuel Performance code	will be an assessed (verified and validated), easy-to-use, multi-dimensional, parallel, extensible fuel performance and safety code, at the continuum- and (limited) grain-scales,
That is	general enough to model a tremendous variety of fuel/reactor configurations with a simple mechanism for incorporating additional material models and a comprehensive approach to sensitivity analysis that incorporates all forms of uncertainties
Which is unlike	legacy fuel performance codes, such as FRAPCON, FALCON, and LIFE,
Because AMP	will be independent of any specific reactor/fuel type, will model three-dimensional physics with substantially less engineering-scale simplifications, will be capable of leveraging high-performance computing hardware, and will incorporate extensive optimization, uncertainty quantification, and sensitivity analysis tools.
and also unlike	research-focused fuel performance codes
Because AMP	will be developed with a focus on rigorous quality assurance to enable its use by the nuclear industry, will be easy-to-use by traditional fuel designers on desktop to leadership-class computational platforms, and will account for all of the physics that occurs within the fuel, even if only as simplified, phenomenological models.

3 STAKEHOLDER DESCRIPTIONS

There are three general forms of stakeholders that will be discussed:

1. the current, external stakeholders (Section 3.1, Table 2),
2. the internal stakeholders (Section 3.2, Table 3), and
3. the potential external stakeholders (Section 3.3, Table 4).

3.1 External Stakeholder Summary

The (current) external stakeholders for the AMP Nuclear Fuel Performance code are shown in Table 2.

Table 2: External Stakeholders

Name	**Description**	**Responsibilities**
NEAMS Leadership	see Introduction.	Agent by which funding is provided; customers of visualization for AMSO program development purposes; providers of high-level requirements through interactions with other DOE/NE programs.
NEAMS Fuels IPSC program manager (Steve Hayes)	Direct-report manager charged with delivering an integrated fuel performance capability that spans the LLS physics and the AMP Nuclear Fuel Performance code .	Technical lead of the integrated fuel performance capability; agent by which funding is provided; customer of visualization for Fuels IPSC program development purposes; provider of requirements for integrated fuel performance capability. Note also that the NEAMS Fuels IPSC program manager is also a Fuel Performance Expert and Primary Stakeholder (see Section 3.2).
NEAMS Fuels IPSC LLS physics researchers	Developers of both integrated and individual atomistic and meso-scale simulation tools, including the MOOSE/Bison/-Marmot code (MBM).	Customers of AMP because they serve as a vehicle to demonstrate the significance of their model/algorithm development work; customer of the AMP sensitivity analyses, which can guide the further development of models/algorithms; providers of software and algorithms (for multi-scale modeling) that may be coupled with, or embedded in, AMP.
CASL	Integrated nominal operation and transient reactor/fuel code suite for Light-Water Reactor applications, with a near-term focus on CRUD prediction, Grid-to-Rod-Fretting, and Pellet-Clad Interaction.	Customer of AMP that would incorporate it in a larger code suite; customers of AMP because it may serve as a vehicle to demonstrate the significance of their LLS model/algorithm development work; customer of the AMP sensitivity analyses to guide the further development of models/algorithms; providers of software and algorithms (for multi-scale modeling) that may be coupled with, or embedded in, AMP.
Fuel Cycle R & D TIO	Technical lead for Fuel Cycle research, Kemal Pasamehmetoglu, and supporting staff, including Cetin Unal.	Indirect sponsor and program manager of the principal DOE/NE fuel research customers; establishes the long-term requirements and evaluates performance with respect to a metric of "usefulness to experimenters."
NEAMS Reactors IPSC element	A program element that incorporates neutronics, thermal-fluid dynamics, and structural mechanics for reactor system and core modeling.	Customer of AMP for integration within their framework; potential provider of requirements for multiphysics coupling and communication.

NEAMS Capability Transfer (CT) Cross-Cutting element	A program element that is focused on technology transfer.	Interfaces with industry and campaign customers on behalf of the NEAMS program to elicit requirements. Potentially providing other services, such as training courses and release/distribution/compilation assistance to users.
NEAMS Enabling Computational Technologies (ECT) Cross-Cutting element	A program element that is focused on fundamental computational technologies, including assistance with foundational computational tools, software development process, and software quality assurance.	Providers of assistance and tools that AMP will leverage; customers of the AMP computational technology requirements; customer because AMP may serve as a vehicle to demonstrate the significance of this cross-cutting activity.
NEAMS Verification, Validation and Uncertainty Quantification (VU) Cross-Cutting element	A program element that provides independent verification, validation, uncertainty quantification, sensitivity analysis, and data assimilation (VVUQSADA) expertise and tools.	Providers of assistance and tools related to VVUQSADA that AMP will leverage; AMP customers primarily focused on demonstrating VVUQSADA (for non-intrusive UQ) applied to nuclear energy problems; provider of requirements for intrusive VVUQSADA.
NEAMS Fundamental Models and Methods (FMM) Cross-Cutting element	A program element that provides fundamental materials, models, and methods that are applicable to multiple IPSCs or are still in the fundamental research stage.	Customer of requirements; potential provider of material models and algorithms for upscaling of LLS physics.
ORNL Management	The management to which the AMP developers at ORNL report, both directly and indirectly.	Customers of visualization for nuclear, computing, and materials program development; invested in the technical success of the project, strategic direction of the software, and financial status of the project.
LANL Management	The management to which the AMP developers at LANL report, both directly and indirectly.	Customers of visualization for nuclear, computing, and materials program development; invested in the technical success of the project, strategic direction of the software, and financial status of the project..
INL Management	The management to which the Fuels ISPC developers and Fuel Performance Experts at INL report, both directly and indirectly.	Customers of visualization for nuclear, computing, and materials program development; invested in the technical success of the project, strategic direction of the software, and financial status of the project..

3.2 Internal Stakeholder Summary

The internal stakeholders for the AMP Nuclear Fuel Performance code are shown in Table 3 and described in more detail in Reference [2].

Table 3: Internal Stakeholders

Role	Name	Responsibilities
Primary Stakeholder	Steve Hayes	Primary interface to current, external stakeholders; lead for gathering requirements from the current, external stakeholders and acceptance testing based on the current, external stakeholder requirements.
Project Manager	Kevin Clarno	Manage the scope, schedule, budget, and risk; secondary interface to external stakeholders; lead for (internal and external) communication, including gathering requirements from internal stakeholders; lead for strategic planning, including gathering requirements from potential, external stakeholders.
Architecture Lead	Bobby Philip	Manage the comprehensive (external and internal) set of software requirements and acceptance testing based on the internal and potential, external requirements; lead the iterative software design process.
Process Lead	Bill Cochran	Lead for defining and overseeing the process to be used in software development and quality assurance; a direct interface to the NEAMS VU and ECT program elements at the technical level.
Fuel Performance Experts		Test the code during development; guide it to become more accurate; apply it to mission-critical applications.
Software Developers		Define and document the development plan; implement and document the software.
Scientific Researchers		Research and evaluate the performance (accuracy, efficiency, scalability) of the software and publish the results; software developers at national laboratories are also scientific researchers.
Post-Doctoral Researchers		As software developers and scientific researchers, it is imperative that they also get established in a field and acquire a job, which requires journal publications.
Student Researchers		As software developers and scientific researchers, it is imperative that they also complete their dissertation and publish.

3.3 Potential Stakeholder Summary

The potential stakeholders for the AMP Nuclear Fuel Performance code are shown in Table 4.

Table 4: Potential Stakeholders

Name	Description	Responsibilities
Nuclear Fuel Industry	GE, Westinghouse, Areva	Must have a very high quality assurance and validation plan for LWRs; also must allow for implementation of proprietary models

Nuclear Regulatory Commission (NRC)	Regulating body of the nuclear fuel industry.	A strategic decision will be required regarding the decision to support either the industry or the regulator, but it is not likely possible to support both.
Naval Reactors (NR)	DOE national laboratories that support the US Nuclear Navy.	Potential customers, but would move AMP Nuclear Fuel Performance code towards a classified tool.

3.4 User Environment

The targeted users for the AMP Nuclear Fuel Performance code are described in detail in Reference [3].

4 PRODUCT OVERVIEW

4.1 Product Perspective

The AMP Nuclear Fuel Performance code is part of the Fuels IPSC, as noted in the introduction (Section 1 and described in more detail in Reference [1], which includes a related software development effort called MOOSE/Bison/Marmot code (MBM). The relationship between the two projects is described in detail in Reference [1], which includes an overview of the relationship as reproduced in Table 5 of this document.

Table 5: Overview of the relationships of AMP and MBM

	MBM	**AMP**	**MBM +AMP**
User Community	SE experimenters, AMP developers	IE experimenters, reactor IPSC developers	novel fuel designers, novel reactor designers
Benefit	Insight into fundamental mechanisms	Evaluation of the performance of prototypic fuel, cladding, and/or structures	Prediction of the performance of nuclear fuel with no empirical database
Relevance of codes to one another	Calibrated, validated correlations and quantified uncertainties for use in AMP	Sensitivity of fundamental mechanisms to guide MBM development	Resolution of nonlinear bidirectional scale cascades
Role of experiment and design community	Provide SE data for validation and calibration	Provide IE data for validation and insight into missing physics and models	Defining novel fuel forms and supporting experiments
Source of input data	DFT and atomistic simulations	Calibrated, validated correlations from mesoscale simulations	DFT and atomistic simulations
Source of validation data	Separate Effects Experiments (SE)	Integral Effects experiments (IE)	n/a

4.2 Assumptions and Dependencies

The following dependencies and assumptions are included in the requirements for the development of the AMP Nuclear Fuel Performance code . It is assumed that the AMP Nuclear Fuel Performance code will get:

- a user interface from NEAMS ECT (NiCE) that will be very nice.
- support from NEAMS CT in user support, training courses, and distribution.
- support from NEAMS ECT in build/configure/test and software quality assurance.
- support from NEAMS VU in independent verification.
- algorithms, data, and maybe code, for grain-scale modeling from the other developers in the Fuels IPSC, including the MOOSE/Bison/Marmot code .
- expert user feedback from friendly users within the Fuels IPSC before any code is openly released.
- consistent funding at, or above, the present level.

If the assumptions prove false, additional scope will be added to this project.

4.3 Needs and Features

The requirements for the AMP Nuclear Fuel Performance code are described in detail in Reference [3].

References

[1] K. Clarno, R. Martineau, G. Dilts, and S. Hayes, NEAMS Integration of the AMP and MBM Fuel Performance Codes for Multi-Scale Fuel Performance Modeling and Simulation, Technical report, Idaho National Laboratory, 2010, Unpublished document delivered to DOE Office of Nuclear Energy as a Milestone reportd.

[2] K. Clarno and B. Philip, Roles and Responsibilities for the AMP Nuclear Fuel Performance Code, Technical report, Oak Ridge National Laboratory, 2010, Within the source documentation of the AMP Nuclear Fuel Performance code.

[3] B. Philip, W. Cochran, K. Clarno, and J. Billings, Requirements Document for the AMP Nuclear Fuel Performance Code, Technical report, Oak Ridge National Laboratory, 2010, Within the source documentation of the AMP Nuclear Fuel Performance code.