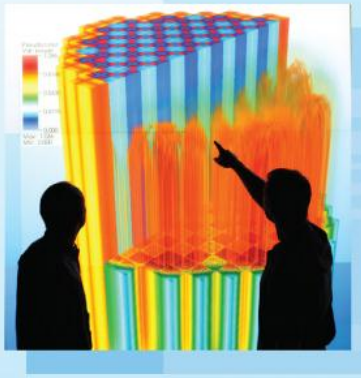
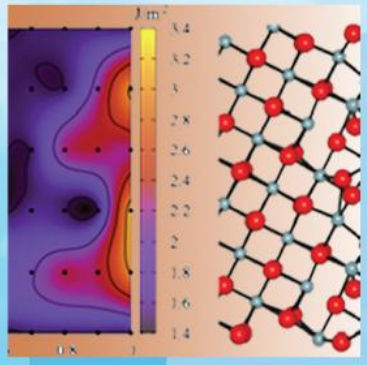
CASL-U-2011-0001-000

Power uprates
and plant life extension



Engineering design
and analysis

Science-enabling
high performance
computing



Fundamental science

Plant operational data

Consortium for Advanced Simulation of LWRs

L3:NFA.ITF.P2.03

Ronaldo Szilard
INL

Completed: 4/30/11

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

NEAMS VU and CASL VUQ:
Strategic Goals, Priorities, and Leveraging Opportunities

Introduction

This document describes at a high level the mission and priorities of the NEAMS VU and CASL VUQ programs. The idea is to clearly align each program with their separate priorities and applications. Differentiation between the two programs is needed, and it should be easy to communicate what the differences are. At the same time, the two programs have a common overarching mission, and thus need to leverage one another and coordinate activities whenever possible. Although the NEAMS and CASL applications are different in scope and timelines, many of the VU tools and capabilities are foundational and cross-cutting in nature. Research results, validation databases, software, and VU processes and methodologies are among the things that will potentially be shared and/or coordinated across both NEAMS VU and CASL VUQ.

Mission At-A-Glance

NEAMS VU and CASL VUQ share a common overarching mission:

To provide essential functions for achieving ***credible, science-based predictive M&S capabilities.***

The essential functions span several dimensions, e.g., capabilities (tools, algorithms), validation databases, processes and methodologies, and credibility assessment.

Achieving science-based predictive M&S capabilities requires advances in the VU-centric capability areas:

- Verification
- Validation
- Calibration through data assimilation
- Sensitivity analysis
- Discretization error analysis and control
- Uncertainty quantification
- Performance and risk assessment

Validation databases will be designed and populated to allow access and potential sharing of data by both programs (when possible). NEAMS VU and CASL VUQ will also develop appropriate V&V/UQ process workflows for achieving, assessing, and communicating the credibility required for the support of licensing applications. The UQ and SA tools will be used to drive ongoing investment priorities within each program.

Scope and Priorities

NEAMS VU and CASL VUQ will support the separate scope and priorities within each of their respective programs. While each will make investments in most or all of the VU capability areas defined above, these investments will be driven and prioritized by the current program needs, likely defined by the challenge problems and timelines that are adopted for solving them. There are also many important opportunities for leveraging between NEAMS VU and CASL VUQ, as described later.

The CASL scope focuses on LWRs. The timeline (for Phase 1) is five years, which, in turn, drives priorities for CASL VUQ. This short timeline implies a larger reliance on legacy physics codes early on in the program, with selective development of new codes and models over the five-year period. The VUQ focus area will follow suit. The early priorities of VUQ will be to deploy existing tools, capabilities, validation databases, and workflows to support CASL challenge problems. VUQ innovations will be driven by the well-defined scope of the program. The research, development and integration of new VUQ capabilities will occur throughout the five year period.

The NEAMS scope includes the entire fuel cycle as well as advanced reactors. The NEAMS timeline is much longer than five years. The larger scope and longer timeline (relative to CASL), in turn, drives different priorities for NEAMS VU. NEAMS VU will focus more strategically and more broadly on V&V/UQ algorithm research and development, process workflow development to include licensing support, and predictive capability assessment methodologies. The scope of required validation data is greater and more complex in NEAMS. Given the diversity of NEAMS applications and the dispersion of the code teams, NEAMS VU must also invest more broadly in partnership models with the code teams to ensure consistency of the VU methodologies employed and successful adoption of the VU capabilities.

Example: The timelines above are driving the integration of DAKOTA into the CASL VERA code within the first six months of CASL. On the other hand, over the first 18 months of NEAMS VU, DAKOTA has not been integrated into a NEAMS IPSC (indeed, there is not a NEAMS IPSC that is ready for this yet).

Leveraging Opportunities

The opportunity for sharing and leveraging between NEAMS VU and CASL VUQ exists in the following areas:

- ***Validation data.*** The VU/VUQ programs will share validation data, where possible (e.g., for common CFD and neutronics models, subject to possible legal restrictions on access). Common validation benchmark problems will

potentially be developed by NEAMS, CASL, and LWRS. NEAMS and CASL will leverage efforts to identify data sources and to define general database specifications and design requirements, and even a common database accessible to both programs. This leveraging is already beginning in FY11 with the creation of the NE-CAMS (Nuclear Energy – Computational Application Management System) project within the NEAMS VU program, led by Kim Mousseau at INL. The NE-CAMS project is being supplemented with a small amount of CASL funds, and the deliverables will be coordinated to benefit both NEAMS and CASL.

- ***V&V plans.*** The development of V&V plans is among the first activities of all NEAMS and CASL code projects. VU/VUQ is playing a central role in each of these activities. Although the plans are tailored to the specific needs of each application area, they will share some content and structure – the role of VU/VUQ is to contribute the common methodology to all plans.
- ***VU workflows.*** Where possible, workflow processes developed for verification, validation, and uncertainty quantification will be shared across programs.
- ***VU assessment best practices.*** Both NEAMS and CASL will explore the use of predictive capability assessment methodologies that are tailored to the application needs. This includes the use of the Predictive Capability Maturity Model (PCMM) and possibly other assessment methodologies. We will share and leverage these, where possible, across NEAMS VU and CASL VUQ. (As explained later, research into new advances in these assessment methodologies will primarily be the role of NEAMS.)
- ***VU software tools.*** New software capabilities that are implemented and released through one program (i.e., NEAMS VU or CASL VUQ) will generally be available for use in the other.
- ***Research results.*** New research findings will be quickly communicated across both programs and leveraged if appropriate.

Investment Priorities

Priorities are driven by different scope and timelines. Respective investments in NEAMS VU and CASL VUQ reflect these differences. The result is that primary ownership of some of the capability and methodology development resides in one or the other of the programs.

Priorities for NEAMS

NEAMS VU will assume primary ownership of the following areas:

- ***Validation database.*** Although this is a highly leveraged activity between NEAMS and CASL, NEAMS will take the lead in ownership (i.e., funding) and direction. The NE-CAMS effort will initially focus on validation database

requirements for CFD, but quickly expand to other applications. NE-CAMS intends to deliver a database that is accessible to the broad Nuclear Energy community.

- ***VU methodology development.*** This includes advancing the current state-of-the-art in methodologies to support both science-based prediction and licensing. It also includes new advances in maturity assessment approaches (e.g., PCMM, PMI, etc.).
- ***Uncertainty quantification R&D for lower-length scales***. This will include subcontinuum scales and effective upscaling techniques that couple with the engineering scales. Each of the NEAMS IPSCs has important physics at the atomistic and molecular scales; UQ at these scales is virtually nonexistent. NEAMS VU has an opportunity and obligation to lead in this area. Major breakthroughs are needed.
- ***Multiple Model Inference R&D for model selection.*** Complex multiphysics codes are almost always equipped with many model alternatives that can be applied to a given phenomenon, such as turbulence, fracture, heat transfer, chemistry, material behavior, etc. The challenge is to objectively assess which model is "best" for a particular purpose. NEAMS VU is making strategic investments in new technologies using ideas from statistics. The goal is to significantly advance the current state-of-the-art and allow for greatly enhanced predictive capabilities for the NEAMS IPSCs.
- ***Code verification capability development.*** NEAMS will invest in new manufactured solution development and other techniques to advance this strategic capability area.

Products of the above activities are expected to be shared with CASL. For example, the predictive maturity assessment capabilities (PCMM, PMI, etc.) will, for the most part, be researched and developed in NEAMS and *used by* CASL. Some capability and methodology development priorities might not necessarily be owned *a priori* by NEAMS VU, but might instead arise in the context of a particular challenge problem driver. For example, shortcomings in certain UQ methods might be identified through a UQ or sensitivity analysis on a NEAMS challenge problem. In this case, investments in new UQ R&D for the particular application area would be given an increased priority within NEAMS.

Priorities for CASL

Early on, CASL will be working more with existing legacy tools than NEAMS will. These codes, when applied to multiphysics problems, are usually tied together in a mathematically loosely coupled manner. This drives the need for new discretization error control methods (and verification methods in general), along with efficient UQ/sensitivity analysis methods (including, for example, new reduced-order models) that are applicable to this structure. Furthermore, the focused model development occurring within CASL requires more immediate capabilities for model calibration through data assimilation. In

general, R&D activities aimed at the CASL core problem set will find an increased priority within CASL.

CASL VUQ will assume primary ownership of the following areas:

- ***Data assimilation R&D.*** This work will advance the state-of-the-art for model calibration, which is necessary for the early timelines of CASL.
- ***Discretization error control capabilities.*** Tools and methodologies are needed for discretization error control and solution verification for the mostly loosely-coupled multiphysics codes that will comprise VERA. Furthermore, issues with proper mathematical convergence with mesh refinement must be dealt with more in CASL than in NEAMS, due to CASL's much heavier use of legacy physics codes and modules.
- ***New reduced-order models for coupled neutronics/T-H.*** The impact will be seen in significant efficiency gains for sensitivity analysis, UQ, and model calibration.
- ***Black-box algorithm and software tool development.*** This includes tools like Percept (formerly called Encore; to support verification/mesh refinement studies) and DAKOTA (for black-box sensitivity analysis, UQ, and model calibration). This is driven by the shorter CASL timelines and heavier use of legacy tools that are difficult to "open up" for integrating intrusive (non-black box) capabilities.

CASL will leverage and apply VU methodologies, workflows, and capability maturity assessment techniques (PCMM, PMI, etc.) developed by NEAMS to the extent possible. It is expected that some tailoring of each of these to the CASL applications will be required, and CASL VUQ will invest in this tailoring and application as appropriate.

Summary

This document describes areas of leveraging between the NEAMS VU and CASL VUQ programs. It also describes the significant differences in the two programs; these differences are driven by different scopes and timelines. The result is that NEAMS VU has a longer-term focus with emphasis on more formal VU methodology development and assessment, as well as ownership of longer-term R&D issues. The CASL VUQ priorities are driven by CASL's shorter timelines. These priorities consist of a balance between innovations in critical areas (e.g., data assimilation) and incorporation of existing black-box tools for UQ/SA. The dual strategies of NEAMS VU and CASL VUQ will result in benefits to each program; the mutual benefits of the FY11 tasks are discussed in detail in the next section.

FY11 Interdependencies

The FY11 tasks in both NEAMS VU and CASL VUQ will deliver products that can benefit the other program over varying time periods. Here is a summary of those tasks.

NEAMS VU FY11 Tasks that Benefit CASL

- ***NE-CAMS Validation Database.*** NEAMS VU will take the lead in funding this effort through a new project led by Kim Mousseau at INL. CASL VUQ will contribute a small amount of funding as well.
- ***VU assessment for Waste IPSC.*** This effort will include a tailoring of the Predictive Capability Maturity Model (PCMM) for the Waste IPSC. A VU assessment will be then performed based on the modified PCMM for a selected Waste challenge problem. A report will be produced. The assessment tools, methodologies, and lessons learned will be beneficial to CASL since the use of PCMM for CASL challenge problems will be explored starting in late FY11.
- ***Predictive Maturity methodology development.*** This task continues exploration and demonstration of the Predictive Maturity Index (PMI) as a means of achieving and communicating adequacy of the calibration/validation process. This project will also provide benefits to CASL since, in conjunction with PCMM, PMI will be explored for possible use in CASL applications.
- ***V&V plan for Reactor IPSC.*** The NEAMS VU team will work with the Reactor IPSC team to produce a V&V plan, due June, 2011. This effort will be synergistic with the CASL V&V plan (led by the AMA focus area with participation from the CASL VUQ team; the initial version was delivered in January, 2011). Although NEAMS and CASL are addressing different types of reactors, it is expected that similar issues will be addressed through the V&V plan; therefore, useful information will flow in each direction between NEAMS and CASL in these activities.
- ***Bayesian methodology development***. This is an R&D project that will investigate methodologies for model selection and assessment, new experiment design strategies for data collection, and improved scalability and efficiency of the algorithms. This project is expected to provide longer-term payoffs to CASL (beyond FY11).
- ***AMP Verification and Validation Support.*** In conjunction with the Fuels IPSC team, NEAMS VU will develop code verification test suites for a large set of the multi-physics capabilities within AMP. These include AMP's thermo-mechanical and diffusion packages, as well as mechanical and thermal contact. Also, NEAMS VU will develop a validation database and assist in the validation demonstration on a selection of transient reactivity insertion accidents. The Predictive Maturity Index (PMI) will also be used in this exercise. This task is expected to have a significant benefit back to the CASL MPO and VUQ focus areas.
- ***Calibration and Validation Investigation for LIFE-IV code.*** This work will explore statistical screening methods for reducing the number of input parameters, using data from approximately 20 pins for the calibration. Advances in the calibration/validation methodology are expected, and this will, in turn, benefit CASL. This task also includes depositing calibration and validation data into the Fuels IPSC database.

- ***VU support for R7***. In FY10, NEAMS VU and the R7 team worked together to interface and demonstrate DAKOTA with R7. This work continues in FY11. Some of DAKOTA's advanced capabilities for UQ and SA will be exercised, along with exploration of DAKOTA's library interface. CASL will benefit from the further maturation of DAKOTA's software and algorithms.

CASL VUQ FY11 Tasks that Benefit NEAMS

- ***Validation data committee and validation data plan.*** In FY11, CASL VUQ is participating in the NE-CAMS (Nuclear Energy – Computational Application Management System), which is being led out of NEAMS VU. CASL VUQ will also be standing up a validation data committee and will eventually coordinate its NE-CAMS activities through this committee. In the shorter term, CASL VUQ will lead development of an initial validation data plan which will focus on specific CASL challenge problem validation needs.
- ***CASL V&V plan.*** VUQ has already played a key role in helping the AMA focus area deliver this plan (which will become a working document for ongoing CASL activities). As mentioned in the previous section, ideas and other information will flow in both directions as CASL and the NEAMS Reactor IPSC each produce V&V plans in FY11.
- ***Verification, Validation, and UQ workflows.*** CASL VUQ is developing and documenting workflows for performing these functions. These workflows will provide input to the more comprehensive VU methodologies being developed by NEAMS VU.
- ***Data Assimilation mathematical framework development.*** This R&D project is expected to advance the current state-of-the-art. Demonstrations of the new capabilities will be performed for benchmark neutronics and T-H problems. This is needed by CASL in the short term, and will benefit NEAMS (and the entire VU community) in the longer term.
- ***Reduced-order models for efficient UQ/SA.*** In FY11, CASL VUQ is supporting implementations of and extensions to the Efficient Subspace Method (ESM), for selected neutronics applications and to nonlinear tightly coupled physics (neutronics/T-H). The ESM library will also be interfaced to DAKOTA. These capabilities should eventually be made available to NEAMS, possibly through DAKOTA's open-source license, although these details have not yet been discussed.
- ***DAKOTA and Percept development***. CASL VUQ is supporting development of capabilities for interfacing Bayesian calibration libraries to DAKOTA. Some advanced UQ capabilities are also under development, including adaptively-refined and adjoint-enhanced Gaussian Process Models and Stochastic Expansions. The Percept library (formerly called Encore) has been incorporated into the Trilinos toolkit as a vehicle for integration into VERA. The NEAMS IPSC's will benefit from these capabilities as they adopt Trilinos and DAKOTA into their respective suites of tools.