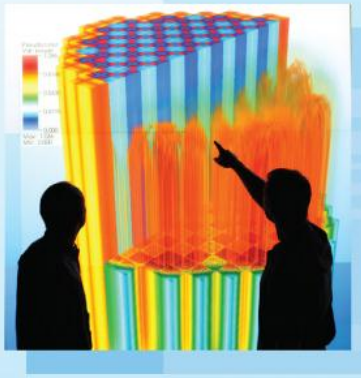
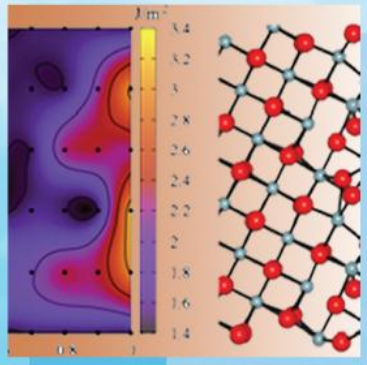
CASL-U-2011-0195-000

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:VUQ.SAUQ.P3.04

Jim Stewart
SNL

Completed: 9/30/11

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

CASL Uncertainty Quantification Roadmap

CASL Milestone L3:VUQ.SAUQ.P3.04

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Version 1

September 30, 2011

Objective

This document is a high-level roadmap for addressing UQ capability challenges that are expected to be encountered in CASL. The UQ capabilities outlined in the roadmap will typically be delivered through CASL milestones, which might take the form of targeted UQ algorithm development, or be rolled into more comprehensive milestones that involve exercising specific VERA modules and/or CASL challenge problems. In all cases, the milestones will be aligned with the evolving needs and priorities of CASL. Thus, the roadmap is a working document, not a set-in-stone plan.

Scope and Challenges

This roadmap is not intended to cover the breadth of VUQ capabilities. Initially the roadmap will be restricted to *uncertainty propagation* through computational models. The technical scope will expand to include verification and validation/calibration (to include *model-form error*) in later versions. This document does explain what model-form error is, but it only describes the forms it takes and the challenges with handling it. Treatment of model-form error requires consideration of experimental data, which is not discussed. The current version of the roadmap describes the capabilities (for uncertainty propagation) that the VUQ Focus Area delivered in FY11 and has planned for FY12.

[1] 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.

CASL-U-2011-0195-000

A number of specific challenges exist with the propagation of uncertainties through CASL's computational models. At the highest level, the challenges are in dealing with the multiphysics, nonlinear, time-dependent, high-dimensional (in dimensions of uncertainty) systems that need to be solved accurately, with confidence, by VERA. CASL's multiphysics systems combine linear or nearly linear models having very large numbers of uncertain parameters with very nonlinear (and possibly nonsmooth) models having (relatively) few numbers of uncertain parameters. Moreover, these parameters can be any mix of aleatory and epistemic types, which present further algorithmic challenges. In general, we think of our systems as very high dimensional, requiring methods for propagating uncertainties that are efficient and scalable. Addressing this "curse of dimensionality" is one of the grand challenges in the UQ research and development community.

The very heterogeneous nature of our multiphysics systems (i.e., mixed linear/nonlinear, varying dimensionality, different physical scales, etc.) requires a toolbox (i.e., hybrid) approach for delivering the most appropriate capability for the problem at hand. The toolbox must include a mix of capabilities spanning deterministic (adjoint) approaches and sampling-based approaches. Within this vast set, there is a continual need for development and improvement of capabilities that must be tailored to the CASL problems.

Here is a summary of challenges that we face for uncertainty propagation in CASL:

- Coupling
  - Single physics
  - Loosely-coupled multi-physics – interface coupling
  - Loosely-coupled multi-physics – overlapping volume
  - Tightly-coupled multi-physics (monolithic system)
- Fidelity
  - Hierarchical multifidelity models
  - Ensemble of models (lacking preference structure → model-form uncertainty)
- Physical scale
  - Continuum/engineering scale models
  - Sub-continuum (lower-length scale) models
  - Coupled sub-continuum/continuum models
- Validation hierarchy
  - Components to sub-systems to full systems
- Mathematical model form
  - Linear vs. Nonlinear
  - Smooth (differentiable) vs. Non-smooth
  - Unimodal vs. Multimodal
- Uncertainty characterization
  - Interface with data: assimilation, inference, inversion
  - Parametric vs. nonparametric distributions
  - Random fields and stochastic processes
- Dimensionality
  - Input Parameter space:

        - Few-to-moderate uncertain (input) dimensions [<O(10-100)]
        - High uncertain (input) dimensions [>>O(100)]
    - State space: High dimension > $O(10^6)$
    - Outputs: (few outputs vs. many outputs)
- Uncertainty form
    - Aleatory (parametric)
    - Epistemic (parametric, model-form, numerical discretization, …)
- Quantity of interest
    - Best estimate plus uncertainty for all models outputs used in support of design, analysis, safety, and operation
    - Risk assessment (tail probability)
- Uncertainty Algorithms
    - Forward (including sampling-based) vs. Adjoint Methods
    - Surrogate-Based vs. Surrogate-Free Methods
    - Hybrid Forward-Adjoint Surrogate-Based Methods

It is evident that CASL cannot address all of these challenges directly. We must leverage what we can, and invest smartly in those areas that deliver the most value to our mission. The FY11 and FY12 activities outlined in this roadmap begin to address some of the most critical challenges listed above.

UQ Problem Description and Definition of Model Error

This section describes the "model error" and the situations in which it arises. We do not address how model error is to be handled in CASL -- that topic will be addressed in a future version of the roadmap.

Consider a single model M (representing a single physics) that maps inputs $\boldsymbol{x}$ and $\boldsymbol{p}$ to outputs $\boldsymbol{u}$ as follows:

$$0 = M(\boldsymbol{x}, \boldsymbol{p}; \boldsymbol{u})$$

where $\boldsymbol{x} = \{x_i;\ i = 1, N_d\}$ are the independent variables (e.g., spatial coordinates, angle, time), $\boldsymbol{p} = \{p_i;\ i=1,\ldots,N_p\}$ are adjustable parameters of the model and/or physical environment, and $\boldsymbol{u} = \{u_i;\ i=1,N_u\}$ represents the N_u unknowns of the problem. Note that M can be linear or nonlinear with respect to $\boldsymbol{u}$. The uncertainties we consider are those of the N_p parameters – these parameters can be any combination of aleatory and epistemic types. Specifically, we are interested in the propagation of the parameter uncertainties through M so that we can compute the uncertainty in $\boldsymbol{u}$. The N_r responses R_i (i.e., the quantities-of-interest) are then computed as

$$R_i = f_i(\boldsymbol{u}),\ i = 1, N_r.$$

In terms of UQ algorithms, situations where N_p and/or N_r are large (e.g., >O(100), depending on the form of M) are challenging because these quantities (i.e., numbers of parameters and responses, respectively) also add to the dimensionality of the problem. Thus, scalable and efficient UQ algorithms are required.

The model (M) itself is likely to have error with respect to the reality that it is attempting to represent. This is the *model error* and is denoted by e_m. It is handled in different ways depending on the context:

- For calibration, e_m is modeled (sometimes referred to as the *model discrepancy term*);
- For validation, e_m is measured (in the units of an accepted validation metric);
- For prediction, e_m is estimated (for the purpose of model interpolation within the validation domain or model extrapolation beyond the validation domain).

In all these situations -- modeling, measuring, or estimating -- e_m requires (single-effects) experimental data (which also has uncertainties). This scenario is depicted in Figure 1.

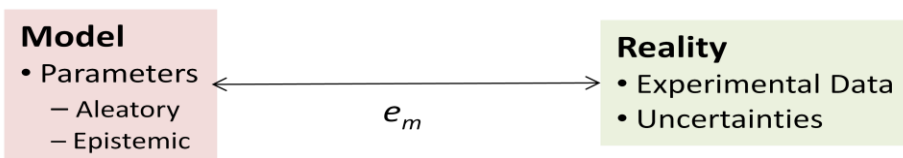

Figure 1. A general computational model with uncertainties in outputs (due to uncertain input parameters) has an error e_m with respect to "reality." The "reality" also has uncertainties due to the inherent uncertainties in the experimental data.

Various layers of complexity can now be added to the model. A simple multi-physics model can be represented as

$$0=Z[M_1(\boldsymbol{x}_1, \boldsymbol{p}_1; \boldsymbol{u}_1), \ldots , M_{Nz}(\boldsymbol{x}_{Nz}, \boldsymbol{p}_{Nz}; \boldsymbol{u}_{Nz})]$$

where N_z is the number of physics and Z is the coupling model. Naturally we could generalize this further to show coupling of these multi-physics models in a hierarchical way (i.e., enumerate Z and combine two or more with higher-level coupling models, etc.). The models M_i individually can be linear or nonlinear. The added complexity in this structure can be realized in several ways. For example, the multiple physics can be mathematically coupled over the entire physical domain (i.e., volumetrically) or at a boundary. They can be coupled in a time-overlapping way or a time-sequenced way. The physics can exhibit radically different spatial and/or time scales. Finally, the coupling model Z can take many forms ranging from a single monolithic (tightly coupled) system to a fully staggered (loose) coupling that requires iterations (in one or all directions) across the individual physics.

We could also parameterize Z but choose not to explicitly show that here. As with each of the single-physics models M_i, Z has a *model error* e_z that we are not addressing in Version 1 of the UQ Roadmap. Modeling, measuring, or estimating e_z would require integrated-effects experimental data.

A further layer of complexity is added when considering *multiple model alternatives* for an individual physics. This is a very common situation – for example in modeling turbulence we often have to choose among many model types (e.g., algebraic, RANS, LES, DNS). To account for this situation, we add a superscript index to our model M (going back to our single-physics model M):

$$0 = M^a(\boldsymbol{x}, \boldsymbol{p}_a; \boldsymbol{u}); 1 <= a <= N$$

where N is the number of model choices. Note also that each model choice M^a will generally have a unique parameterization $\boldsymbol{p}_a$. The multiple model choices can appear in two forms. First, a set of model alternatives could have a clear hierarchy in terms physics fidelity -- we call this *multiple model fidelity*. In the turbulence modeling example above, we would have a hierarchy of four models (M^1 is an algebraic model, M^2 is a RANS model, and so on) that exhibit a sequentially higher resolution of the same physics. This scenario is depicted in Figure 2. Having a clear hierarchy of model fidelity allows one to adaptively control (i.e., reduce) the model error e^a_m. If the model of highest fidelity (M^N) is accurate enough (which would be an assumption), then one could compute a *model error estimate* as follows:

$$e^a_m\,(\text{Est}) = R(\boldsymbol{u})|_{M^N} - R(\boldsymbol{u})|_{M^a}, \text{ where } a < N.$$

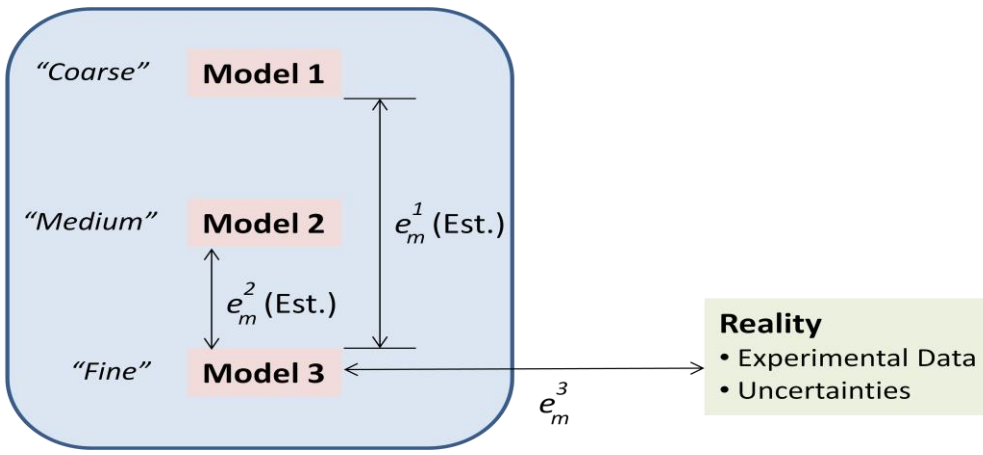

Figure 2. Multiple model alternatives, where the model choices have a clear hierarchy of fidelity. Assuming the "fine" model is significantly more accurate than the lower-fidelity models, then reasonable model error estimates can be computed for the lower-fidelity models. This allows model error to be adaptively controlled.

The above expression states that the estimated model error is the difference in responses between the finest model (M^N) and any coarser model. An adaptive model-error control algorithm would involve switching to a finer model if the estimated error is higher than some tolerance.

The second important case when considering multiple model alternatives is when a clear hierarchy of fidelity does *not* exist. In other words, there is no clear choice in terms of model accuracy that would drive the selection of one model versus the others. This leads to an (epistemic) uncertainty due to the model form. This scenario is depicted in Figure 3. One then could "sample" each model to create a finite set of possible solutions:

$$\{R(\boldsymbol{u})|_{M^1}, \ldots, R(\boldsymbol{u})|_{M^N}\}.$$

Quantitative techniques for *multiple model inference* (MMI) can be developed and applied to determine the "best" model alternative. However, these techniques require the existence of experimental data. Moreover, MMI is still a research area, and different inference methods sometimes give inconsistent

results as to what is the "best" model. Therefore, one must (usually) still account for the epistemic model-form uncertainty to get a complete characterization of the total uncertainty in a given simulation.

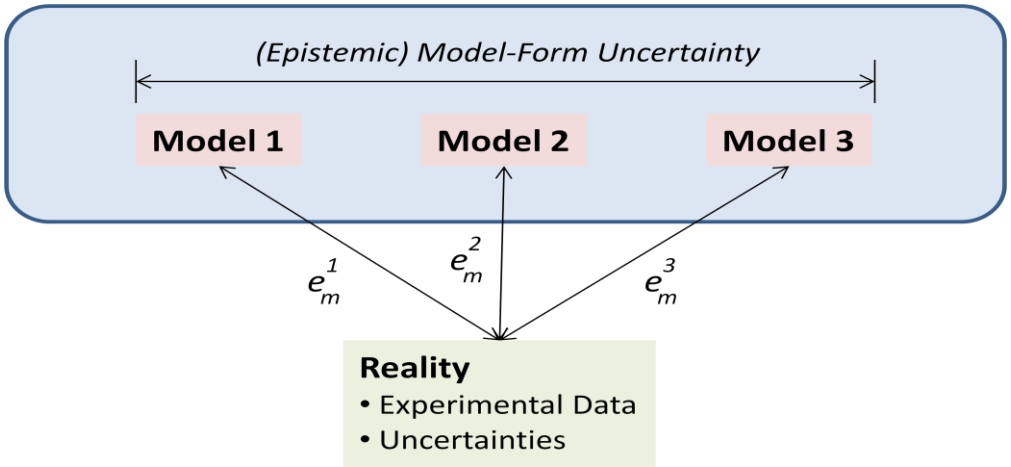

Figure 3. Multiple model alternatives, where no clear hierarchy of model fidelity exists. In this situation, the range of models leads to an epistemic model-form uncertainty. Each model has a potentially different (and unknown unless validated) model error.

There is another layer of complexity in each of the above situations that is due to the *discretization* of the models. Specifically, this is the numerical discretization error that must be estimated as part of the solution verification exercise. The discretization error is another component in the total uncertainty in a given simulation. Thus, there is an important coupling of verification to UQ (as well as to data assimilation) – this topic will be addressed in a future version of the UQ Roadmap.

Finally, we have not discussed the problem of estimating e_m for the purpose of predictions. In general, estimating e_m for predictions (where "Reality" is not known) requires a systematic traversal through the validation hierarchy, where the model error for each piece of the hierarchy is measured through a validation process performed on that piece. The goal is to provide enough information about the model errors at the lower levels to enable the estimation of e_m (through some form of extrapolation and/or scaling) for the full-system quantity-of-interest.

Roadmap for Uncertainty Propagation

We now present how the VUQ Focus Area's FY11 and FY12 milestones map to the situations described in the previous sections. At the time of this writing, the FY12 milestones have not been finalized, so this roadmap is subject to change.

FY11 Roadmap

- *Title:* Enable statistical sensitivity and uncertainty demonstrations for VERA (L2 milestone)

- *Description:* Deploy forward SA and UQ approaches by integrating DAKOTA with VERA modules in an evolutionary approach (initially loosely couple to LIME or individual VERA components).
- *Delivery date:* 3/30/2011
- *Owner:* Brian Adams
- *Model type:* Single physics (VIPRE-W boiling model), nonlinear, steady-state
- *Uncertainties/responses addressed:* Aleatory uncertainties, few parameters (N_p <=$O(10)$), few responses (N_r <= $O(10)$)
- *UQ algorithms exercised:* Latin Hypercube Sampling, Polynomial Chaos Expansions
- *Multiple model alternatives:* No

- *Title:* Uncertainty Management Hybridization Framework (L3 milestone)
  - *Description:* Develop a generalized framework that hybridizes stochastic and deterministic techniques for uncertainty management
  - *Delivery date:* 9/30/2011
  - *Owner:* Hany Abdel-Khalik
  - *Model type:* General coupled physics
  - *Uncertainties/responses addressed:* Aleatory uncertainties, many parameters (N_p >= =$O(100)$), few responses (N_r <= $O(10)$)
  - *UQ algorithms exercised:* Combined global sampling method with local adjoint method
  - *Multiple model alternatives:* No

- *Title:* Scalable UQ Algorithm Deployment (L3 milestone)
  - *Description:* Highlight development of scalable nonlinear UQ algorithms in DAKOTA and deployment of these techniques to probabilistic analysis of Crud.
  - *Delivery date:* 9/30/2011
  - *Owner:* Mike Eldred
  - *Model type:* Single physics (VIPRE-W boiling model), nonlinear, time-dependent
  - *Uncertainties/responses addressed:* Aleatory uncertainties, few parameters (N_p <=$O(10)$), few responses (N_r <= $O(10)$)
  - *UQ algorithms exercised:* Adaptively refined stochastic expansions using generalized sparse grids
  - *Multiple model alternatives:* No

FY12 Roadmap

- *Title:* Two-way coupled-physics UQ in Baseline VERA (L1 milestone, joint with VRI and AMA)
  - *Description:* Demonstrate sensitivity and uncertainty analysis for CIPS-related phenomena with two-way coupled physics as available in VERA at time of execution.
  - Delivery date: 12/16/2011
  - *Owner:* Brian Adams
  - *Model type:* Two-way coupled physics (VIPRE-W, BOA), nonlinear, time-dependent
  - *Uncertainties/responses addressed:* Aleatory uncertainties, few parameters (N_p <=$O(10)$), few responses (N_r <= $O(10)$)
  - *UQ algorithms exercised:* Latin Hypercube Sampling (others TBD)
  - *Multiple model alternatives:* No

- *Title:* Three-way coupled-physics UQ in Baseline VERA (L3 milestone)
  - *Description:* Demonstrate sensitivity and uncertainty analysis for CIPS-related phenomena with three-way coupled physics as available in VERA. This work is an extension of the planned Q1 L1 milestone.
  - *Delivery date:* 3/30/2011
  - *Owner:* Brian Adams and Hany Abdel-Khalik
  - *Model type:* Three-way coupled physics (VIPRE-W, BOA, ANC), linear/nonlinear, time-dependent
  - *Uncertainties/responses addressed:* Aleatory uncertainties, moderate parameters (N_p <=O(100)), few responses (N_r <= O(10))
  - *UQ algorithms exercised:* Latin Hypercube Sampling (others TBD)
  - *Multiple model alternatives:* No

- *Title:* Initial (single-physics) UQ hybridization (mixed stochastic/deterministic) framework demonstration for CIPS or WB-1, using Early Advanced VERA (L3 milestone)
  - *Description:* Demonstrate the framework for a neutronics problem (likely solved with DeCART), where a deterministic approach is exercised.
  - *Delivery date:* 3/30/2012
  - *Owner:* Hany Abdel-Khalik
  - *Model type:* Single physics, linear, time-dependent
  - *Uncertainties/responses addressed:* Aleatory uncertainties, many parameters (N_p >= O(100)), few responses (N_r <= O(10))
  - *Multiple model alternatives:* No

- *Title:* Algorithms for Model-Form Uncertainty Propagation (L3 milestone)
  - *Description:* Demonstrate uncertainty propagation associated with using multiple-model alternatives, for a CIPS problem.
  - *Delivery date:* 6/30/2012
  - *Owner:* Mike Eldred
  - *Model type:* Coupled physics (details TBD), linear/nonlinear, time-dependent
  - *Uncertainties/responses addressed:* Aleatory parameter uncertainties, epistemic model-form uncertainties, few parameters (N_p < =O(10)), few responses (N_r <= O(10))
  - *UQ algorithms exercised:* TBD
  - *Multiple model alternatives:* Yes. Multiple model alternatives that possess a clear hierarchy of fidelity will be studied. Still to be determined is whether multiple model alternatives *without* a hierarchy of fidelity will be included in the milestone scope.

- *Title:* Multi-physics UQ hybridization framework demonstration for CIPS (L2 milestone)
  - *Description:* Demonstrate the framework for a couple neutronics/T-H problem, in which a deterministic approach and a stochastic approach are each exercised within the same problem (and appropriately combined across the physics within the framework)
  - *Delivery date:* 9/30/2012
  - *Owners:* Hany Abdel-Khalik and Mike Eldred
  - *Model type:* Coupled physics, nonlinear, time-dependent,
  - *Uncertainties/responses addressed:* Aleatory uncertainties, many parameters (N_p >= O(100)), few responses (N_r <= O(10))
  - *Multiple model alternatives:* TBD

Summary

The scope of Version 1 of the UQ Roadmap is restricted to uncertainty propagation. It is important that future versions include treatment of the model error term e_m for all three contexts of interest: calibration, validation, and prediction. This will necessitate the inclusion of data assimilation capabilities in the roadmap. We note that the VUQ Focus Area has FY11 and FY12 milestones addressing data assimilation. By extension, the roadmap will also need to include the acquisition of experimental data if the capabilities for calibration and validation are to be exercised on the CASL challenge problems. The roadmap must also include solution verification since numerical discretization errors contribute to the overall simulation uncertainties. The priorities beyond FY12 will be strongly driven by the evolving needs of CASL. One of the primary objectives of VUQ is to provide a SA/UQ-driven process for guiding CASL's R&D investments. Our FY11 and FY12 activities will provide the foundations for enabling sound investment decisions.

Acknowledgements

Thanks to the CASL VUQ team for their dedication in planning and delivering the work described herein. Thanks especially to Hany Abdel-Khalik, Mike Eldred, and Brian Adams for help in producing this roadmap.