Holistic, Hierarchical VVUQ as the Scientific Method for PSAAP (LA-UR-23-32192)

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Verification, validation and uncertainty quantification ("VVUQ") are critical elements within the ASC Program and predictive computational science. At a minimum, VVUQ tests the accuracy of simulation results. At its best, the VVUQ process represents how the scientific method is exercised within computational physics. Predictive scientific computing, for large-scale simulations of interest to decision makers, aims to provide quantifiable uncertainties for simulations. This includes explaining deviations from experimentally observed features. These deviations may be due to model deficiencies in the simulation or due to experimental variability. Quantifiable simulation uncertainties require well tested codes using defensible algorithmic choices balancing speed, robustness and accuracy, while taking into account a variety of physical modeling choices.

Short definitions of VVUQ:
Verification is testing that the modeled equations are implemented correctly and give consistent results on different meshes.
Validation is assessing that the physical models are accurate representations of reality, after relevant parameters have been calibrated. Calibration and validation are often similar activities.
Uncertainty quantification considers input, model and data uncertainties to assess the uncertainty of a predicted quantity.

To help with verification activities, a Python3 package of exact analytic solutions that may be relevant to PSAAP proposals are hosted on GitHub at https://github.com/lanl/ExactPack. External contributions of exact solutions relevant to PSAAP Centers are welcome.

This white paper first briefly discusses VVUQ as the Scientific Method, then describes the idea of Hierarchical VVUQ, and closes by discussing the importance of pulling it all together in a holistic manner.

VVUQ as the Scientific Method

In the simplest terms, the scientific method breaks apart complicated problems into constituent components, tests these in bite-size chunks, and reassembles results to obtain defensible conclusions. VVUQ represents the scientific method for predictive scientific computing. In general, the scientific method helps researchers thoroughly document assumptions, accurately communicate conclusions, and identify potential or probable unknowns in their understanding of both inputs, processes, and outputs. VVUQ helps achieve these objectives for predictive scientific computing by structuring how complicated problems are dissected and analyzed. Aspects of some problems are best broken apart, for example, by focusing on symmetries specific to the problem, and are thus verification efforts. The same problem may lend itself to a different decomposition due either to available experimental results, or a specific lack thereof, which may enhance or impede validation efforts. In both cases, the purpose of breaking the problem apart is the same: understanding relevant uncertainties, quantifying which uncertainties are believed to be the largest, and formally codifying the reasons for those beliefs. Uncertainty quantification ("UQ") helps understand how input uncertainties from data or the problem setup interact with uncertainties from verification and validation analyses. Of course, UQ analyses may further support beliefs, or provide a manner to understand why beliefs were incorrectly held.

Ultimately, VVUQ analyses are done by developing and using diagnostic methods, like analytic solutions, to test code output for failure modes and errors, as well as checking whether, and how well, complicated simulations agree with experimental observations. Verification focuses on mathematical aspects of simulation results, especially grid convergence, and whether simulation results agree or disagree with known solutions and also approach those answers at the correct rate of convergence. Validation uses experimental data for comparison against simulation results to test whether the fidelity of a physical model is sufficient for specific applications, particularly after physical models have been appropriately calibrated. UQ helps establish links between uncertainties associated with algorithms, physical models, and experimental data used in the simulation. For the multi-scale, multi-physics codes and simulations of interest to PSAAP, UQ provides an important tool for estimating the integrated effect of smaller, separable uncertainties on simulations across scales.

Hierarchical VVUQ

The large-scale problems pursued by the NNSA Labs and PSAAP Centers must typically be broken apart many times until they are represented in a manageable form. As such, there are then multiple layers across which "VVUQ as the Scientific Method" is applied. Each layer allows for inspection of different complex and nonlinear phenomena. While uncertainties in adjacent layers may be related, the greater problem lies in understanding how uncertainties across disparate layers inform each other. Similarly, dominant errors and failure modes may change drastically from one layer to another.

For example, an algorithm may show increased accuracy on simple test problems, but prove not to be robust when run on larger multi-physics simulations, or perhaps only one physics submodel breaks its otherwise splendid behavior. Similarly, conclusions intuited by comparing simulations against small-scale experiments may not be preserved when simulations are compared with large-scale experiments. Hierarchical VVUQ helps check the validity of conclusions determined at one level which may not be as strongly supported at a different level, whether going up or down the hierarchy. Moving up and down the hierarchy and pursuing what appears to be conflicting evidence is often what leads to those wonderful "Ah ha!" moments in scientific breakthroughs.

Holistic VVUQ - The sum is greater than the parts

It can be tempting to focus separately on verification or validation or UQ activities when moving up and down the hierarchical levels. Tying those activities together is not easy. However, it is this effort that helps prevent wasting resources later, especially the precious time of students and staff, or the HPC resources afforded by the national labs. If higher-order physics models also require increased mesh resolutions and longer runtimes that prevent sufficient UQ studies, perhaps the model's uncertainty does not warrant the effort; or, perhaps it does! Holistic VVUQ, pulling together the disparate VVUQ elements across hierarchical levels, can help motivate and justify complicated decisions. Choices that may seem like leaps of faith or unwarranted excursions may actually be critical junctures for your Center's success. Again, VVUQ is meant to help apply the scientific method to your specific journey: thoroughly document assumptions, accurately communicate conclusions based on current results, and address unknowns and uncertainties.

VVUQ, taken as separate pieces, may be considered core components of the scientific method for predictive scientific computing. By breaking apart complicated problems into ever-smaller pieces, problems may be efficiently and accurately analyzed, as done so naturally in the scientific enterprise. Some problems must be broken down many times in order to rigorously analyze their most elementary processes. Afterward, the original complicated problem can be synthesized at each level from its constituent parts, reconstructed, and thus better understood. This reconstruction of separate parts also helps decrease model tuning in the final analysis, thereby eliminating "knobs" for tweaking predictions. The process of deconstructing and reconstructing problems often allows for testing hidden assumptions and developing novel and testable hypotheses. Taken together, this helps improve a user's intuition and understanding relative to code output, as well as the appropriate interpretation of simulation results. It is these users who's intuition is strengthened that go on to become relevant subject matter experts.

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Lastly, Aimee Hungerford's presentation at the PSAAP Pre-Proposal Meeting in Houston, on 8 and 9 August, emphasized the importance of inter-personal skills within ASC at the national labs, as well as at PSAAP Centers. Those same inter-personal skills are just as important within any VVUQ team, especially when engaging members who may not be directly affiliated with the VVUQ team. It is always worth emphasizing the importance of kindness and courteous communication between all team members. This can be especially important when PSAAP members are preparing for site visits from NNSA Lab Staff. Please practice kindness daily. It is a practice, and a choice. And it helps all of us be able to get through stressful situations when we have focused in the past on creating and fostering supportive and collaborative environments.