SciDAC Institute – Prospectus

Quantification of Uncertainty in Extreme Scale Computations (QUEST)

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QUEST is a SciDAC Institute that is focused on uncertainty quantification (UQ) in large-scale scientific computations. Our overarching goal is to provide modeling, algorithmic, and general uncertainty quantification (UQ) expertise, together with software tools, to other SciDAC Institutes, SciDAC applications, and Office of Science projects in general—thereby enabling and guiding a broad range of UQ activities in their respective contexts.

QUEST is a collaboration among six institutions with a history of in-depth collaborations on the development, implementation, and use of UQ algorithms/software in challenging high-performance computing (HPC) environments. QUEST members are leading developers of UQ theory, methods, and software in the technical community. They have worked in all aspects of the UQ problem, and have a solid grasp of the challenges and opportunities in this area. They have developed and maintain leading UQ software products that have been applied in HPC environments, with challenging scientific application codes, including climate, geophysics, and combustion.

Key UQ software tools that are included in the QUEST universe are:

- DAKOTA (SNL) (http://dakota.sandia.gov) provides a variety of non-intrusive algorithms for design optimization, model calibration, uncertainty quantification, global sensitivity analysis, solution verification, and parameter studies. It can be used as either a stand-alone application or as a set of library services.

- UQTk (SNL) (http://www.sandia.gov/UQToolkit) is a lightweight C++ library, primarily offering tools for intrusive Galerkin uncertainty propagation. UQTk provides routines for evaluating algebraic expressions and transcendental functions of random variables represented with Polynomial Chaos expansions.

- QUESO (UT) is a MPI/C++ library that provides statistical algorithms for Bayesian inference, model calibration, model validation, and decision making under uncertainty. It naturally maps, into C++ classes, the mathematical entities present in stochastic problems and solution methods, thus enabling the easy integration of new algorithms.

- GPMSA (LANL) focuses on Bayesian inference, using a Gaussian process response surface, trained from an ensemble of forward model runs, to minimize the number of forward model calls required in the inference. It allows for global sensitivity analysis, forward propagation of uncertainty, model calibration/parameter estimation, and predictions with uncertainty.

The vision of QUEST encompasses all aspects of UQ in leadership-class computing. This includes the well-founded setup of the UQ problem; characterization of the input space given available data/information; local and global sensitivity analysis; adaptive dimensionality and order reduction; forward and inverse propagation of uncertainty; handling of application code failures, missing data, and hardware/software fault tolerance; and model inadequacy, comparison, validation, selection, and averaging. The nature of the UQ problem requires the seamless combination of data, models, and information across this whole landscape in a manner that provides a self-consistent quantification of requisite uncertainties in predictions from computational models. Accordingly, our UQ methods and tools span an interdisciplinary space across applied math, information theory, and statistics.

We see our key products as being: (1) delivering expertise, advice, and state of the art UQ tools to SciDAC and Office of Science (SC) math/CS/application projects utilizing large scale computations on leadership-class computational architectures; and (2) shepherding forward our extensive repertoire of UQ theory, algorithms, and software, and enhancing their robustness/effectiveness for relevant benchmark problems in leadership-class computational settings.

The roles of the individual QUEST institutions are designed around the leading strengths and expertise of each institution, while always relying on synergistic coupling among the overall group. The institutional roles are summarized as follows. SNL: forward UQ; UT: inverse UQ; LANL: statistics and Gaussian process surrogates; USC: adaptive probabilistic representations and intrusive methods; JHU: sparse probabilistic representations and non-intrusive methods; MIT: adaptive sampling and statistical inference.

We plan to work collaboratively, via SC Application Partnerships, with SciDAC application projects on the use of UQ in their domains. In this context, we plan to help partner projects in the use of QUEST tools, and to adapt the tools accordingly as needed. We will also work directly with other SciDAC institutes to advise them on incorporating UQ-awareness in their ongoing development of algorithms and software for leadership-class computing. We will conduct periodic tutorials and short courses on various aspects of the UQ problem, and our associated software tools.