Quantification of Uncertainty in Extreme Scale Computations (QUEST)

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Members:

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Goals

QUEST goals include:

- Deliver expertise, advice, and state of the art UQ algorithms and software tools to SciDAC projects utilizing extreme scale computations on advanced computational architectures
- Shepherd forward our extensive repertoire of UQ theory, algorithms, and software, and enhance their robustness/effectiveness for relevant benchmark problems in extreme-scale computational settings.

Scope

The scope of QUEST covers a range of UQ activities including:

- UQ problem setup
- Characterization of the input space
- Local and global sensitivity analysis
- Adaptive stochastic dimensionality and order reduction
- Forward and Inverse UQ
- Fault tolerant UQ methods
- Model comparison and validation

The QUEST team brings together a wide range of expertise in UQ methods and software development covering the above landscape, with application to large-scale computations of physical systems

Key Elements of UQ

- Probabilistic framework
  - Uncertainty is represented using probability theory
- Parameter Estimation, Model Calibration
  - Experimental measurements
  - Regression, Bayesian Inference
- Forward propagation of uncertainty
  - Polynomial Chaos methods
    - Intrusive methods
    - Non-intrusive methods
- Model comparison, selection, and validation
- Model averaging
- Experimental design and uncertainty management

Team Expertise and capabilities

- **SNL** (Najm, Debusschere, Eldred) – Forward and inverse UQ methods, design under uncertainty; DAKOTA, UQTK
- **USC** (Ghanem) – Intrusive UQ methods, probabilistic modeling
- **JHU** (Knio) – Sparse and adaptive forward UQ methods
- **UT** (Ghattas, Moser, Prudencio) – Large scale inverse problems, validation, Inverse UQ; QUESO
- **LANL** (Higdon, Gatticker) – Gaussian Process modeling, inverse UQ; GPMSA
- **MIT** (Marzouk) – Calibration, adaptive sampling, Inverse UQ, experimental design

QUEST UQ Tools – DAKOTA

- http://dakota.sandia.gov/
- Large-Scale Optimization, non-intrusive UQ
- Model calibration, global sensitivity analysis
- Design of Experiments
- solution verification, and parameteric studies
- Over 4000 download registrations
  - govt, industry, academia
- Generic interface to black-box application model
- Java front end
- Used in a wide variety of applications
- GNU LPGL license

QUEST UQ Tools – QUESO

- MPI/C++ library
- Large-scale inverse UQ
- Statistical algorithms for Bayesian inference
- model calibration, model validation,
- decision making under uncertainty
- Parallel multi-chain MCMC
- Used by many investigators at the UT Austin PSAAP center
- Being integrated with DAKOTA

QUEST UQ Tools – UQTK

- http://www.sandia.gov/UQToolkit/
- Lightweight C++ library
- Intrusive Polynomial Chaos UQ methods
- Non-intrusive sparse-quadrature UQ
- Bayesian inference
- Custom representations of uncertain information
- Well suited for prototyping, tutorial/training purposes

QUEST UQ Tools – GPMSA

- Serial matlab code – C++ conversion plans
- Integration with DAKOTA
- Bayesian inference
- Gaussian process surrogates
- Global sensitivity analysis, forward UQ
- Model calibration/parameter estimation
- Statistical models to characterize model discrepancy or structural model error
- Prototyping tool