Quantification of Uncertainty in Extreme Scale Computations (QUEST)

www.quest-scidac.org

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SciDAC PI Meeting, 10–12 Sep 2012, Rockville, MD
Outline

1. Introduction
2. QUEST Overview
3. Technical Progress
4. Closure
Introduction – Motivation

Why Uncertainty Quantification (UQ) ?

- Assessment of confidence in computational predictions
- Validation and comparison of scientific/engineering models
- Design optimization
- Use of computational predictions for decision-support
- Assimilation of observational data and model construction

Why UQ in SciDAC ?

- Explore model response over range of parameter variation
- Enhanced understanding extracted from computations
- Particularly important given cost of SciDAC computations
QUEST Goals

1. Advance the state of the art in UQ theory, methods, and software, addressing UQ challenges with extreme scale computational problems
   - High-dimensionality
   - Nonlinearity
   - Sparse data

2. Provide expertise, advice, and state of the art UQ algorithms and software tools to SciDAC projects
   - UQ software products
   - SciDAC partnerships
   - Outreach: UQ tutorials, summer school, web
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
Key Elements of our UQ strategy

- Probabilistic framework
  - Uncertainty is represented using probability theory
- Parameter Estimation, Model Calibration
  - Experimental measurements
  - Regression, Bayesian Inference
- Forward propagation of uncertainty
  - Polynomial Chaos (PC) Stochastic Galerkin methods
    - Intrusive/non-intrusive
  - Stochastic Collocation methods
- Model comparison, selection, and validation
- Model averaging
- Experimental design and uncertainty management
<table>
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<th>Institution</th>
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<th>Tools</th>
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<td>SNL</td>
<td>Forward and inverse UQ methods, design under uncertainty</td>
<td>DAKOTA UQTK</td>
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<td>USC</td>
<td>Intrusive UQ methods, probabilistic modeling</td>
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<td>Duke</td>
<td>Sparse adaptive forward UQ methods</td>
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<td>UT</td>
<td>Large scale inverse problems validation, inverse UQ</td>
<td>QUESO</td>
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<td>LANL</td>
<td>Gaussian process modeling, inverse UQ</td>
<td>GPMSA</td>
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<tr>
<td>MIT</td>
<td>Calibration, adaptive sampling, inverse UQ, experimental design</td>
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**QUEST UQ Software tools**

**DAKOTA**
- Optimization and calibration
- Non-intrusive UQ
- Global Sensitivity Analysis
- > 10K registered downloads

**QUEST UQ Software tools**

**QUESO**
- Bayesian Inference
- Parallel MultiChain MCMC
- Bayesian Model Analysis
- Model Calibration

**GPMSA**
- Bayesian Inference
- Gaussian Process Emulation
- Model Calibration
- Model discrepancy analysis

**UQTk**
- Intrusive PC UQ
- Non-intrusive sampling
- Customized sparse PCE
- Random fields
# QUEST Partnerships

<table>
<thead>
<tr>
<th>DOE</th>
<th>Project Title</th>
<th>Lead PI</th>
<th>QUEST</th>
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<td>NNSA</td>
<td>Parallel Dislocation Simulator (ParaDiS)</td>
<td>T. Arsenlis</td>
<td>Najm</td>
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<td>LLNL</td>
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<td>FES</td>
<td>Center for Edge Plasma Physics Simulation (EPSI)</td>
<td>C.S. Chang</td>
<td>Moser</td>
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<td>FES</td>
<td>Plasma Surface Interactions: Bridging from the Surface to the Micron Frontier</td>
<td>B. Wirth</td>
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<td>ORNL</td>
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<td>BER</td>
<td>Predicting Ice Sheet &amp; Climate Evolution at Extreme Scales (PISCEES)</td>
<td>P. Jones</td>
<td>Eldred,</td>
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<td>Ghattas</td>
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<td>BER</td>
<td>Multiscale Methods for Accurate, Efficient &amp; Scale-Aware Earth System Modeling</td>
<td>B. Collins</td>
<td>Debusschere</td>
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<td>NP</td>
<td>Nuclear Computational Low Energy Initiative (NUCLEI)</td>
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<td>HEP</td>
<td>Computation-Driven Discovery for the Dark Universe</td>
<td>S. Habib</td>
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<td>HEP</td>
<td>Community Project for Accelerator Science &amp; Simulation (ComPASS)</td>
<td>P. Spentzouris</td>
<td>Prudencio</td>
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Outreach Activities

- **Website**
  - www.quest-scidac.org
  - Production version will be publicly accessible soon

- **UQ Tutorials in workshops/conferences**
  - SAMSI UQ workshop, Raleigh, NC; Sep 7-9, 2011
  - SIAM Conference on UQ, Raleigh, NC; Apr 2-5, 2012

- **UQ Summer School**
  - USC, LA; Aug 22-24, 2012

- **UQ Tools Tutorial**
  - Hands-on practice with UQ software tools
  - Announcements went out in late July
  - [http://cadmus.usc.edu/Quest-Tutorial](http://cadmus.usc.edu/Quest-Tutorial)
    - Some openings still available
M. Eldred, J. Jakeman

- Development of interfaces: QUESO–DAKOTA–GPMSA
  - Ongoing
  - DAKOTA interfaces to both
  - C++ GPMSA implementation using QUESO components

- Stochastic collocation
  - Nodal or hierarchical interpolation on structured grids
  - Interpolants may be local or global
    - value-based or gradient-enhanced
  - Automated refinement
    - uniform, dimension-adaptive, or locally-adaptive
  - Hierarchical surplus error estimates for values and gradients applied to QoI (e.g., response covariance)

- Compressive sensing: basis pursuit and basis denoising
Work with CASL energy innovation hub

PCE/SC with uniform/adaptive refinement vs LHS

\[ n = 4, \text{ smooth, mild anisotropy} \]

\[ n = 10, \text{ discontinuous, high anisotropy} \]
B. Debusschere, C. Safta, K. Sargsyan

- Version 1.0 published under the GNU LGPL
  - Intrusive PC functionality
- New release targeted for Fall 2012
  - Intrusive and non-intrusive utilities
  - User-specified multi-index capabilities
    - Flexible efficient sparse tensor representations
    - Effective for high-dimensional systems
  - Random fields:
    - Covariance matrix estimation (many samples)
    - Karhunen-Loève expansions (KLEs)
- Matlab version
- Example/benchmark problems, tutorial materials
Hierarchical interpolation with generalized sparse grids
  - Gradient-enhancement
  - Error indicators leverage both value and gradient surpluses

Building Sparse PC representations
  - Compressed Sensing (CS) – $\ell_1$ regularization
    - cross validation, tolerances for model choice
  - Bayesian Compressed Sensing (BCS) – Laplace priors
  - BCS/CS comparisons on Genz functions – 5-10d
    - Similar convergence with no. of samples
    - Slightly higher accuracy with CS
    - BCS: $O(100) \times$ reduction in no. of PCE terms

discovery of sparse signals:
SNL: Algorithms: Missing Data
H. Najm, B. Debusschere, C. Safta, K. Sargsyan, K. Chowdhary

Context
- Missing/failed measurements or computational samples
- Partial specification of uncertain information
  - Error bars vs. joint PDF
- Processed data products

Imputation methods
- Existing data $\Rightarrow$ probabilistic prediction of missing data

Data Free Inference (DFI) algorithm
- Given information $\Rightarrow$ probabilistic models of missing data
  - Application in chemical ignition
  - Extension to processed data products
LANL: GPMSA & BART Developments
D. Higdon, J. Gattiker

- New release of GPMSA for sensitivity analysis and computer model calibration using Bayesian methods
  - Tutorial material
  - Range of sample problems
    - sensitivity, calibration, & multivariate output

- Prototype parallel implementation of the Bayesian additive regression tree (BART) for HPC.
  - linear scaling up to $\sim 50p$
  - tests with higher proc counts in progress
UT-Austin: Scalable Parallel Algorithms for Extreme-Scale Stochastic Inverse Problems  
T. Bui-Thanh, O. Ghattas, J. Martin, G. Stadler (also funded by AFOSR and NSF)

Stochastic Inverse Probs:
- PDEs & high-dim parameter spaces (from discretized fields)
- Current methods are prohibitive

Challenges:
- appropriate choice of prior
- consistent discretizations (guarantee convergence to infinite-dim problem)
- scalable parallel MCMC algorithms

Recent accomplishments:
- Consistent discretizations via appropriate mass matrix weightings
- Prior defined by inverse of elliptic operator; carried out by multigrid
- Low rank approximation of Hessian enables sampling of Gaussianized posterior in dimension-independent number of forward solves
- Scaling to 1M parameters and 100K processor cores
Example: Extreme-scale Seismic Inversion
T. Bui-Thanh, O. Ghattas, J. Martin, G. Stadler

- Linearized 3D global seismic inversion
- 1.07M earth model parameters
- 630M wave propagation unknowns
- 100K cores on Jaguar (ORNL)
- $2000 \times$ reduction in effective problem dimension due to low rank approx

- Top row: Prior samples
- Bottom row: Posterior samples
- Difference between rows indicates information gained from (and uncertainty reduced due to) data
- Gordon Bell Prize finalist, SC12
UT-Austin: Software: QUESO
K. C. Estacio-Hiroms, E. E. Prudencio, K. W. Schulz (also funded by NNSA)

- Improvement of QUESO-DAKOTA usability
  - Periodic output of samples
  - Output of extra information
  - Informative output summary

- Implementation of GPMSA models and algorithms
  - QUESO capabilities will be usable through DAKOTA

- Preparation of tutorial material
  - Bayesian inversion, and forward propagation of uncertainty
  - Object-oriented mapping of mathematical concepts
  - Solution of statistical inverse problems with DRAM MCMC
  - Solution of statistical forward problems with Monte Carlo
  - Use of parallel computing for statistical analysis
  - References to Bayesian analysis, MCMC, Monte Carlo, C/C++, MPI
Developed a multiscale Bayesian preconditioning approach
- Demonstrated capability to simultaneously
  - address stiffness and noise
  - represent noisy outputs w/sparse, low-order, PCEs
- Order of magnitude reduction in # of samples / replicas
Developed a sparse adaptive pseudospectral sampling algorithm
  - accommodates arbitrary admissible stencils
  - including a maximal polynomial basis
    - without internal aliasing

Analysis of algorithm performance based on existing Ocean General Circulation Model (OGCM) databases

Demonstrated order-of-magnitude computational savings in simulations of the ocean circulation in the Pacific
MIT: Large-Scale Bayesian Inference
T. Moselhy, Y. Marzouk

Current state of the art

- Markov chain Monte Carlo (MCMC) sampling is the *workhorse algorithm* for Bayesian inference and prediction
- Challenges: enormous computational effort, difficult proposal design, insufficient convergence diagnostics

Inference with optimal maps

- *New approach*: find a deterministic map that *pushes forward* the prior measure to the posterior measure
- Converts inference to an optimization problem, with natural convergence diagnostics
- Outperforms MCMC in efficiency and accuracy on a variety of inference problems, with $10^3$ dimensions or more
(above) sequence of maps yields samples from non-Gaussian posterior in a chemical kinetic system

Current work on map-based inference:
- Hierarchical Bayesian models
- Parallel algorithms for stochastic optimization
- Sequential data assimilation (i.e., filtering and smoothing)
MIT: Optimal Experimental Design
X. Huan, Y. Marzouk

How to choose observations or experimental conditions **optimally**?
- Bayesian approach: maximize *expected information gain* for parameter inference, prediction, model discrimination, etc

Key computational ingredients:
- Surrogates for physical model describing experiments
- Statistical estimators and stochastic optimization methods

Recent accomplishments: **stochastic approximation** and **sample-average approximation** for optimal Bayesian design, using estimators of mutual information gradient
USC: Constrained & Adaptive Constructions
E. Kalligiannaki, R. Tipireddy, G. Ghanem

Develop Constrained Stochastic Representations
- Positive random variables
- More general constraints on either function values or values of nonlinear functionals of the random variables

Develop Bases Adapted to Quantity of Interest
- Scales linearly with stochastic dimension
\[ \mathcal{I} = \{ y(\omega) \in L_2(\Omega, \Sigma(H), P) : y(w) \text{ satisfies constraints } \forall \omega \} \]

The projection of \( y \in L_2 \) on \( \mathcal{I} \):

- Sample from prior PC expansion
- Delete realizations that do not satisfy constraints
- Recompute PC coefficients from remaining realizations

Initial data, \( u(0) = U = 0.2 + U_1 \xi \):

- \( U_1 = 0.08 \), \( N_s = 10^4 \), \( N_t = 150 \)
- \( U_1 = 0.08 \), \( N_s = 10^4 \), \( N_t = 200 \)
- \( U_1 = 0.08 \), \( N_s = 10^4 \), \( N_t = 10 \)
- \( U_1 = 0.08 \), \( N_s = 10^4 \), \( N_t = 0 \)

Improve Convergence of Stochastic ODE

Generator for constrained populations
Expand $u(\xi)$: polynomials in $\eta = A\xi$

- with proper choice of $A$, the measure of the solution is concentrated along leading $\eta_1$ dimension
- $A$ is chosen so that $\eta_1$ contains all Gaussian content of QoI
Closure

- Work on UQ software and algorithms development
  - Computational efficiency
  - Functionality, usability, scalability
  - Adaptivity, sparsity, preconditioning
  - Reduced-order, low-rank
  - Convergence, stability
  - Partial information, missing data

- Robustifying algorithms for large-scale applications
- Software integration well along the way
- Outreach via web, tutorials, and summer school
- SciDAC partnership activities getting off the ground