SAND2017-1578C

An Overview of the QUEST Institute

www.quest-scidac.org

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Sandia National Laboratories,
Livermore, CA

ASCR-SciDAC / BER-BSSD Discussions
Jan 2017

QUEST SciDAC Institute

- QUEST is focused on Uncertainty Quantification (UQ) in extreme scale computations

- Our team includes:
  - Sandia National Labs (SNL), both CA and NM
  - University of Southern California (USC)
  - Los Alamos National Laboratory (LANL)
  - University of Texas at Austin (UT)
  - Duke University (DU)
  - Massachusetts Institute of Technology (MIT)

QUEST Team

Institution	Participants
SNL	**H. Najm**, M. Eldred, B. Debusschere, J. Jakeman, K. Chowdhary, C. Safta, K. Sargsyan, P. Rai
USC	**R. Ghanem**
DU	**O. Knio**, O. Le Maître, J. Winokur
UT	**O. Ghattas**, R. Moser, C. Simmons, A. Alexanderian T. Bui-Thanh, N. Petra, G. Stadler
LANL	**J. Gattiker**, D. Higdon, S. Bhatt, E. Lawrence
MIT	**Y. Marzouk**, P. Conrad, T. Cui, A. Gorodetsky

Team Expertise and Capabilities

Institution	Expertise	Tools
SNL	Forward and inverse UQ methods, design under uncertainty	DAKOTA UQTK
USC	Intrusive UQ methods probabilistic modeling	
DU	Sparse adaptive forward UQ methods	
UT	Large scale inverse problems validation, inverse UQ	QUESO
LANL	Gaussian process modeling, inverse UQ	GPMSA
MIT	Calibration, adaptive sampling, inverse UQ, experimental design	MUQ

QUEST Goals

Advance the state of the art in UQ theory, methods, and software, addressing UQ challenges with extreme scale computational problems

- High-dimensionality
- Large range of scales
- Model complexity and computational costs

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

Why UQ? Why in SciDAC?

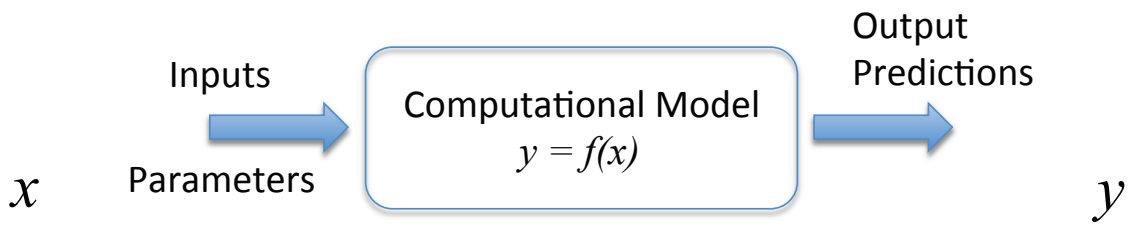
Why UQ?

- 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?

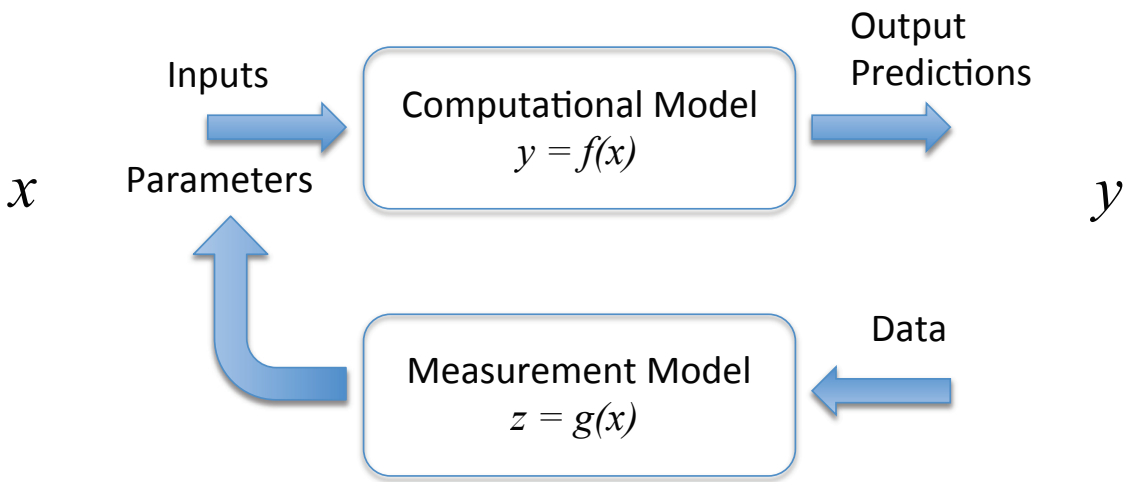
- Explore model response over range of parameter variation
- Enhanced understanding extracted from computations
- Particularly important given **cost** of SciDAC computations

Uncertainty Quantification and Computational Science



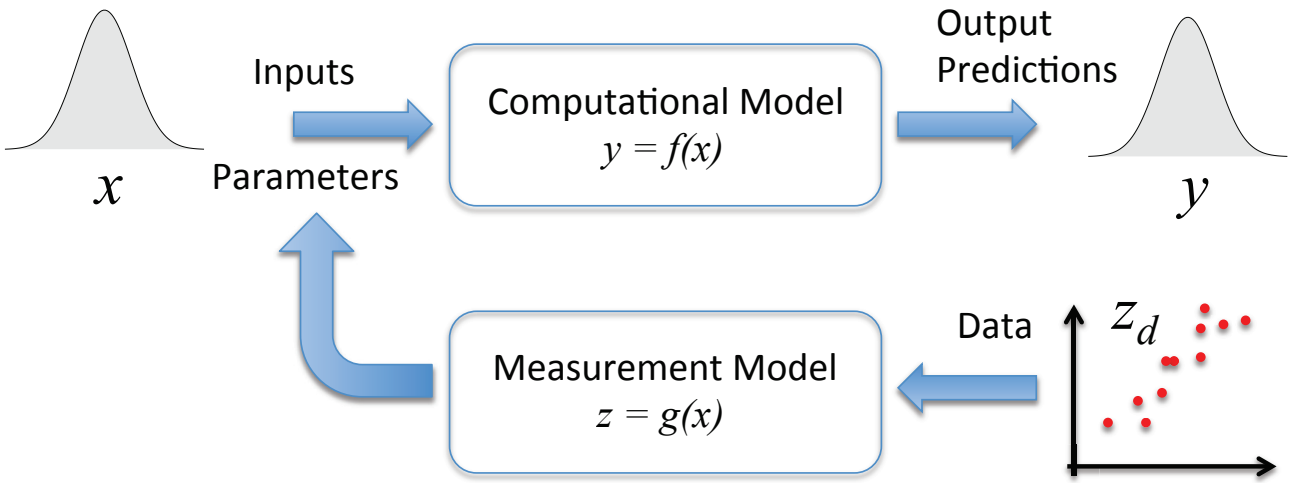
Forward problem

Uncertainty Quantification and Computational Science



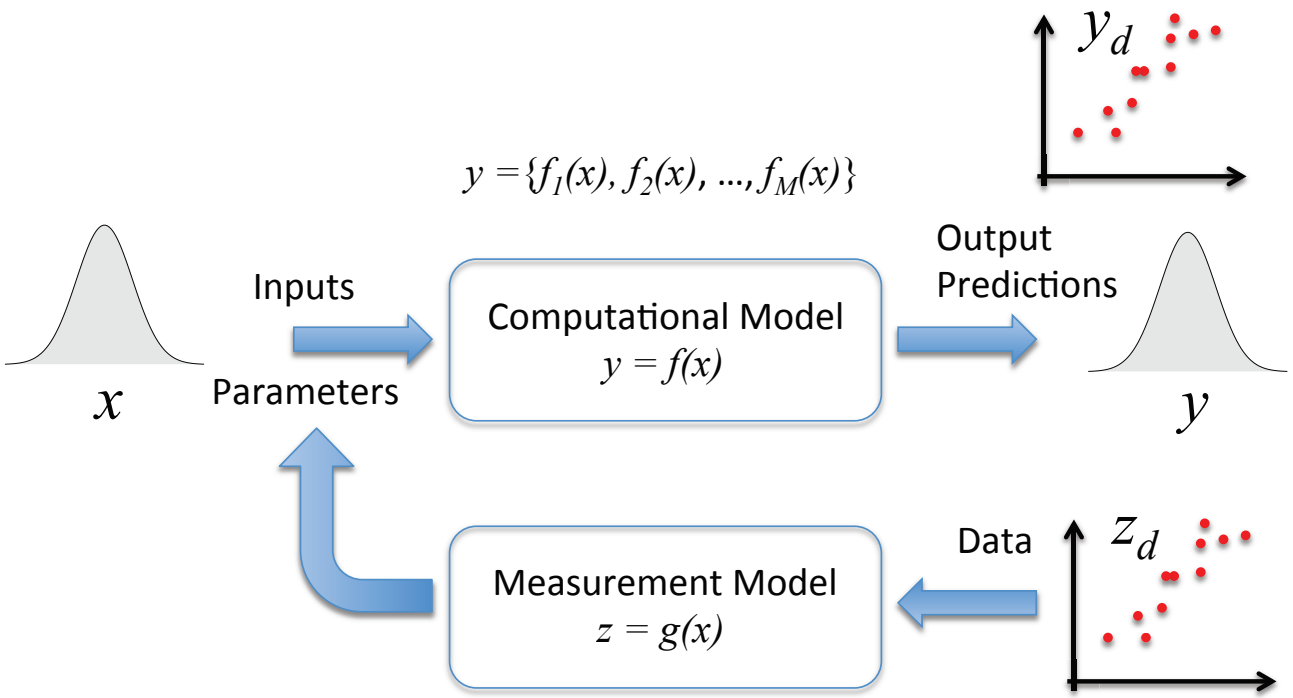
Inverse & Forward problems

Uncertainty Quantification and Computational Science



Inverse & Forward UQ

Uncertainty Quantification and Computational Science



Inverse & Forward UQ

Model validation & comparison, Hypothesis testing

QUEST Scope

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

- 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
- Experimental design and uncertainty management

QUEST UQ Software tools

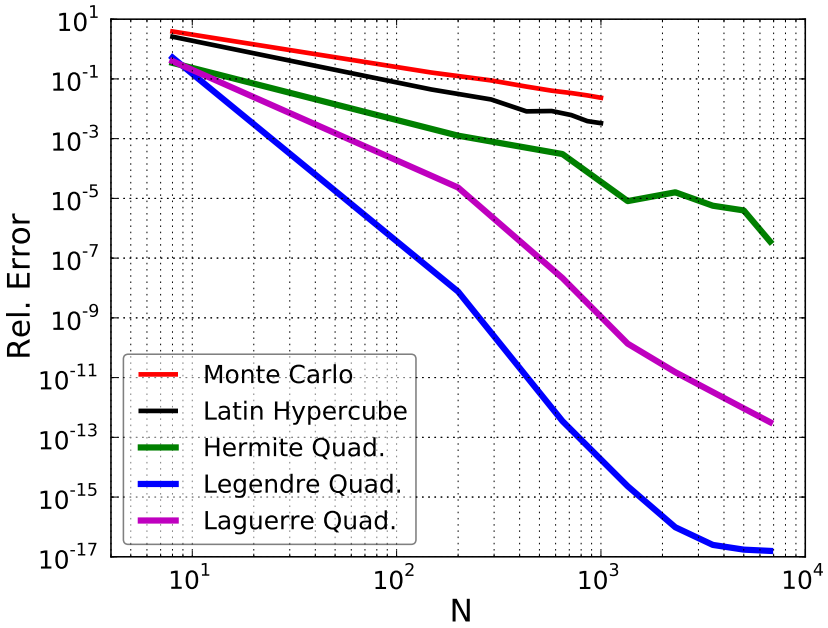
- **DAKOTA:** Optimization and calibration; non-intrusive UQ; global sensitivity analysis; $\sim$10K registered downloads.
- **QUESO:** Bayesian inference; multichain MCMC; model calibration and validation; decision under uncertainty.
- **GPMSA:** Bayesian inference; Gaussian process emulation; model calibration; model discrepancy analysis.
- **UQTk:** Intrusive and non-intrusive forward PC UQ; custom sparse PCE; random fields.
- **MUQ:** Adaptive forward PC UQ; advanced MCMC and variational methods for inference; efficient surrogates.

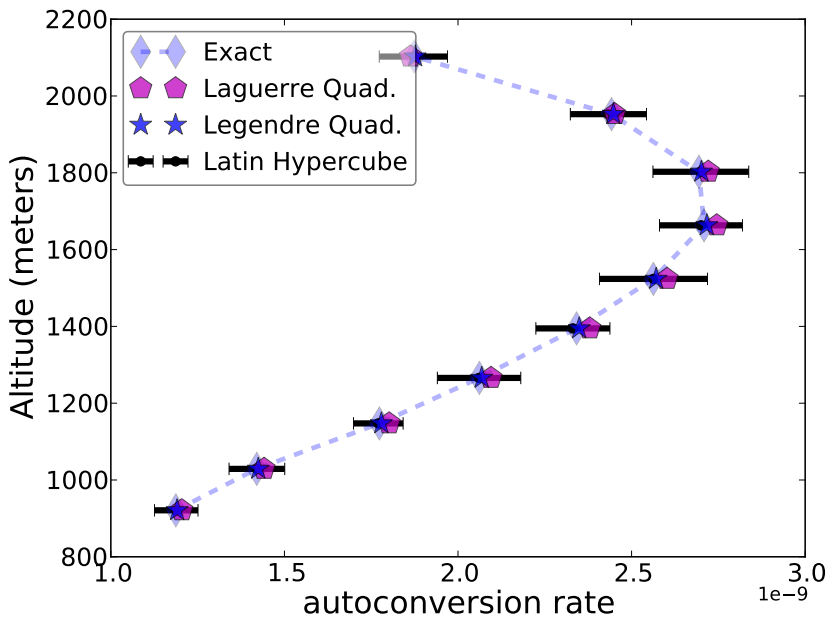
QUEST Partnerships

DOE	Project Title	Lead PI	QUEST
FES	Center for Edge Plasma Physics Simulation (EPSI)	Chang Princeton	Moser UT
FES	Plasma Surface Interactions: Bridging from the Surface to the Micron Frontier	Wirth ORNL	Higdon, Knio LANL, DU
BER	Predicting Ice Sheet & Climate Evolution at Extreme Scales (PISCEES)	Jones LANL	Eldred, Ghattas SNL, UT
BER	Multiscale Methods for Accurate, Efficient & Scale-Aware Earth System Modeling	Collins LBNL	Debusschere SNL
BES	Adaptive Sparse Quadrature Methods for Fast Evaluation of MP2 Integrals (FEMPI)	Hirata UIUC	Najm, Sargsyan SNL
BES	Interfacial Dynamics in Radioactive Environments and Materials (IDREAM)	Clark PNNL	Debusschere SNL
BES	Center for Performance and Design of Nuclear Waste Forms and Containers (WastePD)	Frankel OSU	Najm SNL
BES	Center for Hierarchical Waste Form Materials (CHWM)	zur Loye UofSC	Eldred SNL
NP	Nuclear Computational Low Energy Initiative (NUCLEI)	Carlson LANL	Higdon LANL
HEP	Computation-Driven Discovery for the Dark Universe	Habib ANL	Higdon LANL
HEP	Community Project for Accelerator Science & Simulation (ComPASS)	Spentzouris FNAL	Simmons UT

Impact on Partnership Projects – Earth-System

QUEST tools and expertise have enabled the use of quadrature approaches to **dramatically improve the efficiency and accuracy of integrating microphysics processes** over subgrid variability in atmospheric simulations.

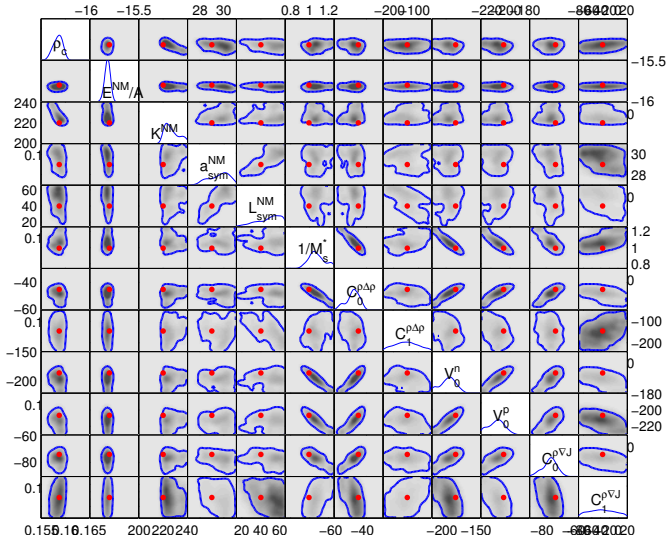




Bert Debusschere, SNL

Impact on Partnership Projects – NUCLEI

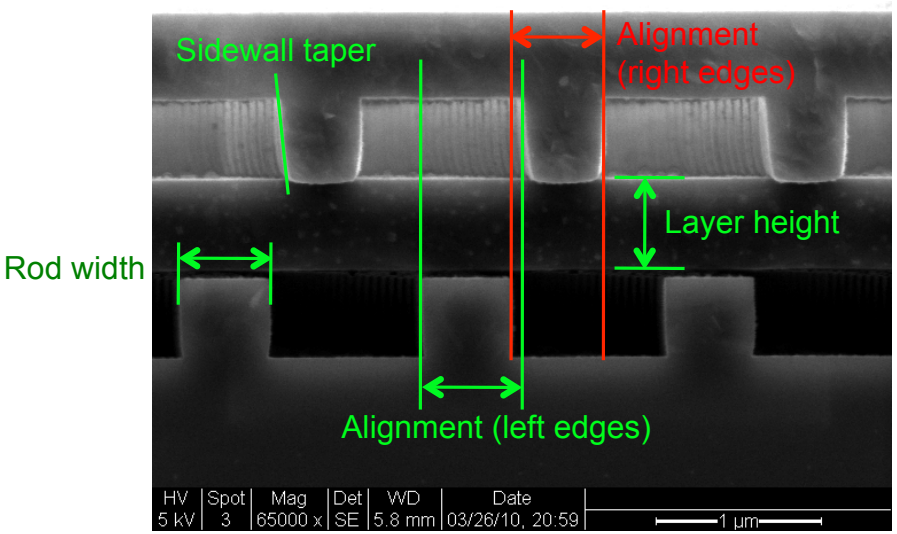
- Quantification of uncertainties in coupling constants in DFT code by combining an ensemble of DFT calculations and experimental measurements
- **Predictions and uncertainties for newly measured mass at Argonne Nat. Lab. (ANL)**
- Assessment of impact of new ANL measurements on prediction and coupling constant uncertainties.

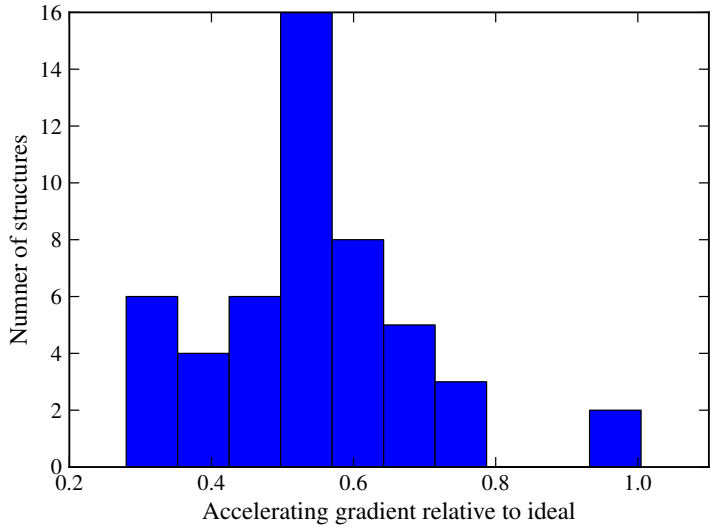


Dave Higdon, LANL

Impact on Partnership Projects – ComPASS

- By applying UQ tools to the simulation of woodpile structures, we have been able to study the effect of lithographic fabrication errors on device performance
- **Progress on fabrication of components for next-generation particle accelerators**





Chris Simmons, UT

QUEST website: www.quest-scidac.org

QUEST
Quantification of Uncertainty in Extreme Scale Computations
A SciDAC Institute funded by the DOE Office of Science

U.S. DEPARTMENT OF ENERGY
Office of Science

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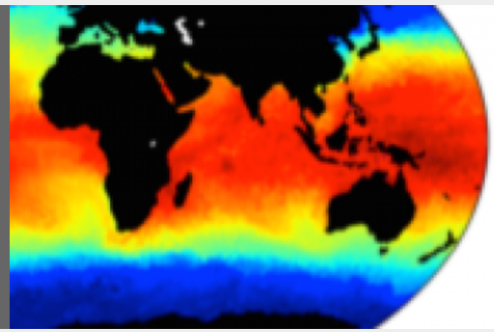
ABOUT QUEST

QUEST is a SciDAC Institute that is focused on uncertainty quantification (UQ) in large-scale scientific computations.



Recent Accomplishments

Low rank approximation based quadrature for fast evaluation of quantum chemistry integrals

January 20, 2017 *Comments are off*

Authors: Prashant Rai, Khachik Sargsyan, Habib Najm, Mathew Hermes and So Hirata Electronic structure calculations have been developed as a powerful tool that are used in several fields including chemical sciences, biochemistry, material and energy sciences. In quantum chemistry, accurate estimation of energy

Continue Reading ?

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Software Menu

- DAKOTA
- UQTk
- QUESO
- GPMSA
- MUQ

Participants

QUEST is comprised of six participating institutions, namely: Sandia National Laboratories, Los Alamos

UQ Methods

A central theme underlying our UQ methods is our use of a probabilistic representation of uncertain quantities, as