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Overview of the QUEST Institute

www.quest-scidac.org

H. Najm

Sandia National Laboratories, Livermore, CA

SciDAC Institutes MidTerm Review Meeting
5–6 May 2014
Washington, DC

Acknowledgement

SNL	M. Eldred, B. Debusschere, J. Jakeman, K. Chowdhary, C. Safta, K. Sargsyan
USC	R. Ghanem
Duke	O. Knio, O. Le Maître, J. Winokur
UT	O. Ghattas, R. Moser, C. Simmons, A. Alexanderian T. Bui-Thanh, N. Petra, G. Stadler
LANL	D. Higdon, J. Gattiker
MIT	Y. Marzouk, P. Conrad, T. Cui, A. Gorodetsky

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- US Department of Energy (DOE), Office of Advanced Scientific Computing Research (ASCR), Scientific Discovery through Advanced Computing (SciDAC)

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Outline

QUEST SciDAC Institute

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

- Our team includes:
  - Sandia National Labs (SNL), both in 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
USC	**R. Ghanem**
Duke	**O. Knio**, O. Le Maître, J. Winokur
UT	**O. Ghattas**, R. Moser, C. Simmons, A. Alexanderian T. Bui-Thanh, N. Petra, G. Stadler
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Team Expertise and Capabilities

Institution	Expertise	Tools
SNL	Forward and inverse UQ methods, design under uncertainty	DAKOTA UQTK
USC	Intrusive UQ methods probabilistic modeling	
Duke	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

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

Why UQ? Why in SciDAC?

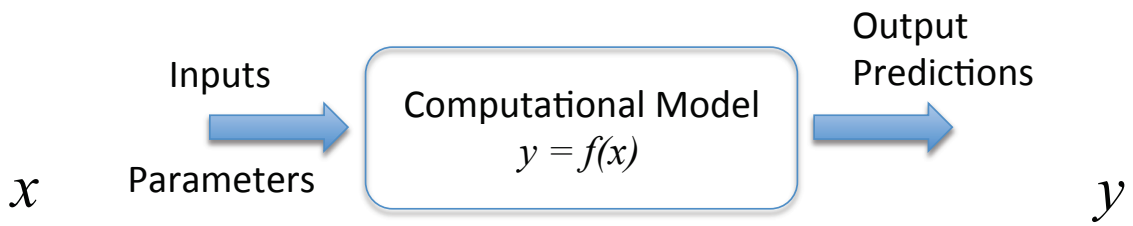
Why Uncertainty Quantification (UQ) ?

- 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 ?

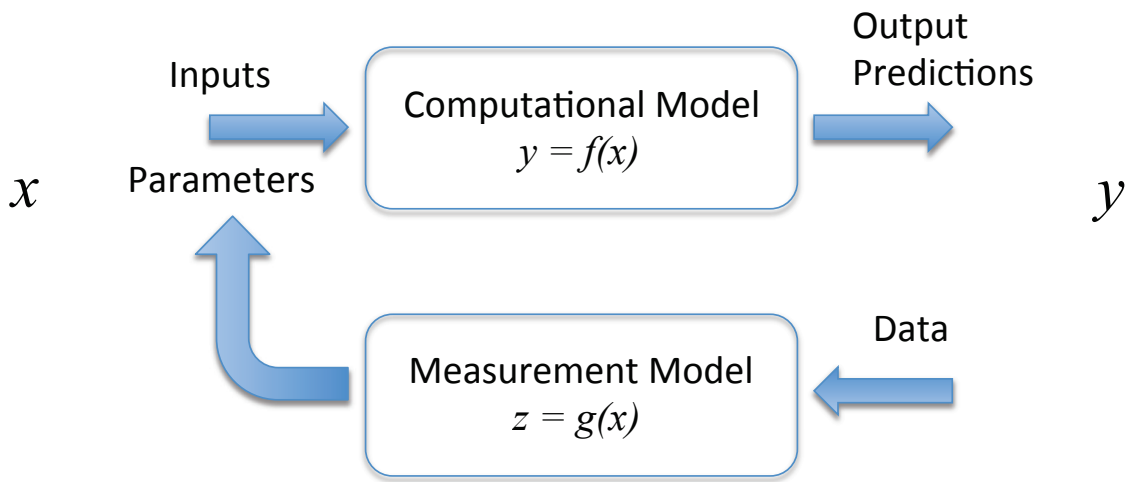
- Explore model response over range of parameter variation
- Enhanced understanding extracted from computations
- Particularly important given *cost* of SciDAC computations

Uncertainty Quantification and Computational Science



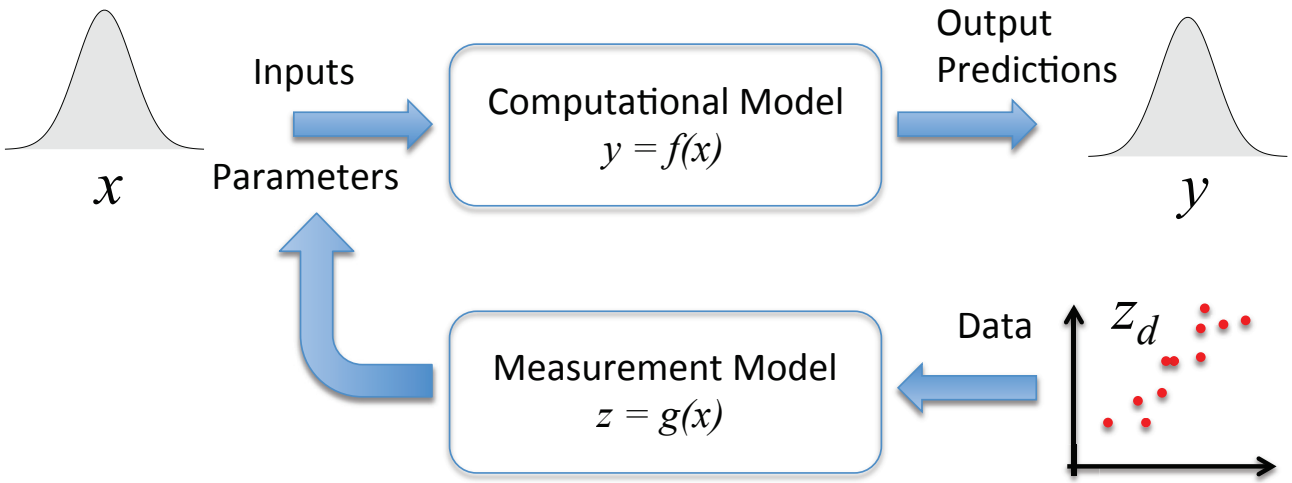
Forward problem

Uncertainty Quantification and Computational Science



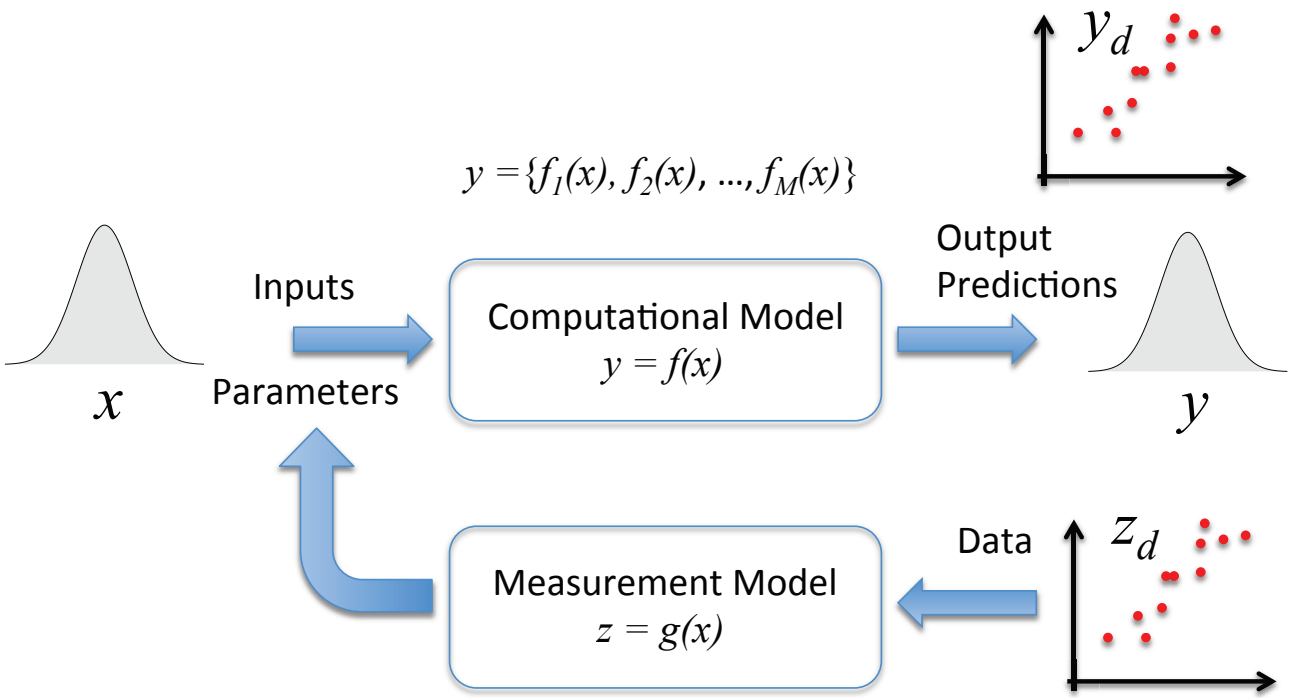
Inverse & Forward problems

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

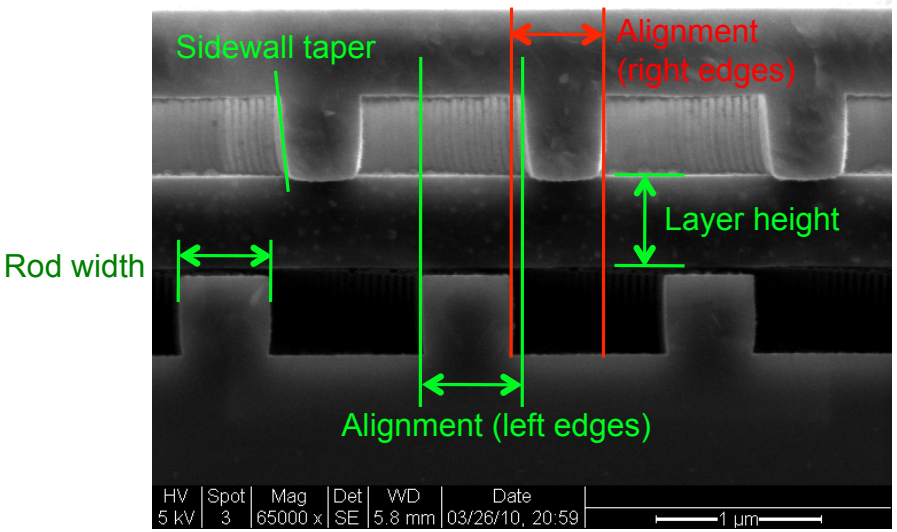
- **DAKOTA:** Optimization and calibration; non-intrusive UQ; global sensitivity analysis; $\sim$10K registered downloads.
- **QUESO:** Bayesian inference; multichain MCMC; model calibration and validation; decision under uncertainty.
- **GPMSA:** Bayesian inference; Gaussian process emulation; model 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.

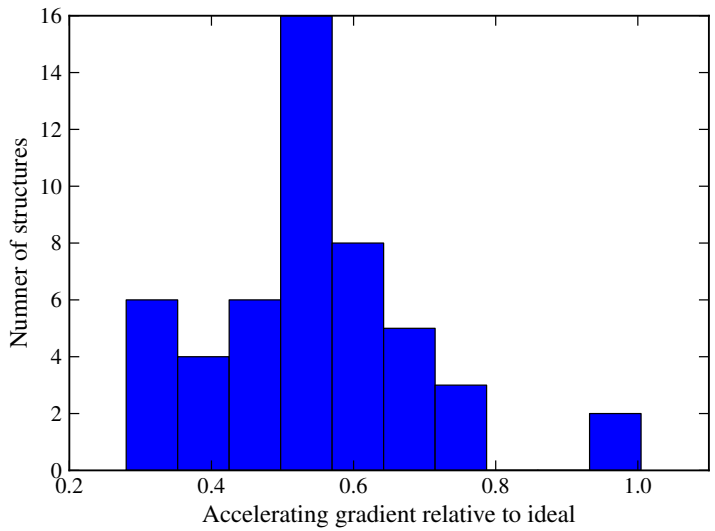
QUEST Partnerships

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 LANL
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
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	Prudencio UT

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**



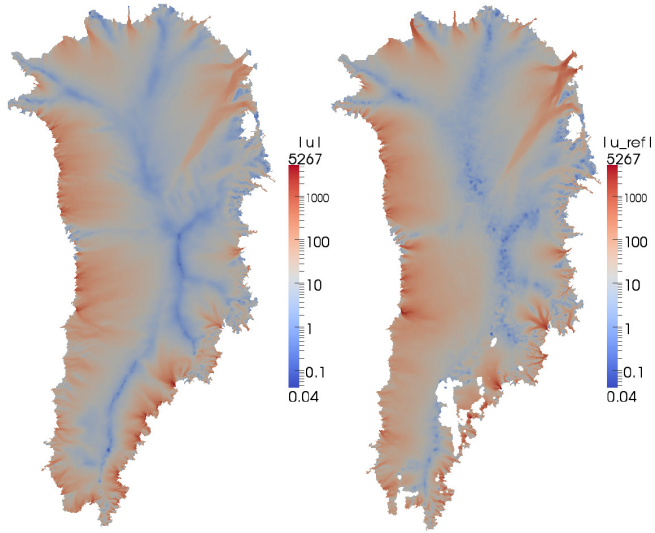


Chris Simmons, UT

Impact on Partnership Projects – PISCEES

- The interactions with QUEST team members have been, and will continue to be, crucial in defining a tractable and defensible UQ workflow, and in **providing scalable algorithms and software for this work**.

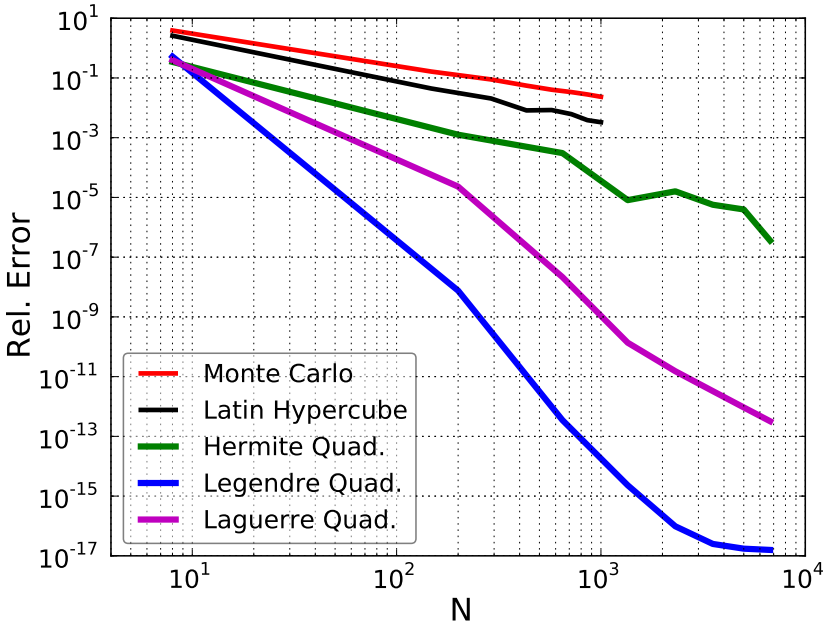
- The software linkage between the QUEST (Dakota, QUESO) and FASTMath (Trilinos) tool sets has **allowed us to overcome software challenges** and leverage their ongoing investments in exploiting both coarse-grained ensemble and fine-grained solver parallelism on leadership class architectures.

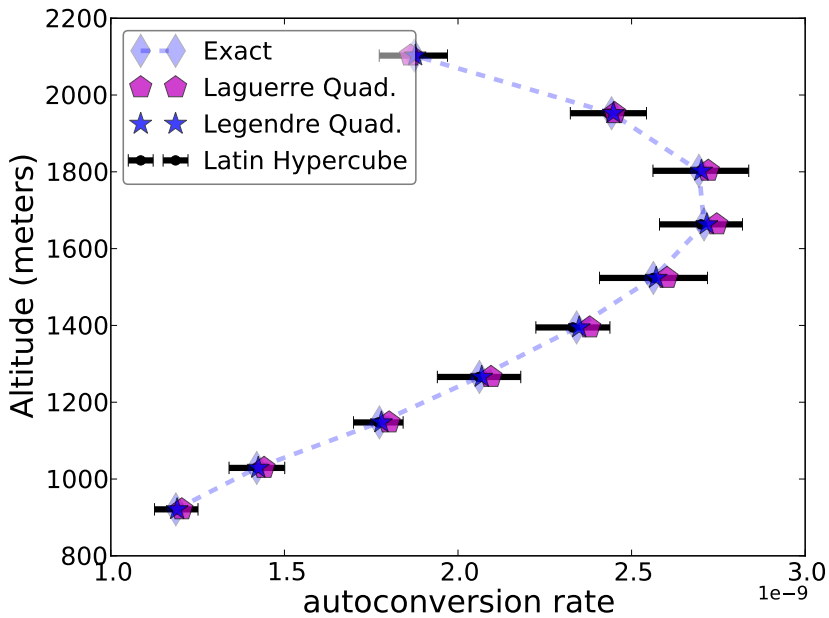


Mike Eldred, SNL

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.

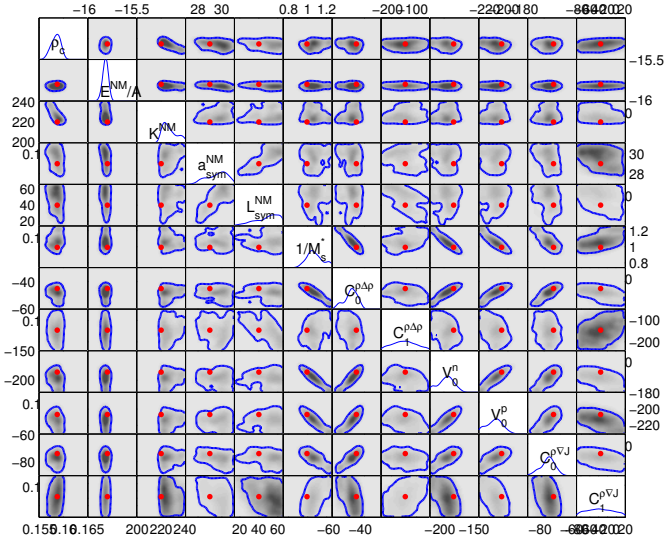




Bert Debusschere, SNL

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 ANL**
- Assessment of impact of new ANL measurements on prediction and coupling constant uncertainties.

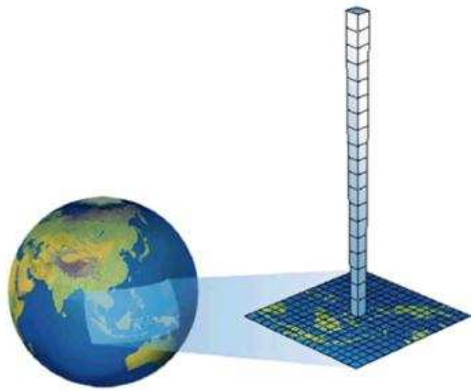


Dave Higdon, LANL

Impact on Partnership Projects – ACES4BGC

- The advances in compressive sensing developed by QUEST have enabled ACES4BGC researchers to design and conduct perturbed parameter climate model ensembles over an extremely high number of UQ dimensions.

- Prior UQ methods limited the dimensionality of climate model ensembles to $O(10)$ UQ parameters.
- QUEST's advances have enabled the push to climate systems with $O(100)$ or more UQ parameters.



Single Column CAM
Don Lucas, LLNL

Impact on DOE research outside of SciDAC

UQTk:

- BES – Chemical Sciences:
  - parameter estimation in hydrocarbon fuel ignition
  - UQ in large eddy simulations of turbulent combustion
- BER – climate research – Community Land Model (CLM)
  - Global sensitivity analysis, sparse surrogate construction

MUQ:

- BES – Mechanical Behavior & Radiation Effects program
  - Model surrogates/emulators
  - Bayesian inference with complex phase-field models of separation and permeation.

Impact on DOE research outside of SciDAC

DAKOTA:

- NNSA/ASC – a broad range of weapon assessment activities within the tri-lab defense programs complex
- EERE A2E, ASCR UQ – wind turbine design
- NE/CASL – light water nuclear reactors
- BER/CSSEF – global climate modeling

QUESO

- NE/CASL – Bayesian inference, parameter estimation
- PSAAP – reentry vehicle modeling

GPMSA

- NNSA/stockpile stewardship
- PSAAP – UMich Radiative shock models

General Impact

- Active publication output in refereed journals – 45 papers
  - Int. J. UQ, Comput. Geosci., SIAM/ASA J. UQ, CMAME, Technometrics, Annals of Nuc. Eng., J. Glaciol. etc ... – www.quest-scidac.org/publications
- Transformational discussions with partnership PIs/staff
  - UQ new to computational scientists and SciDAC
  - Raised awareness of quality/provenance of model inputs
  - Revised attention to data sources, and new data, to better pin-down model inputs (PSI/Xolotl)
- Intensive outreach activities
  - QUEST website – tutorials, information
  - Tutorials in workshops/conferences, short courses
  - USC UQ summer school
  - Invited seminars and plenary lectures

General Impact

- Leadership in the UQ field. QUEST members are:
  - Chairs and organizers of international technical conferences
  - Members of leadership teams of numerous large research collaborations
  - Members of international UQ research centers advisory boards
    - KAUST SRI-UQ, UK EQUIP, SAMSI, MUCM
- Tech transfer, working with industrial partners
  - Pratt & Whitney, Lockheed Martin, GE, Goodyear, Caterpillar
  - Use of UQ for speeding up design & manufacturing

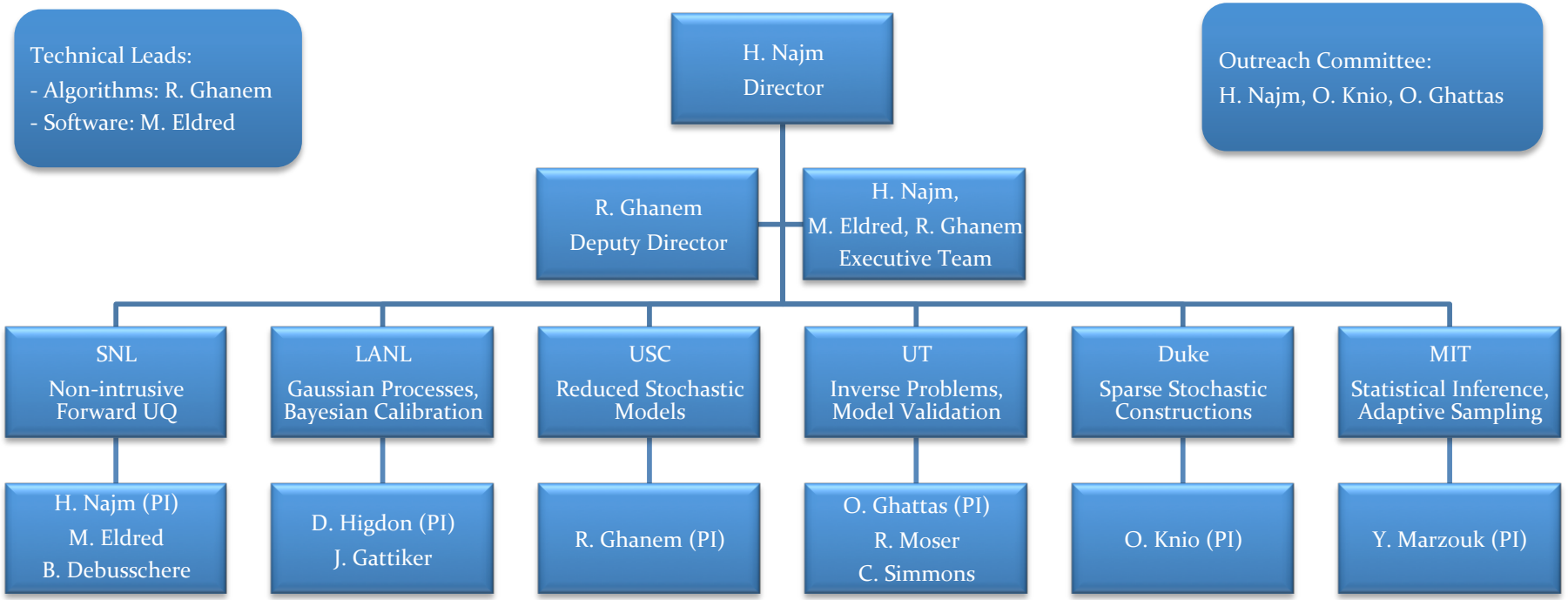
Synergies within QUEST

- MIT/DU: application of adaptive sparse quadrature for UQ in computations of Gulf of Mexico oceanic circulation
  - MIT: algorithms/software
  - DU: performance, benchmarking, large-scale code
- DU/SNL-CA: development of UQTk
  - SNL-CA: C++ libraries; DU: Matlab code
- USC/SNL-CA: model uncertainty, model error embedding
- SNL-CA/NM: benchmarking (Bayesian) compressive sensing methods – sparsity in high-dimensional models
- LANL/UT/SNL-NM: emulator-based Bayesian inference through the integration of GPMSA, QUESO, and DAKOTA

Scope relative to other SciDAC Institutes

- Recognize and make use of synergies with:
- FASTMath: math and algorithms for UQ in computations
  - UQ workflow and Trilinos solvers for large-scale eigenoslvers for random field modeling.
  - Integration of dimension-reduction algorithms in Albany
- FASTMath/SUPER: software for mgmt of concurrent code samples and associated I/O on parallel hardware
  - SUPER: Optimizing UQ workflows; simulation feedback for hard/soft fault tolerance and computational steering
- SDAV: analysis of experimental/computational data
  - Ensemble visualization; integration of UQ in ADIOS
  - Multimodel ensembles; model probability and predictions

QUEST Org Chart



Institute Mgmt

- Guiding set of 5-year milestones
- Key metrics of success:
  - Advancing robust UQ methods/software for extreme-scale applications
  - Addressing UQ challenges presented by partnerships
- Bi-weekly institute-wide telecon
  - Institutional PIs manage internal progress at each institution
- Annual workshop
  - Attendance by delegates from other institutes/partnerships
  - Communicate progress on institute/partnership work
  - Synchronize on collaborative activities

Application Partnership Strategy

- Interactions with proposal teams starting at pre-proposal stage
- Partner-PIs have typically contacted the institute director
- Pairing partnership with a specific QUEST scientist POC employed a well-articulated set of principles
  - Technical match, physical proximity, cost/budget, workload balance
- Director, in consultation with one or more QUEST-PIs, makes the assignments
- We participated in 51 pre-proposals, 29 full proposals, and 7 funded partnerships
- Supplemental requests lead to funding enhancement and a new 8th partnership

Interactions with the other Institutes

- Director-level bi-weekly telecons with DOE
- Mutual invitations to our/their annual workshops
- Existing and growing connections maintained via discussions at SciDAC PI mtg, as well as other scientific conferences of mutual interest

Three Year Roadmap – FY14

1. Fault-tolerant UQ. Benchmark problems. Improve parallel scalability – hybrid MPI+threading, concurrency in iterator recursions, distributed scheduling [SNL]
2. Adaptive basis representations [USC]
3. HPC-aware surrogates in GPMSA; integrate in DAKOTA [LANL]
4. Adaptive capabilities in statistical inversion algorithms and software – multimodal distributions [UT]
5. Stochastic model analysis and reduction. Benchmarks for forward UQ in multiscale time-dependent systems [DU]
6. Develop and implement flexible Bayesian approaches for stochastic input characterization [MIT]

Three Year Roadmap – FY15

1. Effective resource utilization – improved parallel scalability, fault tolerance – UQ in large scale benchmark problems on high end DOE/SC computational platforms [SNL]
2. Stochastic surrogates; PCEs w/random coefficients [USC]
3. Error models accounting for model discrepancy [LANL]
4. Apply statistical inversion and model assessment tools to benchmark large-scale stochastic inverse problems. [UT]
5. Demo combined optimal sampling and representation for large-scale space and time-dependent systems. [DU]
6. Dimensionality reduction algorithms in large-scale statistical inverse problems, leveraging reduced-order stochastic representations for forward UQ. [MIT]

Three Year Roadmap – FY16

1. Eval our success measured by our effectiveness in serving SciDAC partners; Identify areas for improvement. [SNL]
2. Implement algorithms for data-driven basis enrichment and adaptation. [USC]
3. Integrate model discrepancy software into GPMSA. [LANL]
4. Scale up & robustify statistical inversion to exploit massive concurrencies provided by leading edge systems. [UT]
5. Demo sparse representation, stochastic reduction, and inference with extreme-scale model outputs. [DU]
6. Develop large-scale concurrent adaptive sampling strategies for inversion with computationally intensive forward models, fully implemented in MUQ. [MIT]

Closure

Steady progress over the past 2.5 years

- Refining and robustifying QUEST algorithms and software to address UQ challenges in large-scale problems
  - high dimensionality
  - large range of scales
  - complex models and high computational cost
- Addressing UQ needs of SciDAC application partnerships

Roadmap going forward continues to push along these lines

Presentation Plan

This talk covered: Institute Awareness & Management

Following talks:

- Architecture awareness – Eldred
- Application awareness – Higdon
- Science Pipeline – Knio
- Wrap up – Najm