# Uncertainty Quantification Area

FASTMath UQ Team

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FASTMath All-Hands Meeting
Argonne National Lab.
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# Overview

UQ work under FASTMath includes

- Enhancing deployed UQ capabilities in Dakota & UQTk
  - Coupling with MIT UQ library (MUQ)
- Low rank tensor methods for dealing with high-D functions
- Manifold learning
- Adaptive basis
- Bayesian inference
- UQ with model error
- Inference in dynamical systems
- Multilevel Multifidelity methods
- Optimization under uncertainty

ASCR base funding on networks, stochastic dynamical systems, probabilistic computing, etc has contributed to the development and hardening of our UQ software over a number of years

# FASTMath UQ Team

### Sandia – CA

- Habib Najm
- Bert Debusschere
- Cosmin Safta
- Khachik Sargsyan
- Tiernan Casey

### Sandia – NM

- Michael Eldred
- John Jakeman
- Gianluca Geraci

### MIT

- Youssef Marzouk

### USC

- Roger Ghanem

# Partnerships – 1

**Plasma Surface Interactions: Predicting the Performance and Impact of Dynamic PFC Surfaces (PSI2)** [SC-FES]

- Modeling transport of He gas bubbles in ITER divertor material
- Bayesian estimation, global sensitivity analysis (GSA), forward UQ

**Simulation of Fission Gas in Uranium Oxide Nuclear Fuel** [NE]

- Modeling noble gas bubble transport in nuclear fuel rod material
- Bayesian estimation, GSA, forward UQ

**Optimization of Sensor Networks for Improving Climate Model Predictions (OSCM)** [SC-BER]

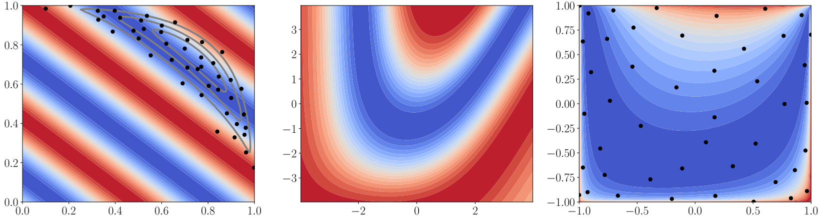
- Energy Exascale Earth System Model (E3SM) Land Component
- Forward UQ and GSA: high-dimensionality challenges
- Bayesian estimation of model parameters with model structural error
- Optimal experimental design for measurement sensor placement

# Partnerships – 2

**Probabilistic Sea Level Projections from Ice Sheet and Earth System Model (ProSPect)** [SC-BER]

- Goal: Estimate uncertainty in predictions of sea-level rise due to ice-sheet evolution
- High-dimensionality (Hi-D) challenges of forward UQ
- Hi-D challenges of Bayesian inference of model parameters
- Moving toward using multi-fidelity algorithms for above tasks

# High Dimensional Function Approximation-Dependence

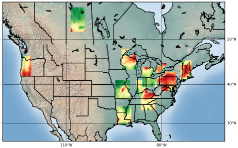



- Efficiently building surrogates of models parameterized by dependent random variables is challenging:
  - Probabilistic transformations introduce non-linearities
  - Approaches not accounting for PDF of variables are inefficient
- Solution:
  - Generate orthonormal polynomial basis and weighted Leja sequence
  - Target accuracy in high-probability regions while maintaining stability

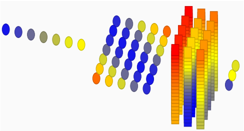
John D. Jakeman, Fabian Franzelin, Akil Narayan, Michael Eldred, Dirk Pflüger, "Polynomial chaos expansions for dependent random variables", *Computer Methods in Applied Mechanics and Engineering*, Volume 351,2019, Pages 643-666, https://doi.org/10.1016/j.cma.2019.03.049.

# High Dimensional Function Approximation - Low Rank

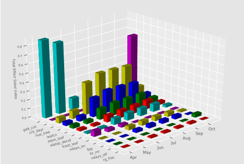
E3SM Simulation




Tensor-train Schematic

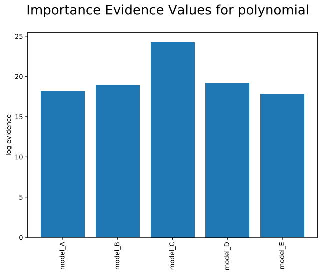


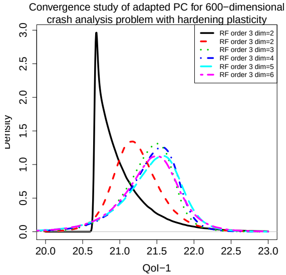
Total Order Sensitivities




- Seek low-rank functional tensor-train representation to reveal couplings in high-dimensional models.
  - Compressed representation, can result in a sample complexity which is only weakly dependent on dimension
  - Can combine local/global approximations in a compact model
- Next Steps:
  - Embed parametric dependencies into a generalized low-rank functional tensor-train decomposition
  - Adaptive sampling of mixed stochastic/physical spaces to target regions of high-probability/non-linear behavior in the joint space

# UQTk Developments




- In-progress integration of new capabilities
  - Coupling between UQTk and MUQ – C++/Python
  - Basis adaptation with error correction
  - Manifold learning and sampling
- Improved User experience
  - Bug fixes, more documentation, better user interfaces
  - New tutorials – *e.g.* Bayesian model selection
- Version 3.1.0 this summer – push to github for easier distribution

# Dakota highlights

- Dakota version 6.10 released May 15, 2019
  - Hardening of multilevel-mutifidelity surrogate approaches
  - Adaptivity through greedy multilevel refinement
- Prototyped integration with Legion AMT for ensemble UQ workflows
  - with Stanford
- Exploited special structure w/functional tensor train approximation
  - Integrated Compressed Continuous Computation (C3) package
    - from Alex Gorodetsky, U. Michigan
  - Multidimensional functions represented in low-rank format
    - sample requirements scale linearly w/dimension $O(dr^2)$
- In progress
  - Integration of MUQ library (w/ MIT and CRREL)
  - Integration of Adaptive Basis for dimension reduction (w/ USC)

# MLMF/OUU Algorithmic highlights

## Advancements on multifidelity/multilevel approaches for UQ

- Surrogate-based approaches
  - Multilevel expansions
    - Polynomial chaos, projection, regression, stoch. collocation
    - Functional tensor train (in progress)
  - Adaptive refinement
    - Isotropic, anisotropic, index set, expanding front
- Sampling-based approaches (more in the poster)
  - *A Generalized Framework for Approximate Control Variates*

(arXiv: 1811.04988v3)

## Optimization Under Uncertainty (OUU)

- Verification cases to test SNOWPAC + MC-based UQ with error est.
- Fall 2019: multifidelity global opt. with GPs (MF EGO)
- 2020: multifidelity OUU for Tokamaks (TDS)

# Advances in Bayesian Methods

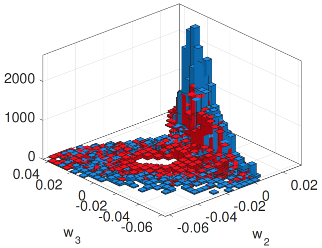
- Systematic framework for embedded **model error** quantification
  - Allows predictive uncertainty attribution into components due to model surrogate construction, data noise and model error
  - Workflow is implemented in UQTk and is employed in DOE and DOD projects, including turbulence modeling, fusion science and land model

(K. Sargsyan, X. Huan, HNN; Int. J UQ 2019)

- MCMC acceleration via **local surrogates**
  - New rate-optimal refinement strategies balance surrogate and sampling error

(Davis, Smith, Pillai, Marzouk 2019)

  - Explicit control of Lyapunov function guarantees convergence for heavier-tailed distributions, broadens robustness and applicability
- **Distance metrics** for likelihood construction for dynamical systems
  - Comparison of chaotic dynamical trajectories using distances between densities defined in manifold coordinates
  - Global diffusion-map distance for constructing Bayesian likelihoods in parameter estimation



# Non-SciDAC Engagement – 1

**SECURE: An Evidence-Based Approach for Cybersecurity**
**C. Safta, J. Jakeman, G. Geraci, B. Debusschere – [SNL Grand Chall. LDRD]**

- Adaptive sampling for quadrature on discrete random variables
  - developed and applied to SECURE relevant models

**Analysis of redox potentials in $H_2$ advanced water splitting materials**
**B. Debusschere – [DOE EERE]**

- Application of UQTk for model comparison and model error computation to water splitting reactions for Hydrogen production.
- Work led to tutorials that have in turn been incorporated in UQTk

**Bayesian Optimal Experimental Design**
**H. Najm – [DOE BES]**

- Application of UQTk surrogate construction and Bayesian capabilities
- Optimal design of a mass spectrometry expt at the ALS

# Non-SciDAC Engagement – 2

## Partnering w/U. Michigan - flood modeling – K. Sargsyan – [NSF]

- Surrogate construction, sensitivity analysis and parameter estimation for the ecohydrologic model using data observed in Manaus, Brazil

M. C. Dwelle, J. Kim,K. Sargsyan, V. Ivanov, "Streamflow, stomata, and soil pits: sources of inference for complex models with fast, robust uncertainty quantification", Advances in Water Resources, Volume 125, pp. 13-31, March, 2019

## Energy Exascale Earth System Model (E3SM) – K. Sargsyan – [SC-BER]

- UQTk is employed for sensitivity analysis and model calibration

D. Ricciuto, K. Sargsyan, P. Thornton, The Impact of Parametric Uncertainties on Biogeochemistry in the E3SM Land Model, Journal of Advances in Modeling Earth Systems, Vol. 10, No. 2, p.297-319, 2018

## Atmosphere to electrons (A2e) – M. Eldred, G. Geraci – [EERE]

- Dakota and multilevel / multifidelity algorithms deployed for forward / inverse UQ and OUU in wind plant applications

# Non-SciDAC Engagement – 3 – R. Ghanem

**Risk assessment for spent fuel containment structures – [NNSA]**

- UQ analysis of a high-fidelity model of a fuel cask system
- UQ models to characterize damage following transport

**Hazard maps for tsunami storm surge – [NSF]**

- Assessment of topography effect on run-up during a tsunami event

**Modeling and design of a lightweight composite car – [DOE]**

- Adaptive basis in very high-dimensional coupled physics problems.

**Probabilistic machine learning (PML) for physics discovery – [DARPA]**

- Integration of manifold sampling with genetic programming to carry symbolic regression for candidate mathematical models.
- Adaptation of PML to large scale OUU; scramjet design optimization