FASTMath UQ Activities

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FASTMath works on advancing the state of the art in UQ methods and software tools, and supporting SciDAC application partnerships.

Dakota

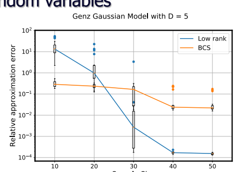
Algorithms for Design Exploration and UQ

- Suite of iterative mathematical and statistical methods that interface to simulations
- Explore computational models and answer system analysis questions:
  - Uncertainty Quantification
  - Design Optimization
  - Model Calibration
  - Sensitivity Analysis
- Foundational components may be combined → Optimization Under Uncertainty, Mixed Integer Non-linear Programming, Mixed Aleatory-Epistemic UQ, et al.
- One simulation interface, many methods: once interface has been created, easily switch among methods and explore different studies
- Scalable parallel computing from desktop to HPC (multilevel parallelism)
- GOAL: provide scientists & engineers a richer perspective on model predictions

DAKOTA
Explore and predict with confidence

Uncertainty Quantification Toolkit (UQTk)

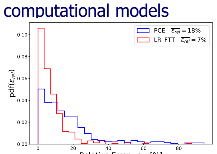
- UQTk provides tools to build a general UQ workflow
  - Intrusive and non-intrusive methods for forward UQ
  - Polynomial Chaos representations of random variables and stochastic processes
  - Sensitivity analysis
  - Sparse surrogate construction
  - Bayesian inference tools
- Open Source LGPL
- http://www.sandia.gov/UQToolkit/
- C++ / Python / Command Line interfaces



Comparison of Low Rank Tensor and Bayesian Compressive Sensing function approximations

High Dimensional Functions

Deployed low-rank functional tensor train (LR-FTT) decomposition algorithms to construct efficient surrogate models for expensive high-dimensional computational models



$$f(x_1, x_2, \ldots, x_d) = \mathcal{F}_1(x_1)\mathcal{F}_2(x_2)\cdots\mathcal{F}_d(x_d)$$

$$\mathcal{F}_k(x_k) = \begin{bmatrix} f_k^{1,1}(x_k) & \cdots & f_k^{1,r_k}(x_k) \\ \vdots & \ddots & \vdots \\ f_k^{r_{k-1},1}(x_k) & \cdots & f_k^{r_{k-1},r_k}(x_k) \end{bmatrix}$$

- LR-FTT surrogates exhibit lower errors compared to sparse regression PCE for selected land model tests

Multilevel-Multifidelity (MLMF) Methods

Monte Carlo methods

- Multilevel methods: exploit variance decay across discretization levels
- Control variate: exploit correlation across model fidelities
- Hybrid methods: multilevel-control variate for multidimensional hierarchies

Stochastic expansion methods:

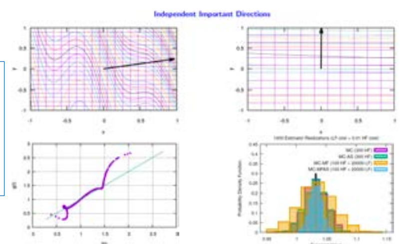
- Polynomial chaos: generalized sparse grids, compressed sensing, tensor train
- Sparse interpolation: nodal, hierarchical

Emphasize foundations that exploit special structure

- Sparsity (compressed sensing), low rank (tensor train), low dimensional (active directions)

Exploiting active directions

- Enhance mathematical relation among models based on principal directions
- Link dissimilar model parameterizations based on shared active variable



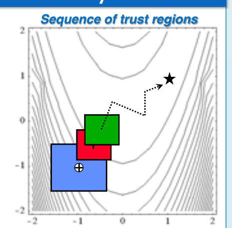
Optimization Under Uncertainty

Achieve desired statistical performance:

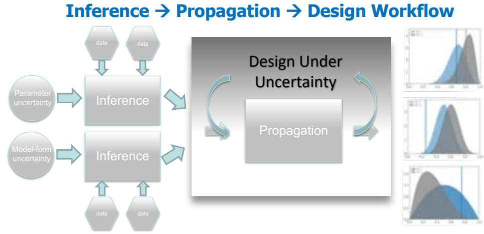
- Robustness → minimize QoI variance
- Reliability → constrain QoI failure probability

Exploit multilevel-multifidelity hierarchies to address computational expense

- From bi-fidelity optimization to recursive trust-region model management (TRMM) with deep multi-dimensional hierarchies



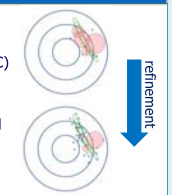
Inference → Propagation → Design Workflow



Bayesian inference in high dimensions

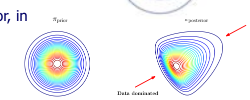
Inference with computationally expensive models:

- Approximations of the likelihood/forward model reduce cost of repeated evaluations (e.g., in Markov chain Monte Carlo (MCMC) sampling of the posterior distribution)
- Errors due to fixed or offline surrogates are difficult to control
- Instead: asymptotically exact surrogates via refinement of local approximations



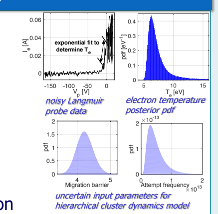
Dimension reduction and sampling:

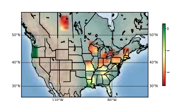
- Data are typically informative, relative to the prior, in a low-dimensional subspace
- New, tailored, dimension reduction methods outperform previous state of the art and yield scalable samplers



Application List

- PSI2: UQ in computational modeling of wall damage processes in plasma facing materials (PFMs), under ITER plasma conditions
- NE: UQ in the computational modeling of noble gas bubble dynamics in nuclear fuel materials
- PROSPECT: quantifying uncertainty in sea-level change due to ice-sheet melt using high-dimensional inference and function approximation methods
- OSCM: deploying advanced techniques for surrogate construction and model error estimation to enable efficient optimization of observational sensor networks (i.e. optimal experimental design)
- Tokamak Disruption: UQ & OUU with Drekar et al.





Net Ecosystem Exchange [gC/m2/day]

Future Plans

- Integrate global sensitivity analysis, sparse PCE construction (employing compressive sensing, MLMF, and basis adaptation concepts) into PSI2 and NE uncertainty propagation efforts across model hierarchies
- MLMF: generalization and unification of multilevel and control variate schemes through relaxation of assumed model relationships
- Bayesian inference: combine global surrogates with local approximation. Integrate a common inference "back end" across main UQ software tools
- High-Dimensional Functional Representations: low-rank representations over mixed physical and stochastic spaces; sampling schemes to reduce ill-conditioning for general probability density functions, targeting both discrete and continuous parameters

More Information: http://www.fastmath-scidac.org or contact Habib Najm, Sandia National Labs, hnnajm@sandia.gov

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