FASTMath: UQ Software

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The SciDAC FASTMath uncertainty quantification (UQ) team works on development of robust UQ methods within high-quality software, providing SciDAC partnership projects with both production deployments at scale and agile prototyping of tailored capabilities.

Dakota (dakota.sandia.gov)

DAKOTA — Explore and predict with confidence. **Version 6.10 released 5/15/19**

C++ toolkit that provides a variety of non-intrusive algorithms for design optimization, model calibration, uncertainty quantification, global sensitivity analysis, and parameter studies. It can be used as either a stand-alone application or as a set of library services, and supports multiple levels of parallelism for scalability on both capability and capacity HPC resources.

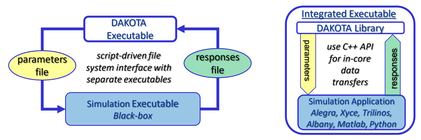
Capabilities:

Core forward UQ components
- **Sampling:** Monte Carlo, Latin hypercube; Incremental, Importance, Adaptive
- **Reliability:** Local (FORM, AMV+, TANA/QMEA); Global (EGRA, GPAIS, POF Darts)
- **Stochastic exp.:** PCE (projection, regression); SC (nodal, hierarchical); FTT (see Algs)
- **Epistemic:** Interval estimation (local, global); Dempster-Shafer

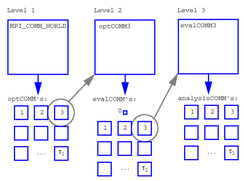
Advanced (multi-component) capabilities
- **Bayesian methods:** QUESO, GPMSA, DREAM, MUQ; Emulator-based MCMC
- **Nested studies:** Mixed aleatory-epistemic UQ; Optimization under uncertainty
- **Multilevel-Multifidelity:** sampling (see Algs poster), surrogates
- **Dimension reduction:** Active subspaces; Adapted basis PCE

Scalable parallelism
- **Multilevel parallelism:** MPI + asynchronous local (system call, fork)
- **Asynchronous many task (AMT):** explore ensemble-based UQ workflows with Legion

Simulation interfacing
- Black box
- Embedded service

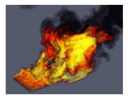


Exploit multiple levels of parallelism
- Recursive partitioning / scheduling with MPI communicators

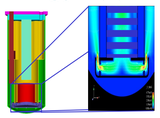


Defense, Science, and Energy Applications

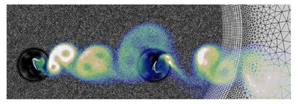
ASC



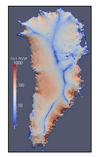
CASL



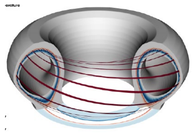
EERE A2e



SciDAC-3



SciDAC-4



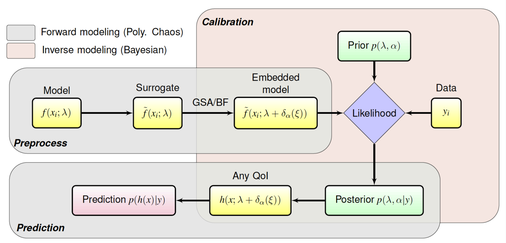
(See TDS poster)

UQTk (www.sandia.gov/UQToolkit)

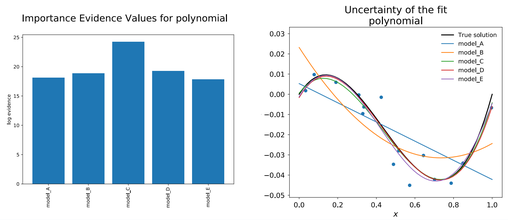
UQTk (http://www.sandia.gov/UQToolkit) is an LGPL open source library of functions for characterization and propagation of uncertainty in computational models.
- Complementary to production tools, UQTk targets:
  - Rapid prototyping
  - Algorithmic research
  - Outreach: Tutorials / Educational
- Version 3.0.4 available at https://github.com/sandialabs/UQTk
- Version 3.1.0 planned for Fall 2019
- Contact: Bert Debusschere: bjdebus@sandia.gov

Capabilities
- PC representations of random variables and stochastic processes
- Intrusive and non-intrusive forward propagation
- Bayesian inference with and without model error
- Bayesian Compressive Sensing
- Low Rank Tensors (v3.1.0)
- Data Free Inference (v3.1.0)
- Tools are flexibly combined into comprehensive workflows.

Simulation interfacing
- Direct linking of C++ lib
- Command Line Apps
- Python interface



Bayes Factors for Model Selection

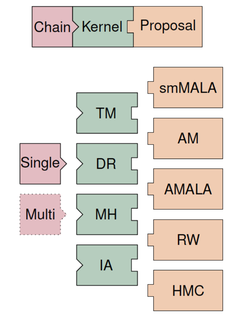


Selected DOE Applications
- BER: OSCM
- FES: PSI-2
- NE: Fission Gas
- BER E3SM
- EERE: HydroGEN

Capability Integration

MUQ

Capabilities:
- Bayesian inference for computationally intensive and high-dimensional models, via a suite of advanced Markov chain Monte Carlo algorithms
- Adaptive surrogate modeling and dimension reduction for scalable inference
- Transport maps for inference and density estimation/stochastic modeling
- Graphical framework (DAGs) to describe complex multi-component statistical models, propagating intrusive (e.g., gradient) information when available



Major components of MCMC: chain, transition kernel, and proposal

Interfacing with Dakota:
- MUQ 2.0 integrated as a TPL in Dakota/packages with management of shared dependencies
- NonDMUQBayesCalibration class defines DAG workflow for inference using MUQ ModPieces

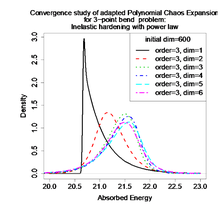
Interfacing with UQTk:
- MUQ can readily be integrated in Python UQTk workflows
- Coupling on C++ library level in progress

Adapted Basis

Capabilities:
- Dimension reduction based on polynomial chaos expansion
- Several algorithms for learning reduction operator, all scale linearly with stochastic dimension
- Accurate high-order approximation achieved along reduced dimensions
- Suitable for input parameters with arbitrary joint probability measures
- Adaptations must be re-learned for each quantity of interest (QoI)

Interfacing with Dakota:
- AdaptedBasisModel performs a low-order PCE approximation (for multiple QoI)
- Rotation defined by first-order PCE
- Can be consumed by other UQ methods as a recast Model with reduced dimensionality

Interfacing with UQTk:
- Iterative scheme discovers converged reduced model
- Convergence acceleration using posterior error analysis
- Interface to random field inputs via Karhunen-Loeve expansion



Inelastic impact mechanics with 600 stochastic dimension.

More Information: http://www.fastmath-scidac.org or contact Mike Eldred, Sandia Labs, mseldre@sandia.gov

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