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UQTk: A C++/Python Uncertainty Quantification Toolkit

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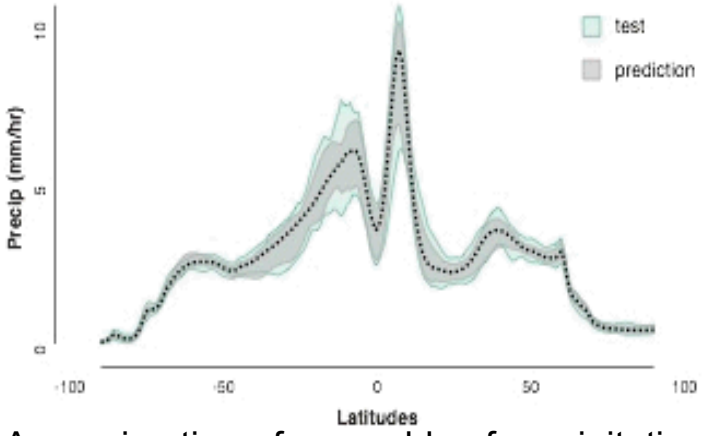
Overview of the technology

- **Technology Area:** Uncertainty Quantification
- **FASTMath Tasks:**
  - FY18: Comparison of low-rank, adaptive quadrature, and Bayesian Compressed Sensing (BCS) for surrogate construction
  - FY19: Support for Machine Learning, and improved interoperability with third party libraries
  - FY20: Performance improvements and enhanced Polynomial Chaos basis types
- **Relevant Software Tools:**
  - UQTk, http://www.sandia.gov/UQToolkit/
- **Applications Impacted (1-3 bullets)**
  - E3SM Climate Modeling
  - Optimization of Sensor Networks for Improving Climate Model Predictions
  - Plasma Surface Interactions
  - Simulation of Fission Gas in Uranium Oxide Nuclear Fuel



Approximation of ensemble of precipitation profiles with PCA and BCS

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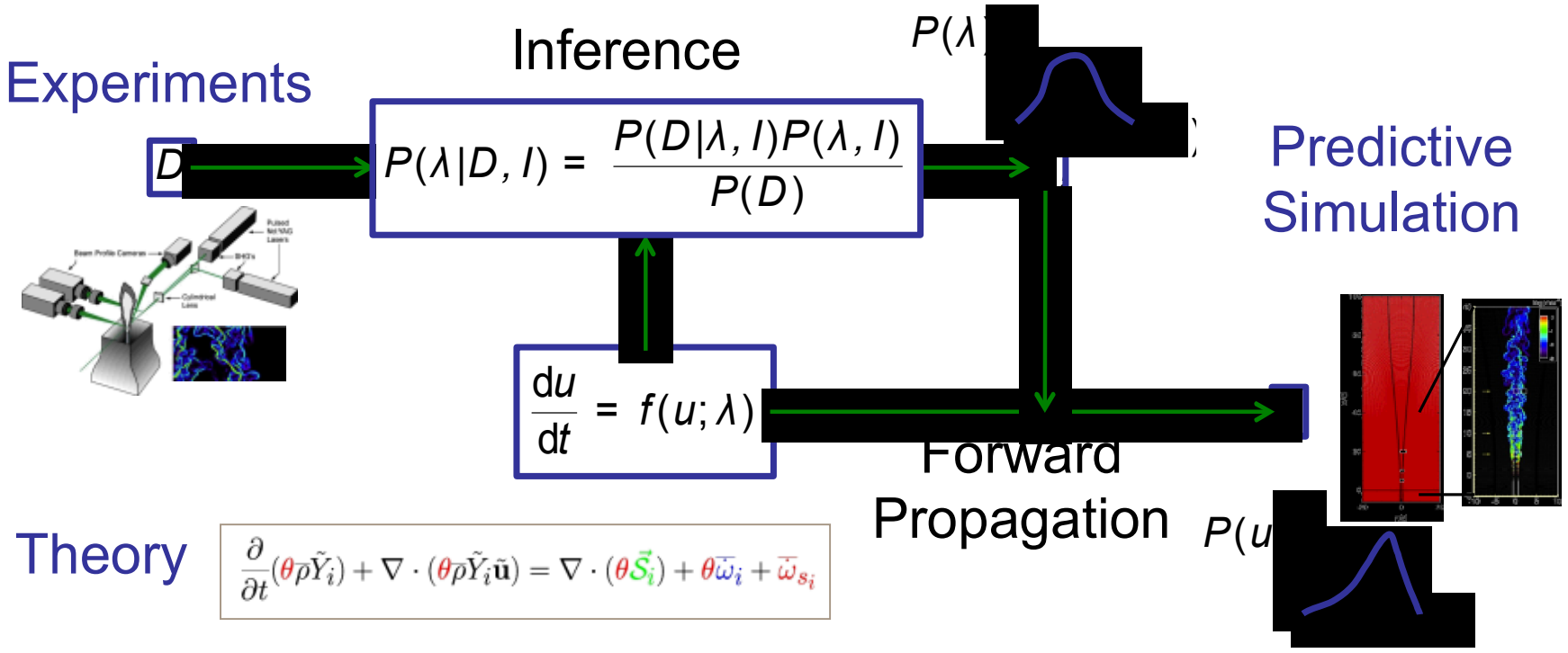
UQTk Description / Technology



- UQTk provides tools to build a general UQ workflow

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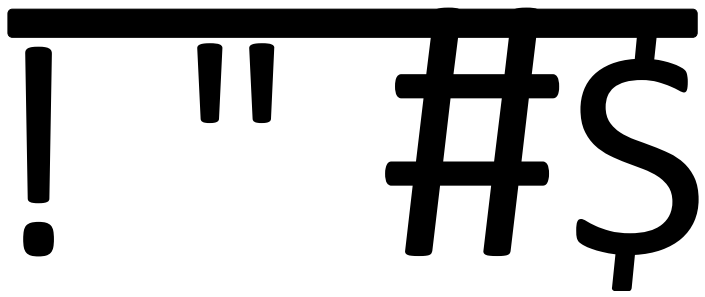
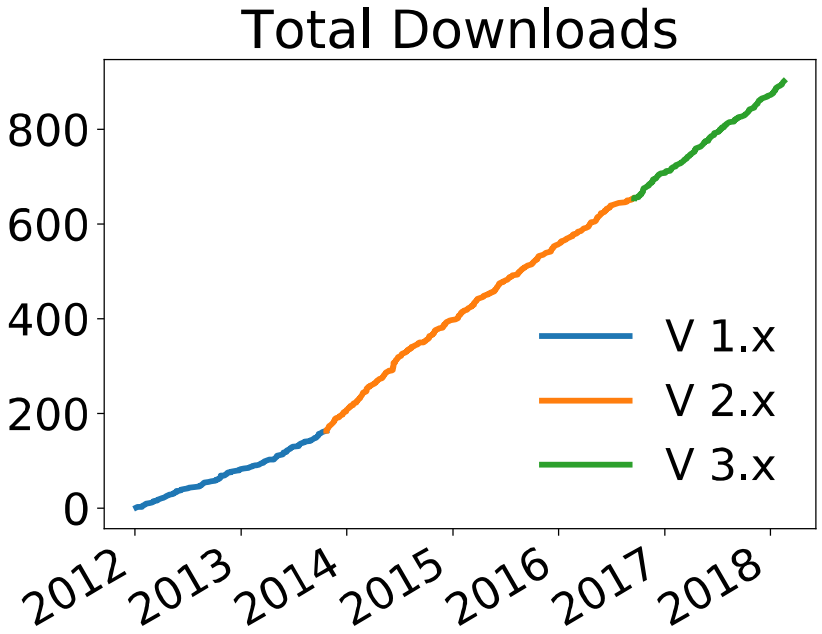
UQTk Description / Technology

- Variety of tools
  - Representation of random variables and stochastic processes (Polynomial Chaos and Karhunen-Loève)
  - Forward UQ (intrusive and non-intrusive)
  - Bayesian Inverse Problems
  - Sensitivity Analysis
  - Bayesian Compressed Sensing
  - Low-Rank approximations
- Tools can be used stand-alone or combined into general workflow
  - C++/Python

UQTk Description / Technology





- Target Usage:
  - Rapid prototyping of UQ workflows
  - Algorithmic research in UQ
  - Tutorials / Educational use

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Proposed work in FASTMath including internal collaborations

- FY18:
  - Enhancements of tools for surrogate construction
    - Low-Rank approximations added
    - Comparison with Bayesian Compressed Sensing (BCS) and Adaptive Quadrature
      - Adaptive Quadrature may be imported from Dakota/Stokhos
  - Enhancements to MCMC libraries
    - Create unified workflow and interface across all MCMC methods
    - Create interface with MUQ (MIT) MCMC methods

Proposed work in FASTMath including internal collaborations

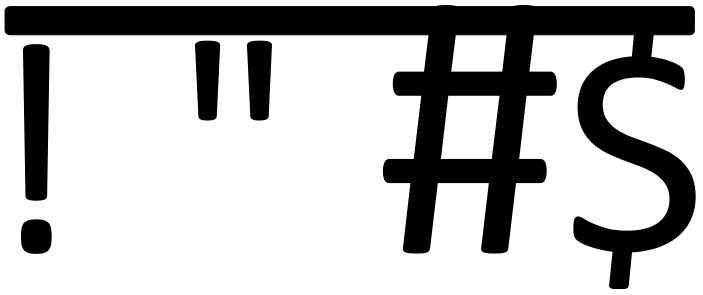
- FY19:
  - Implement interface with Dakota
    - Make Dakota methods available to UQTk users
  - Add Neural Network regression and classification tools
    - From Dakota, other 3rd party libraries, or in-house developed
  - More general interoperability with 3rd party libraries
    - Move away from fixed dependencies
    - Allow users to specify their favorite random number generator

Proposed work in FASTMath including internal collaborations

- FY20:
  - Exploring data types and constructs that better lend themselves to parallelization and GPU usage
    - Work with Kokkos
  - Mixed Polynomial Chaos basis types and associated multi-indices
  - Analysis of computational performance of PC basis ordering schemes

Description of the software tools

- The Uncertainty Quantification Toolkit (UQTk)
  - Intrusive and non-intrusive methods for forward UQ
  - Polynomial Chaos representations of random variables
  - Sensitivity analysis
  - Sparse surrogate construction
  - Bayesian inference tools
- Open Source LGPL
- http://www.sandia.gov/UQToolkit/



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Application interactions

- BER-ASCR partnership: Optimization of Sensor Networks for Improving Climate Model Predictions (OSCM)
  - Led by Daniel Ricciuto (ORNL)
  - Expected impact:
    - Impacts E3SM, DOE's flagship climate modeling effort
    - UQTk is being used for both forward modeling (surrogate construction and GSA) and inverse modeling (parameter tuning, embedded structural error)

Application interactions

- FES-ASCR partnership: Plasma Surface Interactions: Bridging from the Surface to the Micron Frontier through Leadership Computing (PSI2)
  - Led by Brian Wirth (ORNL)
  - Expected impact:
    - Impacts Xolotl, an open-source, high performance plasma-surface interactions simulator that is under development within the DOE's SciDAC program.
    - UQTk has been used for building surrogates and propagating uncertain inputs towards Xolotl predictions.

Application interactions

- NE-ASCR partnership: Simulation of Fission Gas in Uranium Oxide Nuclear Fuel
  - Led by David Andersson (LANL)
  - UQTk is being used for forward and inverse UQ studies
  - Expected impact:
    - Modeling of degradation in nuclear fuel rods
    - Improved understanding of gas bubble diffusion and dynamics in nuclear fuel materials

Application interactions

- BES-ASCR partnership: Predictive Computing for Condensed Matter
  - Partnership led by So Hirata (UIUC)
  - Tool developed : Low rank tensor approximation for multivariate functions.
  - Expected impact:
    - Low rank canonical tensor approximations are used to approximate potential energy surfaces of molecules for estimating anharmonic energy and frequency corrections in quantum chemistry.
  - Relevant publication: Rai P., Sargsyan K., Najm H., Hermes M. and S. Hirata, "Low-rank canonical-tensor decomposition of potential energy surfaces: application to grid-based diagrammatic vibrational Green's function theory", Molecular Physics, 115,17-18, 2120-2134, 2017.