Developing the Next Generation Scalable Exascale Uncertainty Quantification Method

Guang Lin, Nicholas J. Zabaras, Ioannis G. Kevrekidis, Thomas A. Manteuffel, Stephen F. McCormick

Project Introduction
A team of researchers from Pacific Northwest National Laboratory, Cornell University, Princeton University and University of Colorado, Boulder are developing an scalable multifaceted integrated mathematical and computational framework for predictive modeling of high-dimensional multiscale and multi-physics stochastic PDE systems at the exascale. The integrated framework is composed of three synergistic components:

1. Data-driven Stochastic Input Models: Enables to integrate experimental data and underlying physics as stochastic input in numerical models;
2. Scalable Solver for high-dimensional Stochastic PDE Systems: Enables to tackle critical real-world high-dimensional multiscale, and multi-physics stochastic complex systems;
3. Integration of Multiscale Models with Stochastic Analysis: Provide a unified framework for passing uncertain information from the fine scale where heterogeneity is located to macroscopic data.

Problem Definition

Coupling data driven model generation with a Multiscale stochastic modeling framework

Seamlessly couple stochastic analysis with multiscale analysis:
Coupled with a data-driven input model strategy to analyze realistic stochastic multiscale problems.

Scalable Solver for high-dimensional Stochastic PDE Systems

Designing the Next Generation Exascale Statistical Tools

Objectives:
- High-dimensional, Data-driven exploration of PDE-based engineering problems
- Fast implementation and testing of novel statistical algorithms

Key ideas:
- Modularity:
- Efficiency/Scalability:

Features:
- Optimized targeted versions of core statistical models
- Data-based input modeling
- Uncertainty Propagation
- Inverse problems.

Bayesian framework for UQ

Error bars for the Statistics

All Bayesian methods proceed as follows:
- Collect data.
- Construct a probability measure over the possible surrogates.
- Sample from a surrogate and integrate (analytically or via MC) to get a sample of the statistics.
- Repeat the previous step to get confidence intervals for the statistics.

Multiscale Analysis

Coupled with a data-driven input model strategy to analyze realistic stochastic multiscale problems.

Integration of Multiscale Models with Stochastic Analysis:

Scalable Multigrid Methods for Intrusive UQ Approach

Predictive Multiscale Models = Inference in Graphs

Gaussian Mixture Models = Inference in Graphs

Graphical Model Learning

Conclusions

Data-driven model design of heterogeneous media provides many open mathematical challenges
- Need for managing complexity in stochastic multiscale models
- The Bayesian approach offers:
  - Probability measure over surrogates (Into number of samples)
  - Active learning (experimental design)
  - Non-stationary responses (trees of surrogates)
  - Samples of the surrogate distribution can be used for: UQ, Sensitivity Analysis, Model Calibration, ...
- Scalable multigrid methods greatly improve the scalability of non-intrusive UQ methods
- Use of probabilistic graphical models allows stochastic multiscale problems to be addressed as inference problems in graphs

Acknowledgements
This work is supported by the DOE ASCR Applied Mathematics Program

www.pnnl.gov

Proudly Operated by Battelle Since 1965

Pacific Northwest NATIONAL LABORATORY