Forward and Inverse Methods in Uncertainty Propagation and Parameter Calibration

Organizers:
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Abstract

A large variety of phenomena observed in science and engineering are modeled as a relation between a number of input parameters and output quantities of interest (QoIs), methods for forward uncertainty quantification consider variation in the inputs propagating through the model and gives an estimate on the resulting variation in the computed QoIs. On the other hand, inverse problems calibrate parameters to match experimental data or desired design properties. This mini-symposium addresses recent advances in numerical analysis in both areas including methods for high-dimensional approximation, reduced-order modeling, adaptive methods, Bayesian inference and stochastic control/optimization.

Session 1:

- **Speaker:** *Miroslav Stoyanov* (stoyanovmk@ornl.gov), Oak Ridge National Lab,

  Title: Algorithm Resilience with Respect to Hardware Faults

  Abstract: The increase of computational power of modern computer hardware, has been accompanied by a decrease in the hardware reliability, a trend that is most notable in large scale supercomputers. Numerical algorithms are traditionally developed with the implicit assumption that all arithmetic operations can be carried out accurately to within some round-off error; however, this is no longer a safe assumption. We propose a general framework for analyzing the resiliency of algorithms, with respect to errors in basic numerical operations, resulting from soft errors and hardware failures.

- **Speaker:** *Hans-Werner van Wyk* (hvanwyk@fsu.edu), Florida State University,

  Title: Multilevel Methods for Stochastic Quadrature

  Abstract: Multilevel Monte Carlo methods accelerate computations for approximating statistical quantities of interest related to solutions of partial differential equations with random parameters. Sample solutions are approximated at different spatial resolutions and the sample sizes required at each resolution are chosen to minimize the cost, subject to a given error tolerance. We present extensions of this algorithm to stochastic sampling methods, most notably stochastic collocation, and demonstrate its effectiveness by means of a numerical test problem.

- **Speaker:** *Vitor Nunes* (vitor@vt.edu), Virginia Tech,

  Title: Parameter Estimation and Sensitivity Analysis in Groundwater Flow

  Abstract: n this work we use the Fréchet derivative to determine the most significant (deterministic) parametric variations; this is used to generate a low order Karhunen-Loéve expansion of the unknown parameters specific storage and hydraulic conductivity. This expansion is used in the parameter identification problem, which is formulated as an infinite dimensional constrained optimization problem.

  The low order expansion allows us to estimate the infinite dimensional problem by a smooth, albeit high dimensional, deterministic optimization problem, the so-called "finite noise" problem, in the space of functions with bounded mixed derivatives. We will use a power method and sensitivity equations to evaluate the most significant directions, and compute reduced representations of the operator for efficient gradient calculations.

- **Speaker:** *Clayton Webster* (webstercg@ornl.gov), Oak Ridge National Lab,

  Title: A Hierarchical Adaptive Sparse Grid Stochastic Wavelet Collocation Method for PDEs with Random Input Data

  Abstract: Accurate predictive simulations of complex real world applications require numerical approximations to first, oppose the *curse of dimensionality* and second, converge quickly in the presence of steep gradients, sharp transitions, bifurcations or finite discontinuities in high-dimensional parameter spaces. In this talk we present a novel multidimensional multiresolution adaptive (MdMrA) sparse grid stochastic collocation method, that utilizes hierarchical multiscale piecewise Riesz basis functions constructed from interpolating wavelets. The basis for our non-intrusive method forms a stable multiscale splitting and thus, optimal adaptation is achieved. Error estimates and numerical examples will used to compare the efficiency of the method with several other techniques.

Session 2:

- **Speaker:** *Guannan Zhang* (zhangg@ornl.gov), Oak Ridge National Lab,

  Title: A Hyper-Spherical Sparse-Grid Method Discontinuity Detection in Uncertainty Quantification

  Abstract: High-dimensional discontinuity detection is important in UQ area, but conventional adaptive sparse-grid interpolation leads to dense refinement around discontinuities. We propose a novel method for identifying jump discontinuities in by incorporating a hyper-spherical coordinate system (HSCS) into the sparse-grid approximation framework. The basic idea is to transform the Cartesian coordinate system to an N-dimensional HSCS. Then a sparse-grid approximation is constructed in the N-1 dimensional subspace where the discontinuity locations are estimated using bisection method.

- **Speaker:** *Nicholas Dexter* (ndexter@utk.edu), University of Tennessee,

  Title: Stochastic Collocation Techniques Applied to Reactor Criticality

  Abstract: This talk focuses on stochastic collocation method (SCM) applied to a radiation transport problem. We consider a one dimensional model reactor consisting of fuel rods, control rod and coolant, and we study the effects of material cross-section uncertainty on the reactor criticality. We use SCM to compute the statistics of the criticality and we show convergence for a very large range of cross-section uncertainty.

- **Speaker:** *Boris Kramer* (bokr@vt.edu), Virginia Tech,

  Title: Parameter Sensitivity of POD Based Reduced Order Feedback Controllers

  Abstract: With increasing computational power, high fidelity simulation of PDE's is becoming reality. However, reduced order modeling becomes imperative if we want to benefit from prior knowledge of high fidelity simulations to compute feedback controllers. It is understood that reduced order models can only mimic the dynamics obtained in the given data. In this talk, we investigate the sensitivity of a Proper Orthogonal Decomposition(POD) reduced order model with respect to underlying model parameters. In particular, we study the performance of reduced order controllers on the high fidelity model.

- **Speaker:** *Hoang Tran* (hat25@pitt.edu), University of Pittsburgh,

  Title: Stochastic Collocation Method for Fluid Flow Problems with Random Input Data

  Abstract: Stochastic collocation methods prove to be a very efficient approach for solving linear PDEs. In this report, we discuss the performance of these methods to solve two fluid flow problems with random input data: Oseen equations and time dependent Navier-Stokes equations, where the introduce of nonlinear term poses a challenge. Numerical examples are provided to demonstrate the analyses.

Session 3:

- **Speaker:** *Diego Galindo* (galindod@ornl.gov), Oak Ridge National Lab,

  Title: Solving Linear Systems for a Hierarchical Stochastic Collocation Method

  Abstract: We consider stochastic collocation methods for stochastic PDEs that construct a multi-dimensional response surface in a hierarchical way. Each level of the approximation requires that additional linear systems be solved. These linear systems are independent, but have similar structures. This structural similarity and the hierarchy of the collocation are used to inform the solution of the linear systems, resulting in improved convergence of the linear solver.

- **Speaker:** *Nabil Chaabane* (nabil.chaabane@gmail.com), Virginia Tech,

  Title: An Optimal Local Discontinuous Galerkin Method

  Abstract: In this work, we present an error analysis for the local discontinuous Galerkin method for a model of elliptic problem on cartesian grids when polynomials of degree at most k and a special projection of the boundary condition are used. This special projection allows us to achieve an order of convergence of $k+1$ for both the potential and its gradient in the L^2-norm. This method improves the previous estimate of the gradient by a factor $\sqrt{h}$.

- **Speaker:** *Feng Bao* (fzb0005@auburn.edu), Alburn University,

  Title: Numerical Algorithms for Nonlinear Filtering Problem

  Abstract: We consider the classical filter problem where a signal process is modeled by a stochastic differential equation and the observation is perturbed by a white noise. The goal is to find the best estimation of the signal process based on the observation. Kalman Filter, Particle Filter, Zakai equations are some well known approaches to solve optimal filter problems. In this talk, we shall show a new numerical algorithm which we call the implicit algorithm. Both theoretical results and numerical experiments will be presented.

- **Speaker:** *Detelina Stoyanova* (dks10d@fsu.edu), Florida State University,

  Title: A Computational Method for Age-At-Death Estimation Based on Pubic Symphysis

  Abstract: A significant component of forensic science is analyzing bones to assess the age at death of an individual. Forensic anthropologists often include the pubic symphysis in such studies. Subjective methods, such as the Suchey-Brooks method, are currently used to analyze the pubic symphysis. We examines a more objective, quantitative method. The method analyzes 3D surface scans of the pubic symphysis and implements a thin plate spline algorithm which models the bending of a flat plane to approximately match the surface of the bone. Results presented here show that there is a correlation between the minimum bending energy and the age at death of the individual.