International Conference on Uncertainty Quantification in Computational Fluid Dynamics

July 24-26, 2017

601 Pao Yue-Kong Library

Institute of Natural Sciences, Shanghai Jiao Tong University

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1 General Information

Introduction

Fluid dynamics equations use empirical equations of state or constitutive relations thus contain uncertainties. Uncertainties also arise from initial or boundary data, sources, or geometry. Quantifying these uncertainties are important for engineering applications in order to validate and improve the fluid models and conduct more reliable numerical computations. The goal of this conference is to bring in international leaders as well as promising young researchers in order to discuss the cutting-edge research results, and to foster collaborations between overseas and domestic researchers, in this emerging research field.

Date

July 24-26, 2017

Venue

601 Pao Yue-Kong Library

Organizers

- Jianguo Huang, Shanghai Jiao Tong University
- Shi Jin, Shanghai Jiao Tong University
- Hong Liu, Shanghai Jiao Tong University
- Jinglai Li, Shanghai Jiao Tong University
- Min Tang, Shanghai Jiao Tong University
- Lei Zhang, Shanghai Jiao Tong University

2 Schedule

2017-07-24

Time	Speaker	Title
09:00 - 09:45	Dongxiao Zhang	Inverse Modeling and Uncertainty Quantification for Flow in Fractured Reservoirs
09:50 - 10:35	Roger Ghanem	Basis Adaptation for Design Optimization under Uncertainty
10:40 - 11:10		Group Photo and Coffee Break
11:15 - 12:00	Bruno Despres	Properties of Kinetic Polynomials

Time	Speaker	Title
14:00 - 14:30	Guang Lin	From CFD to Uncertainty Quantification and Machine Learning of Fluid Equations
14:35 - 15:05	Xiaoliang Wan	Model the Nonlinear Instability of Wall-Bounded Shear Flows as a Rare Event
15:10 - 15:40		Coffee Break
15:45 - 16:15	Tao Zhou	A Generalized Sampling and Preconditioner Scheme for Constructing Polynomial Chaos Approximations
16:20 - 16:50	Minh Binh Tran	Local Sensitivity Analysis for Viscous Conservation Laws and System of Conservation Laws

2017-07-25

Time	Speaker	Title
09:00 - 09:45	Jan Hesthaven	Reduced Order Modeling for Nonlinear Problems through Neural Networks
09:50 - 10:35	Habib Najm	Bayesian Estimation of Model Error in Physical Systems
10:40 - 11:10		Coffee Break
11:15 - 12:00	Yalchin Efendiev	Bayesian Multiscale Methods for Forward and Inverse Problems

Time	Speaker	Title
14:00 - 14:30	Jingwei Hu	Stochastic Galerkin Methods for the Boltzmann Equation with Uncertainty
14:35 - 15:05	Ruiwen Shu	A Stochastic Asymptotic-Preserving Scheme for a Kinetic-Fluid Model for Disperse Two-Phase Flows with Uncertainty
15:10 - 15:40		Coffee Break
15:45 - 16:15	Xiao Chen	Efficient Stochastic Inversion Using Adjoint Models and Kernel-PCA
16:20 - 16:50	Tiangang Cui	Subspace Acceleration for Large-Scale Bayesian Inverse Problems

2017-07-26

Time	Speaker	Title
09:00 - 09:30	Jinglai Li	Bayesian Inference and Uncertainty Quantification for Infinite Dimensional Bayesian Inverse Problems
09:35 - 10:05	Lijian Jiang	Model Reduction Using Variable-Separation Methods and Some Applications in Uncertainty Quantification
10:10 - 10:40		Coffee Break
10:45 - 11:15	Liu Liu	A gPC Stochastic Galerkin Method for Semiconductor Boltzmann Equations: Analysis on Convergence Rate and Numerics
11:20 - 11:50	Yuhua Zhu	Hypocoercivity and Uniform Regularity for the Vlasov-Poisson-Fokker-Planck System with Uncertainty and Multiple Scales

Time	Speaker	Title
14:00 - 14:45	Olivier Le Maitre	TBA

3 Abstract

3.1 2017-07-24

Inverse Modeling and Uncertainty Quantification for Flow in Fractured Reservoirs

Dongxiao Zhang, Peking University
09:00 - 09:45

Flow in fractured porous media is crucial for production of oil/gas reservoirs and exploitation of geothermal energy. The flow behaviors in such media are mainly dictated by the distribution of the fractures. Measuring and inferring the distribution of fractures is subject to large uncertainty, which, in turn, leads to great uncertainty in the prediction of flow behaviors. Inverse modeling with dynamic data may help to constrain the fracture distributions, thus reducing the uncertainty for the flow prediction. However, inverse modeling for flow in fractured reservoirs is challenging owing to the discrete and non-Gaussian distribution of fractures, as well as the strong nonlinearity in the relationship between the flow responses and the model parameters. In this work, building upon a series of recent advances, an inverse modeling approach is proposed to efficiently update the flow model to match the dynamic data while keeping geological realism in the distribution of fractures. In the approach, the Hough-transform method is employed to parameterize non-Gaussian fracture fields with continuous parameter fields, thus rendering nice properties required in many of the inverse modeling methods. Also, a recently developed forward simulation method, called the embedded discrete fracture model (EDFM), is utilized to model the major fractures while the minor fractures are homogenized with the matrix. The EDFM retains computational efficiency while preserving the ability to capture the geometrical details of major fractures because the matrix (with homogenized fractures) are modeled with a structured grid while the major fractures being handled as planes inserted into the matrix grids. The combination of Hough representation of fractures with the EDFM makes it possible to tune the major fractures (through updating their existence, location, orientation, length and other properties) without requiring either unstructured grids or re-gridding during updating. Such a treatment is amenable to many inverse modeling approaches, such as the iterative inverse modeling method utilized in this study to deal with strong non-linear problems. A series of numerical case studies with increasing complexity are set up to examine the performance of the proposed approach.

Basis Adaptation for Design Optimization under Uncertainty

Roger Ghanem, University of Southern California
09:50 - 10:35

Basis adaptation in the context of polynomial chaos expansions permit the concentration of probabilistic measure of stochastic processes around stochastic dimensions that are adapted to specific quantities of interest. Integrating this machinery with design optimization, the new bases are adapted to the relevant objective and constraint functions, enabling an efficient solution of the associated computational problem. In this presentation, I will demonstrate the application of this methodology to a problem of well placement in a subsurface oil production problem.

Properties of Kinetic Polynomials

Bruno Despres, LJLL/UPMC
11:15 - 12:00

Kinetic polynomials (D. and Perthame, JUQ 2016) have been proposed as a model for uncertainty propagation in kinetic formulations of conservation laws. It appears to be an alternative (or a complement) to the classical moment method, but with stronger theoretical properties in terms of preservation of the maximum principle and the entropy principle. I will review the main properties and explain how to discretize this method.

From CFD to Uncertainty Quantification and Machine Learning of Fluid Equations

Guang Lin, Purdue University
14:00 - 14:30

In this talk, instead of pursuing the numerical solution of fluid equations, our focus is to perform uncertainty quantification and machine learning of fluid equations. First, stochastic piston problem and random roughness problem will be reviewed. Second, motivated by how eagle senses the wind and knows how to fly, compressive sensing based machine learning algorithm is used to determine the flow characteristics around a cylinder from a sparse number of pressure measurements on the cylinder. Using a supervised machine learning strategy, library elements encoding the dimensionally reduced dynamics are computed for various Reynolds numbers. Convex L1 optimization is then used with a limited number of pressure measurements on the cylinder to reconstruct, or decode, the full pressure field and the resulting flow field around the cylinder. Finally, I will present a new data-driven paradigm on learning the fluid equations, particularly, the shallow-water equations and Navier-Stokes equations from noisy measurements. The key idea is to identify the terms in the underlying fluid equations and to approximate the coefficients of the terms with error bars using Bayesian machine learning algorithms only using the available noisy measurement. In particular, Bayesian sparse feature selection and parameter estimation are performed. Numerical experiments show the robustness of the learning algorithms with respect to noisy data and size, and its ability to learn various candidate equations with error bars to represent the quantified uncertainty.

Model the Nonlinear Instability of Wall-Bounded Shear Flows as a Rare Event

Xiaoliang Wan, Louisiana State University
14:35 - 15:05

In this work, we study the nonlinear instability of two-dimensional (2D) wall bounded shear flows from the large deviation point of view. The main idea is to consider the Navier−Stokes equations perturbed by small noise in force and then examine the noise-induced transitions between the two coexisting stable solutions due to the subcritical bifurcation. When the amplitude of the noise goes to zero, the Freidlin−Wentzell (F−W) theory of large deviations defines the most probable transition path in the phase space, which is the minimizer of the F−W action functional and characterizes the development of the nonlinear instability subject to small random perturbations. A recently developed minimum action method for seeking the minimizer of the action functional will also be presented.

A Generalized Sampling and Preconditioner Scheme for Constructing Polynomial Chaos Approximations

Tao Zhou, Institute of Computational Methematics, Chinese Academy of Sciences.
15:45 - 16:15

We propose an least-square algorithm for recovering orthogonal polynomial expansions via collocation. A standard sampling approach for recovering sparse polynomials uses Monte Carlo sampling, from the density of orthogonality, which results in poor function recovery when the polynomial degree is high. Our proposed approach aims to mitigate this limitation by sampling with respect to the weighted equilibrium measure of the parametric domain and subsequently solves a preconditioned least-square problem, where the weights of the diagonal preconditioning matrix are given by evaluations of the Christo el function. Our algorithm can be applied to a wide class of orthogonal polynomial families on bounded and unbounded domains, including all classical families. We present theoretical analysis to motivate the algorithm and numerical results that show our method is superior to standard Monte Carlo methods in many situations of interest. Finally, we show that the framework applies easily to the sparse recovery approach via compressed sensing.

Local Sensitivity Analysis for Viscous Conservation Laws and System of Conservation Laws

Minh Binh Tran, University of Wisconsin Madison
16:20 - 16:50

We develop a local sensitivity analysis for the Cauchy problem of viscous conservation laws and systems of conservation laws. The analysis sheds lights on the long time dependence of solutions with respect to random initial input. The talk is based on my joint works with Prof Shi Jin and Prof Enrique Zuazua.

3.2 2017-07-25

Reduced Order Modeling for Nonlinear Problems through Neural Networks

Jan Hesthaven, Ecole Polytechnique Federale de Lausanne
09:00 - 09:45

The development of reduced order models for complex applications, offering the promise for rapid and accurate evaluation of the output of complex models under parameterized variation, remains a very active research area. Applications are found in problems which require many evaluations, sampled over a potentially large parameter space, such as in optimization, control, uncertainty quantification, and applications where near real-time response is needed.

However, several challenges remain in order to secure the flexibility, robustness, and efficiency needed for general large scale applications, in particular for nonlinear and/or time-dependent problems.

After giving a brief general introduction to reduced order models, we discuss recent attempts to use neural networks to address some of these known challenges, in particular related to the fast evaluation of reduced models for highly nonlinear problems. We shall discuss the motivation behind this, how to construct the reduced models and the associated neural network and also touch on what is achievable in terms of accuracy and robustness of the model.

We shall demonstrate the potential of this approach through a number of examples, including nonlinear Poisson problems, and the incompressible Navier-Stokes equations with geometric variations.

Bayesian Estimation of Model Error in Physical Systems

Habib Najm, Sandia National Laboratories
09:50 - 10:35

When a model is calibrated with respect to data, the goal, from a predictive perspective, is to improve the fidelity of model predictions, relative to the ”truth” behind the data, by estimating best-fit values of model parameters, and using these fitted parameters in subsequent predictions. Often, however, the deficiency in model structure is such, that no combination of parameter values can result in model predictions that agree with the data. In this situation, the improvement in predictive fitness of the model upon calibration can be negligible.

In the context of Bayesian model calibration, statistical model error representations have been employed, whose parameters have been inferred jointly with other model parameters. The calibration of this model error representation provides for a suitably fitted correction on model predictions to bridge the gap with calibration observables. Extending these methods to physical methods has lead to the development of strategies for embedding such model error representations within the model, to ensure satisfaction of various constraints.

This talk will provide an overview of our developments in this regard. I will discuss the basics of the construction, including a number of variants relying on different simplifications, and will outline its utility in different situations including those with or without data noise. I will also present a number of demonstrations in chemical models of increasing complexity, leading up to an application in a large eddy simulation of turbulent flow.

Bayesian Multiscale Methods for Forward and Inverse Problems

Yalchin Efendiev, Texas A&M University, USA
11:15 - 12:00

In this talk, I will describe Bayesian multiscale methods for forward and inverse problems. By representing dominant modes using the Generalized Multiscale Finite Element, I will first describe a Bayesian framework, which provides multiple inexpensive (computable) solutions for a deterministic problem. These approximate probabilistic solutions may not be very close to the exact solutions and, thus, many realizations are needed. We present a rigorous probabilistic description of approximate solutions. Using residual information, we design appropriate prior and posterior distributions. To sample from the resulting posterior distribution, we consider several sampling strategies. The main novel ingredients of our approach consist of: defining appropriate permanent basis functions and the corresponding residual; setting up a proper posterior distribution; and sampling the posteriors. I will also talk about inverse problems.

Stochastic Galerkin Methods for the Boltzmann Equation with Uncertainty

Jingwei Hu, Purdue University
14:00 - 14:30

We develop a stochastic Galerkin method for the Boltzmann equation with uncertainty. The method is based on the generalized polynomial chaos (gPC) approximation, and can handle random inputs from collision kernel, initial data or boundary data. We show that a simple singular value decomposition of gPC related coefficients combined with the fast Fourier spectral method (in velocity space) allows one to compute the collision operator efficiently. To treat high dimensional random inputs, we also propose a sparse grid based Galerkin method using local basis. For both frameworks, the regularity of the solution in random space and an accuracy estimate are established. Several numerical examples will be presented to illustrate the validity of the proposed methods. This is joint work with Shi Jin and Ruiwen Shu.

A Stochastic Asymptotic-Preserving Scheme for a Kinetic-Fluid Model for Disperse Two-Phase Flows with Uncertainty

Ruiwen Shu, University of Wisconsin-Madison
14:35 - 15:05

This is a joint work with Prof. Shi Jin. We consider a kinetic-fluid model for disperse two-phase flows with uncertainty. We propose a stochastic asymptotic-preserving (s-AP) scheme in the generalized polynomial chaos stochastic Galerkin (gPC-sG) framework, which allows the efficient computation of the problem in both kinetic and hydrodynamic regimes. The s-AP property is proved by deriving the equilibrium of the gPC version of the Fokker-Planck operator. The coefficient matrices that arise in a Helmholtz equation and a Poisson equation, essential ingredients of the algorithms, are proved to be positive definite under reasonable and mild assumptions. The computation of the gPC version of a translation operator that arises in the inversion of the Fokker-Planck operator is accelerated by a spectrally accurate splitting method. We prove the uniform regularity in the random space and the spectral accuracy of the gPC-sG method for initial data near equilibrium, by using nonlinear energy estimates and hypocoercivity arguments. Numerical examples illustrate the s-AP property and the efficiency of the gPC-sG method in various asymptotic regimes.

Efficient Stochastic Inversion Using Adjoint Models and Kernel-PCA

Xiao Chen, Lawrence Livermore National Lab, USA
15:45 - 16:15

We have developed an efficient method for the stochastic inversion of the linear elasticity problem in the framework of Bayesian inference. The nonlinear mapping between the observables and parameters leads to non-Gaussian posteriors even with additive noise and Gaussian prior assumptions. The computational cost of the forward model makes the stochastic inversion intractable by using traditional methods such as Markov chain Monte Carlo (MCMC) and polynomial chaos expansion (PCE). Here, we propose a novel stochastic inversion framework, where we first derive a system of continuous adjoint partial differential equations (PDEs) which facilitate efficient computation of the gradient of an objective functional with respect to model parameters. Next, we use a conceptual model representing prior knowledge to generate a series of realizations of the complex structural model. Following that, we construct a relatively low-dimensional feature space where the mesh-dependent and non-linearly spatially correlated model parameters are represented in terms of independent standard Gaussian random variables, using a kernel principle component analysis (KPCA) and an inverse cumulative distribution function (ICDF) transformation. Given the pre-computed gradient with respect to model parameters, we use automatic differentiation to derive an adjoint model of KPCA-based ICDF transformation and obtain the gradient with respect to low-dimensional feature random variables. Finally, we devise an efficient Langevin MCMC scheme to sample the posteriors of the random variables in the feature space and retrieve the mesh-dependent high-dimensional parameter space. This work was performed under the auspices of the U.S. Department of Energy by LLNL under contract DE-AC52-07NA27344 with IM release number LLNL-ABS-702634.

Subspace Acceleration for Large-Scale Bayesian Inverse Problems

Tiangang Cui, Moansh University
16:20 - 16:50

Algorithmic scalability to high dimensional parameters and computational efficiency of numerical solvers are two central challenges in solving large-scale PDE-constrained inverse problems. Here we will investigate the intrinsic dimensionality in both parameter space and model space by exploiting the interaction among various information sources and model structures. We will also discuss various strategies for jointly identifying low-dimensional parameter and model subspaces. The resulting subspaces naturally lead to accelerated sampling methods that can overcome the above-mentioned challenges and demonstrate potential reductions for problems with high-dimensional data.

3.3 2017-07-26

Bayesian Inference and Uncertainty Quantification for Infinite Dimensional Bayesian Inverse Problems

Jinglai Li, Shanghai Jiao Tong University
09:00 - 09:30

Bayesian inference has become increasingly popular as a tool to solve inverse problems, largely due to its ability to quantify the uncertainty in the solutions obtained. In many practical problems such as image reconstructions, the unknowns are often of infinite dimension, i.e., functions of space and/or time. Many existing methods developed for finite dimensional problems may become problematic in the infinite dimensional setting and thus new techniques must be developed to address such problems. In this talk we shall discuss several critical issues associated with the infinite dimensional problems and some efforts made to address them. First we introduce a family of hybrid priors for modeling functions that are subject to sharp jumps. We then present an efficient adaptive MCMC algorithm that is specifically designed for function space inference. Finally, we apply the Bayesian inference methods to a medical image reconstruction problem.

Model Reduction Using Variable-Separation Methods and Some Applications in Uncertainty Quantification

Lijian Jiang, Hunan University
09:35 - 10:05

In the talk, we present a model reduction method based on a novel variable-separation. The idea of the method is applied to obtain the solution in tensor product for stochastic PDEs. The presented variable-separation method has a few advantages over many widely used numerical methods for stochastic PDEs. A hierarchical sparse low rank tensor approximation is used to improve the efficiency for the method and treat high-dimensional stochastic PDEs. The presented method is used for solving a variety of stochastic PDEs and other applications in uncertainty quanfiication.

A gPC Stochastic Galerkin Method for Semiconductor Boltzmann Equations: Analysis on Convergence Rate and Numerics

Liu Liu, University of Wisconsin-Madison
10:45 - 11:15

The author will first talk about a generalized polynomial chaos approach based stochastic Galerkin (gPC-SG) method for semiconductor Boltzmann equation with random inputs and parabolic scaling. A uniform (in the Knudsen number) regularity in the random space, as well as a uniform spectral convergence of the stochastic Galerkin method will be shown. Numerical experiments are conducted to validate the stochastic asymptotic preserving property and efficiency of the proposed method. Lastly, an extended study of exponential convergence to equilibrium for collisional kinetic models with random inputs will also be discussed.

Hypocoercivity and Uniform Regularity for the Vlasov-Poisson-Fokker-Planck System with Uncertainty and Multiple Scales

Yuhua Zhu, University of Wisconsin - Madison
11:20 - 11:50

We study the Vlasov-Poisson-Fokker-Planck system with uncertainty and multiple scales. Here the uncertainy, modeled by random variables, enters the solution through initial data, while the multiple scales lead the system to its high-field or parabolic regimes. With the help of proper Lyapunov-type inequalities, under some mild conditions on the initial data, the regularity of the solution in the random space, as well as exponential decay of the solution to the global Maxwellian, are established under Sobolev norms, which are *uniform* in terms of the scaling parameters. These are the first hypocoercivity results for a nonlinear kinetic system with random input, which are important for the understanding of the sensitivity of the system under random perturbations, and for the establishment of spectral convergence of popular numerical methods for uncertainty quantification based on (spectrally accurate) polynomial chaos expansions.

TBA

Olivier Le Maitre, Univesity of Paris-Saclay, France
14:00 - 14:45

TBA