北京大學
PEKING UNIVERSITY

2017 Young Researchers Workshop: New Trends in Computational and Applied Mathematics

Peking University
December 18-20, 2017

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2017 Young Researchers Workshop: New Trends in Computational and Applied Mathematics

Peking University, December 18-20, 2017

Venue:

Room 77201, Jingchunyuan 78, BICMR, Peking University

Scientific Committee:

- **Weinan E, Princeton University, Peking University**
- **Shi Jin, UW-Madison, Shanghai Jiao Tong University**
- **Pingwen Zhang, Peking University**

Organization Committee:

- **Jun Hu, Peking University**
- **Ruo Li, Peking University**
- **Jianfeng Lu, Duke University**
- **Zhennan Zhou, Peking University**

List of Speakers:

1. **Sona Akopian, Brown University**
2. **Lihui Chai, University of California, Santa Barbara**
3. **Peng Chen, University of Texas at Austin**
4. **Yuwei Fan, Stanford University**
5. **Yuehaw Khoo, Stanford University**
6. **Rongjie Lai, Rensselaer Polytechnic Institute**
7. **Xin Liang, National Chiao Tung University**

8. Huan Lei, Pacific Northwest National Laboratory
9. Lei Li, Duke University
10. Liu Liu, University of Texas at Austin
11. Yulong Lu, Duke University
12. Andre Milzarek, Peking University
13. Ruiwen Shu, University of Wisconsin-Madison
14. Soledad Villar, New York University
15. Haitao Wang, Shanghai Jiao Tong University
16. Alexander Watson, Duke University
17. Hao Wu, Freie Universität Berlin
18. Kailiang Wu, Ohio State University
19. Hai Zhang, Hong Kong University of Science and Technology
20. Jia Zhao, Utah State University

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http://bicmr.pku.edu.cn/meeting/index?id=60

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Schedule

Monday (Dec 18)

Moderator:		
8:30-8:40	**Opening Remark (To be determined)**	
8:40-9:30 **Talk 1**	**Hai Zhang** **Hong Kong University of Science and Technology**	Mathematical theory of wave scattering by subwavelength resonators and applications
9:30-10:20 **Talk 2**	**Alexander Watson** **Duke University**	Wave-packet dynamics in locally periodic media
10:20-10:40	**Coffee Break**	
10:40-11:30 **Talk 3**	**Lei Li** **Duke University**	Some new progress of time fractional differential equations with Caputo derivatives
11:30-12:20 **Talk 4**	**Sona Akopian** **Brown University**	On L^p approximations of solutions of the Landau equation in the Coulomb case
12:00-14:00	**Lunch Break (Lunch boxes provided)**	
Moderator:		
14:00-14:50 **Talk 5**	**Lihui Chai** **University of California, Santa Barbara**	Frozen Gaussian approximation based seismic tomography
14:50-15:40 **Talk 6**	**Yuwei Fan** **Stanford University**	Filtered hyperbolic moment method for Vlasov equation
15:40-16:00	**Coffee Break**	
16:00-16:50 **Talk 7**	**Liu Liu** **The University of Texas at Austin**	Hypocoercivity based Sensitivity Analysis and Spectral Convergence of the Stochastic Galerkin Approximation to Collisional Kinetic Equations with Multiple Scales and Random Inputs
16:50-17:40 **Talk 8**	**Ruiwen Shu** **UW-Madison**	A Stochastic Asymptotic-Preserving Scheme for a Kinetic-Fluid Model for Disperse Two-Phase Flows with Uncertainty
Free Evening		

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Tuesday (Dec 19)

Moderator:		
8:30-9:20 Talk 9	**Kailiang Wu The Ohio State University**	Sequential Function Approximation in High Dimensions
9:20-10:10 Talk 10	**Huan Lei Pacific Northwest National Laboratory**	Data-driven modeling of multiscale multiphysics system
10:10-10:30	**Coffee Break(Group Photo, Approximate number 30)**	
10:30-11:20 Talk 11	**Rongjie Lai Rensselaer Polytechnic Institute**	Geometric PDEs meet matrix completion: Euclidean distance geometry problem and beyond
11:20-12:10 Talk 12	**Yulong Lu Duke University**	Gaussian approximations to probability measures: a variational approach and applications
12:10-14:00	**Lunch Break (Lunch boxes provided)**	
Moderator:		
14:00-14:50 Talk 13	**Soledad Villar New York University**	Quadratic assignment on different data models
14:50-15:40 Talk 14	**Yuehaw Khoo Stanford University**	Convex optimization approach to protein structural calculation from NMR
15:40-16:00	**Coffee Break**	
16:00-16:50 Talk 15	**Peng Chen University of Texas at Austin**	Scalable Approximation of PDE-Constrained Optimization under Uncertainty: Application to Turbulent Jet Flow
16:50-17:40 Talk 16	**Andre Milzarek BICMR, Peking University**	A sub-sampled semi-smooth Newton method for stochastic convex composite problems
18:00	**Conference Banquet (Venue: to be determined)**	

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Wednesday (Dec 20)

Moderator:		
8:30-9:20 **Talk 17**	**Haitao Wang** **Shanghai Jiao Tong University**	Explicit structure of the Fokker-Planck equation with flat confinement
9:20-10:10 **Talk 18**	**Hao Wu** **Freie Universität Berlin**	Variational approach for Markov processes
10:10-10:30	**Coffee Break**	
10:30-11:20 **Talk 19**	**Xin Liang** **National Chiao Tung University**	Eigen-structure behavior of discrete single-curl operator in three-dimensional Maxwell's equations for Pasteur media
11:20-12:10 **Talk 20**	**Jia Zhao** **Utah State University**	Fully Discrete Second-order Linear Schemes for Hydrodynamic Phase Field Models of Binary Viscous Fluid Flows with Variable Densities
12:10-14:00	**Lunch Break (Lunch boxes provided)**	
Afternoon	**Free Discussion**	

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TITLES AND ABSTRACTS

Talk 1

Title: Mathematical theory of wave scattering by subwavelength resonators and applications

Speaker: Hai Zhang, Hong Kong University of Science and Technology

Abstract: In this talk, we will present the recent development of mathematical theory of wave scattering by subwavelength resonators. We will take air-bubble as an example and consider the resonant scattering by a single bubble, a system of dilute bubbles and periodic array of bubbles. For a single bubble, we will derive asymptotic analysis for the Minnaert resonance. For dilute bubbles, we will show how to achieve an effective high contrast media which lead to super-focusing of wave field, and an effective double negative index media which lead to superlensing effect. For periodic bubbles, we will show a subwavelength band-gap opening, and further develop a high frequency homogenization theory for the wave propagation.

Talk 2

Title: Wave-packet dynamics in locally periodic media

Speaker: Alexander Watson, Duke University

Abstract: We study the dynamics of wave-packet solutions of Schrödinger's equation and Maxwell's equations in media with a local periodic structure which varies adiabatically (over many periods of the periodic lattice) across the medium. We focus in particular on the case where symmetries of the periodic structure lead to degeneracies in the Bloch band dispersion surface. We derive systematically and rigorously the 'anomalous velocity' of wave-packets due to the Bloch band's Berry curvature, and the dynamics of a wave-packet incident on a Bloch band degeneracy in one spatial dimension. Joint work with Michael Weinstein and Jianfeng Lu.

Talk 3

Title: Some new progress of time fractional differential equations with Caputo derivatives

Speaker: Lei Li, Duke University

Abstract: In this talk, I will introduce a generalized definition of Caputo derivatives based on a convolution group, and its applications to fractional ODEs, SDEs and PDEs. In particular, for time fractional ODEs, I will talk about the generalized comparison principles under very weak conditions, the monotonicity and blowup behavior for some autonomous fractional ODEs; I will also introduce a fractional SDE model with Caputo derivative and fractional Brownian motion involved to satisfy the fluctuation-dissipation theorem; furthermore, for fractional PDEs, some compactness criteria will be introduced for the existence of weak solutions to time fractional PDEs. This talk is based on a series of work with Jian-Guo Liu, Jianfeng Lu et al.

Talk 4

Title: On L^p approximations of solutions of the Landau equation in the Coulomb case

Speaker: Sona Akopian, Brown University

Abstract: We examine a class of Boltzmann equations with an abstract collision kernel in the form of a singular mass, concentrated at very low collision angles and relative velocities between interacting particles. Like the classical Boltzmann operator, this collision operator also converges to the collision term in the Landau equation as the characterizing parameter ε tends to zero. We will address the existence of L^p solutions to this family of Boltzmann equations and discuss their approximations of solutions to the Landau equation as ε vanishes.

Talk 5

Title: Frozen Gaussian approximation based seismic tomography

Speaker: Lihui Chai, University of California, Santa Barbara

Abstract: We present a systematically introduction to the Frozen Gaussian Approximation (FGA) for high-frequency seismic tomography in 3-D earth models. In the frozen Gaussian approximation (FGA) we approximate the seismic wavefield by a summation of frozen (fixed-width) Gaussian wave-packets propagating along ray paths. One can use a relatively small number of Gaussians to get accurate approximations of the high-frequency wavefield. Meanwhile, FGA algorithm can be

perfectly parallelized, which speeds up the computation drastically with a high-performance computing station. In order to apply FGA to the computation of 3-D high-frequency seismic tomography, first we reformulate the FGA so that one can efficiently compute the Green's functions; and second, we incorporate Snell's law into the FGA formulation, and asymptotically derive reflection, transmission and free surface conditions for FGA to compute high-frequency seismic wave propagation in high contrast media. We successfully apply FGA in the local earthquake inversion and cross-well inversion using travel-time tomography and full-waveform inversion. Our numerical tests show that FGA has a huge advantage in comparison with the classical direct solver such as spectral element method in improving the computational efficiency, parallelizability, and accuracy in the high-frequency regime and large domain simulation.

Talk 6

Title: Filtered hyperbolic moment method for Vlasov equation

Speaker: Yuwei Fan, Stanford University

Abstract: Direct discretization of Vlasov equation usually results an unphysical "recurrence" phenomenon. In this talk, I will propose a novel filtering for the hyperbolic moment method for Vlasov equation. This filtering can prevent the recurrence effects and also preserves a lot of physical properties of hyperbolic moment method, including Galilean transformation invariant, the conservation of mass, momentum and energy. We present two viewpoints to understand the filtering, and show that the filtered hyperbolic moment method can be treated as a solver of Vlasov equation. Numerical results denomenstrate the validity of the filtering.

Talk 7

Title: Hypocoercivity based Sensitivity Analysis and Spectral Convergence of the Stochastic Galerkin Approximation to Collisional Kinetic Equations with Multiple Scales and Random Inputs

Speaker: Liu Liu, The University of Texas at Austin

Abstract: In this talk, a general framework to study general class of linear and nonlinear kinetic equations with random uncertainties from the initial data or collision

kernels, and their stochastic Galerkin approximations--in both incompressible Navier-Stokes and Euler (acoustic) regimes--is provided.

First, we show that the general framework put forth in [C. Mouhot and L. Neumann, Nonlinearity, 19, 969-998, 2006; M. Briant, J. Di. Eqn., 259, 6072-6141, 2005] based on hypocoercivity for the deterministic kinetic equations can be adopted for sensitivity analysis for random kinetic equations, which gives rise to an exponential convergence of the random solution toward the (deterministic) global equilibrium, under suitable conditions on the collision kernel.

Then we use such theory to study the stochastic Galerkin (SG) methods for the equations, establish hypocoercivity of the SG system and regularity of its solution, and spectral accuracy and exponential decay of the numerical error of the method in a weighted Sobolev norm. This is a joint work with Shi Jin.

Talk 8

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

Speaker: Ruiwen Shu, UW-Madison

Abstract: 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.

Talk 9

Title: Sequential Function Approximation in High Dimensions

Speaker: Kailinag Wu, The Ohio State University

Abstract: One of the central tasks in computational mathematics and statistics is to accurately approximate unknown target functions. This is typically done with the help of data--samples of the unknown functions. The recent emergence of big data presents both opportunities and challenges in this field. On one hand, big data introduces more information about the unknowns and, in principle, allows us to create more accurate models. On the other hand, data storage and processing become highly challenging. In this talk, we present a set of sequential algorithms for function approximation in high dimensions with large data sets. The algorithms are of iterative nature and involve only vector operations. They use one data sample at each step and can handle dynamic or streaming data. We present both the numerical algorithms, which are easy to implement, as well as rigorous analysis for their theoretical foundation.

Talk 10

Title: Data-driven modeling of multiscale multiphysics system

Speaker: Huan Lei, Pacific Northwest National Laboratory

Abstract: Computational modeling of multiscale multiphysics systems essentially involves quantifying the uncertainty of quasi-equilibrium properties around individual metastable states as well as prediction of non-equilibrium dynamics over the entire phase space. Due to the implicit knowledge of underlying distribution near individual metastable states, quantifying the quasi-equilibrium properties is centered around constructing a surrogate model with high-dimensional arbitrary random space. We develop a data-driven approach by constructing the sparse representation of the target quantity based on optimization of the basis function as well as transformation of the random variables. The proposed method is demonstrated in quantifying quasi-equilibrium properties such as solvation energy of biomolecule systems. Furthermore, prediction of non-equilibrium dynamics is centered around modeling of the nonlocal spatio/temporal correlations and scale-dependent fluctuations in the target system. Traditional computational models based on those canonical governing principles (e.g., Fick's, Darcy's law) often show limitation. We propose a data-driven approach to

model such system based on efficient parameterization of the generalized Langevin Equation (GLE), where the effects of the smaller scale interactions on the scale of interest (i.e., the scale of the field variable) are properly accounted as the memory kernel of GLE. The approximated kernel formulation satisfies the second fluctuation-dissipation conditions with consistent invariant measure. The proposed method enables us to accurately characterize the challenging non-equilibrium properties such as transition rate where traditional hypothesis-driven modeling equations show limitation.

Talk 11

Title: Geometric PDEs meet matrix completion: Euclidean distance geometry problem and beyond

Speaker: Rongjie Lai, Rensselaer Polytechnic Institute

Abstract: The problem of global understanding of point clouds represented as incomplete inter-point distance has many applications in 3D modeling, sensor network localization as well as protein structuring. Without considering time-consuming global coordinates reconstruction, we propose to only reconstruct manifold locally based on low-rank matrix completion theory and to conduct global understanding using geometric PDEs to link local information and global information. I will demonstrate efficiency and effectiveness of the proposed methods. After that, I will discuss some theoretical analysis of the proposal low-rank matrix completion problem and its extension to understanding matrix completion from sampling under non-orthogonal basis.

Talk 12

Title: Gaussian approximations to probability measures: a variational approach and applications

Speaker: Yulong Lu, Duke University

Abstract: Asymptotic normality is ubiquitous in probability and statistics. Two typical examples are central limit theorems and Bernstein-von Mises theorems. A central limit theorem states that an appropriate averaged sum of a family of random variables tends to a normal distribution. The famous Bernstein-von Mises theorem,

which should be viewed a Bayesian version of CLT, establishes that under some mild assumptions on the prior, the posterior distribution of a Bayesian procedure is close to Gaussian in the limit of large sample size, independent of the specific choice of the prior.
Motivated by the property of asymptotic normality, we study the problem of approximating a (non-Gaussian) probability measure by simple Gaussian families. The key idea is to minimize the Kullback-Leibler divergence between Gaussians and the target measure over a parametric class of Gaussian measures. We also examine the asymptotic behavior of such approximation in some small parameter limit. The theory of KL approximation is demonstrated with two applications: the posterior consistency of Bayesian inverse problems and the typical transition paths in Molecular dynamics. This is in collaboration with Andrew Stuart (Caltech) and Hendrik Weber (Warwick).

Talk 13

Title: Quadratic assignment on different data models

Speaker: Soledad Villar, New York University

Abstract: Quadratic assignment is a very general problem in theoretical computer science. It includes graph matching, the traveling salesman problem, and the Gromov-Hausdorff distance between finite metric spaces as particular cases. Quadratic assignment is in general NP-hard and even hard to approximate, but in fact the problem can be tractable for a large subset of instances. In this talk we present different algorithmic approaches that lead to meaningful results for different data models. A semidefinite relaxation provides a pseudometric that can be computed in polynomial-time and has similar topological properties to the GH distance. A projected power iteration algorithm succeeds at aligning noisy networks. And a graph neural network can actually learn an algorithm to solve network alignment and the traveling salesman problem from solved problem instances.

Talk 14

Title: Convex optimization approach to protein structural calculation from NMR

Speaker: Yuehaw Khoo, Stanford University

Abstract: Nuclear magnetic resonance (NMR) spectroscopy is the most-used technique for protein structure determination besides X-ray crystallography. In this talk, the computational problem of protein structuring from residual dipolar coupling (RDC) will be discussed.
Typically the 3D structure of a protein is obtained through finding the coordinates of atoms subject to pairwise distance constraints. RDC measurements provide additional geometric information on the angles between bond directions and the principal-axis-frame. The optimization problem involving RDC is non-convex and we present a novel convex programming relaxation to it by incorporating quaternion algebra. In simulations we attain the Cramer-Rao lower bound with relatively efficient running time. From real data, we obtain the protein backbone structure for ubiquitin with 1 Angstrom resolution.
This is joint work with Amit Singer and David Cowburn.

Talk 15

Title: Scalable Approximation of PDE-Constrained Optimization under Uncertainty: Application to Turbulent Jet Flow

Speaker: Peng Chen, University of Texas at Austin

Abstract: In this talk, we present a scalable method based on Taylor approximation for PDE-constrained optimal control problems under high-dimensional uncertainty. The computational complexity of the method does not depend on the nominal but only on the intrinsic dimension of the uncertain parameter, thus the curse of dimensionality is broken for intrinsically low-dimensional problems. Further Monte Carlo correction for the Taylor approximation is proposed, which leads to an unbiased evaluation of the statistical moments in the objective function and achieves reduction of variance by several orders of magnitude compared to a Monte Carlo approximation. We apply our method for a turbulence model with infinite-dimensional random viscosity and demonstrate the scalability up to 1 million parameter dimensions.

Talk 16

Title: A sub-sampled semi-smooth Newton method for stochastic convex composite problems

Authors: Andre Milzarek, BICMR, Peking University (Speaker)

Co-Authors:

Xiantao Xiao, School of Mathematical Sciences, Dalian University of Technology

Shicong Cen, Peking University

Zaiwen Wen, BICMR, Peking University

Abstract: In this talk, we present a globalized semi-smooth Newton method for solving stochastic optimization problems involving smooth nonconvex and nonsmooth convex terms in the objective function. More specifically, we assume that the smooth part of the objective function can be written as the expectation of a given smooth loss function. The resulting class of problems that can be solved within our algorithmic framework comprises a large variety of applications such as l1-logistic regression, structured dictionary learning, and other minimization problems arising in machine learning, statistics, or image processing. In practice, since the underlying distribution is often not known or is not completely available, sampling strategies or stochastic first- and second-order oracles have to be used to approximate the expectation terms and to access gradient and Hessian information. The approach we investigate utilizes stochastic second order information and sub-sampled semi-smooth Newton steps for a prox-type fixed-point equation, representing the associated optimality conditions, to accelerate the basic stochastic proximal gradient method for convex composite programming. Approximate growth conditions are introduced to monitor the quality and acceptance of the Newton steps and to combine the two different methods. We prove that our approach converges globally to stationary points in expectation and almost surely. Moreover, under standard assumptions, the proposed algorithm can be shown to locally turn into a pure semi-smooth Newton method and fast local convergence can be established with high probability. Finally, we provide numerical experiments illustrating the efficiency of the stochastic semi-smooth Newton method.

Talk 17

Title: Explicit structure of the Fokker-Planck equation with flat confinement

Speaker: Haitao Wang, Shanghai Jiao Tong University

Abstract: We study the pointwise (in both space and time variables) behavior of the Fokker-Planck Equation with flat confinement. The solution has very accurate description, including the initial singularity, large time behavior and spatially asymptotic behavior. The initial layer is dominated by Kolmogorov-Fokker-Planck solution, the large time behavior is dominated by diffusion fluid wave, and the solution decays exponentially at space-like region. Moreover, the structure of the solution highly depends on the potential function.

Talk 18

Title: Variational approach for Markov processes

Speaker: Hao Wu, Freie Universität Berlin

Abstract: In this talk, we introduce a variational approach for Markov processes (VAMP) that allows us to find optimal feature mappings and optimal Markovian models of the dynamics from given time series data. The key insight is that the best linear model can be obtained from the top singular components of the Koopman operator. This leads to the definition of a family of score functions called VAMP-r which can be calculated from data, and can be employed to optimize a Markovian model. In addition, based on the relationship between the variational scores and approximation errors of Koopman operators, we propose a new VAMP-E score, which can be applied to cross-validation for hyper-parameter optimization and model selection in VAMP. Finally, the combination of VAMP and deep learning is discussed, which provides a powerful tool to analyze dynamic data.

Talk 19

Title: Eigen-structure behavior of discrete single-curl operator in three-dimensional Maxwell's equations for Pasteur media

Speaker: Xin Liang National Chiao Tung University

Abstract: The eigen-structure of the discrete single-curl operator is fundamental and vital for efficient numerical simulations for complex materials, which imply coupling effects between electric and magnetic fields. Here a particular one, namely Pasteur medium (a.k.a. reciprocal chiral medium) is considered. The fields, or equivalently the propagation of electromagnetic waves in the complex materials, is modeled by the

three-dimensional frequency domain source-free Maxwell's equations. Due to the large scale of the problem and the loss of definite property in the strongly-coupled case, lack of theory makes it difficult to guarantee the numerical results are valid and reliable. In this talk, we build several theoretical results on its eigen-structure behavior, of which an amazing one is that we can generate a new state whose energy is smaller than the ground state.

Talk 20

Title: Fully Discrete Second-order Linear Schemes for Hydrodynamic Phase Field Models of Binary Viscous Fluid Flows with Variable Densities

Speaker: Jia Zhao, Utah State University

Abstract: In this talk, we present spatial-temporally second-order, energy stable numerical schemes for two classes of hydrodynamic phase field models of binary viscous fluid mixtures of different densities. One is quasi-incompressible while the other is incompressible. We introduce a novel invariant energy qudratization (IEQ) technique to arrive at fully discrete linear schemes, where in each time step only a linear system needs to be solved. These schemes are then proved to be unconditionally energy stable rigorously so that a large time step is plausible. Both spatial and temporal mesh refinements are conducted to illustrate the second order accuracy of the schemes. Several Numerical examples and conducted, and predictions by the two fluid mixture models are compared and discussed. As a conclusion, we believe the quasi-incompressible model is more reliable than the incompressible one. This is a joint work with Yuezheng Gong (Nanjing University of Aeronautics and Astronautics, China) and Qi Wang (Beijing Computational Science Research Center, China).