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# Workshop on Computation of Kinetic Transport and Related Problems

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June 21-22, 2019



Institute of Natural Sciences, Shanghai Jiao Tong University

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# 1 General Information

## Introduction

This workshop aims at bringing in experts on computation of kinetic transport and related problems, in order to exchange ideas about the numerical simulation, related models or uncertainty quantification of the problem, and to foster future collaborations.

## Acknowledgement

This conference is supported by Institute of Natural Sciences, MOE Key Lab on Scientific and Engineering Computing, Science Challenge Project.

## Date

June 21-22, 2019

## Venue

Room 306, No.5 Science Building, Minhang Campus, Shanghai Jiao Tong University

## Scientific Committee

- Song Jiang, Institute of Applied Physics and Computational Mathematics
- Shi Jin, Shanghai Jiao Tong University

## Organizing Committee

- Jianguo Huang, Shanghai Jiao Tong University
- Min Tang, Shanghai Jiao Tong University
- Wenjun Ying, Shanghai Jiao Tong University

## 2 Schedule

### 2.1 Day 1, 21 June, Friday

Time	Speaker	Title
08:30 - 09:00		Registration
09:00 - 09:40	Guangwei Yuan (袁光伟)	Brief Introduction of Discrete Method for Radiative Heat Conduction in Multifluid Channel
09:40 - 10:20	Ruo Li (李若)	An effective method for the numerical simulation of the strong coupling between radiant transport and electronic energy
10:20 - 10:40		Coffee Break
10:40 - 11:20	Zhongyi Huang (黄忠亿)	Monotone finite point method for non-equilibrium radiation diffusion equations
11:20 - 12:00	Tao Zhou (周涛)	Adaptive multi-fidelity surrogate modeling for Bayesian inference in inverse problems
12:15 - 13:45		Lunch
14:00 - 14:40	Juan Cheng (成娟)	High order positivity-preserving and conservative DG schemes for radiation transfer equations
14:40 - 15:20	Xinghui Zhong (仲杏慧)	Galerkin Method for Stationary Radiative Transfer Equations with Uncertain Coefficients
15:20 - 15:40		Coffee Break
15:40 - 16:20	Yanping Chen(陈艳萍)	Mortar element method for the coupling of Navier-Stokes and Darcy flows
16:20 - 17:00	Shengxin Zhu (朱圣鑫)	Algebraic Acceleration for Transport Problems

## 2.2 Day 2, 22 June, Saturday

Time	Speaker	Title
09:00 - 09:40	Jun Hu (胡俊)	Can We Do Better for Computation of Eigenvalues of PDE Eigenvalue Problems?
09:40 - 10:20	Peng Song (宋鹏)	Introduction to the Numerical Simulation of Radiation Transport in the Laser Indirect-Driven Inertial Confinement Fusion
10:20 - 10:40		Coffee Break
10:40 - 11:20	Ziqing Xie (谢资清)	A Globally Convergent BB-type Local Minimax Method for Finding Multiple Saddle Points
11:20 - 12:00	Weiran Sun (孙蔚然)	Inverse problems for transport equations
12:15 - 13:45		Lunch
14:00 - 14:40	Xinlong Feng (冯新龙)	A difference finite element method for 3D parabolic problem
14:40 - 15:20	Zhen Gao (高振)	Non-intrusive reduced order modeling of convection dominated flows using artificial neural networks with application to Rayleigh-Taylor instability
15:20 - 16:00	Yuhua Zhu (朱裕华)	The Vlasov-Fokker-Planck Equation with High Dimensional Parametric Forcing Term
16:00 - 16:30		Coffee Break

## 3 Abstracts

### 3.1 Day 1, 21 June, Friday

#### **Brief Introduction of Discrete Method for Radiative Heat Conduction in Multifluid Channel**

*Guangwei Yuan (袁光伟) , Institute of Applied Physics and Computational Mathematics  
09:00 - 09:40*

For solving numerically multi-material radiation hydrodynamic problems, a kind of ALE methods named as "multifluid channel method" has been used in some applications.

This talk will describe briefly the research history and some progresses for discrete schemes of radiative heat conduction in multifluid channel.

#### **An effective method for the numerical simulation of the strong coupling between radiant transport and electronic energy**

*Ruo Li (李若) , Peking University  
09:40 - 10:20*

In the low-opacity material, the coupling between radiant transport and electronic energy is strong. The system of radiant transport equation and electronic energy equation represents strong stiffness, which induces difficulties in numerical simulation. In this paper, an effective numerical method for the simulation of the strong coupling between radiant transport and electronic energy is introduced. This method is an integral method based on the ansatz assumption of the electronic temperature. There is no constraint on the time step. Thus the method has high computing efficiency and good accuracy.

#### **Monotone finite point method for non-equilibrium radiation diffusion equations**

*Zhongyi Huang (黄忠亿) , Tsinghua University  
10:40 - 11:20*

In this talk, we propose the monotone tailored-finite-point method for solving the non-equilibrium radiation diffusion equations. Our method satisfies the discrete maximum principle automatically, thus preserves the properties of monotonicity and positivity. Numerical results show that our method can capture the sharp front and also can be accommodated to discontinuous diffusion coefficient.

## **Adaptive multi-fidelity surrogate modeling for Bayesian inference in inverse problems**

*Tao Zhou (周涛) , Chinese Academy of Sciences  
11:20 - 12:00*

The polynomial chaos expansion is widely used as a surrogate model in the Bayesian inference to speed up the Markov chain Monte Carlo calculations. However, the use of such a surrogate introduces modeling errors that may severely distort the estimate of the posterior distribution. In this talk, we present an adaptive procedure to construct a multi-fidelity polynomial surrogate. More precisely, the new strategy starts with a low-fidelity surrogate model, and this surrogate will be adaptively corrected using online high-fidelity data. The key idea is to construct and refine the multi-fidelity surrogate over a sequence of samples adaptively determined from data so that the approximation can eventually concentrate to the posterior distribution. We also introduce a multi-fidelity surrogate based on the deep neural networks to deal with problems with high dimensional parameters. The performance of the proposed strategy is illustrated through two nonlinear inverse problems.

## **High order positivity-preserving and conservative DG schemes for radiation transfer equations**

*Juan Cheng (成娟) , Institute of Applied Physics and Computational Mathematics  
14:00 - 14:40*

Numerical simulation of radiation transfer equations arises in many applications, including astrophysics, inertial confinement fusion, optical molecular imaging, shielding, and so on. The positivity-preserving and conservation-preserving properties are two important and challenging issues for the numerical solution of this kind of equations. In this talk, I will introduce our recent work on high order positivity-preserving and conservative discontinuous Galerkin (DG) schemes solving steady and unsteady radiation transfer equations. The properties such as positivity-preserving and high order accuracy are proven rigorously. One- and two-dimensional numerical results are provided to verify the designed characteristics of our schemes.

## **Galerkin Method for Stationary Radiative Transfer Equations with Uncertain Coefficients**

*Xinghui Zhong (仲杏慧) , Zhejiang University  
14:40 - 15:20*

We study the stationary radiative transfer equation (RTE) with random coefficients. Galerkin type approximation is used, and in random space, orthogonal polynomials associated with the probability distribution of the random variable are utilized as basis functions. Such algorithms have been widely used for kinetic equations with random inputs, but the corresponding numerical analysis is rare. In this talk, we rigorously justify the validity, namely, we study the smoothness of the solution on the random space, and prove the convergence of N-term truncated polynomials under the spectral method framework. The associated numerical tests are conducted to demonstrate our analytical results.

## Mortar element method for the coupling of Navier-Stokes and Darcy flows

*Yanping Chen (陈艳萍) , South China Normal University  
15:40 - 16:20*

In this talk, mortar element method is investigated for the coupling of incompressible flow and porous media flow which is relevant to a variety of physical processes. It consists of three parts: the steady coupling of Navier-Stokes and Darcy flows; the unsteady coupling of Stokes and Darcy flows; the unsteady coupling of Navier-Stokes and Darcy flows. The existence and the uniqueness of the weak solution are proved by Galerkin method. The interface part of Navier-Stokes' boundary is chosen as the mortar. The convergence is proved and numerical results verify theoretical analysis.

## Algebraic Acceleration for Transport Problems

*Shengxin Zhu (朱圣鑫) , Xi'an Jiaotong-Liverpool University  
16:20 - 17:00*

In this talk, we shall present some numerical experiments for simple radiative transport problems, and present some numerical challenges for solving the algebraic problems, and hope to invite advice and suggestions from experts in this filed.

## 3.2 Day 2, 22 June, Saturday

### Can We Do Better for Computation of Eigenvalues of PDE Eigenvalue Problems?

*Jun Hu (胡俊) , Peking University  
09:00 - 09:40*

Finding eigenvalues of operators is important in the mathematical sciences. Many numerical methods have been used to approximate eigenvalue problems of partial differential operators, such as finite difference methods, finite element methods and spectral methods. However, it is well-known that when finite difference methods and finite element methods are applied, only a small portion of numerical eigenvalues can be reliable. Is it possible to improve accuracy for a large number of eigenvalues?

Adaptive finite element methods has been widely used to improve the accuracy of numerical solutions of PDE problems including PDE eigenvalue problems. It is believed to be one of the most efficient discretizations. Is it possible to improve largely adaptive finite element methods of PDE eigenvalue problems?

This talk will try to touch the aforementioned topics.

### Introduction to the Numerical Simulation of Radiation Transport in the Laser Indirect-Driven Inertial Confinement Fusion

*Peng Song (宋鹏) , Institute of Applied Physics and Computational Mathematics  
09:40 - 10:20*

The new-type green energy resource is an important issue in the development of the human's society on earth, as a result of the enormous increasing of the energy requirement. Fusion resource has many advantages, such as high energy density, abundant materials, low environment pollution, etc. Fusion is considered as one of the most possible energy resources for human beings in future. The controllable fusion can supply abundant, economic, safe and clean energy. Laser indirect-driven inertial confinement fusion (ICF) is one way to control fusion in experiment lab. The main process of ICF has four steps. First, laser beams with high energy is generated by the laser facility, and is irradiated into a hohlraum made by high-Z material. Second, high-Z material transforms the laser energy to X-ray, and X-ray transports in the hohlraum, some of which escapes the hohlraum by the hole and some are irradiated on the capsule. Third, the capsule is ablated by X-ray and the center made by nuclear fuel is compressed and a hot spot is formed with high density and high temperature. Finally, the fusion condition is reached in the hot spot and more fuel is ignited, then more energy is released than the laser energy. Laser indirect-driven ICF contains many physical processes. Radiation transport is one of the most important model to describe the energy transform and transport in hohlraum, which determines the radiation spatial and spectral distribution, the driven source's pulse and asymmetry of the capsule. Radiation transport's degree of freedom is so large that the numerical simulation of radiation transport expends more than a half of the computing resource of the entire numerical simulation of ICF, thus how to improve the computing efficiency of radiation transport's numerical method is significant and attractive. This talk will introduce the main process of ICF, and the general numerical methods and difficulties of radiation transport's simulation. More communication and cooperation is expected.

## **A Globally Convergent BB-type Local Minimax Method for Finding Multiple Saddle Points**

*Ziqing Xie (谢资清) , Hunan Normal University  
10:40 - 11:20*

Saddle points, which are unstable critical points, have a widely range of applications in many fields of nonlinear science, such as nonlinear optics, condensed matter physics, chemical reactions, and materials science etc.. Owing to the nonlinearity of model problems, the multiplicity and instability of saddle points, it is extremely challenging to design a stable, efficient and globally convergent numerical algorithm for finding saddle points. In this talk, a globally convergent Barzilai-Borwein-type local minimax method (GBB-LMM) is proposed for finding multiple saddle points of nonconvex functionals in Hilbert space, where the idea of the Barzilai-Borwein gradient method combining with the nonmonotone line search strategy in optimization in Euclidean space is applied to solve a two-level local optimization problem. Actually, the Barzilai-Borwein-type step-size is explicitly constructed as a trial step-size at each iteration step of the local minimax method, and the nonmonotone step-size search rule is introduced to guarantee the global convergence. The feasibility and global convergence of the GBB-LMM are rigorously verified. The GBB-LMM is then implemented to solve several typical nonlinear boundary value problems with variational structures for multiple unstable solutions. The numerical results indicate that our approach may greatly speed up the convergence of traditional local minimax methods.

## Inverse problems for transport equations

*Weiran Sun (孙蔚然) , Simon Fraser University*  
11:20 - 12:00

A classical approach in identifying optical parameters in radiative transfer equations is to apply the singular decomposition to their associated Albedo operators. This approach heavily relies on the specific structure of the equation, and thus could be hard to apply to nonlinear equations. In this talk, we show that by making use of classical analytical tools for kinetic equations, we can recover the absorption and scattering coefficients of a class of equations without resorting to fine details of the Albedo operator. Such tools include the maximum principle, energy estimates, and the celebrated averaging lemma. Since our method is largely based on generic properties of kinetic equations, we can apply it to nonlinear equations whose well-posedness in the forward setting is known. This is a joint work with Qin Li.

## A difference finite element method for 3D parabolic problem

*Xinlong Feng (冯新龙) , Xinjiang University*  
14:00 - 14:40

In this work, we propose a novel difference finite element (DFE) method based on the  $P_1$ -element for the 3D heat equation on a bounded domain  $\Omega = \times(0, L_3)$ . One of novel ideas of this work is to use the second-order backward difference formula (BDF) combining DFE method to overcome the computational complexity of conventional finite element (FE) method for the high-dimensional parabolic problem. The proposed method deduces a numerical solution of the 3D problem on  $\Omega$  into a combination of numerical solutions of a series of 2D problem on  $\Omega_2$ . Finally, numerical tests are presented to show the second-order  $H^1$ -convergence results of the proposed DFE method for the 3D heat equation.

## Non-intrusive reduced order modeling of convection dominated flows using artificial neural networks with application to Rayleigh-Taylor instability

*Zhen Gao (高振) , Ocean University of China*  
14:40 - 15:20

In this talk, a non-intrusive reduced order modeling of convection dominated flows based on the proper orthogonal decomposition (POD) and the artificial neural network (ANN) is designed to simulate the linear and quasi-nonlinear regimes of Rayleigh-Taylor instability (RTI) phenomenon. The temporal and spatial accuracy of the proposed method is demonstrated by solving a high-dimensional parametrized ODE and one-dimensional viscous Burgers' equation with a parameterized diffusion coefficient. The results illustrate that the proposed ROM can achieve a good agreement with the corresponding full-order solutions. Particularly, RTI is simulated by the proposed method, where the amplitude of the small perturbation and time are considered as free parameters. Furthermore, an adaptive sampling method in time is proposed to decrease the number of samples in the parameter space during the linear regime of RTI, which results in the number of snapshots of the full-order solutions required for POD and the training of the ANN is correspondingly reduced. The numerical results show that the adaptive sampling method can achieve an equivalent accuracy and an improved efficiency.

## The Vlasov-Fokker-Planck Equation with High Dimensional Parametric Forcing Term

*Yuhua Zhu (朱裕华) , Stanford University*  
*15:20 - 16:00*

We consider the Vlasov-Fokker-Planck equation with random electric field where the random field is parameterized by countably many infinite random variables due to uncertainty. At the theoretical level, with suitable assumption on the anisotropy of the randomness, adopting the technique employed in elliptic PDEs [5], we prove the best  $N$  approximation in the random space breaks the dimension curse and the convergence rate is faster than the Monte Carlo method. For the numerical method, based on the adaptive sparse polynomial interpolation (ASPI) method introduced in [2], we develop a residual based adaptive sparse polynomial interpolation (RASPI) method which is more efficient for multiscale linear kinetic equation, when using numerical schemes that are time-dependent and implicit. Numerical experiments show that the numerical error of the RASPI  $t$  decays faster than the Monte-Carlo method and is also dimension independent.