Workshop Series on Advances on Scientific and Engineering Computing (II) ——High Performance Computation: Theory and Applications

October 17-18, 2020

上海交通大學 SHANGHAI JIAO TONG UNIVERSITY | 自然科学研究院 Institute of Natural Sciences

Contents

1 General Information

Introduction

Scientific and engineering computing plays a vital role in modern industrial and applied mathematics. Good mathematical models and numerical algorithms can nicely, elegantly or efficiently solve problems which are otherwise difficult and challenging. This workshop aims to bring together leading experts and excellent young researchers inside China to share state of the art research advances in the field of scientific and engineering computing, foster further research collaborations and promote novel and revolutionary research ideas.

Acknowledgement

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

Application and Registration

Please register online.
Preference is given to, but not limited to, applicants with a basic understanding of High Performance Computing. No registration fee.

Date

October 17-18, 2020

Venue

Room 306, No.5 Science Building, Minhang Campus, Shanghai Jiao Tong University
How to arrive: https://ins.sjtu.edu.cn/contact-us

Organizing Committee

- Shi Jin, Shanghai Jiao Tong University
- Min Tang, Shanghai Jiao Tong University
- Wenjun Ying, Shanghai Jiao Tong University

Workshop Series

Workshop on Advances on Scientific and Engineering Computing (I)

2 Schedule

2.1 Day 1, 17 October, Saturday

Time	Speaker	Title
08:30 - 08:40		Opening
08:40 - 09:15	Cheng He/Guiping Zhao	NSFC application
09:15 - 09:25		Group Photo & Break
09:25 - 10:00	Huazhong Tang	High-Order Accurate Entropy Stable Nodal Discontinuous Galerkin Schemes for the Special Relativistic Magnetohydrodynamics
10:00 - 10:35	Hao Wu	Machine Learning for Large-Scale Combinatorial Optimization Problems
10:35 - 10:50		Coffee Break
10:50 - 11:25	Zhongyi Huang	Multi-Phase Segmentation using Modified Complex Cahn-Hilliard Equation
11:25 - 12:00	Zhenli Xu	Highly Scalable Molecular Dynamics Method for Long-Range Particle Systems
12:00 - 14:00		Lunch
14:00 - 14:35	Jialin Hong	Probabilistic Superiority of Stochastic Symplectic Methods via Large Deviations Principle
14:35 - 15:10	Zhennan Zhou	Some Numerical Aspects of Langevin Sampling of the Path Integral Molecular Dynamics
15:10 - 15:30		Coffee Break
15:30 - 16:05	Tiao Lu	Introduction to Simulation of Nano-Scale Semiconductor Devices
16:05 - 16:40	Shipeng Mao	Numerical Methods for Thermally Driven Incompressible Magnetohydrodynamic Problems
16:40 - 17:15	Lihui Chai	Seismic Tomography – Frozen Gaussian Approximation and Stochastic Gradient Reconstruction

2.2 Day 2, 18 October, Sunday

Time	Speaker	Title
09:00 - 09:35	Yajuan Sun	Hamiltonian particle-in-cell methods for simulating Vlasov-Maxwell equations
09:35 - 10:10	Bo Wang	Fast Multipole Method in Layered Media
10:10 - 10:30		Coffee Break
10:30 - 11:05	Qiang Zhang	Superconvergence Analysis on the Runge-Kutta Discontinuous Galerkin Method for Linear Hyperbolic Equation
11:05 - 11:40	Tao Xiong	Conservative Discontinuous Galerkin/Hermite Spectral Method for the Vlasov-Poisson System
12:00 - 14:00		Lunch

3 Abstracts

3.1 Day 1, 17 October, Saturday

NSFC application

Cheng He/Guiping Zhao , National Natural Science Foundation of China
08:40 - 09:15

TBA

High-Order Accurate Entropy Stable Nodal Discontinuous Galerkin Schemes for the Special Relativistic Magnetohydrodynamics

Huazhong Tang, Peking University
09:25 - 10:00

Machine Learning for Large-Scale Combinatorial Optimization Problems

Hao Wu, Tsinghua University
10:00 - 10:35

We will discuss two types of large-scale combinatorial optimization models that arise from practical industrial problems and solve them using machine learning methods.

Multi-Phase Segmentation using Modified Complex Cahn-Hilliard Equation

Zhongyi Huang, Tsinghua University
10:50 - 11:25

In this talk, we propose a novel PDE-based model for the multi-phase segmentation problem by using a complex version of Cahn-Hilliard equations. Specifically, we modify the original complex system of Cahn-Hilliard equations by adding the mean curvature term and the fitting term to the evolution of its real part, which helps to render a piecewise constant function at the stead state. By applying the K-means method to this function, one could achieve the desired multiphase segmentation. To solve the proposed system of equations, a semi-implicit finite difference scheme is employed. Numerical experiments are presented to demonstrate the feasibility of the proposed model and compare our model with other related ones.

Highly Scalable Molecular Dynamics Method for Long-Range Particle Systems

Zhenli Xu, Shanghai Jiao Tong Unviersity
11:25 - 12:00

Probabilistic Superiority of Stochastic Symplectic Methods via Large Deviations Principle

Jialin Hong, Chinese Academy of Sciences
14:00 - 14:35

Plenty of numerical experiments show that stochastic symplectic methods are superior to non-symplectic ones especially in long-time computation, when applied to stochastic Hamiltonian systems. In this talk we first review some basic results on stochastic symplectic methods of stochastic Hamiltonian systems, such as the theory of stochastic generating functions, variational integrators, pseudo-symplectic methods, etc. Then we present the probabilistic superiority of stochastic symplectic methods of stochastic Hamiltonian systems via large deviations principle. (In collaboration with Dr. Chuchu Chen, Dr. Diancong Jin and Dr. Liying Sun)

Some Numerical Aspects of Langevin Sampling of the Path Integral Molecular Dynamics

Zhennan Zhou, Peking University
14:35 - 15:10

We investigate the continuum limit that the number of beads goes to infinity in the ring polymer representation of thermal verages. Studying the continuum limit of the trajectory sampling equation sheds light on

possible preconditioning techniques for sampling ring polymer configurations with large number of beads. We propose two preconditioned Langevin sampling dynamics, which are shown to have improved stability and sampling accuracy. We present a careful mode analysis of the preconditioned dynamics and show their connections to the normal mode, the staging coordinate and the Matsubara mode representation for ring polymers. In the case where the potential is quadratic, we show that the continuum limit of the preconditioned mass modified Langevin dynamics converges to its equilibrium exponentially fast, which suggests that the

finite-dimensional counterpart has a dimension-independent convergence

rate. In addition, the preconditioning techniques can be naturally applied

to the multi-level quantum systems in the nonadiabatic regime and the

interacting quantum particle systems, which are compatible with various numerical approaches, like the surface hopping method and random batch method.

Introduction to Simulation of Nano-Scale Semiconductor Devices

Tiao Lu, Peking University
15:30 - 16:05

As nanomanufacturing technology has been widely used in semiconductor device fabrication, numerical simulation plays a more and more important role in design of new nanoscale devices.

In this talk, I will introduce a platform we developed based on numerical solution of the multi-subband equation which is a quantum-classical hybrid model. The model describes the subbands produced by the quantum confinement in one direction by Schroedinger-Poisson system

and the carrier transport in the channel direction by the Boltzmann equation. The platform is suitable to study not only IV semiconductors such as silicon semiconductors but also III-V compound semiconductors. The influence of various scattering mechanisms and crystal orientations are studied on the platform.

In addition, a method for calibrating the drift-diffusion (DD) model is also proposed so that the quasi-ballistic transport phenomenon can be accurately described by the modified DD model.

Numerical Methods for Thermally Driven Incompressible Magnetohydrodynamic Problems

Shipeng Mao, *University of Chinese Academy of Sciences*
16:05 - 16:40

We study numerical methods for the time-dependent magnetohydrodynamic coupled heat equation through the well-known Boussinesq approximation, in which the Joule effect and Viscous heating are taken into account. To overcome the difficulties of very low regularity of the heat source terms, a regularized weak system is proposed to deal with Joule and Viscous heating terms. We consider an Euler semi-implicit semi-discrete scheme for the regularized system. As both discrete parameter and regularization parameter tend to zero, we prove that the discrete solution converges to a weak solution of the original problem. Next, we consider the fully discrete Euler semi-implicit scheme based on the mixed finite method to approximate the fluid equation and Nedelec edge element to the magnetic induction. The fully discrete scheme requires only solving a linear system per time step. The error estimates for the velocity, magnetic induction and temperature are derived under a proper regularity assumption for the exact solution. Finally, several numerical examples are performed to demonstrate both accuracy and efficiency of our proposed scheme.

Seismic Tomography – Frozen Gaussian Approximation and Stochastic Gradient Reconstruction

Lihui Chai, *Sun Yat-Sen University*
16:40 - 17:15

In this talk, we present some recent developments of using Frozen Gaussian approximation (FGA) in seismic tomography. The FGA is rigorously derived for scalar/elastic wave equation with analysis of its accuracy determined by the ratio of short wavelength over large domain size. We develop the FGA as an efficient parallel asymptotic solver for high-frequency seismic wave propagation and apply it in seismic inversion. In order to overcome the computational difficulty in summing up a large number of Gaussians targeted at a 3-D mesh, we use stochastic sampling techniques to reduce the number of Gaussians and reconstruct "low-resolution" wavefields, but the resulted "stochastic gradient" still preserves necessary information and leads the iteration process converge to the correct velocity model.

This is the joint work with James Hateley (Vanderbilt U), Yixiao Hu (Tsinghua), Zhongyi Huang (Tsinghua), Ping Tong (NTU), Xu Yang (UCSB)

3.2 Day 2, 18 October, Sunday

Hamiltonian particle-in-cell methods for simulating Vlasov-Maxwell equations

Yajuan Sun, University of Chinese Academy of Sciences
09:00 - 09:35

In this talk, we study the Vlasov-Maxwell equations based on the Morrison-Marsden-Weinstein bracket. We develop Hamiltonian particle-in-cell methods for this system by employing finite element methods in space and splitting methods in time. In order to derive the semi-discrete system that possesses a discrete non-canonical Poisson structure, we present a criterion for choosing the appropriate finite element spaces. It is confirmed that some conforming elements, e.g., Nedelec's mixed elements, satisfy this requirement. When the Hamiltonian splitting method is used to discretize this semi-discrete system in time, the resulting algorithm is explicit and preserves the discrete Poisson structure. Some numerical experiments have been performed with help of LSEC Parallel workstation.

Fast Multipole Method in Layered Media

Bo Wang, Hunan Normal University
09:35 - 10:10

A fast multipole method (FMM) is proposed to compute long-range interactions of wave sources embedded in 3-D layered media. The layered media Green's function for the Helmholtz equation, which satisfies the transmission conditions at material interfaces, is decomposed into a free space component and four types of reaction field component from wave reflections and transmissions through the layered media. The proposed algorithm is a combination of the classic FMM for the free space component and FMMs specifically designed for the four types reaction component, made possible by new multipole expansions (MEs) and local expansions (LEs) as well as the multipole-to-local translation (M2L) operators for the reaction field components. The FMMs for the reaction components, which are implemented with the target particles and equivalent polarization sources associated with the reaction field components, are found to be much more efficient than that for the free space component due to the fact that the equivalent polarization sources and the target particles are always separated by a material interface. As a result, the FMM algorithm developed for layered media has a similar computational cost as that for the free space. Numerical results validate the fast convergence of the MEs and the O(N) complexity of the FMM for interaction of wave sources at low wave number in 3-D layered media.

Superconvergence Analysis on the Runge-Kutta Discontinuous Galerkin Method for Linear Hyperbolic Equation

Qiang Zhang, Nanjing University
10:30 - 11:05

In this talk we shall report some convergence results on the Runge-Kutta discontinuous Galerkin (RKDG) method to solve linear constant-coefficient hyperbolic equation. The numerical flux is upwind-biased and the time is advanced by the explicit Runge-Kutta algorithm. First we

present a unified framework to investigate the $L\{2\}$-norm stability performance. The main development is the matrix transferring process based on the temporal differences of stage solutions, which can be employed for any RKDG method with arbitrary stage and order. By the generalized Gauss-Radau projection to the reference functions at time stage, we are able to set up the $L\{2\}$-norm error estimate. This conclusion is optimal in time and space, and is independent of the stage number. Based on the above studies, we can establish the superconvergence results by virtue of the incomplete correction technique to the above reference functions. The conclusion shows that the superconvergence performance of the semi-discrete DG method is perfectly preserved and the time discretization solely produces an optimal error order in time. Finally, some numerical experiments are given.

Conservative Discontinuous Galerkin/Hermite Spectral Method for the Vlasov-Poisson System

Tao Xiong, Xiamen University
11:05 - 11:40

We propose a class of conservative discontinuous Galerkin methods for the Vlasov-Poisson system written as a hyperbolic system using Hermite polynomials in the velocity variable. These schemes are designed to be systematically as accurate as one wants with provable conservation of mass and possibly total energy. Such properties in general are hard to achieve within other numerical method frameworks for simulating the Vlasov-Poisson system. The proposed scheme employs discontinuous Galerkin discretization for both the Vlasov and the Poisson equations, resulting in a consistent description of the distribution function and electric field. Numerical simulations are performed to verify the order of accuracy and conservation properties.