Workshop on Advances on Scientific and Engineering Computing

September 26-27, 2020

Institute of Natural Sciences, Shanghai Jiao Tong University

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.

Date

September 26-27, 2020

Venue

Offline:
9:00-18:00, September 26th, 2020
9:00-12:00, September 27th, 2020
Room 306, No.5 Science Building, Minhang Campus, Shanghai Jiao Tong University

Online—Zoom Info:
9:00-18:00, September 26th, 2020
Zoom ID: 983-662-21975
Code: 790465
Link: https://zoom.com.cn/j/98366221975

9:00-12:00, September 27th, 2020:
Zoom ID: 924-679-68281
Code: 233042
Link: https://zoom.com.cn/j/92467968281

Organizing Committee

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

2 Schedule

2.1 Day 1, 26 September, Saturday

Time	Speaker	Title
08:45 - 09:00		Opening
09:00 - 09:40	Zhijian Yang（杨志坚）	Atomistic-based Stress Evaluation
09:40 - 10:20	Lei Zhang（张磊）	Construct The Solution Landscape on A Complicated Energy Landscape
10:20 - 10:40		Coffee Break
10:40 - 11:20	Junfeng Yin（殷俊锋）	Kaczmarz-type Inner-iteration Preconditioned Flexible GMRES Methods for Consistent Linear Systems
11:20 - 12:00	Zhennan Zhou（周珍楠）	Modeling the Autophagic Effect in Tumor Growth: A Cross Diffusion Model and Its Free Boundary Limit
12:00 - 14:00		Lunch
14:00 - 14:40	Zhonghua Qiao（乔中华）	Exponential Time Difference Methods for Solving Phase Field Equations
14:40 - 15:20	Qiumei Huang（黄秋梅）	Superconvergence of Interpolated Collocation Solutions for Integral Equations of the Second Kind
15:20 - 15:30		Coffee Break
15:30 - 16:10	Xinlong Feng（冯新龙）	Difference finite element method for the 3D penalty Stokes equations
16:10 - 16:50	Xia Ji （季霞）	Inverse Scattering with Multi-frequency Sparse Backscattering Data
16:50 - 17:30	Sihong Shao（邵嗣烘）	Overcoming Sign Problem via Particle Annihilation

2.2 Day 2, 27 September, Sunday

Time	Speaker	Title
09:00 - 09:40	Jiwei Zhang（张继伟）	Uniform Convergence of Nonlocal Approximations to Local PDEs with Nonlocal Horizon Parameters
09:40 - 10:20	Guanghui Hu（胡光辉）	A High-order H-adaptive FVM for Steady Euler Equations on Complex Domain
10:20 - 10:40		Coffee Break
10:40 - 11:20	Zuoqiang Shi（史作强）	Point Integral Method: A Novel Numerical Method for Poisson Equation on Point Cloud
11:20 - 12:00	Kai Jiang（蒋凯）	Computing the Stationary States of Phase Field Crystal Models: Efficient Numerical Methods and Simulations

3 Abstracts

3.1 Day 1, 26 September, Saturday

Atomistic-based Stress Evaluation

Zhijian Yang (杨志坚), *Wuhan University*
09:00 - 09:40

Constitutive relation is one of the most important properties of materials. Either experiments or massive MD/MC simulations are needed to get such material properties. In this talk, I will discuss different aspects of atomistic-based stress evaluation. I will talk about effective and practical algorithms for both homogeneous and inhomogeneous system, with and without temperature effects, with and without defects. Some theoretical results will also be provided.

Construct The Solution Landscape on A Complicated Energy Landscape

Lei Zhang (张磊), *Peking University*
09:40 - 10:20

How do we search for the entire family tree of possible intermediate states, without unwanted random guesses, starting from a stationary state on the energy landscape all the way down to energy minima? Here we introduce a general numerical method that constructs the pathway map, which guides our understanding of how a physical system moves on the energy landscape. The method identifies the transition state between energy minima and the energy barrier associated with such a state. As an example, we solve the Landau-deGennes energy incorporating the Dirichlet boundary conditions to model a liquid crystal confined in square box; we illustrate the basic concepts by examining the multiple stationary solutions and the connected pathway maps of the model. The joint work with Pingwen Zhang (PKU), Jianyuan Yin (PKU), Jeff Z.Y. Chen (Waterloo).

Kaczmarz-type Inner-iteration Preconditioned Flexible GMRES Methods for Consistent Linear Systems

Junfeng Yin (殷俊锋), *Tongji University*
10:40 - 11:20

We propose using greedy and randomized Kaczmarz inner-iterations as preconditioners for the right-preconditioned flexible GMRES method to solve consistent linear systems, with a parameter tuning strategy for adjusting the number of inner iterations and the relaxation parameter. We also present theoretical justifications of the right-preconditioned flexible GMRES for solving consistent linear systems. Numerical experiments on overdetermined and underdetermined linear systems show that the proposed method is superior to the GMRES method preconditioned by NE-SOR inner iterations in terms of total CPU time.

Modeling the Autophagic Effect in Tumor Growth: A Cross Diffusion Model and Its Free Boundary Limit

Zhennan Zhou（周珍楠）, *Peking University*
11:20 - 12:00

In this work, we propose two macroscopic tumor growth models to incorporate and investigate the spatial effects of autophagy. The cells are classified into two phases: normal cells and autophagic cells, whose dynamics are also coupled with the nutrients. First, we construct a fluid mechanical model describing the evolution of cell densities, where the drift is determined by the negative gradient of the joint pressure, and the reaction terms manifest the unique mechanism of autophagy. Next, in the incompressible limit, such a cell density model naturally connects to a free boundary model, describing the geometric motion of the tumor region. Analyzing the free boundary model in a special case, we show that the ratio of the two phases of cells exponentially converges to a "well-mixed" limit. Within this "well-mixed" limit, we obtain an analytical solution of the free boundary model which indicates the exponential growth of the tumor size in the presence of autophagy in contrast to the linear growth without it. We also provide extensive numerical simulations to illustrate the properties of the tumor models and explore with specially designed experiments the effects of autophagy, such as the enhancement of survivability.

Exponential Time Difference Methods for Solving Phase Field Equations

Zhonghua Qiao（乔中华）, *Hong Kong Polytechnic University*
14:00 - 14:40

Exponential time differencing (ETD) method is an efficient time integration method for differential equations. A comprehensive discussion on this method could be found in a review article M. Hochbruck and A. Ostermann. Exponential integrators. Acta Numer., 19:209–286, 2010.

In this talk, we will introduce several widely used ETD schemes and their applications in the simulation of phase field equations.

Superconvergence of Interpolated Collocation Solutions for Integral Equations of the Second Kind

Qiumei Huang（黄秋梅）, *Beijing University of Technology*
14:40 - 15:20

In this talk, we first introduce integral equations of the second kind, we then propose the interpolation postprocessing technique based on the (hybrid) collocation solutions and get the superconvergence of the new "interpolated" solutions. Numerical experiments are provided to verify the theoretical results.

Difference finite element method for the 3D penalty Stokes equations

Xinlong Feng（冯新龙）, *Xinjiang University*
15:30 - 16:10

In this paper, a penalty difference finite element (PDFE) method is presented for the 3D Stokes equations by using the FE pair $(\{\mathbf{P}\}\_\{\mathbf{1},\mathbf{1}\},\mathbf{P}\_\{\mathbf{0},\mathbf{1}\})$. This new method consists of transmitting the FE solution of the 3D Stokes equations in the direction (x,y,z) into a series of the FE solution pair $(w\_hk,p\_h\{k\})$ based on the FE space pair $W\_h\times M\_h$ of the 2D penalty Stokes equations and the FE solution $u\_\{3h\}k$ based on the FE space $S\_h\cap H1\_0()$ of the elliptic equation, where $u\_h=\sum\{l\_3-1\}\_\{k=1\}u\_hk\phi\_k(z)$ and $p\_h=\sum\{l\_3\}\_\{k=1\}p\_h\{k\}\psi\_k(z)$ with $u\_hk=(w\_hk,u\_\{3h\}k)\{\top\}$ and $w\_hk=(u\_\{1h\}k,u\_\{2h\}k)$ and $\phi\_k(z)$ is P_1-nodal point basis functions related to point z_k and $\psi\_k(z)$ is P_0-piecewise constant basis functions related to element $(z\_\{k-1\},z\_k)$ in the direction z. Here, the finite element space pair $W\_h\times M\_h$ is only required to satisfy the inf-sup condition.

Inverse Scattering with Multi-frequency Sparse Backscattering Data

Xia Ji （季霞）, *Chinese Academy of Sciences*
16:10 - 16:50

In this talk, we will introduce a direct sampling method for inverse scattering problems, which uses multi-frequency backscattering far field data taken at sparse directions. The underlying object could be point-like scatterers, small scatterers, or extended inhomogeneities and obstacles. Both the theoretical basis and numerical simulations will be presented.

Overcoming Sign Problem via Particle Annihilation

Sihong Shao（邵嗣烘）, *Peking University*
16:50 - 17:30

The infamous numerical sign problem poses a fundamental obstacle to long-time stochastic Wigner simulations in high dimensional phase space. Although the existing particle annihilation via uniform mesh (PAUM) significantly alleviates the sign problem when dimensionality D < 5, the setting of regular grids gives rise to another challenge in data storage when D > 5 due to the curse of dimensionality. To this end, we developed an adaptive particle annihilation algorithm, termed sequential-clustering particle annihilation via discrepancy estimation (SPADE), which consists of adaptive clustering of particles via controlling their number-theoretic discrepancies and independent random matching in each group, and may learn the minimal amount of particles that can accurately capture the oscillating nature of the Wigner function. Both deterministic error bounds by the Koksma-Hlawka inequality and non-asymptotic random error bounds by concentration inequalities are proved to be affected by two factors. One factor measures the irregularity of point distributions and reflects their discrete nature. The other relies on the variation of test function and is influenced by the continuity. Only the latter implicitly depends on dimensionality D, implying that SPADE can be immune to the curse of dimensionality for a wide class of test functions. Combining SPADE with a recently proposed variance reduction technique via the stationary phase approximation (SPA), we make the first attempt to simulate the transitions of hydrogen energy levels in 6-D phase space, where the feasibility of PAUM with sample sizes about 109-1010 has also been explored as a comparison.

3.2 Day 2, 27 September, Sunday

Uniform Convergence of Nonlocal Approximations to Local PDEs with Nonlocal Horizon Parameters

Jiwei Zhang（张继伟）, *Wuhan University*
09:00 - 09:40

In this talk we focus on the uniform convergence rates from nonlocal models to the corresponding local models, and presents a necessary condition to guarantee the first-order and

second-order convergence rate with respect to a nonlocal horizon parameter δ without extra assumptions on the regularity of nonlocal solutions. To do so, we first revisit the maximum principle for nonlocal models, and present the uniqueness of the nonlocal solutions. After that, we give the methodology to address the truncated errors on the volume constrains or Neumann BCs, and then combine the resulting errors from boundary layers with the maximum principle to obtain the uniform convergence order. Our analysis shows that the constant value continuation of the boundary conditions of local problems only leads to first-order convergence rate. And if we expect to have second-order convergence rate, the information of first-order derivatives for local problems on the boundaries is required. One and two dimensional numerical examples are given to verify the effectiveness of our theoretical analysis.

A High-order H-adaptive FVM for Steady Euler Equations on Complex Domain

Guanghui Hu（胡光辉）, *University of Macau*
09:40 - 10:20

In this talk, we introduce our recent work on developing high-order h-adaptive finite volume methods for steady Euler equations in the complex domain. Numerical challenges such as high order representation of the curved boundary, high order reconstruction of the numerical solution, would be introduced, and our solutions for these challenges will also be provided. In addition, a goal-oriented adaptive mesh method is introduced for improving the performance of the method. Numerical results successfully show the high-order accuracy and the robustness of the proposed method.

Point Integral Method: A Novel Numerical Method for Poisson Equation on Point Cloud

Zuoqiang Shi（史作强）, *Tsinghua University*
10:40 - 11:20

Partial differential equations on manifolds have been widely studied and play a crucial role in many subjects. In this talk, we will present a novel numerical method, point integral method to solve elliptic equations on point cloud. This method is based on an nonlocal approximation of elliptic operators. Then the elliptic equation can be transfered to an integral equation which is easy to discretize on unstructured point cloud. We will also present a high order nonlocal approximation for Dirichlet problem.

Computing the Stationary States of Phase Field Crystal Models: Efficient Numerical Methods and Simulations

Kai Jiang（蒋凯）, *Xiangtan University*
11:20 - 12:00

Phase field crystal (PFC) models are an efficient methodology to simulate phases and phase transitions in many physical systems. In this talk, a class of gradient based approaches, which is the so-called adaptive accelerated Bregman proximal gradient (AA-BPG) methods, will be presented and the convergence property is established without the global Lipschitz constant requirements. One key feature of our algorithms is that the energy dissipation and mass conservation properties hold during the iteration process. Moreover, we develop a hybrid acceleration framework to accelerate the AA-BPG methods and most of existing approaches through coupling with the practical Newton method. Extensive numerical experiments demonstrate that our approaches lead to a significant acceleration over many existing methods, especially in computing complex periodic crystals and quasicrystals. We also apply our approaches to simulate a class of PFC models, and find some new physical phenomena.