Titles and Abstracts

1. Yongyong Cai, School of Mathematical Sciences, Beijing Normal University

Title: Ground states of Bose-Einstein condensates with higher order interaction

Abstract: We analyze the ground state of a Bose-Einstein condensate in the presence of higher-order interaction (HOI), modeled by a modified GrossPitaevskii equation (MGPE). Due to the appearance of HOI, the ground state structures become very rich and complicated. We establish the existence and non-existence results under different parameter regimes, and obtain their limiting behaviors and/or structures with different combinations of HOI and contact interactions.

2. Lihui Chai, Sun Yat-sen University

Title: Frozen Gaussian Approximation Based Seismic Tomography

Abstract: In this talk, we present some recent applications 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. Similar to other ray-based beam methods (e.g. Gaussian beam methods), one can use relatively small number of Gaussians to get accurate approximations of high-frequency wavefield. The algorithm is embarrassingly parallel, which can drastically speed up the computation with a multicore-processor computer station. We develop the FGA as an efficient parallel asymptotic solver for high-frequency seismic wave propagation and apply it in full-waveform seismic inversion. Results on synthetic test of the imaging and earthquake location problems are presented. This is the joint work with James Hateley (Vanderbilt U), Zhongyi Huang (Tsinghua), Yijia Tang (SJTU), Ping Tong (NTU), Hao Wu (Tsinghua), Xu Yang (UCSB)

3. Weiguo Gao, School of Mathematical Sciences, Fudan University

Title: An Alternating SDP Algorithm for Biclustering

Abstract: We propose a convex model and an alternating SDP algorithm for biclustering which is an extension of the standard clustering. By using some random matrix results, we show that one step iteration achieves the exact solution without noise and still gets very good approximation when noise is presented. Further iterations improve the result in the noise case. The theoretical bound we obtained is better than the existing bounds. Numerical experiments demonstrate the efficiency of our proposed method. This is joint work with Xiuyuan Cheng and Yuxin Ma.

4. Xingyu Gao, Institute of Applied Physics and Computational Mathematics

Title: The self-consistent field iteration for the Kohn-Sham equation of inhomogeneous systems

Abstract: Solving the Kohn-Sham equation is most computationally demanding in the first-principles calculations. The self-consistent field (SCF) iteration is used to solve such a nonlinear eigenvalue problem. The Kerker preconditioner, based on the dielectric function of homogeneous electron gas, is designed to accelerate the SCF iteration. However, a question still remains regarding its applicability to the inhomogeneous systems. We develop a modified Kerker preconditioner that captures the long-range screening behavior of inhomogeneous systems. The efficiency is shown by the tests on long-z slabs of metals, insulators and metal-insulator contacts.

5. Qiaolin He, College of Mathematics, Sichuan University

Title: The Fictitious Domain Method Based on Navier Slip Boundary Condition for Simulation of Flow-Particle Interactions

Abstract: In this article, we develop a least–squares/fictitious domain method for direct simulation of fluid particle motion with Navier slip boundary condition at the fluid-particle interface. Let Ω and B be two bounded domains of $\mathbf{R}^d$ such that $\overline{B} \subset \Omega$. The motion of solid particle B is governed by Newton's equations. Our goal here is to develop a fictitious domain method where one solves a variant of the original problem on the full Ω, followed by a well-chosen correction over B and corrections related to translation velocity and angular velocity of the particle. This method is of the virtual control type and relies on a least-squares formulation making the problem solvable by a conjugate gradient algorithm operating in a well chosen control space. Since the fully explicit scheme to update the particle motion using Newton's equation is unstable, we propose and implement an explicit-implicit scheme in which, at each time step, the position of the particle is updated explicitly, and the solution of Navier-Stokes equations and particle velocities are solved by the the least–squares/fictitious domain method implicitly. Our numerical results match with that in [**?**], which means that the anisotropy parameter p in Jeffery orbit theory increases with the increasing slip length.

6. Kai Jiang, School of Mathematics and Computational Science, Xiangtan University

Title: Efficient methods for computing the stationary states of phase field crystal models

Abstract: In this talk, we will present efficientmethodsto compute the stationary states of phase field crystal models. These approaches consist two parts: (1) an efficient and accurate numerical method is proposed to evaluate the ordered structures, including quasicrystals and periodic crystals; (ii) a class of novel methods are developed to compute the stationary states by combining numerical PDE methods and the modern optimization approaches.The efficiency and robustness of the proposed methods will be demonstrated by some numerical experiments. Meanwhile,somenew physical phenomena will be presented.

7. Shi Jin, School of Mathematical Sciences and Institute of Natural Sciences, Shanghai Jiao Tong University

Title: Random Batch Methods for Interacting Classical and Quantum Particles

Abstract: We develop random batch methods for interacting particle systems with large number of particles. These methods use small but random batches for particle interactions, thus the computational cost is reduced from $O(N^2)$ per time step to $O(N)$, for a system with N particles with binary interactions. For one of the methods, we give a particle number independent error estimate under some special interactions.

For quantum $N-$body Schrodinger equation, we obtain, for pair-wise random interactions, a convergence estimate for the Wigner transform of the single-particle reduced density matrix of the particle system at time t that is uniform in $N > 1$ and independent of the Planck constant $\hbar$. To this goal we need to introduce a new metric specially tailored to handle at the same time the difficulties pertaining to the small $\hbar$ regime (classical limit), and those pertaining to the large N regime (mean-field limit).

The classical part was a joint work with Lei Li and Jian-Guo Liu, while the quantum part was with Francois Golse and Thierry Paul.

8. Lei Li, Shanghai Jiao Tong university

Title: Two sampling methods using random batches

Abstract: I will talk about two sampling methods: a splitting Monte Carlo and the Stein Variational Gradient Descent. The former can be viewed as a special case of the Metropolis MCMC method while the latter is a nonparametric variational inference method. We then apply the random batch ideas to reduce the computational cost for these two methods, yielding efficient sampling methods. The random mini-batch idea is famous for its application in SGD and recently has been used by Jin et al to interacting particle systems.

9. Yvon Maday, Laboratoire Jacques-Louis Lions, Université Pierre et Marie Curie

Title: TBA

Abstract: TBA

10. Sihong Shao, School of Mathematical Sciences, Peking University

Title: Lovsz extension and graph cut

Abstract: A firm bridge between discrete data world and continuous math field should be tremendously helpful in data analysis. Along this direction, the Lovsz extension provides a both explicit and equivalent continuous optimization problem for a discrete optimization problem, for instance, the Cheeger cut problem. In this talk, we report a set-pair Lovsz extension which provides not only an answer to the dual Cheeger cut, anti-Cheeger cut, and max 3-cut problems, all of which cannot be handled by the Lovsz extension, but also works for the Cheeger cut and maxcut problems. In particular, the set-pair Lovsz extension enlarges the feasible region of resulting equivalent continuous optimization problems from a half space (resulted from the Lovsz extension) to the entire space for the Cheeger cut and maxcut problems. On the other hand, it provides new possibilities for designing continuous optimization algorithms for combination problems on the practical side, too. As an illustration, we propose a simple continuous iterative algorithm for the maxcut problem which converges to a local optimum in finite steps. Here simple means the inner subproblem is

solved analytically and thus no optimization solver is called. Numerical experiments on G-set demonstrate the performance. In particular, the ratios between the best cut values achieved by the simple iterative algorithm and the best known ones are at least 0.986 and can be further improved to at least 0.997 by a preliminary attempt to break out of local optima.

11. Zhiqiang Sheng, Laboratory of Computational Physics, Institute of Applied Physics and Computational Mathematics, Beijing

Title: Construction and analysis of nonlinear finite volume scheme preserving maximum principle on distorted meshes problems

Abstract: The maximum principle is one of the key requirements to discretization schemes, and can ensure that there is no spurious oscillations for the numerical solution and preserve physical bounds of problem. In this talk, we first introduce a new nonlinear finite volume scheme satisfying the maximum principle for the diffusion equation on distorted meshes, and then introduce the corresponding theoretical analysis including the coercivity, existence and convergence. Numerical results are presented to demonstrate the properties of our scheme.

12. Huazhong Tang, Center for Applied Physics and Technology, HEDPS and LMAM, School of Mathematical Sciences, Peking University

Title: High-order accurate entropy stable schemes for special relativistic hydrodynamics

Abstract: We develop the high-order accurate entropy stable nite difference schemes for one- and two-dimensional special relativistic hydrodynamic equations. The schemes are built on the entropy conservative ux and the weighted essentially non-oscillatory (WENO) technique as well as explicit Runge-Kutta time discretization. The key is to technically construct the affordable entropy conservative ux of the semi-discrete second-order accurate entropy conservative schemes satisfying the semi-discrete entropy equality for the found convex entropy pair. As soon as the entropy conservative ux is derived, the dissipation term can be added to give the semi-discrete entropy stable schemes satisfying the semi-discrete entropy inequality with the given convex entropy function. The WENO reconstruction for the scaled entropy variables and the high-order explicit Runge-Kutta time discretization are implemented to obtain the fully-discrete high-order entropy stable schemes. Several numerical tests are conducted to validate the accuracy and the ability to capture discontinuities of our entropy stable schemes.

We also develop the high-order accurate entropy stable nite difference schemes for the special relativistic magnetohydrodynamic equations.

13. Min Tang, Institute of Natural Science and Department of Mathematics, Shanghai Jiao Tong University

Title: Accurate front capturing asymptotic preserving scheme for nonlinear gray radiative transfer equation

Abstract: We develop an asymptotic preserving scheme for the nonlinear gray radiative transfer equation. Two asymptotic regimes are considered: one is a diffusive regime described by a nonlinear diffusion equation for the material temperature; the other is a free streaming regime with zero opacity. To alleviate the restriction on time step and capture the correct front propagation in the diffusion limit, an implicit treatment is crucial. However, this often involves a large-scale nonlinear iterative solver as the spatial and angular dimensions are coupled. Our idea is to introduce an auxiliary variable that leads to a "redundant" system, which is then solved with a three-stage update: prediction, correction, and projection. The benefit of this approach is that the implicit system is local to each spatial element, independent of angular variable, and thus only requires a scalar Newton's solver. We also introduce a spatial discretization with a compact stencil based on even-odd decomposition. Our method preserves both the nonlinear diffusion limit with correct front propagation speed and the free streaming limit, with a hyperbolic CFL condition.

14. Yanli Wang, Beijing Computational Science Research Center

Title: Approximation of the Boltzmann Collision Operator Based on Hermite Spectral Method

Abstract: Boltzmann equation is adopted to describe the statistical behavior of gas molecules. The numerical simulation for this six-dimensional equation is one significant topic after the invention of computers. The difficulty comes partly from its high dimensionality, and partly from its complicated integral operator modeling the binary collision of gas molecules. This work aims at an affordable way to model and simulate the binary collision between gas molecules. Our new attempt is an intermediate approach between a direct discretization of the quadratic Boltzmann collision operator and simple modelling methods like BGK-type operators. In detail, we first focus on the relatively important physical quantities, which are essentially the first few coefficients in the Hermite expansion, and use an intricate and accurate way to describe their evolution. The strategy comes from the discretization of the quadratic collision operator. For the less important moments, we borrow the idea of the BGK-type operators and let these moments converge to the equilibrium at a constant rate. Although the first part is computationally expensive, we can restrict the number of degrees of freedom such that the computational cost is acceptable. The accuracy of such a model depends apparently on the size of the accurately modelled part. Our numerical examples show that this method can efficiently capture the evolution of lower order moments in the spatially homogeneous Boltzmann equation.

15. Haijun Wu, Department of Mathematics, Nanjing University

Title: TBA

Abstract: TBA

16.Yinhua Xia, School of Mathematical Sciences, USTC

Title: Invariant preserving discontinuous Galerkin methods for nonlinear wave equations

Abstract: In this talk, we will present and analyze the invariant preserving discontinuous Galerkin (DG) discretizations for nonlinear wave equations, e.g. the Korteweg-de Vries (KdV) type equations, Camassa-Holm and Degasperis-Procesi type equations, short pulse type equation, etc. The conservative and dissipative schemes will be constructed systematically. The conservative schemes can preserve some discrete Hamiltonian invariant, while the dissipative ones guarantee the corresponding stability. Also we will introduce how to deal with the non-classical solution for some wave equations, such as peakon- and cuspon-soliton solutions, loop-solition and breather solutions, and shock solutions. Numerical experiments in different circumstances are provided to illustrate the accuracy and capability of these schemes.

17. Xiaoping Xie, School of Mathematics, Sichuan University

Title: Numerical analysis of a semilinear fractional diffusion equation

Abstract: We consider the numerical analysis of a semilinear fractional diffusion equation with nonsmooth initial data. A new Grönwall's inequality and its discrete version are proposed. By the two inequalities, error estimates in three Sobolev norms are derived for a spatial semi-discretization and a full discretization, which are optimal with respect to theregularity of the solution. A sharp temporal error estimate on graded temporal grids is also rigorouslyestablished. In addition, the spatial accuracy $O(h^2(t^{-\alpha} + \ln(1/h)))$ in the pointwise $L^2(\Omega)$-norm is obtained for a spatial semi-discretization.Finally, several numerical results are provided to verify the theoretical results. This is joint work with Binjie Li and Tao Wang.

18. Ziqing Xie, LCSM, School of Mathematics and Statistics, Hunan Normal University

Title: Some bifurcation properties of several semilnear PDEs

Abstract: In this talk ,we will discuss some interesting bifurcation properties for several semilinear PDES due to the change of some parameters. Some results can be proved strictly and others are just belong to discovery from the point of computation and its theoretical verfication is still open.

19. Yan Xu, University of Science and Technology of China

Title: Higher order structure-preserving numerical schemes for nonlinear time-dependent problems

Abstract: In this talk, we discuss local discontinuous Galerkin (LDG) method for solving the nonlinear equations which contain nonlinear high order deriva- tives. The discretization results in an extremely local, element based dis- cretization, which is beneficial for parallel computing and maintaining high order accuracy on unstructured meshes. We also develop a novel semi- implicit spectral deferred correction (SDC) time marching method. The method can be used in a large class of problems, especially for highly non- linear ordinary differential equations (ODEs) without easily separating of stiff and non-stiff components, which is more general and efficient compar- ing with traditional semi-implicit SDC methods. The proposed semi-implicit SDC method is based on low order time integration methods and corrected iteratively.

The order of accuracy is increased for each additional iteration. This SDC method is intended to be combined with the method of lines, which provides a flexible framework to develop high order semi-implicit time marching methods for nonlinear partial differential equations (PDEs). Cou- pled with the LDG spatial discretization, the fully discrete schemes are all high order accurate in both space and time, and stable numerically with the time step proportional to the spatial mesh size. Using Lagrange mul- tipliers the conditions imposed by the positivity preserving limiters are di- rectly coupled to a DG discretization combined with implicit time integration method. The positivity preserving DG discretization is then reformulated as a Karush-Kuhn-Tucker (KKT) problem. We therefore develop an efficient active set semi-smooth Newton method that is suitable for the KKT formu- lation of time-implicit positivity preserving DG discretizations. Convergence of this semi-smooth Newton method is proven using a specially designed quasi-directional derivative of the time-implicit positivity preserving DG dis- cretization. Numerical experiments are carried out to illustrate the accuracy and capability of the proposed method.

20. Zhenli Xu, Institute of Natural Science and Department of Mathematics, Shanghai Jiao Tong University

Title: Modified Poisson-Nernst-Planck model for charge transport at nanoscale

Abstract: Coulomb and hard-sphere correlations play important role in many soft matter and electrochemical energy systems at the nano/micro scale, which are ignored in the classical mean-field theory. We develop a modified Poisson-Nernst-Planck model to include these many-body properties in electrolytes, which also takes the ion-size effect into account and is expected to provide more accurate prediction for ion dynamics for problems with nanoscale confinement. Issues related to mathematical analysis and numerical algorithms will be discussed in this talk. Simulation results are given to show the performance of this model.

21. Qingzhi Yang, School of Mathematics, Nankai University ,

Title: The numerical methods for a class of nonlinear eigenvalue problem

Abstract: In this talk, we are going to discuss the numerical algorithms for a class of nonlinear eigenvalues, which arises in the Bose-Einstein condensation problem. We show that the minimal eigenvalue of the problem can be obtained by solving an optimization over the unit circle. We propose a kind of semidefinite programming relaxation of the optimization and prove it is tight. With suitable transformation, we illustrate that alternating direction multipliers method (ADMM) for a class of separate optimization may be used to solve the optimization problem. Some numerical experiments for finding the minimal eigenvalue are presented using semidefinite programming method, ADMM and a function of Matlab for constrained optimization. In addition, we show that using a polynomial optimization method, all real eigenvalues can be found under certain assumptions. Some small-scale numerical examples are presented.

22. Wenjun Ying, School of Mathematical Sciences and Institute of Natural Sciences Shanghai Jiao Tong University

Title: An Extreme Value Preserving Scheme for Nonlinear Hyperbolic Conservation Laws

Abstract: In this talk, I will present an extreme value preserving total variation diminishing (TVD) scheme for nonlinear hyperbolic conservation laws. Numerical examples with the Euler equations in both triangle and tetrahedral grids will be presented.

23. Tieyong Zeng, Chinese University of Hong Kong

Title: TBA

Abstract: TBA

24. Kai Zhang, Mathematics School and Institute of Jilin University

Title: Numerical method for random interface Maxwell's equation

Abstract: A robust numerical method via the shape derivatives and low-rank approximation is developed for computations of three-dimensional Maxwell's equations with random interfaces. Based on a shape calculus, we estimate the statistical moments of the stochastic Maxwell equations in terms of perturbation magnitude. In order to capture the oscillations with high resolution near the interface, we adopt the adaptive edge element with third order polynomials to solve the deterministic equations approximating the expectation. For the second moment, an efficient low-rank approximation based on pivoted Cholesky decomposition is proposed to compute the two-point correlation function to approximate the variance of stochastic Maxwell's equations. Numerical experiments are presented to illustrate our theoretical results.

25. Lei Zhang, Beijing International Center for Mathematical Research, Peking University

Title: Construct the Solution Landscape on a complicated energy landscape

Abstract: 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-de Gennes 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).

26. Wensheng Zhang, LSEC, ICMSEC, Academy of Mathematics and Systems Science, Chinese Academy of Sciences

Title: Time domain full waveform inversion for velocity and density

Abstract: The full waveform inversion is a method for estimating media parameters such as the velocity and density by using the waveform data including traveltime, phase and amplitude observed on surface. It has the advanrage of high imaging accuracy. However, it is a typical nonlinear and ill-posed problem and the solution is nonunique. The full waveform inversion can be completed in the time domain or in the frequency domain. In the time domain, the forward problem can be solved effectinelly by the finite difference method. The inverse inversion is an optimization iterative process based on numerical optimizational algorithms. In this talk, I will present the numerical methods for the inverse problem of velocity and density. Numerical results for the benchmark model are also presented.

27. Douglas Zhou, School of Mathematical Sciences and Institute of Natural Sciences, Shanghai Jiao Tong University

Title: A brain-spired spiking neural model for artificial intelligence

Abstract: Spiking neural networks are widely applied to simulate cortical dynamics in the brain, and are regarded as the next generation of machine learning. Therefore, as a first step, it is important to model single-neuron dynamics quantitatively. However, the existing point neuron models fail to capture dendritic effects, which are crucial for neuronal information processing. We derive an effective point neuron model, which incorporates an additional synaptic integration current arising from the nonlinear interaction between synaptic currents across spatial dendrites. Our model captures the somatic voltage response of a realistic neuron with complex dendrites and provides some insight into the construction of basic unit in artificial neural networks.

28. Xiang Zhou, Department of Mathematics, City University of Hong Kong

Title: Gentlest Ascent Dynamics

Abstract: Gentlest Ascent Dynamics (GAD) is the first nonlinear dynamical system locally converging to saddle point. In this talk I will review the theoretic and algorithmic understanding of this dynamics as well as its wide applications in rare event studies and phase space explorations.

In addition, I will offer a rethinking of GAD through three aspects
(1) geometricunderstanding (min-mode)
(2) the Hamiltonian dynamics of the exit problem
(3) the optimal control for active particle.

29. Zhennan Zhou, Beijing International Center for Mathematical Research

Title: Numerical methods for some nonlinear transport equations in biology.

Abstract: In the first part, we first introduce a semi-discrete scheme for 2D Keller-Segel equations based on a symmetrization reformation, which is equivalent to the convex splitting method and is free of any nonlinear solver. We show that, this new scheme is stable as long as the initial condition does not exceed certain threshold, and it asymptotically preserves the quasi-static limit in the transient regime. Furthermore, we show that the fully discrete scheme is conservative and positivity preserving, which makes it ideal for simulations. In the second part, we propose a positivity preserving

scheme for a class of Fokker Planck equations for neurons networks: the nonlinear noisy integrate and fire neuron models. We show that the semi-discrete scheme satisfies the relative entropy estimates, which matches the few known results from PDE analysis.