Titles and Abstracts

1. Yongyong Cai, Beijing Computational Science Research Center, China

Title: Non-relativistic limit of the nonlinear Dirac equation and its numerical methods

Abstract: We consider the (nonlinear) Dirac equation in the non-relativistic limit regime, involving a small parameter inversely proportional to the speed of light. The (nonlinear) Dirac equation converges to the (nonlinear) Schrodinger equation in the non-relativistic limit. By a careful analysis, we obtain a semi-relativistic limit of the nonlinear Dirac equation, which enables a design of uniformly accurate multi-scale numerical method. The major difficulty of the problem is that the solution has a rapid oscillation in time depending on the small parameter.

2. Eric Cances, Ecole des Ponts ParisTech, France

Title: Numerical analysis of linear and nonlinear eigenvalue problems

Abstract: In this talk, I will review some recent advances on the numerical analysis of linear and nonlinear elliptic eigenvalue problems. I will first present the derivation of accurate, fully computable, lower and upper bounds of the exact eigenvalues of the Laplace operator on a polyhedral bounded domain with Dirichlet boundary conditions, for both conforming and non-conforming discretization methods. I will then focus on the nonlinear Gross-Pitaevskii and Kohn-Sham equations, and show that a priori error analysis results can be used to construct more efficient numerical schemes for computing ground states of interacting quantum bosonic and fermionic systems.

3. Ionut Danaila, University of Rouen Normandy, France

Title: Newton and Sobolev gradient methods for nonlinear fluid and superfluid flow problems

Abstract: In the first part of the talk, we present new numerical methods for the direct minimization of the Gross-Pitaevskii energy functional with rotation. We derive new Newton and conjugate-gradient methods combining concepts from Riemannian Optimization and Sobolev gradient theory. The capabilities of the methods are illustrated by computing vortex configurations of superfluid rotating Bose-Einstein condensates [1].

The second part of the talk will be devoted to phase-change systems governed by the Navier-Stokes equations with Boussinesq approximation for the heat transfer. We present a new single domain numerical approach with mesh adaptivity, using a fully linearized Newton algorithm for the time integration of the system of equations. The advantage of our adaptivity method is to allow accurate and simultaneous tracking of different interfaces in the system [2].

[1] I. Danaila, B. Protas, Computation of Ground States of the Gross-Pitaevskii Functional via Riemannian Optimization, to appear in SIAM J. Sci. Computing, 2017.

[2] I. Danaila, R. Moglan, F. Hecht, S. Le Masson, A Newton method with adaptive finite elements for solving phase-change problems with natural convection, J. of Computational Physics, 274, p. 826-840, 2014.

4. Yana Di, Institute of Computational Mathematics and Scientific/Engineering Computing, Chinese Academy of Sciences, China

Title: Numerical simulations on adsorption of the surfactant

Abstract: The research of surfactant systems is one of the important areas in soft condensed matter physics. The surfactant behaviors result in various kinds of interface/surface phenomena and also effect greatly on the physical characters of complex fluid systems. Here, we treat these problems in a physical way, and simulate the interface wetting and spreading phenomena of polydimethylsiloxane oil/surfactant solution systems. We try to understand how the electrostatic/volume effect related to surface change the wetting status.

5. Weiguo Gao, Fudan University, Shanghai, China

Title: TBA

Abstract: TBA

6. Jun Hu, Peking University, Beijing, China

Title: High Accurate Approximations for Eigenvalues By Nonconforming Elements

Abstract: For both the Raviart-Thomas element and the Crouzeix-Raviart element, we prove the full second order superconvergence rate of the recovery operator. Based on these results, by using the canonical interpolation of the first order Raviart-Thomas element, we derive an asymptotic expansion for eigenvalues by the Crouzeix-Raviart and the enriched Crouzeix-Raviart element. Also, we construct asymptotically exact a posteriori error estimators for eigenvalues solved by the Crouzeix-Raviart element and the enriched Crouzeix-Raviart element. Based on these estimators, we propose two ways to improve accuracy for eigenvalue approximations.

7. Jianguo Huang, School of Mathematical Sciences, Shanghai Jiao Tong University

Title: The generalized Arrow-Hurwicz method with applications to fluid computation

Abstract: In this talk, we will first discuss the existence and uniqueness of a class of nonlinear saddle-point problems, which are frequently encountered in physical models. Then, a generalized Arrow-Hurwicz method is introduced to solve such problems. For the method, the convergence rate analysis is established under some reasonable conditions. It is also applied to solve three typical discrete methods in fluid computation, with the computational efficiency demonstrated by a series of numerical experiments. This is a joint work with Binbin Du from Shanghai Jiao Tong University.

8. Jingfang Huang, Department of Mathematics, the University of North Carolina at Chapel Hill

Title: A Fast Hierarchical Algorithm for Computing High Dimensional Truncated Multivariate Gaussian Probabilities and Expectations

Abstract: Multivariate Gaussian distribution is one of the most important continuous distributions. If some components are restricted to an interval, either finite or semi-finite, it is referred to as the truncated multivariate normal (TMVN) distribution. Many statistical algorithms rely on the evaluation of some expectations with respect to a TMVN, especially in the expectation-maximization (EM) type algorithms. In this talk, we present a fast hierarchical algorithm to reduce the computational complexity of evaluating the p-dimensional TMVN probability and expectation integrals to the asymptotically optimal $O(p)$, by utilizing the low-rank and low-dimensional structures in the inverse of the covariance matrix, and by processing the compressed information efficiently on a hierarchical tree. The principles in the hierarchical algorithm can be generalized to create a numerical framework for more general high-dimensional big datasets.

9. Chang-Ock Lee, Department of Mathematical Sciences, KAIST, Korea

Title: A Finite Element Approach for the Dual Total Variation Minimization and Its Nonoverlapping Domain Decomposition Methods

Abstract: We propose a finite element discretization for the dual Rudin-Osher-Fatemi (ROF) model using a Raviart-Thomas basis for $H_0(\text{div};\Omega)$. The proposed discretization naturally adopts the existing solvers for the ROF model using either dual or primal-dual approaches, like the FISTA (Fast Iterative Shrinkage Thresholding Algorithm) and the primal-dual algorithm. Since the proposed discretization has the splitting property for the energy functional, which is not satisfied for the existing finite difference based discretization, it is more adequate for designing domain decomposition methods. A primal domain decomposition method is proposed, which resembles the classical Schur complement method for the second order elliptic problems. The proposed primal domain decomposition method achieves $O(1/n^2)$ convergence. A primal-dual domain decomposition method based on the method of Lagrange multipliers on the subdomain interfaces is also considered. The local problems of the proposed primal-dual domain decomposition method can be solved in linear convergence rate. Numerical results for the proposed methods are provided.

10. Yvon Maday, Laboratoire Jacques-Louis Lions, Universit Pierre et Marie Curie, France

Title: A Reduced Basis Technique for Long-Time Unsteady Turbulent Flows

Abstract: We present a reduced basis technique for long-time integration of parametrized incompressible turbulent flows. The new contributions are threefold. First, we propose a constrained Galerkin formulation that corrects the standard Galerkin statement by incorporating prior information about the long-time attractor. For explicit and semi-implicit time discretizations, our statement reads as a constrained quadratic programming problem where the objective function is the Euclidean norm of the error in the reduced Galerkin (algebraic) formulation, while the constraints correspond to bounds for the maximum and minimum value of the coefficients of the N-term expansion. Second, we propose an a posteriori error indicator, which corresponds to the dual norm of the residual associated with the time-averaged momentum equation. We demonstrate that the error indicator is highly-correlated with the error in

mean flow prediction, and can be efficiently computed through an offline/online strategy. Third, we propose a Greedy algorithm for the construction of an approximation space/procedure valid over a range of parameters; the Greedy is informed by the a posteriori error indicator developed in this paper. We illustrate our approach and we demonstrate its effectiveness by studying the dependence of a two-dimensional turbulent lid-driven cavity flow on the Reynolds number.

This is a joint work with Lambert Fick, Anthony T Patera and Tommaso Taddei.

11. Ulrich Rüde, Cauerstrasse 11, Lehrstuhl für Simulation FAU Erlangen-Nürnberg, 91058 Erlangen, Germany; CERFACS, Toulouse, France

Title: Parallel Algorithms for Complex Flows

Abstract: This talk will report about recent progress to simulate complex flow problems using finite element methods or advanced kinetic methods, highlighting their differences and advantages when implemented on modern supercomputer systems.

The finite element method for incompressible flows often requires the solution of systems with saddle point structure. We will present our experience with a parallel multigrid algorithm using hierarchical hybrid grids . For a geophysical application, the simulation of Earth Mantle convection, we will demonstrate that the solution of FE systems with in excess of 10^{12} degrees of freedom is feasible on current petascale class supercomputers .The highest efficiency is achieved for novel matrix-free techniques where the stiffness matrix is not stored but recomputed using suitably constructed approximations in every step of the iterative multigrid solver .

Kinetic schemes, such as the Lattice Boltzmann method (LBM) are structurally different since they are explicit time stepping schemes. Though this poses time step restrictions, these methods can often benefit from being parallelizable with only nearest neighbor communication. Du to their structural simplicity, LBM methods are sometimes also more flexible and more extensible . One particular strength of the LBM is the simulation of suspensions and multiphase flows via a direct numerical simulation, i.e. when each particle, droplet, or bubble, are fully resolved. As one example we will present efforts to simulate the sediment transport in a river bed with fully resolved and geometrically modeled grains. Here we rely on the LBM methods realized in the waLberla framework that exhibit not only excellent scalability, but that are also carefully optimized using hybrid parallelization for node level parallelism and they are aggressively vectorized. Consequently, they are significantly faster than conventionally implemented lattice Boltzmann methods on the same architecture. We will showcase parallel flow simulations on up to a million parallel threads.

12. Sihong Shao, Peking University, China

Title: Towards First-Principle Quantum Dynamics beyond the Born-Oppenheimer Approximation

Abstract: The first-principle quantum dynamics is crucial in investigating physical or chemical properties of molecules. The Born-Oppenheimer molecule dynamics, as the most popular one, treats the electrons quantum-mechanically by the density functional theory, but the nuclei as the Newtonian particles. That is, the Born-Oppenheimer molecule dynamics is not a truly first-principle quantum dynamics,

especially in the situation that the quantum effect of nuclei may not be neglected. Set against such background, my group aims at developing a truly first-principle quantum dynamics beyond the Born-Oppenheimer approximation and the mathematical formalism of quantum mechanics we choose is the Wigner function approach. In this talk, we will report the recent progress we have made in this direction.

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

Title: A nonlinear finite volume scheme preserving maximum principle

Abstract: For the construction of nonlinear finite volume schemes preserving maximum principle for diffusion equations on distorted meshes, the nonlinear weighted method is a common-used approach. In this talk, we introduce three finite volume schemes preserving maximum principle based on nonlinear weighted methods, in which a conservative flux is constructed by using three kinds of weighted combination of nonconservative flux. We perform an elementary analysis to compare the errors of flux for these weighted methods. Numerical results are presented to demonstrate the accuracy and properties of these schemes.

14. Huazhong Tang, School of Mathematical Sciences, Peking University, Beijing 100871, PR China; School of Mathematics and Computational Science, Xiangtan University, Xiangtan 411105, Hunan Province, PR China

Title: A stochastic Galerkin method for first-order quasilinear hyperbolic systems with uncertainty

Abstract: This talk is concerned with generalized polynomial chaos (gPC) approximation for first-order quasilinear hyperbolic systems with uncertainty. The one-dimensional (1D) hyper-bolic system is first symmetrized with the aid of left eigenvector matrix of the Jacobian matrix. Then the gPC stochastic Galerkin method is applied to derive a provably symmet-rically hyperbolic equations for the gPC expansion coefficients. The resulting deterministic gPC Galerkin system is discretized by a path-conservative finite volume WENO scheme in space and a third-order total variation diminishing Runge-Kutta method in time. The method is further extended to two-dimensional (2D) quasilinear hyperbolic system with uncertainty, where the symmetric hyperbolicity of the one-dimensional gPC Galerkin sys-tem is carried over via an operator splitting technique. Several numerical experiments are conducted to demonstrate the accuracy and effectiveness of the proposed gPC stochastic Galerkin method.

15. Min Tang, Shanghai Jiao Tong University, China

Title: The fractional diffusion limit of a kinetic model with biochemical pathway

Abstract: Kinetic-transport equations that take into account the intra-cellular pathways are now considered as the correct description of bacterial chemotaxis by run and tumble. Recent mathematical studies have shown their interest and their relations to more standard models. Macroscopic equations of Keller-Segel type have been derived using parabolic scaling. Due to the randomness of receptor methylation or intra-cellular chemical reactions, noise occurs in the signaling pathways and aects the

tumbling rate. Then, comes the question to understand the role of an internal noise on the behavior of the full population. In this paper we consider a kinetic model for chemotaxis which includes biochemical pathway with noises. We show that under proper scaling and conditions on the tumbling frequency as well as the form of noise, fractional diusion can arise in the macroscopic limits of the kinetic equation. This gives a new mathematical theory about how long jumps can be due to the internal noise of the bacteria.

16. Ping Tong, Nanyang Technological University, Singapore

Title: Numerical methods for partial differential equations and the applications in seismic imaging

Abstract: In this talk we focus on several partial differential equations and their roles in seismic imaging from the global to industrial scales. Numerical methods for Eikonal equation, acoustic wave equation, and elastic wave equation will be discussed. If only the traveltime information of primary or secondary seismic phases is used in seismic imaging, Eikonal equation is well suited for tracing the 3-D travelling path of a single phase. Imaging results obtained by solving Eikonal equation in the Sumatra region (Indonesia) will be presented. However, if we want to use the full information embedded in the waveforms, 3-D acoustic wave equation or elastic wave equation should be numerically and efficiently solved. Numerical results of synthetic tests and in Tibet (China) will be shown.

17. Hanquan Wang, Yunnan University of Finance and Economics, China

Title: Coherent Pulse Progression of Mid-Infrared Quantum-Cascade Lasers Under Group-Velocity Dispersion and Self-Phase Modulation

Abstract: The effect of group-velocity dispersion (GVD) and self-phase modulation (SPM) on the coherent pulse progression in mid-infrared quantum-cascade lasers (QCLs) is investigated. The background saturable absorber (SA) effect is included in this paper. In this case, the lasing pulses can be built up from the instable continuous wave operation condition related to both SA effect and GVD under the influence of a small initial disturbance. The theoretical model is built based on the MaxwellBloch formulism accounting for the couplings among the electric field, the polarization, and the population inversion. The pulse evolution in time-spatial domains is simulated by the finite difference method with prior nondimensionalization, which is necessary for convergent solution. It is found that the anomalous GVD, which receives less attention in the study of QCL dynamics, can significantly narrow the spectrum splitting between side modes. The SPM can broaden the linewidth of the spectral modes. Their combined effects can lead the possibility of forming solitons.

18. Wei-Cheng Wang, National Tsing Hua University

Title: TBA

Abstract: TBA

19. Xiaoping Wang, Hong Kong University of Science and Technology

Title: TBA

Abstract: TBA

20. Yanli Wang, Peking University

Title: Filtered Hyperbolic Moment Method for the Vlasov Equation

Abstract: Landau damping is one of the fundamental problems in the applications of the Vlasov-Poisson equations. However, in the numerical simulations of Landau damping, it is observed that an unphysical phenomenon called recurrence occurs for most grid-based solvers. In this paper, we study the unphysical recurrence phenomenon arising in the numerical simulation of the VP equations using hyperbolic moment method from a mathematical point of view. It is rigorously proven that all the non-constant modes are damped exponentially by the filters, and formally shown that the filter does not affect the damping rate of the electric energy in the linear Landau damping problem. Moreover, we propose a novel quasi time-consistent filter to suppress the numerical recurrence effect numerically. The filter preserves a lot of physical properties of hyperbolic moment equations (HME). Two viewpoints, collisional viewpoint and dissipative viewpoint, are presented to dissect the filter, and show that the filtered hyperbolic moment method can be treated as a solver of Vlasov equation. Numerical simulations of the linear Landau damping and two stream instability are tested to demonstrate the effectiveness of the filter.

21. Haijun Wu, Nanjing University

Title: TBA

Abstract: TBA

22. Hao Wu, Tsinghua University, China

Title: The quadratic Wasserstein metric for earthquake location

Abstract: In [Engquist et al., Commun. Math. Sci., 14(2016)], the Wasserstein metric was successfully introduced to the full waveform inversion. We apply this method to the earthquake location problem. For this problem, the seismic stations are far from each other. Thus, the trace by trace comparison [Yang et al., arXiv(2016)] is a natural way to compare the earthquake signals.

Under this framework, we have derived a concise analytic expression of the Frèchet gradient of the Wasserstein metric, which leads to a simple and efficient implementation for the adjoint method. We square and normalize the earthquake signals for comparison so that the convexity of the misfit function with respect to earthquake hypocenter and origin time can be observed numerically. To reduce the impact of noise, which can not offset each other after squaring the signals, a new control parameter is introduced. Finally, the LMF (Levenberg-Marquardt-Fletcher) method is applied to solve the resulted optimization problem. According to the numerical experiments, only a few iterations are required to converge to the real earthquake hypocenter and origin time. Even for data with noise, we can obtain reasonable and convergent numerical results.

23. Yang Xiang, Hong Kong University of Science and Technology

Title: Energy and Dynamics of Grain Boundaries Based on the Underlying Microstructure

Abstract: Grain boundaries are the interfaces of grains with different orientations in polycrystalline materials. Energetic and dynamic properties of grain boundaries play essential roles in the mechanical and plastic behaviors of the materials. These properties of grain boundaries strongly depend on their microscopic structures. We present continuum models for the energy and dynamics of grain boundaries based on the continuum distribution of the line defects (dislocations or disconnections) on them. The long-range elastic interaction between the line defects is included in the continuum models to maintain stable microstructure on grain boundaries during the evolution. The continuum models is able to describe both normal motion and tangential translation of the grain boundaries due to both coupling and sliding effects that were observed in atomistic simulations and experiments.

24. Xiaoping Xie, School of Mathematics, Sichuan University, Chengdu 610064, China

Title: High-order temporal accuracy algorithms for two types of fractional partial differential equations

Abstract: We consider the numerical solution to two types of fractional partial differential equations, i.e. time fractional wave problems and modified anomalous subdiffusion problems. For the time fractional wave problems, we develops a high-accuracy algorithm which employs a spectral method in the temporal discretization and a finite element method in the spatial discretization. For the modified anomalous subdiffusion problems with two time fractional derivatives of orders α and β $(0 < \alpha < \beta < 1)$, we use a time-stepping discontinuous Galerkin method in the temporal discretization and a finite element method in the spatial discretization. Stability and convergence of the algorithms are derived. Numerical experiments are performed to verify the theoretical results.

This is a joint work with Binjie Li and Hao Luo.

25. Ziqing Xie, Hunan Normal University

Title: Finding excited states of Bose-Einstein condensates by a constrained gentlest ascent dynamics

Abstract: A constrained gentlest ascent dynamics (CGAD) is proposed for finding excited states of Bose-Einstein condensates (BECs) by considering them as constrained saddle points of the Gross-Pitaevskii energy functional. First the formulation of the CGAD is carefully designed to search for a constrained saddle point with any specified index, and its linear stability analysis is provided. Then an effective time-splitting strategy of the CGAD based on a discrete orthonormalization is presented to simplify the numerical implementation. Further a fully discrete semi-implicit backward Euler sine-pseudospectral approximation is introduced. Finally, extensive numerical results are reported to show the efficiency of our methods. Some of them are consistent with theoretical and computational results which are already predicted in the literature, and others show some new interesting physical phenomena but still open to be verified.

26. Liwei Xu, School of Mathematical Sciences, University of Electronic Science and Technology of China

Title: Regularization of hyper-singular boundary integral operators of elastic waves

Abstract: As computing the exterior or transmission problems of scattering waves with the boundary integral equation methods, one usually needs to compute the corresponding hypersingular boundary integral operators. In this talk, we will present some new regularized formulations of hyper-singular boundary integral operators associated with the elastic waves in two and three dimensions, and thermal elastic waves in three dimensions. These formulas are derived using the tool of Gunter derivatives and are equivalent to the original hyper-singular boundary integral formulations in mathematics. Furthermore, turning to the Galerkin scheme, one simply needs to compute weakly singular kernels which could be evaluated analytically under the proper assumptions. We will apply these formulations to numerically investigate such problems as the fluid-solid interaction problems, eigenvalue problems etc.. Numerical examples are presented to verify and validate the theoretical results.

27. Guangwei Yuan, Institute of Applied Physics and Computational Mathematics, P. O. Box 8009, Beijing, 100088,China

Title: Numerical methods preserving physical features for nonlinear energy equations

Abstract: In the numerical simulations of engineering application problems, it is necessary to establish mathematical models satisfying physical constraints, and design accurate and efficient discrete methods for solving numerically the models. This talk will discuss the energy transfer process in radiation hydrodynamics problems. This process is described by the nonlinear energy equation, in which the main physical features include energy conservation, energy density positivity, and finite propagation speed, etc. To meet the requirement of practical simulation, it is important to preserve main physical features in constructing discrete schemes and linearized methods for the nonlinear energy equations.Numerical results are presented to demonstrate the performance of some numerical methods preserving important physical features.

The work is supported by the National Natural Science Foundation of China (11571048).

28. Lei Zhang, Beijing International Center for Mathematical Research, Center for Quantitative Biology, Peking University

Title: Recent Developments in Numerical Methods of Finding Saddle Points and its Applications in Liquid Crystal

Abstract: Nucleation is one of the most common physical phenomena in physical, chemical, biological and materials sciences. Due to the difficulties and challenges in making direct experimental observation, many computational methods have been developed to model and simulate various nucleation events. In my talk, I will provide a sampler of some newly developed numerical algorithms that are widely applicable to many nucleation and phase transformation problems. I first describe some recent progress on the design of efficient numerical methods for computing saddle points and minimum energy paths, and then show an application of finding transition pathways of nematic liquid crystal. I will show that a combination of the Landau-de Gennes

model and the string method can successfully compute the minimum energy path and the transition state configuration of defects in liquid crystals.

29. Zhennan Zhou, Peking University

Title: An accurate front capturing scheme for tumor growth models with a free boundary limit

Abstract: In this talk, I will present some recent work on the tumor growth equation along with various models for the nutrient component, including the in vitro model and the in vivo model. At the cell density level, the spatial availability of the tumor density n is governed by the Darcy law via the pressure $p(n) = n^m$. As m goes to infinity, the cell density models formally converge to Hele-Shaw flow models, which determine the free boundary dynamics of the tumor tissue in the incompressible limit. We derive several analytical solutions to the Hele-Shaw flow models, which serve as benchmark solutions to the geometric motion of tumor front propagation. Also, we develope a numerical scheme based on a novel prediction-correction reformulation that can accurately approximate the front propagation even when the nonlinearity is extremely strong. We show that the semi-discrete scheme naturally connects to the free boundary limit equation as m goes to infinity, and with proper spacial discretization, the fully discrete scheme has improved stability, preserves positivity, and implements without nonlinear solvers. This is a joint work with Jian-Guo Liu, Min Tang and Li Wang.