Focus Activity on Mathematical and Computational Methods for Quantum and Kinetic Problems

June 7-10, 2017 (summer school); June 11-14, 2017 (workshop)

Conference Room II, 3rd Floor, summer school
Conference Room I, 1st Floor, workshop
CSRC Home Building

http://www.csrc.ac.cn/en/event/workshop/2017-01-25/69.html

Sponsorship: Beijing Computational Science Research Center

Contents

Introduction

Quantum and kinetic problems arise in many areas of sciences, engineering and industry applications. Analysis and simulation are two basic tools for the study of mathematical models in quantum and kinetic problems. This workshop will bring applied and computational mathematicians as well as physicists together to exchange the latest developments in the study of quantum and kinetic problems, identify future directions and unsolved questions, and actively initiate collaborations. The activities have two parts. Part I, June 7–June 10, the summer school for local graduate students and junior researchers to learn the state-of-the-art knowledge in quantum and kinetic problems as well as their applications; part II, June 11–June 14, workshop for researchers to exchange ideas and new trends in the area.

Organizing Committee

Weizhu BAO	National University of Singapore and Beijing Computational Science Research Center *matbaowz@nus.edu.sg*
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Schedule Overview


Focus Activity on Mathematical and Computational methods for Quantum and Kinetic Problems
Summer School: June 7 - June 10, Beijing, China
June 6 Tuesday
June 7 (Wednesday)
June 8 (Thursday)
June 9 (Friday)
June 10 (Saturday)
8:00
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18:00
18:30
Registration
Openning
Eric Cances
Weizhu Bao
Lorenzo Pareschi
Break
Lunch
Jose A Carrillo

Focus Activity on Mathematical and Computational methods for Quantum and Kinetic Problems
Workshop: June 11 - June 14, Beijing, China

	June 10 (Saturday)	June 11 (Sunday)	June 12 (Monday)	June 13 (Tuesday)	June 14 (Wednesday)
8:00		Registration	Registration	Registration	Registration
8:30					
9:00		Openning			
9:30		*Pingwen Zhang*	*Avy Soffer*	*Jialin Hong*	*Jie Shen*
10:00		*Emmanuel Lorin*	*Yujin Guo*	*Qi Wang*	*Yan Xu*
10:30		*Break*	*Break*	*Break*	*Break*
11:00		*Wuming Liu*	*Alexander Ostermann*	*Florian Mehats*	*Huazhong Tang*
11:30					
12:00		*Carlo Barenghi*	*Zhongyi Huang*	*Mohammed Lemou*	*Ruo Li*
12:30					
13:00		Lunch	Lunch	Lunch	Lunch
13:30					
14:00		*Aihui Zhou*	*Anton Arnold*	*Liqun Cao*	*Ionut Danaila*
14:30					
15:00		*Zaiwen Wen*	*Chunxiong Zheng*	*Jiwei Zhang*	*Guanghui Hu*
15:30		*Break*	*Break*	*Break*	*Break*
16:00	Registration	*Eric Cances*	*Karolina Kropielnicka*	*Zhimin Zhang*	*Nicolas Crouseilles*
16:30					
17:00		*Huajie Chen*	*Yongyong Cai*	*Jingrun Chen*	*Qinglin Tang*
17:30					Closing Remark
18:00		Banquet, bus leaves at 17:35			
18:30					

Schedule with Titles and Talks

Part I. Summer School

Venue: Conference Room II, 3rd Floor, CSRC Home Building

June 7, 2017 (Wednesday)	
8:30 - 9:20	Registration
9:20 - 9:30	Opening Remarks by Organizers
9:30 - 10:30	**Eric Cancès** Density Functional Theory: models and numerical methods - I
10:30 - 11:00	Coffee & Tea Break
11:00 - 12:00	**Eric Cancès** Density Functional Theory: models and numerical methods - II
12:00 - 14:00	Lunch
14:00 - 15:00	**Weizhu Bao** Computational methods and their analysis for the nonlinear Schrödinger equations - I
15:00 - 15:30	Coffee & Tea Break
15:30 - 16:30	**Weizhu Bao** Computational methods and their analysis for the nonlinear Schrödinger equations – II
June 8, 2017 (Thursday)	
8:30 - 9:30	Registration
9:30 - 10:30	**Weizhu Bao** Computational methods and their analysis for the nonlinear Schrödinger equations - III
10:30 - 11:00	Coffee & Tea Break
11:00 - 12:00	**Weizhu Bao** Computational methods and their analysis for the nonlinear Schrödinger equations - IV
12:00 - 14:00	Lunch
14:00 - 15:00	**Lorenzo Pareschi** Numerical schemes for multiscale kinetic equations: asymptotic-preserving and hybrid methods - I
15:00 - 15:30	Coffee & Tea Break
15:30 - 16:30	**Lorenzo Pareschi** Numerical schemes for multiscale kinetic equations: asymptotic-preserving and hybrid methods - II

June 9, 2017 (Friday)	
8:30 - 9:30	Registration
9:30 - 10:30	**Lorenzo Pareschi** Numerical schemes for multiscale kinetic equations: asymptotic-preserving and hybrid methods - III
10:30 - 11:00	Coffee & Tea Break
11:00 - 12:00	**Lorenzo Pareschi** Numerical schemes for multiscale kinetic equations: asymptotic-preserving and hybrid methods - IV
12:00 - 14:00	Lunch
14:00 - 15:00	**José A Carrillo** Minimizing interaction energies: nonlocal potentials and nonlinear diffusions - I
15:00 - 15:30	Coffee & Tea Break
15:30 - 16:30	**José A Carrillo** Minimizing interaction energies: nonlocal potentials and nonlinear diffusions – II
June 10, 2017 (Saturday)	
8:30 - 9:30	Registration
9:30 - 10:30	**Eric Cancès** Density Functional Theory: models and numerical methods - III
10:30 - 11:00	Coffee & Tea Break
11:00 - 12:00	**Eric Cancès** Density Functional Theory: models and numerical methods - IV
12:00 - 14:00	Lunch
14:00 - 15:00	**José A Carrillo** Minimizing interaction energies: nonlocal potentials and nonlinear diffusions - III
15:00 - 15:30	Coffee & Tea Break
15:30 - 16:30	**José A Carrillo** Minimizing interaction energies: nonlocal potentials and nonlinear diffusions - IV

Part II. Workshop

Venue: Conference Room I, 1st Floor, CSRC Home Building

June 11, 2017 (Sunday)

8:00 - 8:45	Registration
8:45 - 9:00	Opening Remarks by Organizers
9:00 - 9:45	**Pingwen Zhang** Boundary problems for the fractional operators
9:45 - 10:30	**Emmanuel Lorin** Convergence analysis of Schwarz waveform relaxation domain decomposition methods for the Schrödinger equation
10:30 - 11:00	Coffee & Tea Break
11:00 - 11:45	**Wuming Liu** Topological excitations and dynamics of Bose-Einstein Condensates in the synthetic gauge field
11:45 - 12:30	**Carlo Barenghi** Quantum vortex reconnections and quantum turbulence
12:30 - 14:00	Lunch
14:00 - 14:45	**Aihui Zhou** Adaptive finite element approximations for density functional models
14:45 - 15:30	**Zaiwen Wen** Electronic structure calculation using semidefinite programs
15:30 - 16:00	Coffee & Tea Break
16:00 - 16:45	**Eric Cancès** Incommensurate and disordered quantum systems
16:45 - 17:30	**Huajie Chen** Numerical analysis of finite temperature DFT
From 17:35	Banquet

June 12, 2017 (Monday)

8:00 - 9:30	Registration
9:00 - 9:45	**Avy Soffer** A new multi-time scale method for dispersive waves
9:45 - 10:30	**Yujin Guo** Theory and applications of L^2-critical constraint variational problems
10:30 - 11:00	Coffee & Tea Break
11:00 - 11:45	**Alexander Ostermann** Low regularity exponential-type integrators for nonlinear Schrödinger equations
11:45 - 12:30	**Zhongyi Huang** Bloch decomposition-based stochastic Galerkin/collocation method for Schrödinger equation with random inputs
12:30 - 14:00	Lunch
14:00 - 14:45	**Anton Arnold** A hybrid WKB-based method for the stationary Schrödinger equation in the semi-classical limit
14:45 - 15:30	**Chunxiong Zheng** Extended-WKB analysis for the high-frequency linear wave equations
15:30 - 16:00	Coffee & Tea Break
16:00 - 16:45	**Karolina Kropielnicka** Exponential splitting, Lie algebra, and commutator-free Magnus based methods for the linear Schrödinger equation
16:45 - 17:30	**Yongyong Cai** Non-relativistic limit of the (nonlinear) Dirac equations and their numerical methods

June 13, 2017 (Tuesday)

8:00 - 9:30	Registration
9:00 - 9:45	**Jialin Hong** Stochastic symplectic methods and multi-symplectic methods for two stochastic Hamiltonian partial differential equations
9:45 - 10:30	**Qi Wang** Kinematics and dynamics of active matter systems
10:30 - 11:00	Coffee & Tea Break
11:00 - 11:45	**Florian Méhats** Highly oscillatory problems: application of averaging techniques to a uniformly accurate numerical method
11:45 - 12:30	**Mohammed Lemou** Averaging and approximation of highly oscillatory transport equation with time-space dependent frequency
12:30 - 14:00	Lunch
14:00 - 14:45	**Liqun Cao** FEM analysis and multiscale algorithms for Maxwell-Schrödinger system in nanostructures
14:45 - 15:30	**Jiwei Zhang** The construction of artificial boundary conditions for nonlocal models
15:30 - 16:00	Coffee & Tea Break
16:00 - 16:45	**Zhiming Zhang** A new approach for solving the time-dependent Ginzburg—Landau superconductivity model
16:45 - 17:30	**Jingrun Chen** Multiscale modeling of current-driven magnetization dynamics

June 14, 2017 (Wednesday)

8:00 - 9:30	Registration
9:00 - 9:45	**Jie Shen** A new and robust approach to construct energy stable schemes for gradient flows
9:45 - 10:30	**Yan Xu** An h-adaptive local discontinuous Galerkin method for phase transition problem
10:30 - 11:00	Coffee & Tea Break
11:00 - 11:45	**Huazhong Tang** Globally hyperbolic moment model of arbitrary order for special relativistic Boltzmann equation
11:45 - 12:30	**Ruo Li** Stability of hyperbolic moment models for Boltzmann equation
12:30 - 14:00	Lunch
14:00 - 14:45	**Ionut Danaila** Computation of stationary states of rotating Bose-Einstein condensates via Riemannian Optimization
14:45 - 15:30	**Guanghui Hu** On adaptive finite element simulations of high harmonic generation with time-dependent density functional theory
15:30 - 16:00	Coffee & Tea Break
16:00 - 16:45	**Nicolas Crouseilles** Uniformly accurate particle-in-cell method for the long time behavior of the 2d Vlasov Poisson equation with uniform strong magnetic field
16:45 - 17:30	**Qinglin Tang** Computing ground states of spin 2 Bose-Einstein condensates by the normalized gradient flow
17:30 - 17:45	Closing Remark

Titles and Abstracts

Part I. Summer School

Computational methods and their analysis for the nonlinear Schrödinger equations

Weizhu Bao

National University of Singapore, Singapore

In this tutorial, I begin wtih the nonlinear Schrödinger/Gross-Pitaevskii equations (NLSE/GPE) for modeling Bose-Einstein condensation (BEC), nonlinear optics, quantum physics and chemistry, etc., and review some dynamical properties of NLSE/GPE including conserved quantities, dispersion relation, center-of-mass dynamics, soliton solutions and semiclassical limits. Different numerical methods will be presented including finite different time domain (FDTD) methods and time-splitting spectral method, and their error estimates and comparison will be discussed. Extensions to NLSE/GPE with an angular momentum rotation term and/or non-local dipole-dipole interaction as well as multi-component will be presented. Finally, applications to soliton interactions, collapse and explosion of BEC, quantum transport and quantized vortex interaction will be investigated.
References:

[1]. W. Bao and Y. Cai, Mathematical theory and numerical methods for Bose-Einstein condensation, Kinet. Relat. Mod., 6 (2013), pp. 1-135.

[2]. X. Antoine W. Bao and C. Besse, Computational methods for the dynamics of the nonlinear Schrödinger/Gross-Pitaevskii equations, Comput. Phys. Commun., 184 (2013), pp. 2621-2633.

[3]. W. Bao, Q. Tang and Z. Xu, Numerical methods and comparison for computing dark and bright solitons in the nonlinear Schrödinger equation, J. Comput. Phys., 235 (2013), pp. 423-445.

[4]. W. Bao, D. Jaksch and P. A. Markowich, Numerical solution of the Gross-Pitaevskii equation for Bose-Einstein condensation, J. Comput. Phys., 187 (2003), pp. 318-342.

Density functional theory: models and numerical methods

Eric Cancès

Ecole des Ponts and INRIA, France

First-principle molecular simulation based on electronic structure calculation has become an essential tool in chemistry, condensed matter physics, molecular biology, materials science, and nanosciences. In this lecture, I will focus on Density

Functional Theory and the Kohn-Sham model, which is to date the most widely used approach in electronic structure calculation, since it provides the best compromise between accuracy and computational efficiency. The Kohn-Sham model is a constrained optimization problem, whose Euler-Lagrange equations have the form of a coupled system of nonlinear elliptic eigenvalue problems. I will explain how to derive the Kohn-Sham model from the N-body Schrödinger equation, comment on the approximations made, and present some numerical methods to solve this problem.

Minimizing interaction energies: nonlocal potentials and nonlinear diffusions

José A. Carrillo
Imperial College London, UK

In these lectures we will discuss several recent works regarding the minimization of nonlocal interaction energies. Understanding how qualitative properties of local minimizers are related to potentials will be the first goal. We will discuss the existence of global minimizers of free energies and its relation to obstacle problems. Finally, we will show different scaling regimes for homogeneous functionals with nonlinear diffusion and we will discuss the diffusion dominated case where no critical parameter appears. We show that all dynamics are controlled by a unique compactly supported stationary state.

Numerical schemes for multiscale kinetic equations: asymptotic-preserving and hybrid methods

Lorenzo Pareschi
University of Ferrara, Italy

Many applications involve kinetic equations with multiple space-time scales. Numerically resolving such scales may be computationally prohibitive and therefore one resorts on the use of some asymptotic analysis in order to derive reduced fluid-dynamic models which are valid in the small scales regime. The derivation of numerical schemes which are capable to describe correctly such asymptotic behavior without resolving the small scales has attracted a lot of attention in the recent years leading to the so-called asymptotic-preserving (AP) methods. A typical AP method permits the use of the same numerical scheme for the multiscale kinetic equation and its small scale limit, with fixed discretization parameters. This allows to match regions where the perturbation parameters have very different orders of magnitude without adopting a multi-physics approach that couples different physical models at different scales. In these lectures we first survey the basic concepts

of AP methods for kinetic equations, next we consider the design principles of AP techniques based on exponential, Runge-Kutta and linear multistep methods and present some representative examples. The last part of the lectures will be devoted to the construction of hybrid AP methods which combine a stochastic solver for the kinetic equation with a deterministic solver for the reduced fluid-dynamic model.
References:

[1]. G.Dimarco, L.Pareschi, Numerical methods for kinetic equations, Acta Numerica 23 (2014), 369–520.

[2]. J. Hu, Q. Li, L. Pareschi, Asymptotic-preserving exponential methods for the quantum Boltzmann equation with high-order accuracy. J. Sci. Comput. 62 (2015), no. 2, 555–574.

[3]. G. Dimarco, L. Pareschi, Implicit-explicit linear multistep methods for kinetic equations, to appear on SIAM J. Num. Anal. arxiv: 1603.00102.

Part II. Workshop

A hybrid WKB-based method for the stationary Schrödinger equation in the semi-classical limit

Anton Arnold
Technische Universitat Vienna, Austria

We are concerned with the efficient numerical integration of ODEs of the form $\epsilon^2\psi_{xx} + a(x)\psi = 0$ for $0 < \epsilon << 1$ on coarse grids, but still yielding accurate solutions. In particular we study the numerical coupling of the highly oscillatory regime (i.e. for given $a(x) > 0$) with evanescent regions (i.e. for $a(x) < 0$). In the oscillatory case we use a marching method that is based on an analytic WKB-preprocessing of the equation. And in the evanescent case we use a FEM with WKB-ansatz functions.

We present a full convergence analysis of the coupled method, showing that the error is uniform in ϵ and second order w.r.t. h. We illustrate the results with numerical examples for scattering problems for a quantum-tunnelling structure.

This is a joint work with Claudia Negulescu.

References:

[1]. A. Arnold, C. Negulescu: Stationary Schrödinger equation in the semi-classical limit: numerical coupling of oscillatory and evanescent regions, submitted to Numer. Math. 2017.

[2]. A. Arnold, N. Ben Abdallah, C. Negulescu: WKB-based schemes for the oscillatory 1D Schrödinger equation in the semi-classical limit, SIAM J. Numer. Anal. 49, No. 4 (2011) 1436-1460.

Quantum vortex reconnections and quantum turbulence

Carlo Barenghi
Newcastle University, UK

Superfluids (such as liquid helium and atomic Bose-Einstein condensates) are remarkable because of two properties: the absence of viscosity and the discrete nature of the vorticity (which is concentrated in thin quantized filaments). These properties have profound implications for the turbulence which is easily generated when a superfluid is stirred. Recent work has identified two turbulence regimes in quantum fluids: the first has properties which are similar to ordinary (classical) turbulence, the latter is different. I shall review this evidence and discuss

vortex reconnections. Vortex reconnections are fundamental in turbulence. They are localized, dramatic events which take place when two vortex filaments collide, exchange'heads' and 'tails' and change the flow's topology. In particular, I shall describe recent combined experimental and theoretical work which has revealed new forms of quantum vortex interactions and reconnections in trapped atomic Bose-Einstein condensates.

References:

[1]. S. Serafini, L. Galantucci, E. Iseni, T. Bienaime, R.N. Bisset, C.F. Barenghi, F. Dalfovo, G. Lamporesi and G. Ferrari,Vortex reconnections and rebounds in trapped atomic Bose–Einstein condensates,to published in Phys. Rev. X (2017), arXiv:1611.01691

[2]. G.W. Stagg, N.G. Parker, and C.F. BarenghiSuperfluid boundary layer, Phys. Rev. Lett. 118, 135301 (2017)

[3]. C.F. Barenghi, Y.A.Sergeev and A.W.Baggaley,Regimes of turbulence without an energy cascade,Nature Scientific Reports 6, 35701 (2016)

[4]. C.F. Barenghi, V. L'vov, and P.-E. Roche,Experimental, numerical and analytical velocity spectra inturbulent quantum fluid, Proc. Nat. Acad. Sciences USA, 111 (suppl. 1) 4683 (2014)

Non-relativistic limit of the (nonlinear) Dirac equations and their numerical methods

Yongyong Cai

CSRC, China

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) Schrödinger equation in the non-relativistic limit. Using superposition and multiscale decomposition, we designed a uniformly accurate scheme for solving the Dirac equation in the non-relativistic limit. For the nonlinear case, 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.

Incommensurate and disordered quantum systems

Eric Cancès

Ecole des Ponts and INRIA, France

After recalling the standard mathematical formalism used to model disordered materials such as doped semiconductors, alloys, or amorphous materials, and classical results about random Schrödinger operators (Anderson localization), I will present a tight-binding model for computing the electrical conductivity of multilayer 2D materials. All these models fall into the scope of the mathematical framework, based on non-commutative geometry, introduced by Bellissard to study the electronic properties of aperiodic systems. I will finally present some numerical simulations.

FEM analysis and multiscale algorithms for Maxwell-Schrödinger system in nanostructures

Liqun Cao

Chinese Academy of Science, China

When the size of physical devices reaches the wavelength of an electron, quantum effects become important even dominant and can not be neglected. To analyze and model such physical devices, coupled numerical simulations of Maxwell and Schrödinger equations with the effective mass approximation (EMA) need to be performed. Maxwell-Schrödinger system originates from the interaction of the matter field and the electromagnetic field in nanostructures. In this talk, we will introduce our recent advances in the FEM analysis and the multiscale algorithms for Maxwell-Schrödinger system. First, we will briefly talk about the fundamental physical questions and the mathematical models such as gauge invariance, topological invariance and so forth. Meanwhile, we will introduce some important studies about the analysis and computation of Maxwell-Schrödinger system. Second, we focus on discussing the Crank-Nicolson finite element methods and the error analysis for the Maxwell-Schrödinger system under some gauge conditions. Third, the homogenization method and the multiscale asymptotic method for the Maxwell-Schrödinger system with rapidly oscillating discontinuous coefficients which rises in heterogeneous nanostructures are presented under the Weyl gauge and for the electric dipole approximate model. Finally, the numerical results and some unsolved questions are advanced.

This talk is based on the joint work with Dr. Chupeng Ma and Dr. Lei Zhang.

Numerical analysis of finite temperature DFT

Huajie Chen

Beijing Normal University, China

We study finite dimensional approximations of the Mermin-Kohn-Sham equation, which is derived from the finite temperature DFT model. For general numerical discretization methods, we prove the convergence of the finite dimensional approximations and derive the optimal a priori error estimates. We also provide numerical simulations for several molecular systems that support our theory.

Multiscale modeling of current-driven magnetization dynamics

Jingrun Chen
Soochow University, China

Understanding magnetization dynamics in magnetic materials under external current control plays a vital role in magnetic storage devices, such as magnetoresistance random access memories and race-track memories. In this presentation, we will discuss how to model such a phenomenon at different spatial and temporal scales. Consequently, a series of models is obtained with increasing accuracy. Efficient numerical methods are also proposed and applied to a couple of prototypical devices, which produces consistent results with experiments. Of physical and technological interests, 1D surrogate model is also derived using the method of matched asymptotics, which explains the Walker's breakdown. The gap between the 1D model and the original model will also be discussed.

Uniformly accurate particle-in-cell method for the long time behavior of the 2d Vlasov Poisson equation with uniform strong magnetic field

Nicolas Crouseilles
University of Rennes 1, France

In this talk, we focus on the numerical resolution of the 4D phase space Vlasov-Poisson system subject to a strong external uniform magnetic field. To do so, we consider a Particle-In-Cell based method, for which the characteristics are reformulated by means of the two-scale formalism, which is well-adapted to handle highly-oscillatory equations. Then, a numerical scheme is derived for the two-scale equations. The so-obtained scheme enjoys a uniform accuracy property, meaning that its accuracy does not depend on the small parameter. Several numerical results illustrate the capabilities of the method.

Computation of stationary states of rotating Bose-Einstein condensates via Riemannian Optimization

Ionut Danaila

University of Rouen Normandy, France

We combine in this work concepts from Riemannian Optimization [1] and Sobolev gradient theory [2] to derive a new conjugate-gradient method for the direct minimization of the Gross-Pitaevskii energy functional with rotation. The method is derived at a continuous level, applying the optimize-then-discretize principle instead of the usual "discretize-then-differentiate" technique. The conservation of the number of particles of the system imposes a spherical constraint. Consequently, appropriate Riemannian retraction and transport are applied to maintain the iterates on the spherical manifold. We first derive a Riemannian gradient method and then a nonlinear conjugate-gradient method. The new method greatly improves the convergence rate to a stationary solution, when compared to existing methods. We illustrate the capabilities of the method by computing vortex configurations of rotating Bose-Einstein Condensates for difficult cases, with high values of the non-linear interaction constant and very high rotation rates.

This is a joint work with B. Protas, McMaster University, Canada.

References:

[1]. P.-A. Absil, R. Mahony, R. Sepulchre, Optimization algorithms on matrix manifolds, Princeton University Press, 2008.

[2]. J. W. Neuberger, Sobolev gradients, Springer, 2010.

[3]. I. Danaila, B. Protas, Computation of Ground States of the Gross-Pitaevskii Functional via Riemannian Optimization, arXiv:1703.07693v1, 2017.

Theory and applications of L^2-critical constraint variational problems

Yujin Guo

Wuhan Institute of Physics and Mathematics

L^2-constraint variational problems often arise in quantum many-body systems. Even though L^2-noncritical cases have been tackled a lot since the celebrated works of [P. L. Lions, Poincare Anal., 1984], L^2-critical cases have not been investigated too much until recent years. The main purpose of this talk is to discuss the recent progresses on the theory and applications of L^2-critical constraint variational problems.

Stochastic symplectic methods and multi-symplectic methods for two stochastic Hamiltonian partial differential equations

Jialin Hong
Chinese Academy of Sciences, China

In this talk we review some results on stochastic symplectic methods for stochastic Hamiltonian systems, including stochastic generating functions and stochastic Hamilton-Jacobi theory. We investigate the canonical form and the stochastic symplectic structure of stochastic nonlinear Schrödinger equations (SSEs), and show that the symplectic Runge-Kutta semi-discretization for SSEs in time preserves charge conservation law. We present stochastic multi-symplectic methods for stochastic Maxwell equations, and show that these methods preserve physical properties of equations.

On adaptive finite element simulations of high harmonic generation with time-dependent density functional theory

Guanghui Hu
University of Macau, China

High harmonic generation (HHG) plays an important role in the emerging attosecond physics, and has applications on developing novel techniques such as imaging of molecular orbitals. There are several challenges on numerical study of HHG. In this talk, HHG as well as theoretical and numerical challenges on its study will be introduced. Then a numerical framework of adaptive finite element solutions of Kohn-Sham and time-dependent Kohn-Sham equations for HHG simulations will be described in detail. Numerical results will show the effectiveness of the proposed method.

Bloch decomposition-based stochastic Galerkin/collocation method for Schrödinger equation with random inputs

Zhongyi Huang
Tsinghua University, China

In this talk, we focus on the analysis and numerical methods for the Schrödinger equation with lattice potential and random inputs. Here we recall the well-known

Bloch decomposition-based split-step pseudo-spectral method where we diagonalize the periodic part of the Hamilton operator so that the effects from dispersion and periodic lattice potential are computed together. Meanwhile, for the random non-periodic external potential, we utilize the generalize polynomial chaos with Galerkin procedure to form an ode system which can be solved analytically. Furthermore, we analyse the convergence theory of the stochastic collocation method for the linear Schrödinger equation with random inputs. We provide sufficient conditions on the random potential and initial data to ensure the spectral convergence.

This is a joint work with Zhizhang Wu.

Keywords: Schrödinger equation; uncertainty quantification; Bloch decomposition; stochastic Galerkin/collocation methods.

Exponential splitting, Lie algebra, and commutator-free Magnus based methods for the linear Schrödinger equation

Karolina Kropielnicka

University of Gdańsk and Polish Academy of Sciences, Poland

The discretization of a linear Schrödinger equation is difficult due to the presence of a small parameter which induces high oscillations. A standard approach consists of a spectral semi-discretization, followed by an exponential splitting. This, however, is sub-optimal, because the exceedingly high precision in space discretization is married by low order of the time solver.

In this talk we sketch an alternative approach.

Our analysis commences not with semi-discretization, but with the investigation of the Lie algebra generated by differentiation and by multiplication with the interaction potential: it turns out that this algebra possesses a structure which renders it amenable to a very effective form of asymptotic splitting: exponential splitting where consecutive terms are scaled by increasing powers of the small parameter. The semi-discretization in deferred to the very end of computations.

We will focus on the method for the time dependent linear Schrödinger equation with potential non-depending on time, however we will also discuss the difficulties that appear with time dependent potential and will briefly propose the remedy to that stage of an affair, a commutator-free Magnus based method.

Averaging and approximation of highly oscillatory transport equation with time-space dependent frequency

Mohammed Lemou

University of Rennes 1, France

A general strategy will be presented to deal with highly oscillatory transport equations with varying frequencies. A smooth change of time is used to bring down the problem to a constant-frequency one. Then standard averaging techniques can be applied and uniformly accurate (with respect to the frequency) numerical schemes will be constructed. Some applications in quantum mechanics and plasma physics will be presented.

Stability of hyperbolic moment models for Boltzmann equation

Ruo Li

Peking University, China

Grad's moment models for Boltzmann equation were recently regularized to globally hyperbolic systems, and thus the regularized models attain local well-posedness for Cauchy data. The hyperbolic regularization is only related to the convection term in Boltzmann equation. We in this paper studied the regularized models with the presentation of collision terms. It is proved that the regularized models are linearly stable at the local equilibrium and satisfy Yong's first stability condition with commonly used approximate collision terms, and particularly with Boltzmann's binary collision model.

Topological excitations and dynamics of Bose-Einstein Condensates in the synthetic gauge field

Wuming Liu

Chinese Academy of Sciences, China

We will review our research on topological excitations and dynamics in Bose-Einstein Condensates (BECs) with the synthetic gauge field. We investigate topological excitation in the Rashba SOC BECs. Our results show that the weak SOC leads to the emergence of monopoles with the polar-core vortex that are long-lived, and the strong SOC leads to the emergence of monopoles with the square lattice in spinor BECs. It is found that increasing the strength of the interaction can induce a cyclic phase transition from Dirac monopoles with a polar-core vortex to those with a Mermin-Ho vortex. Such monopoles can be detected by the time-of-flight absorption imaging technique [1]. We also investigate nonlinear matter waves and topological spin textures in atomic-molecular BECs. we obtain two

kinds of Jacobi elliptic solutions and a family of rational solutions of the atomic-molecular BECs with space-modulated nonlinearity. In addition, we find a way of creating a Rashba-Dresselhaus SOC in atomic-molecular BECs, which can induce the emergence of carbon-dioxide-like skyrmion. The skyrmion can be detected by measuring the vortices structures using the time-of-flight absorption imaging technique in real experiments [2, 3]. We investigate topological excitation in SU(3) spin-orbit-coupled Bose gases. It is found that the SU(3) SOC and spin-exchange interaction play important roles in determining the ground-state phase diagram. Our simulations show that in the case of effective ferromagnetic spin interaction, the SU(3) SOC induces a threefold degeneracy to the magnetized ground state. In particular, the SU(3) SOC allows the spontaneous emergence of double-quantum spin vortices in the antiferromagnetic case. This exotic topological defect can be readily observed by the current magnetization-sensitive phase-contrast imaging technique [4]. From now on, we will review our research on the dynamics in BECs. We examine the dynamics of vortex quadrupoles in a trapped two-dimensional BECs. It is found that the movement of these vortex-clusters fall into three distinct regimes which are fully described by the radial positions of the vortices in a isotropic harmonic trap, or by the major radius (minor radius) of the elliptical equipotential lines decided by the vortex positions. Our simulations show that In the recombination and exchange regimes the quadrupole structure maintains, while the vortices annihilate each other permanently in the annihilation regime. We further find that the mechanism of the charge flipping in the exchange regime and the disappearance of the quadrupole structure in the annihilation regime are both through an intermediate state where two vortex dipoles connected through a soliton ring [5]. Motion of solitons in one-dimensional spin-orbit-coupled Bose-Einstein condensates is studied. We demonstrate that the spin dynamics of solitons is governed by a nonlinear Bloch equation. The spin dynamics affects the orbital motion of solitons leading to spin-orbit effects in the dynamics of macroscopic quantum objects (mean-field solitons). The latter perform oscillations with a frequency determined by the SOC, Raman coupling, and intrinsic nonlinearity. These findings reveal unique features of solitons affected by the SOC, which are confirmed by analytical considerations and numerical simulations of the underlying Gross-Pitaevskii equations [6].

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Convergence analysis of Schwarz waveform relaxation domain decomposition methods for the Schrödinger equation

Emmanuel Lorin

Carleton University, Canada

This talk is dedicated to the asymptotic estimation of the convergence rate for the Classical and quasi-Optimal Schwarz waveform relaxation domain decomposition methods applied to the computation of i) the stationary states to the one- and two-dimensional linear and nonlinear Schrödinger equations by the "imaginary time method", and of ii) to the time-dependent Schrödinger equation with non-constant potential. The analysis will extensively use to the theory of inhomogeneous pseudodifferential operators. Some numerical experiments will illustrate the accuracy of theoretical estimates, and some applications in quantum chemistry will also be presented.

This is a joint work with X. Antoine (IECL).

Highly oscillatory problems: application of averaging techniques to a uniformly accurate numerical method

Florian Méhats

University of Rennes 1, France

I will present averaging techniques applied to highly oscillatory models (an ODE example and the nonlinear Klein-Gordon equation in the nonrelativistic regime). Then I will show how these results can be used to construct a micro/macro model which is well-fitted to design uniformly accurate numerical methods.

This is a joint work with P. Chartier, M. Lemou and G. Vilmart.

Low regularity exponential-type integrators for nonlinear Schrödinger equations

Alexander Ostermann

University of Innsbruck, Austria

Nonlinear Schrödinger equations are usually solved by pseudo-spectral methods, where the time integration is performed by splitting schemes or exponential integrators. Notwithstanding the benefits of this approach, its successful application requires additional regularity of the solution. In this talk, we introduce as an alternative low regularity exponential-type integrators. For such methods, first-order convergence only requires the boundedness of one additional derivative of the solution. This allows us to impose lower regularity assumptions on the data than for instance required for classical splitting or exponential integration schemes. For one-dimensional quadratic Schrödinger equations we can even prove first-order convergence without any loss of regularity. Numerical experiments underline the favorable error behavior of the newly introduced exponential-type integrators for low regularity solutions compared to classical splitting and exponential integration schemes.

This is joint work with Katharina Schratz (KIT, Karlsruhe).

References:

[1]. A. Ostermann, K. Schratz. Low regularity exponential-type integrators for semilinear Schrödinger equations. To appear in Found. Comput. Math. (2017).

A new and robust approach to construct energy stable schemes for gradient flows

Jie Shen

Purdue University, USA and Xiamen University, China

We propose a new technique dealing with nonlinear terms in the numerical schemes of gradient flows. By introducing a scalar auxiliary variable, we construct second-order schemes unconditionally energy stable based on the Crank–Nicolson (CN) or the BDF scheme for the linear part. The scheme is not restricted to specific forms of the nonlinear part of the free energy, and only requires to solve decoupled linear equations which are independent of the nonlinear terms.

We use this technique to deal with several challenging applications which can not be easily handled by existing approaches, and present convincing numerical results to show that our schemes are not only much more efficient and easy to implement, but also can better capture the physical properties in these models.

A new multi-time scale method for dispersive waves

Avy (Avraham) Soffer
Rutgers Univeristy, USA

I will describe a new approach to multi-scale time averaging technique, which allows to inductively construct averaged hamiltonians, which approximates the full dynamics to arbitrary order in the inverse of the adiabatic parameter. I will show applications to adiabatic theorems in QM, and in scattering theory, as well as numerical schemes to solve dispersive equations for long times.

Globally hyperbolic moment model of arbitrary order for special relativistic Boltzmann equation

Huazhong Tang
Peking University and Xiangtan University, China

We first extend the model reduction method by the operator projection to the 1D special relativistic Boltzmann equation. The derivation of arbitrary order globally hyperbolic moment system is built on our careful study of two families of the complicate Grad type orthogonal polynomials depending on a parameter. We derive their recurrence relations, calculate their derivatives with respect to the independent variable and parameter respectively, and study their zeros and coefficient matrices in the recurrence formulas. Some properties of the moment system are also proved. They include the eigenvalues and their bound as well as eigenvectors, hyperbolicity, characteristic fields, linear stability, and Lorentz covariance. A semi-implicit numerical scheme is presented to solve a Cauchy problem of our hyperbolic moment system in order to verify the convergence behavior of the moment method. The results show that the solutions of our hyperbolic moment system converge to the solution of the special relativistic Boltzmann equation as the order of the hyperbolic moment system increases.

Now we are also deriving the globally hyperbolic moment model of arbitrary order for the 3D special relativistic Boltzmann eq. Moreover, it is interesting to develop robust, high order accurate numerical schemes for the moment system, find other basis for the derivation of moment system with some good property, e.g. non-negativity, and investigate the relativistic effects by using the moment system.

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Computing ground states of spin 2 Bose-Einstein condensates by the normalized gradient flow

Qinglin Tang

National University of Singapore, Singapore

In this talk, an efficient and accurate numerical method will be proposed to compute the ground state of spin-2 Bose-Einstein condensates (BECs) by using the normalized gradient flow (NGF) or imaginary time method (ITM). The key idea is twofold. One is to find the five projection or normalization conditions that are used in the projection step of NGF/ITM,while the other one is to find a good initial data for the NGF/ITM.Based on the relations between chemicalpotentials and the two physical constraints given by the conservation of the total massand magnetization, these five projection or normalization conditions can be completely anduniquely determined in the context of the discrete scheme of the NGF discretized by back-Euler finite difference (BEFD) method, which allows one to successfully extend the powerful and popular NGF/ITM to compute the ground state of spin-2 BECs.Additionally, the structures and properties of the ground states in a uniform system areanalysed so as to construct efficient initial data for NGF/ITM. Numerical results will be reported to show the efficiency of our methodand to demonstrate some interesting physical phenomena.

Kinematics and dynamics of active matter systems

Qi Wang

CSRC, China and University of South Carolina, USA

Active matter systems can be described using a set of stochastic differential equations with a well-chosen random fluctuations for specific active characteristics. This SDE system is equivalent to a phase or configuration space kinetic model. In this talk, I will discuss first the active matter system modeled by an SDE system, demonstrating the long-time collective motion on a flat substrate surface and on a curvy surface. Then, I will discuss how a phase space kinetic theory can be used to describe the active suspension system with a viscous solvent.

Electronic structure calculation using semidefinite programs

Zaiwen Wen

Peking University, China

Electronic structure calculation can be modeled by a variational approach where the two-body reduced density matrix (RDM) is the unknown variable. It can lead to an extremely large-scale semidefinite programming (SDP) problem. This talk will present a practically efficient second-order type method.

An h-adaptive local discontinuous Galerkin method for phase transition problem

Yan Xu

University of Science and Technology of China, China

The goal of this talk is to present a local discontinuous Galerkin (LDG)discretization of the (non)-isothermal Navier-Stokes-Korteweg (NSK) equations in conservative form. These equations are used to model the dynamics of a compressible fluid exhibiting liquid-vapour phase transitions. The NSKequations are closed with a Van der Waals equation of state and contain third order nonlinear derivative terms. These contributions frequently cause standard numerical methods to violate the energy dissipation relation and require additional stabilization terms to prevent numerical instabilities. In order to address these problems we first develop an LDG method for the isothermal NSK equations using discontinuous finite element spaces combined with a time-implicit Runge-Kutta integration method. Next, we extend the LDG discretization to the non-isothermal NSK equations. An important feature of the LDG discretizations presented in this article is that they are relatively simple, robust and do not require special regularization terms. To save computing time and to capture the thin interfaces more accurately, we extend the LDG discretization with a mesh adaptation method. Given the current adapted mesh, a criterion for selecting candidate elements for refinement and coarsening is adopted based on the locally largest value of the density gradient. A strategy to refine and coarsen the candidate elements is then provided. We emphasize that the adaptive LDG discretization is relatively simple and does not require additional stabilization. The use of a locally refined mesh in combination with an implicit Runge-Kutta time method is, however, non-trivial, but results in an efficient time integration method for the NSK equations. Computations, including cases with solid wall boundaries, are provided to demonstrate the accuracy, efficiency and capabilities of the adaptive LDG discretizations.

The construction of artificial boundary conditions for nonlocal models

Jiwei Zhang
CSRC, China

The numerical solutions of nonlocal models such as nonlocal heat and wave equations on unbounded domains are considered. Differing from local models, the nonlocal effect makes the design of absorbing boundary conditions (ABCs) more difficult since it breaks up the symmetry of the operator and requires an artificial layer to limit the bounded computational domain of interest. In this talk, we will report the recent progress on this topic.

These works are jointed with Prof. Qiang Du, Prof. Houde Han and Prof. Chunxiong Zheng and so on.

Boundary problems for the fractional operators

Pingwen Zhang
Peking University, China

For characterizing the Brownian motion in a bounded domain, it is well-known that the boundary conditions of the classical diffusion equation just rely on the given information of the solution along the boundary of a domain; on the contrary, for the Levy flights or temperedLevy flights in a bounded domain, it involves the information of a solution in the complementary set of domain, with the potential reason that paths of the corresponding stochastic process are discontinuous. Guided by probability intuitions and the stochastic perspectives of anomalous diffusion, we show the reasonable ways, ensuring the clear physical meaning and well-posedness of the partial differential equations (PDEs), of specifying 'boundary' conditions for space fractionalPDEs modeling the anomalous diffusion. Some properties of the operators are discussed, and the well-posednesses of the PDEs with generalized boundary conditions are proved.

A new approach for solving the time-dependent Ginzburg–Landau superconductivity model

Zhiming Zhang
CSRC, China and Wayne State University, USA

The time-dependent GinzburgLandau system models superconductivity in material science. We prove well-posedness of such a system in a non-convex polygonal domain, and decompose the solution as a regular part plus a singular part. We see

that the magnetic potential is not in H^1 in general, and a direct use of the standard finite element method may give incorrect solutions. To remedy this situation, we reformulate the equations into an equivalent system of elliptic and parabolic equations based on the Hodge decomposition, which avoids direct calculation of the magnetic potential. The essential unknowns of the reformulated system admit H^1 solutions and can be solved correctly by finite element methods. We then propose a decoupled and linearized algorithm to solve the reformulated equations and present error estimates based on proved regularity of the solution. Numerical examples are provided to support our theoretical analysis and show the efficiency of the method.

Extended-WKB analysis for the high-frequency linear wave equations

Chunxiong Zheng
Tsinghua University, China

WKB analysis plays an important role in the high-frequency asymptotics for wave equations. However, it faces the break-down problem due to the appearance of caustics. In the last few years, we have developed a novel high-frequency asymptotic theory, called extended WKB analysis. This method is blind to the traditional caustics, and works for any kind of linear wave equations, either scalar or vectorial. It presents an asymptotic approximation of the wave field with uniform accuracy. In this talk, we will report the basic idea and some main results.

Adaptive finite element approximations for density functional models

Aihui Zhou
Chinese Academy of Science, China

Density functional models are powerful, widely used approaches for computation of ground state electronic energies and densities in chemistry, materials science, biology, and nanosciences. In this presentation, we will talk about adaptive finite element approximations of orbital-free and Kohn-Sham density functional models, including the construction and analysis of the residual type a posteriori error estimators as well as the convergence and complexity of the adaptive finite element approximations. We will demonstrate several typical numerical experiments that show the robustness and efficiency of the adaptive finite element computations in electronic structure calculations.

This presentation is based on some joint works with H. Chen, X. Dai, X. Gong, and L. He.

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Part II. June 11 – June 14, Workshop, Invited Speakers

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   - ✧ Time: 9:30~17:30 (July 6, Wednesday)
2. **Summer School Venue**: Conference Room II, 3rd Floor (中心三层第二会议室)
3. **Workshop Venue**: Conference Room I, 1st Floor (中心一层第一会议室)
4. **Lunch Place**: Canteen, B1 Floor (中心地下一层餐厅)
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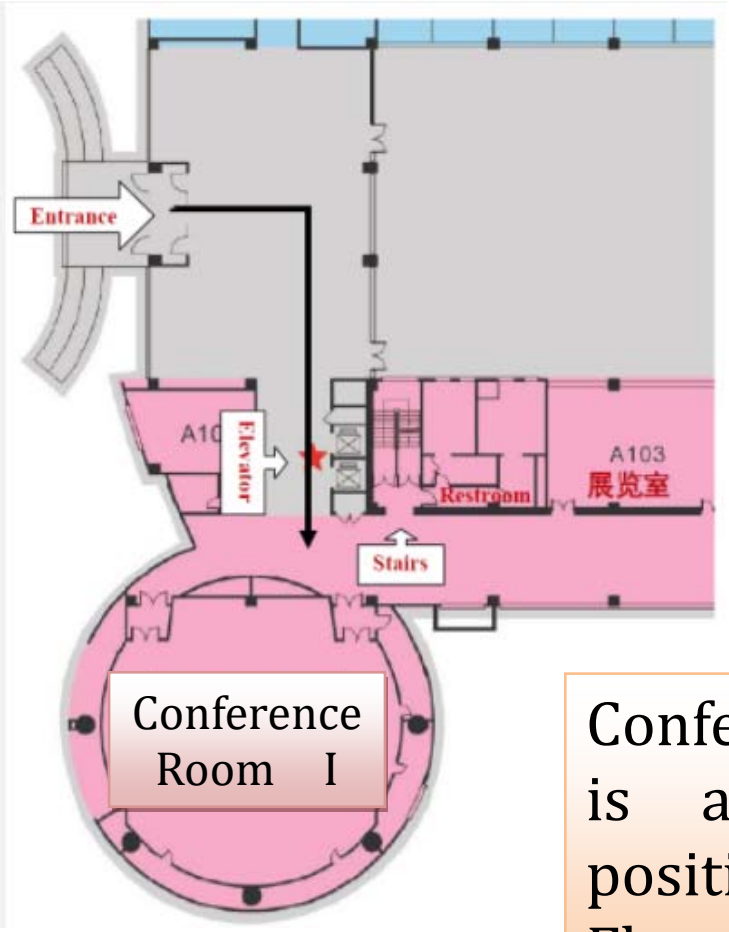

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2) From Beijing Railway Station (北京站): The cost is about 100 RMB (80 mins).

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