Quick information

Conference Venue: School of Mathematics and Statistics (SMS), Wuhan University.

Accommodation: Fengyi Hotel

Breakfasts: Fengyi Hotel

Lunchs: Mei Yuan restaurant in Wuhan University.

Dinner (expect 05/17): Fengyi Hotel

Banquet(05/17): Kang Long Tai Zi restaurant

Transportation: Shuttle bus between Fengyi Hotel and conference venue is available.

Shuttle Bus Information

May 16th	**07:30, Fengyi – SMS**
	12:20, SMS – Meiyuan
	13:30, Fengyi – MeiYuan -- SMS
	18:30, SMS – Fengyi
May 17th	**07:30, Fengyi – SMS**
	11:50, SMS – Meiyuan
	13:30, Fengyi – MeiYuan -- SMS
	17:30, SMS – Kang Long Tai Zi
May 18th	**07:30, Fengyi – SMS**
	12:30, SMS – Meiyuan
	13:50, Fengyi – MeiYuan -- SMS
	18:10, SMS -- Fengyi
May 19th	**07:30, Fengyi – SMS**
	11:50, SMS – Meiyuan
	13:30, Fengyi – City Tour

Conference Schedule

May 15th, Wednesday, Afternoon
Registration

May 16th, Thursday, Morning	
	Session S1 (1st Floor)
	Chair: Chen, Hua
08:00 – 08:20	Opening Ceremony (1st Floor)
08:20 – 09:00	Shi, Zhongci
09:00 – 09:40	Tang, Tao
09:40 – 10:10	Photo and Tea break
	Chair: Wei, Guowei
10:10 – 10:50	Shen, Jie
10:50 – 11:30	Zhang, Pingwen
11:30 – 12:10	Zhang, Zhimin
Lunch	

May 16th, Thursday, Afternoon		
	Session P1 (1st Floor)	Session P2 (2nd Floor)
	Chair: Shen, Zuowei	Chair: Zhang Zhimin
14:00 – 14:40	Yuan, Guangwei	Han, Weimin
14:40 – 15:20	Li, Ruo	Li, Zhihui
15:20 – 16:00	Lu, Xiliang	Liang, Dong
16:00 – 16:20	Tea break	
	Chair: Tang, Tao	Chair: Lin, Ping
16:20 – 17:00	Ye, Xiu	Chen, Duan
17:00 – 17:40	Ju, Lili	Li, Xiaofan
17:40 – 18:20	EBANSHU presentation	
Dinner		

May 17th, Friday, Morning	
	Session S3 (1st Floor)
	Chair: Shu, Chi-wang
08:00 – 08:40	Sheen, Dongwoo
08:40 – 09:20	Dai, Yuhong
09:20 – 10:00	Ren, Weiqing
10:00 – 10:20	Tea break
	Chair: Dai, Yuhong
10:20 – 11:00	Cai, David
11:00 – 11:40	Lin, Ping
Lunch	

May 17th, Friday, Afternoon	
	Session S2 (1st Floor)
	Chair: Shen, Jie
14:00 – 14:40	Shu, Chi-wang
14:40 – 15:20	Jiang, Song
15:20 – 15:40	Tea break
	Chair: Zhang, Pingwen
15:40 – 16:20	Baker, Nathan A.
16:20 – 17:00	Wei, Guowei
May 17th, Friday, Evening	
Banquet (18:30)	

May 18th, Saturday, Morning	
	Session S4 (1st Floor)
	Chair: Jiang, Song
08:00 – 08:40	Shen, Zuowei
08:40 – 09:20	Jin, Shi
09:20 – 10:00	Tang, Huazhong
10:00 – 10:20	Tea break
	Chair: Zou, Jun
10:20 – 11:00	Du, Qiang
11:00 – 11:40	Wang, Xiaoping
11:40 – 12:20	Chen, Zhiming
Lunch	

May 18th, Saturday, Afternoon		
	Session P3 (1st Floor)	Session P4 (2nd Floor)
	Chair: Ren, Weiqing	Chair: Tang, Huazhong
14:20 – 15:00	Xu, Kun	Zhou, Yongcheng
15:00 – 15:40	Xiang, Yang	Zhang, Shangyou
15:40 – 16:20	Wang, Xiaoming	Tu, Xuemin
16:20 – 16:40	Tea break	
	Chair: Wang, Xiaoping	Chair: Lu, Xiliang
16:40 – 17:20	Wu, Xiaoqun	Xiang, Hua
17:20 – 18:00	Wang, Yanqiu	Sun, Tong
Dinner		

May 19th, Sunday, Morning	
	Session S5 (1st Floor)
	Chair: Ye, Xiu
08:00 – 08:40	Lin, Haiqing
08:40 – 09:20	Liu, Jianguo
09:20 – 10:00	Cai, Wei
10:00 – 10:20	Tea break
	Chair: Yang, Zhijian
10:20 – 11:00	Bai, Zhongzhi
11:00 – 11:40	Zou, Jun
Lunch	

May 19th, Sunday, Afternoon
City Tour

Detailed Program

Thursday, May 16, 2013

Morning Session (1st floor)

Chair: Chen, Hua

08:00-08:20 Opening Ceremony

08:20-09:00 Shi, Zhongci

Nonconforming Finite Elements

09:00-09:40 Tang, Tao

High-Order and Adaptive Time Stepping Methods for Energy Gradient Flows

09:40-10:10 Photo and Tea break

Chair: Wei, Guowei

10:10-10:50 Shen, Jie

Some recent advances on phase-field models for multiphase complex fluids

10:50-11:30 Zhang, Pingwen

The Small Deborah Number Limit of the Doi-Onsager Equation to the Ericksen-Leslie Equation

11:30-12:10 Zhang, Zhimin

Polynomial Preserving Recovery: Recent Development and Application

Afternoon Session

Parallel Session (P1, 1st floor)

Chair: Shen, Zuowei

14:00-14:40 Yuan, Guangwei

Approximation Models of Radiation Transport Problems

14:40-15:20 Li, Ruo

From discrete velocity model to moment method

15:20-16:00 Lu, Xiliang

Primal Dual Active Set Algorithm for Compressive Sensing

16:00-16:20 Tea break

Chair: Tang, Tao

16:20-17:00 Ye, Xiu

An introduction of new finite element methods: Weak Galerkin finite element methods

17:00-17:40 Ju, Lili

A Parallel Computational Model for Three-Dimensional Thermo-Mechanical Stokes Flow Simulations of Glaciers and Ice Sheets

17:40-18:20 EBANSHU presentation

Parallel Session (P2, 2nd floor)

Chair: Zhang, Zhimin

14:00-14:40 Han, Weimin

Mathematical Studies of Models in X-ray Dark-field Tomography

14:40-15:20 Li, Zhihui

Study on the Gas-Kinetic Unified Algorithm for Multi-Scale Flows from Free-Molecule to Continuum Regimes Solving Boltzmann Model Equation

15:20-16:00 Liang, Dong

High-Order Energy-Conserved S-FDTD Schemes for Computational Electromagnetics

16:00-16:20 Tea break

Chair: Lin, Ping

16:20-17:00 Chen, Duan

Proton transport and its role in cancer research: mathematical modeling and numerical simulations

17:00-17:40 Li, Xiaofan

A Conservative Finite Difference Scheme for Poisson-Nernst-Planck Equations

Friday, May 17, 2013

Morning Session (1st floor)

Chair: Shu, Chi-wang

08:00-08:40 Sheen, Dongwoo

A class of nonparametric DSSY(Douglas-Santos-Sheen-Ye) elements

08:40-09:20 Dai, Yuhong

Unconstrained Optimization Models for Computing Several Extreme Eigenpairs of Real Symmetric Matrices

09:20-10:00 Ren, Weiqing

The climbing string method for saddle points search

10:00-10:20 Tea break

Chair: Dai, Yuhong

10:20-11:00 Cai, David

TBA

11:00-11:40 Lin, Ping

A Multiscale Method for Crystalline Materials With A Complex Lattice Structure

Afternoon Session (1st floor)

Chair: Shen, Jie

14:00-14:40 Shu, Chi-Wang

Discontinuous Galerkin method for hyperbolic equations with singularities

14:40-15:20 Jiang, Song

Nonlinear Rayleigh-Taylor instability for nonhomogeneous incompressible viscous magnetohydrodynamic flows

15:20-15:40 Tea break

Chair: Zhang, Pingwen

15:40-16:20 Baker, Nathan A

Geometric flow for biomolecular solvation

16:20-17:00 Wei, Guowei

Multiscale multiphysics and multidomain models for biomolecules

Saturday, May 18, 2013

Morning Session (1st floor)

Chair: Jiang, Song

08:00-08:40 Shen, Zuowei

Image Restoration: Wavelet Frame Approach, Total Variation and Beyond

08:40-09:20 Jin, Shi

Semiclassical computational methods for quantum dynamics with band-crossing

09:20-10:00 Tang, Huazhong

Numerical Methods and Solutions of Nonlinear Dirac Equations

10:00-10:20 Tea break

Chair: Zou, Jun

10:20-11:00 Du, Qiang

Nonlocal calculus, nonlocal balance laws and their numerical discretization

11:00-11:40 Wang, Xiaoping

Modeling and simulation of three-component flows on solid surface

11:40-12:20 Chen, Zhiming

Reverse Time Migration for Extended Obstacles: Acoustic and Electromagnetic Waves

Afternoon Session

Parallel Session (P3, 1st floor)

Chair: Ren, Weiqing

14:20-15:00 Xu, Kun

Direct Modeling for Computational Fluid Dynamics

15:00-15:40 Xiang, Yang

Continuum models for dislocation structure, energy and dynamics of dislocation arrays and low angle grain boundaries

15:40-16:20 Wang, Xiaoming

Phase Field models for two phase flows in karstic geometry

16:20-16:40 Tea break

Chair: Wang, Xiaoping

16:40-17:20 Wu, Xiaoqun

Inferring Topologies of Complex Networks

17:20-18:00 Wang, Yanqiu

An a posteriori error estimation for coupled Darcy-Stokes equations

Parallel Session (P4, 2nd floor)

Chair: Tang, Huazhong

14:20-15:00 Zhou, Yongcheng

High order exponentially fitted methods for drift-diffusion equations

15:00-15:40 Zhang, Shangyou

On minimal symmetric conforming and nonconforming finite elements for linear elasticity equations on n-rectangular grids

15:40-16:20 Tu, Xuemin

Implicit particle filters and an application to an elliptic inverse problem

16:20-16:40 Tea break

Chair: Lu, Xiliang

16:40-17:20 Xiang, Hua

Communication-Avoiding Matrix Algorithms Using Tournament Pivoting

17:20-18:00 Sun, Tong

Numerical smoothness for PDE error analysis

Sunday, May 19, 2013

Morning Session (1st floor)

Chair: Ye, Xiu

08:00-08:40 Lin, Haiqing

Superconductivity: Modeling and Computation

08:40-09:20 Liu, Jianguo

Global weak solution for kinetic models of active swimming and passive suspensions

09:20-10:00 Cai, Wei

Accuracy and efficiency in computing electrostatic potential for an ion channel model in layered dielectric/electrolyte media

10:00-10:20 Tea break

Chair: Yang, Zhijian

10:20-11:00 Bai, Zhongzhi

Block Alternating Splitting Implicit Iteration Methods for Saddle Point Problems from Time-Harmonic Eddy Current Models

11:00-11:40 Zou, Jun

Overlapping Domain Decomposition Methods for Linear and Nonlinear Inverse Problems

Abstracts

Block Alternating Splitting Implicit Iteration Methods for Saddle Point Problems from Time-Harmonic Eddy Current Models

Zhongzhi Bai

Institute of Computational Mathematics and Scientific/Engineering Computing

For the saddle-point problems arising from the finite element discretizations of the hybrid formulations of the time-harmonic eddy current problems, we establish a class of block alternating splitting implicit iteration methods and demonstrate its unconditional convergence. Experimental results are given to show the feasibility and effectiveness of this class of iterative methods when they are employed as preconditioners for Krylov subspace methods such as GMRES and BiCGSTAB.

Geometric flow for biomolecular solvation

Nathan A. Baker

Pacific Northwest National Laboratory

Implicit solvent models are important components of modern biomolecular simulation methodology due to their efficiency and dramatic reduction of dimensionality. However, such models are often constructed in an ad hoc manner with an arbitrary decomposition and specification of the polar and nonpolar components. In this talk, we review current implicit solvent models and suggest a new free energy functional which combines both polar and nonpolar solvation terms in a common self-consistent framework. Upon variation, this new free energy functional yields the traditional Poisson-Boltzmann equation as well as a new geometric flow equation. These equations are being used to calculate the solvation energies of small polar molecules to assess the performance of this new methodology. Optimization of this solvation model has revealed strong correlation between pressure and surface tension contributions to the nonpolar solvation contributions and suggests new ways in which to parameterize these models.

Accuracy and efficiency in computing electrostatic potential for an ion channel model in layered dielectric/electrolyte media

Wei Cai

University of North Carolina at Charlotte & Shanghai Jiaotong University

In this talk, we will present the study of the numerical accuracy and efficiency in computing the electrostatic potential for a finite cylinder, used in an explicit/implicit hybrid solvation model for ion channel, embedded in a layered dielectric/electrolyte medium representing a biological membrane and ionic solvents. A charge locating inside the cylinder cavity, where ion channel proteins and ions are given explicit atomistic representations, will be influenced by the polarization field of the surrounding implicit dielectric/electrolyte medium. Two numerical techniques, a specially designed boundary integral equation method and image charge methods, will be investigated and compared in terms of accuracy and efficiency for computing the electrostatic potential. While the boundary integral equation method based on layered Green's functions provides an highly accurate solution suitable for producing a benchmark reference solution, the image methods are found to give reasonable accuracy while being highly efficient and viable for using the fast multipole method (FMM) for interactions of a large number of charges in the atomistic region of the hybrid model. (Joint work with Prof. Tang huazhong and Ms. Lin Huiming at Peking University)

Proton transport and its role in cancer research: mathematical modeling and numerical simulations

Duan Chen

Ohio State University

Ion channels are special proteins with holes down in their middle and embedded in membranes of various cells. They exchange information/materials for intra- and extra-cellular environments by selectively conducting ions such as sodium, calcium, or potassium. As a topic in structural biology, this type of membrane proteins has drawn much attentions in applied mathematics recently.

In this talk I will present a multiscale and multiphysics model for proton transport through membrane proteins--a special form of ion channels conducting hydrogen ions. The model is in form of a total energy functional and then governing equations are derived via variational principle. High performance numerical algorithms are developed to handle challenges in simulations and the major tools include interface problem solver, iterative method for nonlinear PDEs and accelerating techniques.

I will also briefly introduce the role of proton transport in tumor development(e.g. angiogenesis) and chemical dynamics within cancer cells. Proton transporter inhibitors

have been concluded as a potentially effective therapeutic treatment for various cancers. The related drug design of those inhibitors will heavily depend on the molecular structure of proton transporters, thus our model and methodology could play a significant role in this area. Some preliminary work on modeling and mathematical analysis are included.

Augmented Immersed Finite Element Methods for Elliptic PDEs with Interfaces and Irregular Domains

Jinru Chen

Nanjing Normal University

Augmented immersed finite element methods (AIFEM) are proposed in this paper to solve elliptic interface problems with piecewise discontinuous coefficients and non-homogeneous jump conditions; and Poisson equations on irregular domain. Based on the framework of the immersed finite element method (IFEM), a uniform triangulation is used so that a fast Poisson solver can be used. The non-homogeneous jump conditions in the solution and the flux are treated as source terms using the source removal technique. For the piecewise constant but discontinuous coefficient,we use the augmented approach to precondition the partial differential equation to a Poisson equation with different flux jump condition as the augmented variable. Then the GMRES iteration is used to solve the augmented variable which is one dimensional lower than the solution. The core of each GMRES iteration involves solving a Poisson equation using a fast Poisson solver and an interpolation scheme to interpolate the flux jump condition. Numerical experiments showed that the number of the GMRES iteration is independent of the mesh size and the jump in the coefficient, which agrees with theoretical analysis in the literature. The AIFEM developed for interface problems has also been extended to Poisson equations on irregular domains with some slight modifications.

Reverse Time Migration for Extended Obstacles: Acoustic and Electromagnetic Waves

Zhiming Chen

Institute of Computational Mathematics and Scientific/Engineering Computing

We consider the resolution of the single frequency reverse time migration (RTM) method for extended targets without the assumption of the validation of geometric optics approximations. The resolution analysis, which applies in both penetrable and non-penetrable obstacles with sound soft or impedance boundary condition on the obstacle, implies that the imaginary part of the cross-correlation imaging functional is

always positive and thus may have better stability properties. Numerical experiments are included to illustrate the powerful imaging quality and to confirm our resolution results. This is joint work with Junqing Chen and Guanghui Huang.

Unconstrained Optimization Models for Computing Several Extreme Eigenpairs of Real Symmetric Matrices

Yuhong Dai

Institute of Computational Mathematics and Scientific/Engineering Computing

This paper considers the problem of computing several extreme eigenpairs of real symmetric matrices. Based on the variational principles, we put forward some new unconstrained models for this classical problem and further analyze some signi_cant properties. It is shown that the extreme eigenpairs of any real symmetric matrix can be recovered from the global minimizers of our unconstrained quartic and β-order models. The alternate Barzilai-Borwein method with the adaptive nonmonotone line search is then utilized for solving the unconstrained models. The preliminary numerical results indicate that our approach is promising. This is a joint work with Bo Jiang and Chunfeng Cui.

Nonlocal calculus, nonlocal balance laws and their numerical discretization

Qiang Du

Pennsylvania State University & Beijing Computational Science Research Center

We exploit the use of a recently developed nonlocal vector calculus to study a class of constrained value problems on bounded domains associated some nonlocal balance laws. The nonlocal vector calculus provides striking analogies between nonlocal model and classical local PDE models as well as the notion of local and nonlocal fluxes. We also consider finite-dimensional approximations using both quadrature based difference methods and discontinuous or continuous Galerkin finite element methods. Results on convergence, error analysis and condition number estimates are presented in both nonlocal setting and in local limit.

Mathematical Studies of Models in X-ray Dark-field Tomography

Weimin Han

University of Iowa

X-ray mammography is currently the most prevalent imaging modality for screening and diagnosis of breast cancers. However, its success is limited by the poor contrast between healthy and diseased tissues in the mammogram. A potentially prominent imaging modality is based on the significant difference of x-ray scattering behaviors between tumor and normal tissues. Driven by major practical needs for better x-ray imaging, exploration into contrast mechanisms other than attenuation has been active for decades, e.g., in terms of scattering, which is also known as dark-field tomography. In this talk, a theoretical study is provided for the x-ray dark-field tomography (XDT) assuming the spectral x-ray detection technology.

The radiative transfer equation (RTE) is usually employed to describe the light propagation within biological medium. It is challenging to solve RTE numerically due to its integro-differential form and high dimension. For highly forward-peaked media, it is even more difficult to solve RTE since accurate numerical solutions require a high resolution of the direction variable, leading to prohibitively large amount of computations. For this reason, various approximations of RTE have been proposed in the literature. A family of differential approximations of the RTE is introduced and analyzed.

Nonlinear Rayleigh-Taylor instability for nonhomogeneous incompressible viscous magnetohydrodynamic flows

Song Jiang

Institute of Applied Physics and Computational Mathematics

We investigate the nonlinear instability of a smooth Rayleigh-Taylor steady-state solution (including the case of height heavier density with increasing height) to the three-dimensional incompressible nonhomogeneous magnetohydrodynamic equations of zero resistivity in the presence of a uniform gravitational field. We first analyze the equations obtained from linearization around the steady-state solution. Then we construct solutions of the linearized problem that grow in time in the Sobolev space H^k, thus leading to a instability result for the linearized problem. With the help of the constructed unstable linear solutions and a local well-posedness result of classical solutions to the original nonlinear problem, we can show the instability of the nonlinear problem from the dynamics point of view. Moreover, we find that the third component of the velocity already induces the nonlinear instability.

(joint-work with Fei Jiang and Weiwei Wang)

Semiclassical computational methods for quantum dynamics with band-crossing

Shi Jin

Shanghai Jiaotong University & University of Wisconsin-Madison

Band-crossing is a quantum dynamical behavior that contributes to important physics and chemistry phenomena such as quantum tunneling, Berry connection, chemical reaction etc. In this talk, we will discuss several recent works in developing semiclassical methods for band-crossing, including examples from surface hopping, Schrodinger equation with periodic potentials, and high frequency solutions of linear hyperbolic systems with polarized waves.

A Parallel Computational Model for Three-Dimensional Thermo-Mechanical Stokes Flow Simulations of Glaciers and Ice Sheets

Lili Ju

University of South Carolina

In this talk we focuses on the development of an efficient, three-dimensional, thermo-mechanical, nonlinear-Stokes flow computational model for ice sheet simulation. The model is based on the parallel finite element model developed by Leng et. al (2012) which features high-order accuratefinite element discretizations on variable resolution grids. Here, we add an improved iterative solution method for treating the nonlinearity of the Stokes problem, a new highorder accurate finite element solver for the temperature equation, and a new conservative finite volume solver for handling change of ice thickness. The result is an accurate and efficient numerical model for thermo-mechanical glacier and ice-sheet simulations. We demonstrate the improved efficiency of the Stokes solver using the ISMIP-HOM Benchmark experiments and a realistic test case for the Greenland ice-sheet. We also apply our model to the EISMINT-II benchmark experiments and demonstrate stable thermomechanical ice sheet evolution on both structured and unstructured meshes.

From discrete velocity model to moment method

Ruo Li

Peking University

In the numerical approaches for Boltzmann equation, the discrete velocity model and the moment method are formally very different. The difference is so big that the communities working on the two approaches are in certain hostile relation. In this talk, I will try to show the intrinsic connection between these two approaches. Precisely, the Grad type moment method with appropriate closure can be regarded as a discrete velocity model with some daptivities in setup of the velocity points. The globally hyperbolic regularization of the moment method plays an essential role in connecting both approaches together.

A Conservative Finite Difference Scheme for Poisson-Nernst-Planck Equations

Xiaofan Li

Illinois Institute of Technology

A macroscopic model to describe the dynamics of ion transport in ion channels is the Poisson-Nernst-Planck(PNP) equations. In this talk, we will present a finite-difference method for solving PNP equations, which is second-order accurate in both space and time. We use the physical parameters specifically suited toward the modelling of ion channels. We introduce a simple iterative scheme to solve the system of nonlinear equations resulting from discretizing the equations implicitly in time, which converges in a few iterations. We place emphasis on ensuring numerical methods to have the same physical properties that the PNP equations themselves also possess, namely conservation of total ions and correct rates of energy dissipation. Further, we illustrate that, using realistic values of the physical parameters, the conservation property is critical in obtaining correct numerical solutions over long time scales.

Study on the Gas-Kinetic Unified Algorithm for Multi-Scale Flows from Free-Molecule to Continuum Regimes Solving Boltzmann Model Equation

Zhihui Li

China Aerodynamics Research and Development Center

The Boltzmann equation can describe the molecular transport phenomena for the full spectrum of flow regimes and act as the main foundation for the study of complex gas

dynamics. However, the difficulties encountered in solving the full Boltzmann equation are mainly associated with the nonlinear multidimensional integral nature of the collision term, and an exact solution of the Boltzmann equation is impractical for the analysis of practical complex flows. From the kinetic-molecular theory of gases, numerous statistical or relaxation kinetic model equations resembling various order of moments of the original Boltzmann equation have been put forward. Thus, instead of solving the full Boltzmann equation, one solves the nonlinear kinetic model equations and probably finds a more economical and efficient numerical method for complex gas flows over a wide range of Knudsen numbers.

In this work, we are essentially concerned with developing the gas-kinetic unified algorithm (GKUA) for the direct solution of the Boltzmann kinetic relaxation model equation, in which the unified Boltzmann model equation for describing the complex multi-scale flows covering various flow regimes can be deduced and translated into hyperbolic conservation systems with nonlinear source terms in physical space and time by first developing the discrete velocity ordinate (DVO) method in the gas kinetic theory. Then the gas-kinetic numerical schemes are constructed by using the time-splitting method for unsteady equation and the finite-difference technique. In the earlier papers (Int. J. Numer. Meth. Fluids 42,361-382,2003, J. Comput. Phys. 193,708-738,2004 and J. Comput. Phys. 228,1116-1138,2009), the GKUA has been successively presented and applied to the one-, two- and three-dimensional flow problems from highly rarefied free-molecule to continuum flow regimes. In this report, the GKUA will be further extended and developed to investigate complex hypersonic flows with wide range of Mach numbers covering the full spectrum of flow regimes for possible engineering applications.

Based on the Boltzmann model equation describing the gas transfer phenomena, the colliding relaxation parameters and the local equilibrium distribution function can be integrated with the macroscopic flow parameters, the molecular viscosity transport coefficients, the thermodynamic effect, the molecular power law models, and the flow states from various flow regimes. The unified velocity distribution function equation can be presented with the non-dimensional form in the Cartesian coordinates, as follows

$$\frac{\partial}{\partial t} f\left(t,\vec{r},\vec{V}\right)+\vec{V}\cdot\frac{\partial}{\partial\vec{r}} f\left(t,\vec{r},\vec{V}\right)=\nu\left[f^{N}\left(t,\vec{r},\vec{V}\right)-f\left(t,\vec{r},\vec{V}\right)\right] \quad (1)$$

$$f^{N}=f_{M}\cdot[1+(1-\mathrm{Pr})\vec{c}\cdot\vec{q}\left(2c^{2}/T-5\right)/(5PT/2)] \quad (2)$$

$$f_{M}=n/(\pi T)^{3/2}\exp[-c^{2}/T]$$

$$\nu=\frac{2\alpha(5-2\omega)(7-2\omega)}{5(\alpha+1)(\alpha+2)\sqrt{\pi}}\cdot\frac{1}{Kn_{\infty}}\cdot nT^{(1-\chi)} \quad , \quad Kn_{\infty}=\lambda_{\infty}/L \quad (3)$$

The equation (1) represents the time dependence of the molecular velocity distribution function on position space $\vec{r}=(x,y,z)$ and velocity space $\vec{V}=(V_x,V_y,V_z)$ and provides the statistical description of gas flows from the level of the kinetic theory of gases. All of the macroscopic flow variables of gas dynamics, such as the density of the gas ρ, the flow

velocity $\vec{U}$, the temperature T, the pressure p, the viscous stress tensor τ and the heat flux vector $\vec{q}$, can be evaluated by the moments of the velocity distribution function over the velocity space.

In order to replace the continuous dependency of f on the velocity space, the discrete velocity ordinate method can be employed to discretize the finite velocity region removed from $\vec{U}$. The single velocity distribution function equation can be transformed into hyperbolic conservation equations with nonlinear source terms at each of discrete velocity ordinate points. In view of the unsteady characteristics of molecular convective movement and colliding relaxation, the time-splitting numerical method can be adopted so that the discrete velocity distribution function equation can be decomposed into the colliding relaxation equations with the nonlinear source terms and the convective motion equations in three directions of the position space. The integration of the source term of colliding relaxation is solved by the second-order Runge-Kutta method, and the NND-4(a) scheme based on primitive variables is applied to the convective equations, respectively. The second-order finite difference scheme directly solving the six-dimensional discrete velocity distribution functions can be constructed.

Once the discrete velocity distribution functions $f_{\sigma,\delta,\theta}$ are solved, the macroscopic flow moments at any time in each point of the physical space can be computed and updated by the appropriate discrete velocity quadrature method, in which the evaluation points of the integration are related to the determined discrete velocity ordinate points. In this study, the new Gauss-type integration method with the weight function $2/\pi^{1/2}\exp(-V^2)$ will be further developed and applied to attack hypersonic flows with different Mach numbers.

In the GKUA, it is the most time-consuming process that the discrete velocity distribution functions are numerically solved at each of discrete velocity ordinate points, which needs to use the six-dimensional array to store the information of the discrete velocity distribution functions with the six-layer loop operations. To resolve the difficulty on the vast computer memory and runtime needed by the current method in solving three-dimensional complex flows and to well exploit the power of massively parallel computers, the multi-processing strategy and parallel implementation technique suitable for the GKUA has been developed.

To validate the reliability of the present GKUA in solving the high Mach number problems from free-molecule flow to rarefied transition and continuum flows, the complex flows around sphere and complex bodies are computed and studied with different Mach numbers $3 < M_\infty < 20$ under various Knudsen numbers $0.0001 < Kn_\infty < 10$ and angles $0 \le \alpha \le 30°$ of attack. The computational results are found in high resolution of the flow fields and good agreement with the relevant theoretical, DSMC, N-S and experimental results. As the general remarks, it can be tested from this study that the gas-kinetic

numerical method directly solving the Boltzmann simplified velocity distribution function equation may provide an important and feasible way that complex hypersonic aerothermodynamic problems and flow mechanisms in the whole flow regimes from the continuum to the free molecule flow can be effectively studied from the view of mesoscopic theory by directly tracing the time evolution of the velocity distribution function, which is completely different from molecular particle transport methods or macroscopic fluid dynamics solvers.

High-Order Energy-Conserved S-FDTD Schemes for Computational Electromagnetics

Dong Liang

York University

In computational electromagnetics, for problems requiring long-time integration and problems of wave propagations over longer distances, it has led to the development of high-order FDTD schemes which produce smaller dispersion or phase errors for a given mesh resolution. However, some delevoped high-order FDTD schemes are conditionally stable and require large computational memory and huge computational cost. On the other hand, during the propagation of electromagnetic waves in lossless media without sources, the electromagnetic energy keeps constant for all time, which explains the physical feature of conservation of electromgnemtic energy in long term behavior. In this talk, we will present our new high-order energy-conserved S-FDTD schemes for Maxwell's equations. We will show theoretical results on energy conservation, unconditional stability and optimal convergence. We will also present numerical experiments to confirm our theoretical results.

Superconductivity: Modeling and Computation

Haiqing Lin

Beijing Computational Science Research Center

Since the first discovery of superconductivity in 1911, it has been an endless search for superconductors with high transition temperature. Various mechanisms and techniques were proposed, yet it remains a great challenge to scientists. In this talk, I will present a few examples to illustrate difficulties in modeling and computation of superconductivity. In particular, I highlight places where we need helps from mathematicians.

A Multiscale Method for Crystalline Materials With A Complex Lattice Structure

Ping Lin

University of Dundee

Many scientific systems such as materials may have to be modeled by an atomistic model when atomistic defects occur. In the atomistic model the material is considered as a system of a large number of atoms, where an atom is interacted with any other through, for example, a pair potential energy. The equillibrium configuration is a minimizer of the total energy of the system. The computational cost is extremely high due to the large number of atoms.

Much attention has been paid to a so-called quasicontinuum (QC) approximation which can significantly reduce degrees of freedom through a multiscale (coupled atomistic and continuum) model and may be seen as an approximate representation of the atomistic model. In the talk we will briefly introduce the idea of the QC approximation for materials with both simple and complex lattice structures. Then we will present our recent results which identify the equivalence between the QC and a discrete homogenization process for materials with complex lattice structure but without defects and then analyze the approximate error for the complex-lattice QC method. The talk is based on joint works with A Abdulle and A Shapeev.

Global weak solution for kinetic models of active swimming and passive suspensions

Jian-guo Liu

Duke University

Bacterium swimming, acting as a force dipole, in fluid is modeled by a coupled Fokker-Planck equation and incompressible (Navier-)Stokes equation. According to the mechanism for swimming, bacterium can be classified into pusher and puller. The local flow generated by the pusher outward force dipole increases the local straining flow, and hence reduces the effective viscosity and enhance flow-mixture, known in physics literature as long wave instability. This instability can be explained by the fact that there is no entropy-dissipation relation for the pusher suspensions of coupled Fokker-Planck-(Navier-)Stokes system. Nonetheless, with some careful estimates, we are able to control the entropy and obtain the existence of global weak entropy solution for both pusher and puller system.

Polymer suspensions is commonly modeled by suspension of extensible rods. There exists a spring force resisting to the rod extension which effectively increases the viscosity. We will present some shape compactness embedding theorems used in the relative entropy

estimates for both Hookean and FENE models and we will present some global existence results.
This is a joint work with Xiuqing Chen of Beijing University of Posts and Telecommunications

Primal Dual Active Set Algorithm for Compressive Sensing

Xiliang Lu

Wuhan University

The success and popularity of Compressed Sensing (CS) depends essentially on the ability of efficiently finding an approximated sparse solution of an underdetermined linear system. There are two categories of algorithms: convex relaxation algorithm and greedy algorithm. In this talk we present a primal dual active set strategy for both convex relaxation optimization problem and greedy algorithm. The locally superlinearly convergence for PDAS for convex relaxation problem is proved. Several numerical examples are given to show the efficiency of the PDAS algorithms, both for convex relaxation problem and l_0-minimization problem. This method can be extended to the inverse problems or other problems without RIP for the measurement matrix.

The climbing string method for saddle points search

Weiqing Ren

National University of Singapore

Many problems arising from applied sciences can be abstractly formulated as a system that navigates over a complex energy landscape of high or infinite dimensions. Well known examples include nucleation events during phase transitions, conformational changes of bio-molecules, chemical reactions, etc. The string method was designed for finding minimum energy paths between two minima of a potential (or free) energy. In this talk, I will discuss how the string method can be modified to compute saddle points using the minimum as the only input. Numerical examples of the diffusion of a 7-atom cluster on a substrate and the wetting transition on a rough surface will be presented.

A class of nonparametric DSSY(Douglas-Santos-Sheen-Ye) elements

Dongwoo Sheen

Seoul National University

In 1999 Douglas-Santos-Sheen-Ye (DSSY) [3] introduced (parametric) nonconforming quadrilateral element which are of four DOFs for rectangular (and parallelogram) meshes, but are of five DOFs for quadrilateral meshes [1]. Differently from the Rannacher-Turek quadrilateral element [5], one of the special characteristics of the DSSY element is the edgewise mean value property, which is fulfilled also by the Crouzeix-Raviart nonconforming simplicial element [2]. In this talk, we introduce a class of nonparametric DSSY elements of four DOFs for quadrilateral meshes [4]. We will also discuss applications of thses elements to Stokes and elasticity problems. Error estimates and numerical results will be presented.

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Some recent advances on phase-field models for multiphase complex fluids

Jie Shen

Purdue University & Xiamen University

I shall present some recent work on phase-field model for multiphase complex fluids. Particular attention will be paid to develop models which are valid for problems with large density ratios and obey an energy dissipation law. I shall present efficient and accurate numerical schemes for solving the coupled nonlinear system for the multiphase complex fluid. In many cases, these schemes are decoupled and energy stable. I'll also provide ample numerical results which not only demonstrate the effectiveness of the numerical schemes, but also validate the flexibility and robustness of the phase-field model.

Image Restoration: Wavelet Frame Approach, Total Variation and Beyond

Zuowei Shen

National University of Singapore

This talk is about the wavelet frame-based image and video restorations. We start with some of main ideas of wavelet frame based image restorations. Some of applications of wavelet frame based models image analysis and restorations will be shown. Examples of such applications include image and video inpainting, denoising, decomposition, image deblurring and blind deblurring, segmentation, CT image reconstruction and etc. In all of these applications, spline wavelet frames derived from the unitary extension principle are used. This allows us to establish a connection between wavelet frame base method and the total variation based method. In fact, we will show that when spline wavelet frames are used, a special model of a wavelet frame method can be viewed as a discrete approximation at a given resolution to the total variation based method. A convergence analysis in terms of objective functionals and their approximate minimizers as image resolution increases will be discussed.

Nonconforming Finite Elements

Zhongci Shi

Institute of Computational Mathematics and Scientific/Engineering Computing

Discontinuous Galerkin method for hyperbolic equations with singularities

Chi-wang Shu

Brown University

Discontinuous Galerkin (DG) methods are finite elementmethods with features from high resolution finite differenceand finite volume methodologies and are suitable for solving hyperbolic equations with nonsmooth solutions. In this talk we will first give a survey on DG methods, then we will describe our recent work on the study of DG methods for solving hyperbolic equations with singularities in the initial condition, in the source term, or in the solutions. The type of singularities include both discontinuities and δ-functions. Especially for problems involving δ-singularities, many numerical techniques rely on modifications with smooth kernels and hence may severely smear such singularities, leading to large errors in the approximation. On the other hand,

the DG methods are based on weak formulations and can be designed directly to solve such problems without modifications, leading to very accurate results. We will discuss both error estimates for model linear equations and applications to nonlinear systems including the rendez-vous systems and pressureless Euler equations involving δ-singularities in their solutions. This is joint work with Qiang Zhang, Yang Yang and Dongming Wei.

Numerical smoothness for PDE error analysis

Tong Sun

Bowling Green State University

Numerical smoothness is an innovative concept proposed by the speaker. It will fundamentally improve the understanding about the error analysis of numerical PDEs, especially for time-dependent problems. The talk will explain (1) the concept of numerical smoothness; (2) the necessity of numerical smoothness in PDE error analysis; and (3) the relationship between numerical smoothness and numerical stability. Some error analysis results on nonlinear conservation laws will be presented, which will show the advantages of the error analysis methodology based on the numerical smoothness concept. New research results will be presented along with a list of open research topics.

Numerical Methods and Solutions of Nonlinear Dirac Equations

Huazhong Tang

Peking University

The Dirac equation is a relativistic wave equation in particle physics, formulated in 1928, and describes fields corresponding to elementary spin-½ particles (such as the electron) as a vector of four complex numbers (a bispinor), in contrast to the Schrödinger equation which described a field of only one complex value. It implied the existence of a new form of matter, antimatter, hitherto unsuspected and unobserved, and actually predated its experimental discovery.

This talk concentrates on a (1+1)-dimensional nonlinear Dirac (NLD) equation with a general self-interaction, which is a linear combination of the scalar, pseudoscalar, vector and axial vector self-interactions to the power of the integer k. The solitary wave solutions to the NLD equation are analytically derived, and the number of solitary humps in the charge and energy densities is proved in theory. The results show that for a given integer k, the number of solitary humps for the charge density is not bigger than 4, while the number of solitary humps for the energy density is not bigger than 3.

This talk also presents a numerical study of the interaction dynamics for the solitary waves of nonlinear Dirac equation with scalar self-interaction by using a fourth order accurate Runge–Kutta discontinuous Galerkin method. Some new interaction phenomena are observed: (a) a new quasi-stable long-lived oscillating bound state from the binary collisions of a single-humped soliton and a two-humped soliton; (b) collapse in binary and ternary collisions; (c) strongly inelastic interaction in ternary collisions; and (d) bound states with a short or long lifetime from ternary collisions.

High-Order and Adaptive Time Stepping Methods for Energy Gradient Flows

Tao Tang

Hong Kong Baptist University

The key idea of the phase-field methodology is to replace sharp interfaces by thin transition regions where interfacial forces are smoothly distributed. One of the main reasons for the success of the phase-field methodology is that it is based on rigorous mathematics and thermodynamics. Most phase-field models satisfy a nonlinear stability relationship, usually expressed as a time-decreasing free-energy functional, which is called energy gradient stability. To obtain accurate numerical solutions of such problems, it is desirable to use high-order approximations in space and time. Yet because of the difficulties introduced by the combination of nonlinearity and stiffness, most computations have been limited to lower-order in time, and in most cases to constant time-stepping. On the other hand, numerical simulations for many physical problems require large time integration; as a result large time-stepping methods become necessary in some time regimes.

To effectively solve the relevant physical problems, the combination of higher-order and highly stable temporal discretizations becomes very useful. In this talk, we will describe some adaptive time stepping approach for phase-field problems, which inherits the energy gradient stability of the continuous model. Particular attention will be given to effectively resolve both the solution dynamics and steady state solutions.

Implicit particle filters and an application to an elliptic inverse problem

Xuemin Tu

University of Kansas

In this talk, I will give a brief introduction of implicit sampling that finds samples of multidimensional probability densities. This implicit sampling strategy generates a particle (sample) beam which is focused towards on the high probability region of the target pdf

and the focusing makes the number of particles required manageable even if the state dimension is large. The efficiency and accuracy of the algorithm is illustrated by an application to an elliptic inverse problem.

Phase Field models for two phase flows in karstic geometry

Xiaoming Wang

Florida State University

Multiphase flow phenomena are ubiquitous. Common examples include coupled atmosphere and ocean system (air and water), oil reservoir (water, oil and gas), cloud and fog (water vapor, water and air). Multiphase flows also play an important role in many engineering and environmental science applications. In some applications such as flows in unconfined karst aquifers, karst oil reservoir, proton membrane exchange fuel cell, multiphase flows in conduits and in porous media must be considered together. Geometric configurations that contain both conduit (or vug) and porous media are termed karstic geometry. Despite the importance of the subject, little work has been done on multi-phase flows in karstic geometry.

In this talk we present a family of phase field models for two phase flow in karstic geometry. These models together with the associated interface boundary conditions are derived utilizing Onsager's extremum principle. The models derived enjoy physically important energy laws. Numerical schemes that preserve these energy laws will be presented as well.

Modeling and simulation of three-component flows on solid surface

Xiaoping Wang

Hong Kong University of Science and Technology

We propose a phase field model for the study of three-component immiscible flows with boundary. The model is a generalization of the two-component model. We first study certain consistency conditions for the forms of the bulk free energy and surface energy. We then develop an adaptive mesh refinement(AMR) technique to solve the system in order to improve the efficiency of the problem. Several numerical results are given, including the liquid lens spreads between two phases, the buoyancy-driven droplet through a fluid-fluid interface, spreading of a compound droplet on a stationary substrate, and shear flows of a compound droplet on a channel.

An a posteriori error estimation for coupled Darcy-Stokes equations

Yanqiu Wang

Oklahoma State University

Kanschat and Riviere has recently proposed an H(div) conforming mixed finite element method for the coupled Darcy-Stokes flow, which uses a unified discretization for both the Stokes side and the Darcy side. In their method, the discrete velocity field is continuous in the normal direction across the Stokes-Darcy interface, which we refer to as a "strong coupling". Many other numerical methods use a "weak coupling" scheme. That is, the normal continuity of the velocity field across the Darcy-Stokes interface is imposed weakly by introducing a Lagrange multiplier. Here, we develop an a posteriori error estimator for the H(div) conforming, "strongly coupled" mixed formulation. Due to the strong coupling on the interface, special techniques need to be employed in the proof of its global reliability and efficiency. This is the main difference between our work and the previous work by Babuska and Gatica (2010), in which they considered a weakly coupled interface condition.

Multiscale multiphysics and multidomain models for biomolecules

Guowei Wei

Michigan State University

A major feature of biological sciences in the 21st Century will be their transition from phenomenological and descriptive disciplines to quantitative and predictive ones. However, the emergence of complexity in self-organizing biological systems poses fabulous challenges to their quantitative description because of the excessively high dimensionality. A crucial question is how to reduce the number of degrees of freedom, while preserving the fundamental physics in complex biological systems. We discuss a multiscale multiphysics and multidomain paradigm for biomolecular systems. We describe macromolecular system, such as protein, DNA, ion channel, membrane, etc., by a number of approaches, including static atoms, molecular mechanics, quantum mechanics and elastic mechanics; while treating the aqueous environment as a dielectric continuum or fluid mechanics. We use differential geometry to couple various microscopic and macroscopic domains on an equal footing. Based on the variational principle, we derive coupled Poisson-Boltzmann, Nernst-Planck, Kohn-Sham, Laplace-Beltrami, Newton, elasticity and/or Navier-Stokes equations for the structure, dynamics and transport of protein, protein-ligand binding and ion-channel systems.

Inferring Topologies of Complex Networks

Xiaoqun Wu

Wuhan University

Network topology plays a crucial role in determining the network's intrinsic dynamics and function, thus understanding and modeling the topology of a complex network will lead to a better knowledge of its evolutionary mechanisms and to a better cottoning on its behaviors. In the past few years, topology identification of complex networks has received increasing interest and wide attention. Many approaches have been developed for this purpose, such as the synchronization-based identification, information-theoretic methods, and intelligent optimization algorithms. However, how to infer the interaction patterns from observed dynamical time series is still challenging as an inverse problem, especially in the absence of the knowledge of nodal dynamics and in the presence of system noise. In this talk we will present some of our related work on inferring topologies of complex networks, including those based on adaptive control, optimization, as well as Granger causality test.

Communication-Avoiding Matrix Algorithms Using Tournament Pivoting

Hua Xiang

Wuhan University

Since the cost of communication greatly exceeds the cost of float-point arithmetic on current and future computing platforms, we are motivated to devise algorithms that communicate as little as possible, even if they do slightly more arithmetic. To achieve this goal, we use a new pivoting strategy, which we refer to as tournament pivoting. We will discuss two typical communication-avoiding matrix algorithms. That is, a communication-avoiding LU factorization (CALU), and a communication-avoiding rank revealing QR factorization (CARRQR).

We will show that CALU does an optimal amount of communication, and asymptotically less than Gaussian elimination with partial pivoting (GEPP). Generally the entire CALU process is equivalent to GEPP on a large, but very sparse matrix, formed by entries of A and zeros. Hence we expect that CALU will behave as GEPP and it will also be numerically stable. Extensive experiments on random matrices and a set of special matrices show that CALU is stable in practice.

We will show that CARRQR minimizes data transfer, modulo polylogarithmic factors, on both sequential and parallel machines, while previous QR factorization with column pivoting (QRCP) is communication sub-optimal and requires asymptotically more

communication. CARRQR reveals the numerical rank of a matrix in an analogous way to QRCP. Although the upper bound of a quantity involved in the characterization of a rank revealing factorization is worse for CARRQR than for QRCP, our numerical experiments on a set of challenging matrices show that this upper bound is very pessimistic, and CARRQR is an effective tool in revealing the rank in practical problems.
This is the joint with J. W. Demmel, L. Grigori, and M. Gu; and the talk is based on our two joint papers.

Continuum models for dislocation structure, energy and dynamics of dislocation arrays and low angle grain boundaries

Yang Xiang

Hong Kong University of Science and Technology

We present continuum models for dislocation structure, energy and dynamics of dislocation arrays and low angle grain boundaries which may be nonplanar and nonequilibrium. In our continuum model, we define a dislocation potential function on the dislocation array surface or grain boundary to describe the orientation dependent continuous distribution of dislocation in a very simple and accurate way. The continuum formulations of energy and dynamics are derived from the discrete dislocation model, and include the long-range interaction of constituent dislocations, local line tension effect of dislocations, and the cooperative motion of dislocations. Applications to low angle grain boundaries are presented.

Direct Modeling for Computational Fluid Dynamics

Kun Xu

Hong Kong University of Science and Technology

All partial differential equations (PDEs) for the description of flow motion have their intrinsic valid physical modeling scales, and these scales may not be compatible with the numerical mesh size scale. Theoretically, it is problematic in the numerical PDE methodology, where the PDE is directly discretized in the hope of developing reliable and consistent CFD methods. In this talk, I will introduce a new concept about direct modeling for the development of CFD method, where the physical modeling will be done directly in a discretized space. The construction of the unified gas-kinetic scheme (UGKS) is an example under the above CFD principle, where the flow behavior from rarefied to continuum in different scales can be captured in a single computation.

An introduction of new finite element methods: Weak Galerkin finite element methods

Xiu Ye

University of Arkansas at Little Rock

Newly developed weak Galerkin finite element methods will be introduced for solving partial differential equations. Their applications to different partial differential equations will be discussed such as the biharmonic equations and the Brinkman equations.

Approximation Models of Radiation Transport Problems

Guangwei Yuan

Institute of Applied Physics and Computational Mathematics

In this talk some approximate models of radiation transport problems are discussed, which are widely used for numerical simulating radiation hydrodynamic problems in many fields such as astrophysics and inertial confinement fusion (ICF). Since the computational cost of solving fully radiation transport equation is extremely expensive, we have to consider its approximate and simplified models. There are some well-known approximate models such as radiation heat conduction, including multi-temperatures models, and multi-group diffusion, P1 and M1 etc. A special case is the equilibrium radiation heat conduction, which leads to one-temperature model. In applications it is necessary that different radiation physical models are adopted in different physical domains, and then formulating the well-posed coupling models and investigating their basic properties are very important for accurate and efficient numerical solutions.

The Small Deborah Number Limit of the Doi-Onsager Equation to the Ericksen-Leslie Equation

Pingwen Zhang

Peking University

We present a rigorous derivation of the Ericksen-Leslie equation starting from the Doi-Onsager equation. As in the fluid dynamic limit of the Boltzmann equation, we first make the Hilbert expansion for the solution of the Doi-Onsager equation. The existence of the Hilbert expansion is connected to an open question whether the energy of the Ericksen-Leslie equation is dissipated. We show that the energy is dissipated for the

Ericksen-Leslie equation derived from the Doi-Onsager equation. The most difficult step is to prove a uniform bound for the remainder in the Hilbert expansion. This question is connected to the spectral stability of the linearized Doi-Onsager operator around a critical point. By introducing two important auxiliary operators, the detailed spectral information is obtained for the linearized operator around all critical points. However, these are not enough to justify the small Deborah number limit for the inhomogeneous Doi-Onsager equation, since the elastic stress in the velocity equation is also strongly singular. For this, we need to establish a precise lower bound for a bilinear form associated with the linearized operator. In the bilinear form, the interactions between the part inside the kernel and the part outside the kernel of the linearized operator are very complicated. We find a coordinate transform and introduce a five dimensional space called the Maier-Saupe space such that the interactions between two parts can been seen explicitly by a delicate argument of completing the square. However, the lower bound is very weak for the part inside the Maier-Saupe space. In order to apply them to the error estimates, we have to analyze the structure of the singular terms and introduce a suitable energy functional.
Furthermore, we prove the local well-posedness of the Ericksen-Leslie system, and the global well-posednss for small initial data under the physical constrain condition on the Leslie coefficients, which ensures that the energy of the system is dissipated. Instead of the Ginzburg-Landau approximation, we construct an approximate system with the dissipated energy based on a new formulation of the system.

On minimal symmetric conforming and nonconforming finite elements for linear elasticity equations on n-rectangular grids

Shangyou Zhang

University of Delaware

A family of conforming and another family of nonconforming mixed finite elements are proposed for solving the first order system of linear elasticity equations in any space dimension, where the stress field is approximated by symmetric finite element tensors. The nonconforming element has a perfect match between the stress components and the displacement: The discrete spaces for the normal stress σ_{ii}, the shear stress σ_{ij} and the displacement u_i are $span\{1,x_i\}$, $span\{1, x_i, x_j\}$ and $span\{1\}$, respectively, on rectangular grids. For the conforming element, the normal stresses are approximated by quadratic polynomials $span\{1, x_i, x_i^2\}$, the shear stresses by bilinear polynomials $span\{1, x_i, x_j, x_ix_j\}$, and the displacements by linear polynomials $\operatorname{span}\{1, x_i \}$. As a result of these choices, the theoretical analysis is independent of the spatial dimension as well.
The total degrees of freedom per element for the new nonconforming element is 7 plus 2 in 2D, or 15 plus 3 in 3D. The previous record of the least degrees of freedom is, 13 plus 4 in 2D, and 54 plus 12 in 3D, on the rectangular grid. For the conforming element, the

number of total degrees of freedom per element is 10 plus 4 in 2D, or 21 plus 6 in 3D, while the previous record for conforming element is 17 plus 4 in 2D, and 72 plus 12 in 3D. The well-posedness condition and the optimal a priori error estimate are proved. Numerical tests in 2D and 3D are presented to show a superiority of the new elements over others, as a superconvergence is surprisingly exhibited.

Polynomial Preserving Recovery: Recent Development and Application

Zhimin Zhang

Beijing Computational Science Research Center & Wayne State University

Gradient recovery is a post-processing technique in finite element methods, which is widely used in commercial softwares such as Ansys, MCS/Nastran, Pro/Mechanica, etc. In this talk, we will discuss a gradient recovery method called polynomial preserving recovery (PPR) and its recent development on reconstructing the Hessian matrix and application in mesh refining and in the commercial software COMSOL-MultiPhysics.

High order exponentially fitted methods for drift-diffusion equations

Yongcheng Zhou

Colorado State University

It is known that the numerical solutions of the drift-diffusion equation may suffer from the instability for strong field. Here we report a class of high-order exponentially fitted finite element methods that can achieve both numerical stability and efficiency in solving 2-D drift-diffusion equations. We find that by utilizing the one-one correspondence between continuous piecewise polynomial space of degree k+1 and the divergence-free vector space of degree k, one can construct arbitrarily high-order 2-D exponentially fitted basis functions that are strictly interpolative at a selected node set but are discontinuous on edges in general, spanning nonconforming finite element spaces. Convergence up to forth order measured in L-infty norm is observed in our numerical experiments, suggesting promising applications of the methods to drift-diffusion problems arising in simulating semiconductor devices and biomolecular electrodiffusion.

Overlapping Domain Decomposition Methods for Linear and Nonlinear Inverse Problems

Jun Zou

Chinese University of Hong Kong & Wuhan University

In this talk we shall discuss some efficient overlapping domain decomposition methods for a class of linear and nonlinear inverse problems. This is a joint work with Xiao-Chuan Cai (UC Boulder), Hui Feng (Wuhan University) and Daijun Jiang (Huazhong Normal University).

This work was substantially supported by Hong Kong RGC grants (Projects 405110 and 404611).

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