2016 年同济大学计算数学青年学者论坛会议日程

会议地点：同济大学综合楼 1002 会议室

日期	时　间	内　　容
12 月 3 日（星期六）	**09:00－09:15**	开幕式
	09:15－09:30	合影
	09:30－10:30	**主持人：许学军**
	09:30－10:00	**应文俊：A simple method for computing singular or nearly singular integrals on closed surfaces**
	10:00－10:30	**陈景润： Towards a unified macroscopic description of exciton diffusion in organic semiconductors**
	10:30－10:50	茶　歇
	10:50－11:50	**主持人： 陈景润**
	10:50－11:20	**陈旻昕： Efficient and Qualified Mesh Generation for Gaussian Molecular Surface Using Piecewise Trilinear Polynomial**
	11:20－11:50	**郭 玲： Stochastic collocation methods via compressive sampling and its applications in UQ**
	11:50－14:00	午　餐：学苑餐厅
	14:00－15:30	**主持人： 周解勇**
	14:00－14:30	**郭 谦： Explicit methods for nonlinear stochastic differential equations**
	14:30－15:00	**胡 丹： Optimization, Adaptation, and Initiation of Biological Transport Networks**
	15:00－15:30	**廖奇峰： Reduced Basis ANOVA Methods for Partial Differential Equations with High-Dimensional Random Inputs**
	15:30－16:00	茶　歇
	16:00－17:30	**主持人： 王增琦**
	16:00－16:30	**潘建瑜：Preconditioned iterative methods for finite volume discretization of steady-state space-fractional diffusion equations**
	16:30－17:00	**吴钢：The convergence of harmonic Ritz vectors and harmonic Ritz values---A Revisit**
	17:00－17:30	**吴语茂： The new methods for calculating the scattered fields from the nano-periodic structures and high frequency**
	18:00－19:30	晚　宴：三好坞 3 楼

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	09:00－09:30	陆帅：**Filter based methods for statistical linear inverse problems**
	09:30－10:00	徐振礼：**Modified Poisson-Nernst-Planck equations with many-body effects**
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	10:30－11:00	易利军：**Some recent progress in the hp-version time-stepping methods for initial value problems**
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	13:30－14:00	何晓明：**Decoupled, linear, and energy stable finite element method for the Cahn-Hilliard-Navier-Stokes-Darcy phase field model**
	14:00－14:30	刘东杰：**Nonconforming FEMs for an Optimal Design Problem**
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	16:00－16:30	许威：**Jacobian-Free Implicit Inner-Iteration Preconditioner for Nonlinear Least Squares Problems**
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报告摘要信息：（按姓氏字母顺序排列）

陈旻昕（苏州大学）

Title: Efficient and Qualified Mesh Generation for Gaussian Molecular Surface Using Piecewise Trilinear Polynomial Approximation

Abstract: Recent developments for mathematical modeling and numerical simulation of biomolecular systems raise new demands for qualified, stable, and efficient surface meshing, especially in implicit-solvent modeling. In our former work, we have developed an algorithm for manifold triangular meshing for large Gaussian molecular surfaces, TMSmesh. In this talk, I will introduce our recent work on a new algorithms to greatly improve the meshing efficiency and qualities, and implement into a new program version, TMSmesh 2.0. In TMSmesh 2.0, in the first step, a new adaptive partition and estimation algorithm is proposed to locate the cubes in which the surface are approximated by piecewise trilinear surface with controllable precision. Then, the piecewise trilinear surface is divided into single valued pieces by tracing along the fold curves, which ensures that the generated surface meshes are manifolds. Numerical test results show that TMSmesh 2.0 is capable of handling arbitrary sizes of molecules and achieves ten to hundreds of times speedup over the previous algorithm. The result surface meshes are manifolds and can be directly used in boundary element method (BEM) and finite element method (FEM) simulation.

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Title: Towards a unified macroscopic description of exciton diffusion in organic semiconductors

Abstract: Exciton diffusion length is an important parameter to characterize the efficiency of organic solar cells. Diffusion model, Monte-Carlo method, Stern-Volmer formula, and exciton-exciton annihilation model have been used to calculate exciton diffusion lengths of different materials under photoluminescence and photocurrent measurements. In this talk, I will discuss the relations between different models from a modeling viewpoint with mathematical justification and experimental verification.

郭玲（上海师范大学）

Title: Stochastic collocation methods via compressive sampling and its applications in UQ

Abstract: Stochastic computation has received intensive attention in recent years, due to the pressing need to conduct uncertainty quantification (UQ) in practical computing. One of the most widely used techniques in UQ is generalized polynomial chaos. In this talk, we will discuss collocation method via compressive sampling for recovering sparse polynomial chaos expansions (PCE) using randomized quadratures. The framework includes both the bounded measures such as the uniform and the Chebyshev measure, and the unbounded measures which include the Gaussian measure. We also consider the gradientenhanced l1-minimization, where the

derivatives (besides the function values) of a quantity of interest with respect to the underlying variables are used to accelerate the identification of the PCE coefficients.

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题目：Explicit methods for nonlinear stochastic differential equations

摘要：Comparing with traditional explicit methods, implicit methods have better stability properties, but this comes with implementation costs dominated by the iteration scheme required to solve the implicit stage equations at each time step. In this talk, we introduce a class of explicit schemes, including truncated Euler method, truncated Milstein method, etc., for solving nonlinear stochastic differential equations under Khasminskii-type condition.

Xiaoming He (Department of Mathematics and Statistics, Missouri University of Science and Technology)

Title: Decoupled, linear, and energy stable finite element method for the Cahn-Hilliard-Navier-Stokes-Darcy phase field model

Abstract: In this presentation, we discussan efficient numerical approximation for a phase field model of the coupled two-phase free flow and two-phase porous media flow. This model consists of Cahn-Hilliard-Navier-Stokes equations in the free flow region and Cahn-Hilliard-Darcy equations in the porous media region that are coupled by seven interface conditions. The coupled system is decoupled based on the interface conditions and the solution values on the interface from the previous time step. A fully discretized scheme with finite elements for the spatial discretization is developed to solve the decoupled system. In order to deal with the difficulties arising from the interface conditions, the decoupled scheme needs to be constructed appropriately for the interface terms and a modified discrete energy is introduced with an interface component. Furthermore, the scheme is linearized and energy stable. Hence, at each time step one only needs to solve a linear elliptic system for each of the two decoupled equations. Stability of the model and the proposed method is proved. Numerical experiments are presented to illustrate the features of the proposed numerical method and verify the theoretical conclusions.

胡丹（上海交通大学）

Title: Optimization, Adaptation, and Initiation of Biological Transport Networks

Abstract: Blood vessel systems and leaf venations are typical biological transport networks. The energy consumption for such a system to perform its biological functions is determined by the network structure. In the first part of this talk, I will discuss the optimized structure of vessel networks, and show how the blood vessel system adapts itself to an optimized structure. Mathematical models are used to predict pruning vessels in the experiments of zebra fish. In the second part, I will discuss our recent modeling work on the initiation process of transport networks.

Simulation results are used to illustrate how a tree-like structure is obtained from a continuum adaptation equation system, and how loops can exist in our model. Possible further application of this model will also be discussed.

廖奇峰（上海科技大学）

Title: Reduced Basis ANOVA Methods for Partial Differential Equations with High-Dimensional Random Inputs

Abstract: We present a reduced basis ANOVA approach for partial deferential equations (PDEs) with random inputs. The ANOVA method combined with stochastic collocation methods provide model reduction in high-dimensional parameter space through decomposing high-dimensional inputs into unions of low-dimensional inputs. In this work, to further reduce the computational cost, we investigate spatial low-rank structures in the ANOVA-collocation method, and develop efficient spatial model reduction techniques using hierarchically generated reduced bases. We present a general mathematical framework of the methodology, validate its accuracy and demonstrate its efficiency with numerical experiments. This is joint work with Prof. Guang Lin of Purdue University.

刘东杰（上海大学）

Title: Nonconforming FEMs for an Optimal Design Problem

Abstract: Some optimal design problems in topology optimization eventually lead to a degenerate convex minimization problem with possibly multiple minimizers, but with a unique stress。 This talk proposes the discrete Raviart-Thomas mixed finite element method (dRT-MFEM) and establishes its equivalence with the Crouzeix-Raviart nonconforming finite element method (CR-NCFEM). The convergence analysis combines a priori convergence rate of CFEM with the efficient a posterior error control of MFEM. Numerical experiments provide empirical evidence that the proposed dRT-MFEM overcomes the reliability-efficiency gap for the first time.

陆帅（复旦大学）

Title: Filter based methods for statistical linear inverse problems

Abstract: Ill-posed inverse problems are ubiquitous in applications. Understanding of algorithms for their solution has been greatly enhanced by a deep understanding of the linear inverse problem. In the applied communities ensemble-based filtering methods have recently been used to solve inverse problems by introducing an artificial dynamical system. This opens up the possibility of using a range of other filtering methods, such as 3DVAR and Kalman based methods, to solve inverse problems, again by introducing an artificial dynamical system. The aim of this talk is to analyze such methods in the context of the ill-posed linear inverse problem.

Statistical linear inverse problems are studied in the sense that the observational

noise is assumed to be derived via realization of a Gaussian random variable. We investigate the asymptotic behavior of filter based methods for these statistical linear inverse problems. Rigorous convergence rates are established for 3DVAR and for the Kalman filters, including minimax rates in some instances. Blowup of 3DVAR and its variant form is also presented, and optimality of the Kalman filter is discussed. These analyses reveal close connection between (iterative) regularization schemes in deterministic inverse problems and filter based methods in data assimilation. It is a joint work with Dr. M. A. Iglesias (U. of Nottingham, UK), Dr. K. Lin (Fudan U., China) and Prof. A. M. Stuart (Caltech, USA).

Kun Du, Junmei Ma(上海财经大学*), Qiang Zhao, Guiding Gu

Importance Sampling for Pricing Financial Derivatives: Based on the Least Square Approach

Abstract: This paper develops an efficient importance sampling Monte Carlo method for variance reduction when it is used to price financial derivatives. A general class of Exponential change of measure is well discussed and applied to determine the formulation of the new optimal importance sampling density. Then the least square approach is properly used to find the new drift vector and covariance matrix of the Gauss vector simultaneously. The method proposed by the paper has little smoothness requirements for the payoff functions and doesn't rely on the initial values. It is illustrated that this method is high efficient for pricing financial derivatives, such as Asian options, Straddle options, Volatility swaps and Variance options. Furthermore, this method can be naturally applied to more general importance sampling densities such as non-Gaussian or multi-modal distributions.

潘建瑜（华东师范大学）

题目：Preconditioned iterative methods for finite volume discretization of steady-state space-fractional diffusion equations

摘要：

许威（同济大学）

题目：Jacobian-Free Implicit Inner-Iteration Preconditioner for Nonlinear Least Squares Problems

摘要：Nonlinear least squares (NLS) problems arise in many applications.
The common solvers require to compute and store the corresponding Jacobian matrix explicitly, which is too expensive for large problems. Recently, some Jacobian-free (or matrix free) methods were proposed, but most of these methods are not really Jacobian free since the full or partial Jacobian matrix still needs to be computed in some iteration steps. In this paper, we propose an effective {\em real} Jacobian free method especially for large NLS problems, which is realized by the novel combination of using automatic differentiation for $J({\bf x}){\bf v}$ and $J({\bf

x})^T{\bf v}$ along with the implicit iterative preconditioning ideas. Together, they yield a new and effective three-level iterative approach. In the outer level, the dogleg/trust region method is employed to solve the NLS problem. At each iteration of the dogleg method, we adopt the iterative linear least squares (LLS) solvers, CGLS or BA-GMRES method, to solve the LLS problem generated at each step of the dogleg method as the middle iteration. In order to accelerate the convergence of the iterative LLS solver, we propose an implicit inner iteration preconditioner based on the weighted Jacobi method. Compared to the existing Jacobian-free methods, our proposed three-level method need not compute any part of the Jacobian matrix explicitly in any iteration step. Furthermore, our method does not rely on the sparsity or structure pattern of the Jacobian, gradient or Hessian matrix. In other words, our method also works well for dense Jacobian matrices. Numerical experiments show the superiority of our proposed method.

徐振礼（上海交通大学）

题目：Modified Poisson-Nernst-Planck equations with many-body effects

摘要：Dielectric-boundary and ion correlation effects play important role in many soft matter and electrochemical energy systems at the nano/micro scale. We develop a modified Poisson-Nernst-Planck model to include these many-body properties in electrolytes, which also takes the ion-size effect into account and is expected to provide more accurate prediction for ion dynamics with microscopic confinement. We discuss asymptotic and numerical strategies to solve the resulted PDEs, validate the model by Monte Carlo particle simulations, and report the study on the effect of ion correlation and dielectric boundary in different applications, particularly, an application for a blue energy device.

吴钢（中国矿业大学）

Title: The convergence of harmonic Ritz vectors and harmonic Ritz values---A Revisit

Abstract: We are interested in computing a simple eigenpair $(\lambda,{\bf x})$ of a large non-Hermitian matrix A, by using a general harmonic Rayleigh-Ritz projection method. Given a search subspace $\mathcal{K}$ and a target point τ that is not an eigenvalue of A, we focus on the convergence of the harmonic Ritz vector $\widetilde{\bf x}$ and the harmonic Ritz value $\widetilde{\lambda}$.
In [{Z. Jia}, {\em The convergence of harmonic Ritz values, harmonic Ritz vectors, and refined harmonic Ritz vectors}, Math. Comput., 74 (2004), pp. 1441-1456.], Jia showed that for the convergence of the harmonic Ritz vector and the harmonic Ritz value, it is essential to assume a certain Rayleigh quotient matrix is {\it uniformly nonsingular} as $\angle({\bf x},\mathcal{K})\rightarrow 0$. However, this assumption can not be guaranteed both in theory and in practice, and the Rayleigh quotient matrix can be singular or near singular even if τ is not close to λ. In this work, we abolish this constraint and derive new bounds for the

convergence of harmonic Rayleigh-Ritz projection methods. We show that as the distance between ${\bf x}$ and $\mathcal{K}$ tends to zero, the harmonic Ritz value converges, and the harmonic Ritz vector converges if $\frac{1}{\lambda-\tau}$ is uniformly bounded away from the other Ritz values of A in $(A-\tau I)\mathcal{K}$.

吴新明（复旦大学）

Title: A Regularized Newton Method for Computing Ground States of Bose-Einstein Condensates

Abstract: In this paper, we compute ground states of Bose-Einstein condensates (BECs), which can be formulated as an energy minimization problem with a spherical constraint. The energy functional and constraint are discretized by either the finite difference, or sine or Fourier pseudospectral discretization schemes and thus the original infinite dimensional nonconvex minimization problem is approximated by a finite dimensional constrained nonconvex minimization problem. Then we present a feasible gradient type method to solve this minimization problem, which is an explicit scheme and maintains the spherical constraint automatically. To accelerate the convergence of the gradient type method, we approximate the energy functional by its second-order Taylor expansion with a regularized term at each Newton iteration and adopt a cascadic multigrid technique for selecting initial data. It leads to a standard trust-region subproblem and we solve it again by the feasible gradient type method.
The convergence of the regularized Newton method is established by adjusting the regularization parameter as the standard trust-region strategy. Extensive numerical experiments on challenging examples, including a BEC in three dimensions with an optical lattice potential and rotating BECs in two dimensions with rapid rotation and strongly repulsive interaction, show that our method is efficient, accurate and robust.

吴语茂 **(复旦大学)**

Title: The new methods for calculating the scattered fields from the nano-periodic structures and high frequency electrically large scatterers

Abstract: In this talk, the operator marching method for the scattering problems of nano-periodic structures is introduced. The scattered fields are fast calculated with high accuracy. Then, the surface integral equation method for analyzing the scattered electromagnetic fields on diffraction grating structures will be presented. Next, we propose the numerical steepest descent path method for solving the high frequency scattered fields. Numerical results on the engineering scatterer models illustrate that the proposed method is frequency independent in computational cost and error controllable in accuracy.

易利军（上海师范大学）

Title: Some recent progress in the hp-version time-stepping methods for initial

value problems

Abstract: In this talk we shall present some recent progress in the hp-version continuous Galerkin and spectral collocation time-stepping methods for initial value problems for ordinary differential equations, delay differential equations, and integro-differential equations. Numerical examples are presented to illustrate the theoretical results. This talk is based on joint work with Benqi Guo (University of Manitoba) and Zhongqing Wang (University of Shanghai for Science and Technology).

应文俊（上海交通大学）

题目：A simple method for computing singular or nearly singular integrals on closed surfaces

摘要：In this talk, I will present a simple, accurate method for computing singular or nearly singular integrals on a smooth, closed surface, such as layer potentials for harmonic functions evaluated at points on or near the surface. The integral is first computed with a regularized kernel and then discretized with a new quadrature using surface points which project onto grid points in coordinate planes. Leading order terms of the regularization and discretization errors are computed from asymptotic analysis near the singular point and added to the computed value so that the result has high order accuracy. The method does not require coordinate charts on the surface or special treatment of the singularity other than the corrections. The method is accelerated by the treecode algorithm of Duan and Krasny for Ewald summation. I will also present numerical examples with different surfaces.

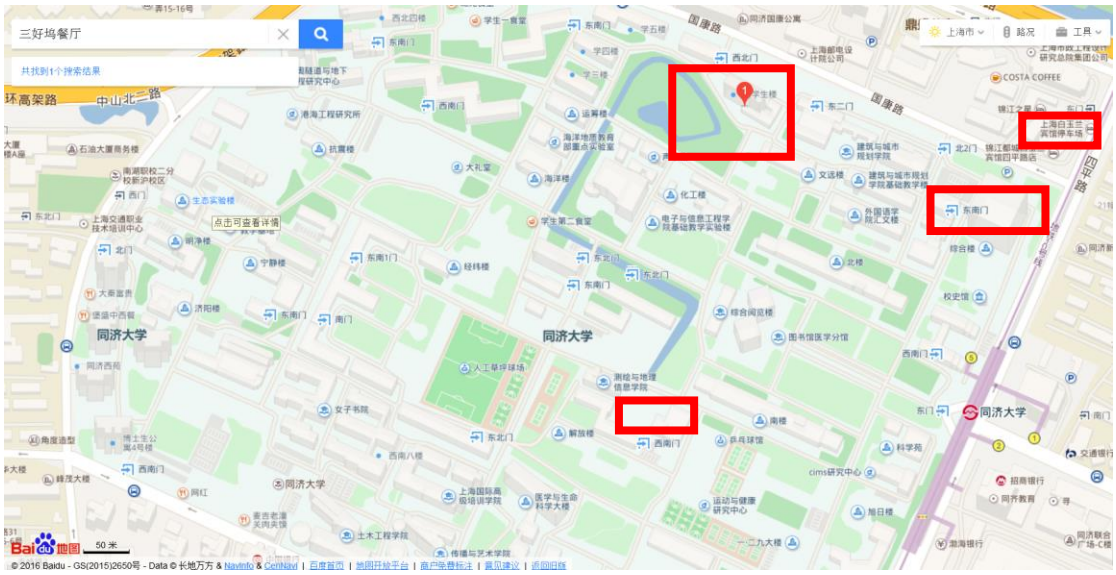
周圣高（苏州大学）

题 目 ： Stochastic Level-Set Variational Implicit-Solvent Approach to Solute-Solvent Interfacial Fluctuations

摘要：In this talk, we present a theory in the form of Langevin geometrical flow to incorporate solute-solvent interfacial fluctuations into the VISM. Such fluctuations are crucial to biomolecular conformational changes and binding process. We also develop a stochastic level-set method to numerically implement such a theory. We describe the interfacial fluctuation through the ``normal velocity'' that is the solute-solvent interfacial force, derive the corresponding stochastic level-set equation in the sense of Stratonovich so that the surface representation is independent of the choice of implicit function, and develop numerical techniques for solving such an equation and processing the numerical data. We apply our computational method to study the dewetting transition in the system of two hydrophobic plates and a hydrophobic cavity of a synthetic host molecule. Numerical simulations demonstrate that our approach can describe an underlying system jumping out of a local minimum of the free-energy functional and can capture dewetting transitions of hydrophobic systems. In the case of two hydrophobic plates, we find that the wavelength of interfacial fluctuations has a strong influence to the dewetting transition. In addition,

we find that the estimated energy barrier of the dewetting transition scales quadratically with the inter-plate distance, agreeing well with existing studies of molecular dynamics simulations. Our work is a first step toward the inclusion of fluctuations into the VISM and understanding the impact of interfacial fluctuations on biomolecular solvation with an implicit-solvent approach. This is a joint work with Li-Tien Cheng, Bo Li, J. A. McCammon and many others.

附一：地图：同济大学综合楼（会议）、白玉兰宾馆（住宿）、学苑餐厅（用餐）、三好坞餐厅(用餐)



2016年同济大学计算数学青年学者研讨会通讯录

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周圣高	苏州大学	sgzhou@suda.edu.cn	

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16:

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Xiaoming He (Department of Mathematics and Statistics, Missouri University of Science and Technology)

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胡丹（上海交通大学）

Title: Optimization, Adaptation, and Initiation of Biological Transport Networks

Abstract: Blood vessel systems and leaf venations are typical biological transport networks. The energy consumption for such a system to perform its biological functions is determined by the network structure. In the first part of this talk, I will discuss the optimized structure of vessel networks, and show how the blood vessel system adapts itself to an optimized structure. Mathematical models are used to predict pruning vessels in the experiments of zebra fish. In the second part, I will discuss our recent modeling work on the initiation process of transport networks. Simulation results are used to illustrate how a tree-like structure is obtained from a continuum adaptation equation system, and how loops can exist in our model. Possible further application of this model will also be discussed.

廖奇峰（上海科技大学）

Title: Reduced Basis ANOVA Methods for Partial Differential Equations with High-Dimensional Random Inputs

Abstract: We present a reduced basis ANOVA approach for partial deferential equations (PDEs) with random inputs. The ANOVA method combined with stochastic collocation methods provide model reduction in high-dimensional parameter space through decomposing high-dimensional inputs into unions of low-dimensional inputs. In this work, to further reduce the computational cost, we investigate spatial low-rank structures in the ANOVA-collocation method, and develop efficient spatial model reduction techniques using hierarchically generated reduced bases. We present a general mathematical framework of the methodology, validate its accuracy and demonstrate its efficiency with numerical experiments. This is joint work with Prof. Guang Lin of Purdue University.

刘东杰（上海大学）

Title: Nonconforming FEMs for an Optimal Design Problem

Abstract: Some optimal design problems in topology optimization eventually lead to a degenerate convex minimization problem with possibly multiple minimizers, but with a unique stress 。 This talk proposes the discrete Raviart-Thomas mixed finite element method (dRT-MFEM) and establishes its equivalence with the Crouzeix-Raviart nonconforming finite element method (CR-NCFEM). The convergence analysis combines a priori convergence rate of CFEM with the efficient a posterior error control of MFEM. Numerical experiments provide empirical evidence that the proposed dRT-MFEM overcomes the reliability-efficiency gap for the first time.

陆帅（复旦大学）

Title: Filter based methods for statistical linear inverse problems

Abstract: Ill-posed inverse problems are ubiquitous in applications. Understanding of algorithms for their solution has been greatly enhanced by a deep understanding of the linear inverse problem. In the applied communities ensemble-based filtering methods have recently been used to solve inverse problems by introducing an artificial dynamical system. This opens up the possibility of using a range of other filtering methods, such as 3DVAR and Kalman based methods, to solve inverse problems, again by introducing an artificial dynamical system. The aim of this talk is to analyze such methods in the context of the ill-posed linear inverse problem.

Statistical linear inverse problems are studied in the sense that the observational

noise is assumed to be derived via realization of a Gaussian random variable. We investigate the asymptotic behavior of filter based methods for these statistical linear inverse problems. Rigorous convergence rates are established for 3DVAR and for the Kalman filters, including minimax rates in some instances. Blowup of 3DVAR and its variant form is also presented, and optimality of the Kalman filter is discussed. These analyses reveal close connection between (iterative) regularization schemes in deterministic inverse problems and filter based methods in data assimilation. It is a joint work with Dr. M. A. Iglesias (U. of Nottingham, UK), Dr. K. Lin (Fudan U., China) and Prof. A. M. Stuart (Caltech, USA).

Kun Du, Junmei Ma(上海财经大学*), Qiang Zhao, Guiding Gu
Importance Sampling for Pricing Financial Derivatives: Based on the Least Square Approach
Abstract: This paper develops an efficient importance sampling Monte Carlo method for variance reduction when it is used to price financial derivatives. A general class of Exponential change of measure is well discussed and applied to determine the formulation of the new optimal importance sampling density. Then the least square approach is properly used to find the new drift vector and covariance matrix of the Gauss vector simultaneously. The method proposed by the paper has little smoothness requirements for the payoff functions and doesn't rely on the initial values. It is illustrated that this method is high efficient for pricing financial derivatives, such as Asian options, Straddle options, Volatility swaps and Variance options. Furthermore, this method can be naturally applied to more general importance sampling densities such as non-Gaussian or multi-modal distributions.

潘建瑜（华东师范大学）
题目：Preconditioned iterative methods for finite volume discretization of steady-state space-fractional diffusion equations
摘要：

徐振礼（上海交通大学）
题目：TBC
摘要：

吴钢（中国矿业大学）
Title: The convergence of harmonic Ritz vectors and harmonic Ritz values---A Revisit
Abstract: We are interested in computing a simple eigenpair $(\lambda,{\bf x})$ of a large non-Hermitian matrix A, by using a general harmonic Rayleigh-Ritz projection method.
Given a search subspace $\mathcal{K}$ and a target point τ that is not an

eigenvalue of A, we focus on the convergence of the harmonic Ritz vector $\widetilde{\bf x}$ and the harmonic Ritz value $\widetilde{\lambda}$.
In [{Z. Jia}, {\em The convergence of harmonic Ritz values, harmonic Ritz vectors, and refined harmonic Ritz vectors}, Math. Comput., 74 (2004), pp. 1441-1456.], Jia showed that for the convergence of the harmonic Ritz vector and the harmonic Ritz value, it is essential to assume a certain Rayleigh quotient matrix is {\it uniformly nonsingular} as $\angle({\bf x},\mathcal{K})\rightarrow 0$.
However, this assumption can not be guaranteed both in theory and in practice, and the Rayleigh quotient matrix can be singular or near singular even if τ is not close to λ.
In this work, we abolish this constraint and derive new bounds for the convergence of harmonic Rayleigh-Ritz projection methods. We show that as the distance between ${\bf x}$ and $\mathcal{K}$ tends to zero, the harmonic Ritz value converges, and the harmonic Ritz vector converges if $\frac{1}{\lambda-\tau}$ is uniformly bounded away from the other Ritz values of A in $(A-\tau I)\mathcal{K}$.

吴新明（复旦大学）

Title: A Regularized Newton Method for Computing Ground States of Bose-Einstein Condensates

Abstract: In this paper, we compute ground states of Bose-Einstein condensates (BECs), which can be formulated as an energy minimization problem with a spherical constraint. The energy functional and constraint are discretized by either the finite difference, or sine or Fourier pseudospectral discretization schemes and thus the original infinite dimensional nonconvex minimization problem is approximated by a finite dimensional constrained nonconvex minimization problem. Then we present a feasible gradient type method to solve this minimization problem, which is an explicit scheme and maintains the spherical constraint automatically. To accelerate the convergence of the gradient type method, we approximate the energy functional by its second-order Taylor expansion with a regularized term at each Newton iteration and adopt a cascadic multigrid technique for selecting initial data. It leads to a standard trust-region subproblem and we solve it again by the feasible gradient type method.
The convergence of the regularized Newton method is established by adjusting the regularization parameter as the standard trust-region strategy. Extensive numerical experiments on challenging examples, including a BEC in three dimensions with an optical lattice potential and rotating BECs in two dimensions with rapid rotation and strongly repulsive interaction, show that our method is efficient, accurate and robust.

吴语茂 **(复旦大学)**

Title: The new methods for calculating the scattered fields from the

nano-periodic structures and high frequency electrically large scatterers

Abstract: In this talk, the operator marching method for the scattering problems of nano-periodic structures is introduced. The scattered fields are fast calculated with high accuracy. Then, the surface integral equation method for analyzing the scattered electromagnetic fields on diffraction grating structures will be presented. Next, we propose the numerical steepest descent path method for solving the high frequency scattered fields. Numerical results on the engineering scatterer models illustrate that the proposed method is frequency independent in computational cost and error controllable in accuracy.

易利军（上海师范大学）

Title: Some recent progress in the hp-version time-stepping methods for initial value problems

Abstract: In this talk we shall present some recent progress in the hp-version continuous Galerkin and spectral collocation time-stepping methods for initial value problems for ordinary differential equations, delay differential equations, and integro-differential equations. Numerical examples are presented to illustrate the theoretical results. This talk is based on joint work with Benqi Guo (University of Manitoba) and Zhongqing Wang (University of Shanghai for Science and Technology).

应文俊（上海交通大学）

题目：A simple method for computing singular or nearly singular integrals on closed surfaces

摘要：In this talk, I will present a simple, accurate method for computing singular or nearly singular integrals on a smooth, closed surface, such as layer potentials for harmonic functions evaluated at points on or near the surface. The integral is first computed with a regularized kernel and then discretized with a new quadrature using surface points which project onto grid points in coordinate planes. Leading order terms of the regularization and discretization errors are computed from asymptotic analysis near the singular point and added to the computed value so that the result has high order accuracy. The method does not require coordinate charts on the surface or special treatment of the singularity other than the corrections. The method is accelerated by the treecode algorithm of Duan and Krasny for Ewald summation. I will also present numerical examples with different surfaces.

周圣高（苏州大学）

题 目 ： Stochastic Level-Set Variational Implicit-Solvent Approach to

Solute-Solvent Interfacial Fluctuations

摘要：In this talk, we present a theory in the form of Langevin geometrical flow to incorporate solute-solvent interfacial fluctuations into the VISM. Such fluctuations are crucial to biomolecular conformational changes and binding process. We also develop a stochastic level-set method to numerically implement such a theory. We describe the interfacial fluctuation through the ``normal velocity'' that is the solute-solvent interfacial force, derive the corresponding stochastic level-set equation in the sense of Stratonovich so that the surface representation is independent of the choice of implicit function, and develop numerical techniques for solving such an equation and processing the numerical data. We apply our computational method to study the dewetting transition in the system of two hydrophobic plates and a hydrophobic cavity of a synthetic host molecule. Numerical simulations demonstrate that our approach can describe an underlying system jumping out of a local minimum of the free-energy functional and can capture dewetting transitions of hydrophobic systems. In the case of two hydrophobic plates, we find that the wavelength of interfacial fluctuations has a strong influence to the dewetting transition. In addition, we find that the estimated energy barrier of the dewetting transition scales quadratically with the inter-plate distance, agreeing well with existing studies of molecular dynamics simulations. Our work is a first step toward the inclusion of fluctuations into the VISM and understanding the impact of interfacial fluctuations on biomolecular solvation with an implicit-solvent approach. This is a joint work with Li-Tien Cheng, Bo Li, J. A. McCammon and many others.

附一：地图：同济大学综合楼（会议）、白玉兰宾馆（住宿）、学苑餐厅（用餐）、三好坞餐厅(用餐)

2016年同济大学计算数学青年学者研讨会通讯录

（按姓氏字母顺序排列）

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