



The Sixth Chinese-German Workshop on Computational and Applied Mathematics

Shanghai, China October 9-13, 2017

Program & Abstracts

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Sponsor

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General Information

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•	Jun Hu	Peking University
•	Carsten Carstensen	Humboldt University of Berlin
•	Dolf Donnochon	University of Usidelhang
	Kon Kannacher	University of Heidelberg

Date

October 9-13, 2017

Conference venue

Room 1002, Tongji University Multi-Functional Building

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Wei Gong	Chinese Academy of Sciences
Jianguo Huang	Shanghai Jiao Tong University
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Chunxiong Zheng	Tsinghua University
Jiwei Zhang	Beijing Computational Science Research Center
Qingsong Zou	Sun Yat-sen University
Ran Zhang	Jilin University
Xuying Zhao	Chinese Academy of Sciences

German Participants

Malte Braack	Christian-Albrechts-University of Kiel
Carsten Carstensen	Humboldt University of Berlin
Lars Diening	University of Bielefeld
Dietmar Gallistl	Karlsruhe Institute of Technology
Christiane Helzel	Heinrich-Heine-University
Michael Hinze	University Hamburg
Dietmar Kröner	Albert-Ludwigs-University of Freiburg
Guido Kanschat	Heidelberg University
Ralf Kornhuber	Free University of Berlin
Daniel Peterseim	University of Augsburg
Malte A. Peter	University of Augsburg
Katharina Schratz	Karlsruhe Institute of Technology
Mira Schedensack	Humboldt University of Berlin

Monday, October 9, 2017

Opening Ceremony

08:30 - 09:00

Talks

	Chair: Zhongci Shi
Carsten Carstensen	09:00 - 09:40
Title:	Adaptivite Least Squares Finite Element Methodology
Yunqing Huang	09:40 - 10:20
Title:	Hill-Climbing Algorithm with a Stick for Unconstrained Optimization Problems
Tea Break	10:20 - 10:50
	Chair: Ralf Kornhuber
Dietmar Kröner	10:50 - 11:30
Title:	Numerical treatment of interfaces
Huazhong Tang	11:30 - 12:10
Title:	High-Order Accurate Physical-Constraints-Preserving Schemes for Special Relativistic Hydrodynamics
Lunch	12:30 - 14:00
Talks	
Wanhin Chan	Chair: Dietmar Kroner $14.00 - 14.40$
	Optimal Convergence Analysis of a Mixed Finite Flement Methods for Fourth-
Title:	order Elliptic Problems
Malte Braack	14:40 - 15:20
Title:	Local projection stabilization for saddle-point problems with non Dirichlet conditions
Xuejun Xu	15:20 - 16:00
Title:	Local Multigrid for Biharmonic Equation
Tea Break	16:00 - 16:30
	Chair: Danping Yang
Lars Diening	16:30 - 17:10
Title:	Local estimates for the discrete p-harmonic functions for fully adaptive meshes
Yanping Chen	17:10 - 17:50
Title:	Analysis of two-grid methods for miscible displacement problem by mixed finite element methods
Ran Zhang	17:50 - 18:30
Title:	Recent advance in the weak Galerkin method for eigenvalue problems

Tuesday, October 10, 2017

Talks

	Chair: Carsten Carstensen
Jun Hu	09:00 - 09:40
Title:	Adaptive and Multilevel Mixed Finite Element Methods
Haijun Wu	09:40 - 10:20
Title:	Polynomial preserving recovery of linear FEM for Helmholtz equation with high wave number
Tea Break	10:20 - 10:50
	Chair: Huazhong Tang
Christiane Helzel	10:50 - 11:30
Title: Chuanju Xu	High-Order Finite Volume methods for Hyperbolic PDEs on Cartesian Grids 11:30 - 12:10
Title:	Muntz Spectral Methods with Applications to Some Singular Problems
Lunch	12:10 - 14:00
Talks	
	Chair: Yunqing Huang
Michael Hinze	14:00 - 14:40
Title:	Optimal control of surface PDEs
Xiaoping Xie	14:40 - 15:20
Title:	Robust a posteriori error estimation for a weak Galerkin finite element discretization of Stokes equations
Yan Xu	15:20 - 16:00
Title:	Efficient high order semi-implicit time discretization and local discontinuous Galerkin methods for highly nonlinear PDEs
Tea Break	16:00 - 16:30
	Chair: Haijun Wu
Malte A. Peter	16:30- 17:10
Title:	A two-scale Stefan problem arising in a model for tree-sap exudation
Shipeng Mao	17:10 - 17:50
Title:	Adaptive finite element method for incompressible magnetohydrodynamics
Ruo Li	17:50 - 18:30
Title:	Finding 13-Moment System Beyond Grad
Banquet	

Wednesday, October 11, 2017

Talks

	Chair: Jun Hu
Ziqing Xie	09:00 - 09:40
Title:	Two methods for Finding Multiple Solutions of Semilinear PDEs
Ralf Kornhuber	09:40 - 10:20
Title:	Numerical homogenization of fault networks
Tea Break	10:20 - 10:50
	Chair: Michael Hinze
Jianguo Huang	10:50 - 11:30
Title:	A continuous DG time stepping method and its adaptive algorithms for second order evolution problems
Huoyuan Duan	11:30 - 12:10
Title:	Finite element approximation of singular solution and singular data of time- harmonic Maxwell equations by Riesz-lifting
Lunch	12:10 - 14:00

Excursion

Thursday, October 12, 2017

Talks

	Chair: Xuejun Xu	
Pingbing Ming	09:00 - 09:40	
Title:	A hybrid method for multiscale PDEs	
Guido Kanschat	09:40 - 10:20	
Title:	Multilevel domain-decomposition methods for radiation diffusion and radiation transport	
Tea Break	10:20 - 10:50	
~	Chair: Lars Diening	
Danping Yang	10:50 - 11:30	
Title:	Adaptive finite element iterative approximation of optimal control governed by PDEs	
Jinru Chen	11:30 - 12:10	
Title:	A Conforming Enriched Finite Element Method for Elliptic Interface Problems	
Lunch	12:10 - 14:00	
Talks		
	Chair: Jianguo Huang	
Katharina Schratz	14:00 - 14:40	
Title:	Exponential-type time integrators for nonlinear Schrödinger, Korteweg-de Vries and Klein-Gordon type equations	
Qingsong Zou	14:40 - 15:20	
Title:	The immersed finite volume method for elliptic interface problems	
Jiwei Zhang	15:20 - 16:00	
Title:	Efficient algorithm for nonlocal/time-fractional models	
Tea Break	16:00 - 16:30	
	Chair: Malte Braack	
Chunxiong Zheng	16:30 - 17:10	
Title:	Extended WKB analysis for the high-frequency linear wave equations	
Mira Schedensack	17:10 - 17:50	
Title:	Error analysis of a variational multiscale stabilization for convection- dominated diffusion equations	
Wei Gong	17:50 - 18:30	
Title:	Convergence of adaptive finite element method for elliptic optimal control problems	

Friday, October 13, 2017

Talks

	Chair: Christiane Helzel	
Daniel Peterseim	09:00 - 09:40	
Title:	Numerical simulation of Bose-Einstein-Condensates	
Xuying Zhao	09:40 - 10:20	
Title:	Decomposition of nonlocal norms and quantitative dependence analysis for nonlocal diffusion models	
Tea Break	10:20 - 10:50	
	Chair: Guido Kanschat	
Dietmar Gallistl	10:50 - 11:30	
Title:	A posteriori error analysis of equations in nondivergence form with Cordes coefficients	
Manman Ma	11:30 - 12:10	
Title:	A fast numerical method for simulating ion structure near core-shell dielectric nanoparticle	
Lunch	12:10 - 14:00	

Excursion

Abstracts

Adaptivite Least Squares Finite Element Methodology

Carsten Carstensen Humboldt University of Berlin

The leasts squares finite element schemes are popular because they lead to symmetric and positive definite discrete problems with seemingly no stability conditions. Although their similarity with mixed finite element methods has been observed in [1], the natural choice of the localized least squares residual as an mesh-refining criterion is not justified. It has been observed that the associated adaptive algorithm it is convergence for a bulk parameter very large close to one [2]. This is in contradiction to the methodology of optimal rates where this parameter has to be sufficiently small [3, 4]. One remedy in the analysis of mixed finite element schemes, of leasts squares finite element schemes and for the discontinuous Petrov-Galerkin methodology is the usage of separate marking and alternative a posteriori error estimates as in [5]. Mixed finite element methods with flux errors in H(div)-norms and div-least-squares finite element methods require the separate marking strategy in obligatory adaptive mesh-refining. The refinement indicator $\sigma_{\ell}^2(K) = \eta_{\ell}^2(K) + \mu^2(K)$ of a finite element domain K in a triangulation $\tau \ell$ on the level ℓ consists of some residual-based error estimator $\eta \ell$ with some reduction property under local mesh-refining and some data approximation error $\eta\ell$. Separate marking [Safem] means either Dörfler marking (or bulk chasing) if $\mu_{\ell}^2 \leq$ $\kappa \eta_{\ell}^2$ and otherwise an optimal data approximation algorithm run with controlled accuracy [4, 5].

The presentation explains the setting and results of more practical applications for the Stokes problem [6, 7] and linear elasticity [8] and ends with an outlook on the possibilities for nonlinear problems. [1] J. Brandts, Y. Chen, and J. Yang, A note on least-squares mixed finite elements in relation to standard and mixed finite elements, IMA J. Numer. Anal., 26 (2006), pp. 779–789, doi:10.1093/imanum/dri048.

[2] P. Bringmann, C. Carstensen, and E. J. Park. Convergence of natural adaptive least-squares finite element methods. Numer. Math. (2017) doi:10.1007/s00211-017-0866-x
[3] C. Carstensen, M. Feischl, M. Page, and D. Praetorius. Axioms of adaptivity. Comput. Methods Appl. Math., 67(6):1195--1253, 2014.

[4] C. Carstensen and H. Rabus. Axioms of adaptivity for separate marking. arXiv:1606.02165v1.

[5] C. Carstensen and E.-J. Park. Convergence and optimality of adaptive least squares finite element methods. SIAM J. Numer. Anal., 53:43--62, 2015.

[6] P. Bringmann and C. Carstensen. An adaptive least-squares FEM for the Stokes equations with optimal convergence rates. Numer. Math., 135(2):459-492, 2017.

[7] P. Bringmann and C. Carstensen. h-adaptive least-squares finite element method for the 2d stokes equations of any order with optimal convergence rates. Computers and Mathematics with Appications, 2017

[8] P. Bringmann, C. Carstensen, and G. Starke. An adaptive least-squares fem for linear elasticity with optimal convergence rates, 2017 to appear.

Hill-Climbing Algorithm with a Stick for Unconstrained

Optimization Problems

Huang Yunqing and Jiang Kai Xiangtan University

Inspired by the behavior of the blind for hill-climbing using a stick to detect a higher place by drawing a circle, we propose a heuristic direct search method to solve the unconstrained optimization problems. Instead of searching a neighbourhood of the current point as done in the traditional hill-climbing, or along specified search directions in standard direct search methods, the new algorithm searches on a surface with radius determined by the motion of the stick. The significant feature of the proposed algorithm is that it only has one parameter, the search radius, which makes the algorithm convenient in practical implementation. The developed method can shrink the search space to a closed ball, or seek for the final optimal point by adjusting search radius. Furthermore our algorithm possesses multi-resolution feature to distinguish the local and global optimum points with different search radii. Therefore, it can be used by itself or integrated with other optimization methods flexibly as a mathematical optimization technique. A series of numerical tests, including high-dimensional problems, have been well designed to demonstrate its performance.

Numerical Treatment of Interfaces

Dietmar Kröner Albert-Ludwigs-University of Freiburg

In this contribution we will consider moving interfaces and partial differential equation on moving interfaces in different contexts. First we will present the existence, uniqueness and numerical experiments for solutions of nonlinear conservation laws on moving surfaces [2], [3]. In addition to the "hydrodynamical" shocks, geometrically induced shocks will appear. In the second part we study the compressible two phase flow with phase transition on the bases of the Navier-Stokes-Korteweg- and a phasefield model [4], [1]. It turns out that it is extremely important for the numerical schemes of both models that they satisfy a discrete energy inequality to satisfy the second law of thermodynamics. Different numerical experiments will be presented. In the third part we will report on recent research on our experience of the application of the volume of fluid method (VOF) for the resolution of interfaces. The main advantage compared to level set methods is, that the VOF method is mass conserving. We will show different numerical experiments of droplets on solid walls. These results have been obtained together with S. Burbulla, D. Diehl, J. Gerstenberger, M. Kr änkel, T. Malkmus, T. M üller, M. Nolte, C. Rohde.

[1] K. Hermsdörfer, C. Kraus, and D. Kröner, *Interface conditions for limits of the Navier-Stokes-Korteweg model*, Interfaces Free Bound. 13 (2011), no. 2, 239–254.

[2] G. Dziuk, D. Kröner, and T. Müller, *Scalar conservation laws on moving hypersurfaces*, Interfaces Free Bound. 15 (2013), no. 2, 203–236.

[3] D. Kröner, T. Müller, and L. M. Strehlau, *Traces for functions of bounded variation on manifolds with applications to conservation laws on manifolds with boundary*, SIAM J. Math. Anal. 47 (2015), no. 5, 3944–3962.

[4] D. Diehl, J. Kremser, D. Kröner, and Ch. Rohde, *Numerical solution of Navier-Stokes-Korteweg systems by local discontinuous Galerkin methods in multiple space dimensions*, Appl. Math. Comput. 272 (2016), part 2, 309–335.

High-Order Accurate Physical-Constraints-Preserving

Schemes for Special Relativistic Hydrodynamics

Huazhong Tang Peking University and Xiangtan University

Relativistic hydrodynamics (RHD) plays an essential role in many fields of modern physics, e.g. astrophysics. Relativistic flows appear in numerous astrophysical phenomena from stellar to galactic scales, e.g. active galactic nuclei, super-luminal jets, core collapse super-novae, X-ray binaries, pulsars, coalescing neutron stars and black holes, micro-quasars, and gamma ray bursts, etc. The relativistic description of fluid dynamics should be taken into account if the local velocity of the flow is close to the light speed in vacuum or the local internal energy density is comparable (or larger) than the local rest mass density of the fluid. It should also be used whenever matter is influenced by large gravitational potentials, where the Einstein field theory of gravity has to be considered. The dynamics of the relativistic systems requires solving highly nonlinear equations and the analytic treatment of practical problems is extremely difficult. Hence, studying them numerically is the primary approach.

We develop high-order accurate physical-constraints-preserving finite difference WENO schemes for special relativistic hydrodynamical (RHD) equations, built on the local Lax-Friedrich splitting, the WENO reconstruction, the physical-constraintspreserving flux limiter, and the high order strong stability preserving time discretization. They are formal extensions of the existing positivity-preserving finite difference WENO schemes for the non-relativistic Euler equations. However, developing physicalconstraints-preserving methods for the RHD system becomes much more difficult than the non-relativistic case because of the strongly coupling between the RHD equations, no explicit expressions of the conservative vector for the primitive variables and the flux vectors, and one more physical constraint for the fluid velocity in addition to the positivity of the rest-mass density and the pressure. The key is to prove the convexity and other properties of the admissible state set and discover a concave function with respect to the conservative vector replacing the pressure which is an important ingredient to enforce the positivity-preserving property for the non-relativistic case.

Several numerical examples are used to demonstrate accuracy, robustness, and effectiveness of the proposed physical-constraints-preserving schemes in solving relativistic problems with large Lorentz factor.

Optimal Convergence Analysis of a Mixed Finite Element

Methods for Fourth-order Elliptic Problems

Wenbin Chen Fudan University

In this talk, a class of fourth-order elliptic problems arising from solving various gradient systems is analyzed. The well-posedness of the problem is based on an abstract framework. The optimal error estimate is obtained from a super-close relation, which presents a closer approximation of the finite element solution, to the Ritz projection of the PDE solution. Compared to standard interpolation error estimates, such closer approximation is one order higher in convergence accuracy. As a result, the new estimates have greatly improved the original ones in literature, which were derived by super-convergence technique. Numerical results well agree with theoretical analysis for P_1 , P_2 and P_3 elements on three different meshes.

Local projection stabilization for saddle-point problems with

non Dirichlet conditions

Malte Braack

Christian-Albrechts-University of Kiel

The local projection stabilization (LPS) method is already an established method for stabilizing saddle-point problems and convection-diffusion problems. The a priori error analysis is usually done for homogeneous Dirichlet data. However, it turns out that without Dirichlet conditions the situation is more involved. Even in the case of Stokes stabilization without Dirichlet conditions on the entire boundary, the standard approach has to be modified. This is due to some integration by parts needed in the analysis. In the non-Dirichlet case, additional boundary integrals appear which can not be absorbed by available quantities. Therefore, the LPS method must be adapted in this case.

In this work, we explain the differences of the Dirichlet and non-Dirichlet case. A possible modification and an a priori error estimate will be presented. Applications arise in many standard flow applications but also e.g. in coupled Darcy-Stokes problems, where interior layers (interfaces) may arise and require such algorithmic adaptations of standard methods.

[1] G.S. Beavers and D. D. Joseph. Boundary conditions at a naturally permeable wall, J. Fluid Mech. 30, 197-207, 1967.

[2] R. Becker and M.Braack. A finite element pressure gradient stabilization for the Stokes equations based on local projections. Calcolo, 38(4):173-199, 2001.

[3] M. Braack and E. Burman. Local projection stabilization for the Oseen problem and its interpretation as a variational multiscale method. SIAM J. Numer. Anal., 43(6):2544-2566, 2006.

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Local Multigrid for Biharmonic Equation

Xuejun Xu

School of Mathematical Sciences, Tongji University and Institute of Computational Mathematics, AMSS, CAS, Beijing

In this talk, we shall present some local multigrid methods (LMG) to solve the linear algebraic systems resulting from the application of adaptive conforming Bogner-Fox-Schmit (BFS) rectangular element and nonconforming Adini rectangular element approximations to the biharmonic problem. The abstract Schwarz framework is applied to verify the uniform convergence of the local multilevel methods featuring Jacobi and Gauss-Seidel smoothing only on local nodes associated with the local refinements. By the abstract framework, convergence estimate may also be derived from the stability of the space splitting and its strengthen Cauchy-Schwarz inequality.

Local estimates for the discrete p-harmonic functions for

fully adaptive meshes

Lars Diening University of Bielefeld

It is well known that harmonic functions and p-harmonic functions have higher interior regularity, see for example [Uhl77]. In 1957 De Giorgi introduced in [DG57] a new technique that allows for example to estimate the maximum of the solution on a ball by a mean integral of the solution on an enlarged ball. In particular, we showed that every harmo function satisfies

$$\max_{B} |u|^{2} \le c \quad \frac{1}{|2B|} \quad \int_{2B} |u|^{2} dx.$$

A similar result holds for p-harmonic functions. The proof is based on subtle Cacciopoli estimates using truncation operators.

In this talk we present similar estimates for discretely harmonic and p- harmonic functions. Our solutions can be scalar valued as well as vector valued, which makes a big difference for p-harmonic functions.

Such estimates are of strong interest, since these estimates provide an alternative approach to $L\infty$ -estimates of the error u–uh, which is future project. Various results already exist in this direction for harmonic functions, e.g. [SW95]. However, the main obstacle in this direction even in the linear case is adaptivity. All of the results obtained so far, require that the mesh size does not vary too much locally. This puts certain undesired assumptions on the refinement algorithm.

Our approach differs in such that we allow for arbitrary highly graded meshes (still shape regular). However, our approach uses certain properties of the Lagrange basis functions. This restrict our approach at the moment to acute meshes and linear elements. The proof of our result is based on a discretized version of the De Giorgi technique. We use a few novel estimates, that have not been available before.

Let us mention also that there is a strong relation to the discrete maximum principle. In particular, in the case of p-harmonic functions, similar truncation operators and similar mesh requirements (non-obtuse) appear, see [DKS13].

The talk is based on a joint project with Toni Scharle from Oxford university. References

[DG57] Ennio De Giorgi, Sulla differenziabilità e l'analiticità delle estremali degli integrali multipli regolari, Mem. Accad. Sci. Torino. Cl. Sci. Fis. Mat. Nat. (3) 3 (1957), 25–43.

[DKS13] L. Diening, Ch. Kreuzer, and S. Schwarzacher, Convex hull property and maximum principle for finite element minimisers of general convex functionals, Numer. Math. 124 (2013), no. 4, 685–700.

[SW95] A. H. Schatz and L. B. Wahlbin, Interior maximum-norm estimates for finite element methods. II, Math. Comp. 64 (1995), no. 211, 907–928.

[Uhl77] K. Uhlenbeck, Regularity for a class of non-linear elliptic systems, Acta Math. 138 (1977), no. 3-4, 219-240.

Analysis of two-grid methods for miscible displacement

problem by mixed finite element methods

Yanping Chen South China Normal University

The miscible displacement of one incompressible fluid by another in a porous medium is governed by a system of two equations. One is elliptic form equation for the pressure and the other is parabolic form equation for the concentration of one of the fluids. Since only the velocity and not the pressure appears explicitly in the concentration equation, we use a mixed finite element method for the approximation of the pressure equation. In order to find a stable finite element discretization method, we use different discretization method for the concentration equation, such as finite element method with characteristic; mixed finite element method with characteristic; expanded mixed finite element method with characteristic etc. To linearize the discretized equations, we use one (two) Newton iterations on the fine grid in our methods. Firstly, we solve an original non-linear coupling problem. Then, solve a linear system on the fine grid and while in second method we make a correction on the coarse grid between one (two) Newton iterations on the fine grid. We obtain the error estimates of two-grid method, it is shown that coarse space can be extremely coarse and we achieve asymptotically optimal approximation. Finally, numerical experiment indicates that two-grid algorithm is very effective.

Recent advance in the weak Galerkin method for eigenvalue

problems

Ran Zhang Jilin University

This talk is devoted to introducing eigenvalue problem of PDEs by the weak Galerkin (WG) finite element method with an emphasis on obtaining lower bounds. The WG method uses discontinuous polynomials on polygonal or polyhedral finite element partitions. As such it is more robust and flexible in solving eigenvalue problems since it finds eigenvalue as a min-max of Rayleigh quotient in a larger finite element space. We demonstrate that the WG methods can achieve arbitrary high order convergence. This is in contrast with classical nonconforming finite element methods which can only provide the lower bound approximation by linear elements with only the second order convergence. Numerical results are presented to demonstrate the efficiency and accuracy of the WG method.

Adaptive and Multilevel Mixed Finite Element Methods

Jun Hu

Peking University

In the first part, we developed a block diagonal preconditioner with the minimal residual method and a block triangular preconditioner with the generalized minimal residual method for the mixed finite element methods of linear elasticity. They are based on a new stability result of the saddle point system in mesh-dependent norms. The mesh-dependent norm for the stress corresponds to the mass matrix which is easy to invert while the displacement it is spectral equivalent to Schur complement. A fast auxiliary space preconditioner based on the \$H^1\$ conforming linear element of the linear elasticity problem is then designed for solving the Schur complement. For both diagonal and triangular preconditioners, it is proved that the conditioning numbers of the preconditioned systems are bounded above by a constant independent of both the crucial Lam\'{e} constant and the mesh-size. Numerical examples are presented to support theoretical results.

In the second part, we proposed a posteriori error estimators for the symmetric mixed finite element methods for linear elasticity problems of Dirichlet and mixed boundary conditions. In particular, we proved reliability and efficiency of the estimators.

Polynomial preserving recovery of linear FEM for Helmholtz

equation with high wave number

Haijun Wu Nanjing University

We study superconvergence property of the linear finite element method with the polynomial preserving recovery (PPR) for the two dimensional Helmholtz equation. The H^1-error estimate with explicit dependence on the wave number k is derived. First, we prove that under the assumption $k(kh)^2 <= C_0$ and certain mesh condition, the estimate between the finite element solution and the linear interpolation of the exact solution is superconvergent under the H1-seminorm, where h is the mesh size. Second, we prove a similar result for the recovered gradient by PPR and explain the effect of PPR on the pollution error. Furthermore, we estimate the error between the finite element gradient and recovered gradient. All theoretical findings are verified by numerical tests.

High-Order Finite Volume methods for Hyperbolic PDEs on

Cartesian Grids

Christiane Helzel Heinrich-Heine-University

Hyperbolic partial differential equations (PDEs) modelling wave propagation arise in the description of dynamical processes in many diff t disciplines, ranging from engineering applications to geophysical flow to the description of biological processes. Many of these PDEs are in divergence form, i.e. are initial value problems of the form

> $\partial tq + \partial x 1 f1(q) + \ldots + \partial x d fd(q) = 0$ in $\Omega \times (0, T)$ q(x, 0) = qO(x) in Ω ,

where $\Omega \subset \text{Rd}$, $q: \text{Rd} \times \text{R}^+ \to \text{Rm}$ is a vector of conserved quantities and $f1, \ldots, fd$: $\text{Rm} \to \text{Rm}$ are vector valued flow functions. The Euler equations of gas dynamics, which describe conservation of mass, momentum and energy, are a prominent example. The construction of accurate and robust numerical methods for hyperbolic problems is an active research field. From the mathematical point of view, the difficulties arise due to the nonlinear flux functions, which lead to non-smooth solution structures such as shock waves. We restrict our considerations to finite volume schemes. Some of the most successful methods are multidimensional high resolution Godunov-type methods based on the use of Riemann solvers and nonlinear limiters. Such second-order methods may often be a good choice in terms of balance between computational cost and desired resolution, especially for problems with solutions dominated by shock waves or contact discontinuities and relatively simple structures between these discontinuities. However, for problems containing complicated smooth solution structures, where the accurate resolution of small scales is required, schemes with a higher order of accuracy are more efficient and computationally affordable.

I will present two of our recent contributions devoted to the development of high order accurate finite volume methods. The first approach is concerned with the construction of high order WENO finite volume methods on adaptively refined Cartesian grids and was recently published in [1, 2]. Our second part of the talk will be devoted to current work in progress towards the construction of a third order accurate wave propagation algorithm for acoustics problems.

[1] P. Buchmüller and C. Helzel, Improved accuracy of high-order WEMO finite volume methods on Cartesian rids, J. Sci. Comput., 2, pp. 343-368, 2014.

[2] P. Buchmüller, J. Dreher and C. Helzel, Finite volume WENO methods for hyperbolic conservation laws on Cartesian grids with adaptive mesh refinement, Appl. Math. Comput., 272, pp. 460-478, 2016.

Muntz Spectral Methods with Applications to Some Singular

Problems

Chuanju Xu Xiamen University

In this talk we will present a fractional spectral method for a class of equations with non-smooth solutions. The proposed method makes new use of the classical fractional polynomials, also known as Muntz polynomials. We will show how to construct efficient fractional spectral methods for some integro-differential equations which can achieve spectral accuracy for solutions with limited regularity. A detailed convergence analysis will be provided. The potential application of this method covers a large number of problems, including integro-differential equations with weakly singular kernels, fractional differential equations, and so on.

Optimal control of surface PDEs

Michael Hinze University Hamburg

Surface PDEs become increasingly important for e.g. the description, simulation, and control of diffusion processes on cell membranes. In this talk we introduce an optimal control approach for surface PDEs with special emphasis on its tailored discretization. We build our approach upon the discretization of the Laplace-Beltrami operator proposed by Dziuk in [1]. We numerically analyze the errors stemming from the discretization of the surface and of the finite element discretization of the surface PDE [2] and also consider pointwise control and/or state constraints [3]. We also present results for parabolic surface PDEs based on the work of Elliott and Dziuk [4], on Vierling [5], and Kr öner and the author [6]. Finally, we present numerical experiments which support our analytical findings.

[1] Dziuk, G. (1988) Finite elements for the Beltrami operator on arbitrary surfaces. Partial Differential Equations and Calculus of Variations (S. Hildebrandt & R. Leis eds). Lecture Notes in Mathematics, vol. 1357. Berlin: Springer, pp. 142–155.

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Robust a posteriori error estimation for a weak Galerkin

finite element discretization of Stokes equations

Xiaoping Xie Sichuan University

We propose a robust residual-based a posteriori error estimator for a weak Galerkin finite element method for Stokes equations in two and three dimensions. The estimator consists of two terms. The first term characterizes the difference between the \$L^2\$-projection of the velocity approximation on the element interfaces and the corresponding numerical trace, and the second term is related to the jump of the velocity approximation between the adjacent elements. We show that the estimator is reliable and efficient through two estimates of global upper and global lower bounds, up to two data oscillation terms caused by the source term and the nonhomogeneous Dirichlet boundary condition. The estimator is also robust in the sense that the constant factors in the upper and lower bounds are independent of the viscosity coefficient. Numerical results are provided to verify the theoretical results.

Efficient high order semi-implicit time discretization and local discontinuous Galerkin methods for highly nonlinear PDEs

Yan Xu

University of Science and Technology of China

In this talk, we present a high order semi-implicit time discretization method for highly nonlinear PDEs, which consist of the surface diffusion and Willmore flow of graphs, the phase field models, etc. These PDEs are high order in spatial derivatives, which motivates us to develop implicit or semi-implicit time marching methods to relax the severe time step restriction for stability of explicit methods. In addition, these PDEs are also highly nonlinear, fully implicit methods will incredibly increase the difficulty of implementation. In particular, we can not well separate the stiff and non-stiff components for these problems, which leads to traditional implicit-explicit methods nearly meaningless. In this paper, a high order semi-implicit time marching method and the local discontinuous Galerkin (LDG) spatial method are coupled together to achieve high order accuracy in both space and time, and to enhance the efficiency of the proposed approaches, the resulting linear or nonlinear algebraic systems are solved by multigrid solver. Numerical simulation results in one and two dimensions are presented to illustrate that the combination of the LDG method for spatial approximation, semi-implicit temporal integration with the multigrid solver provides a practical and efficient approach when solving this family of problems.

A two-scale Stefan problem arising in a model for tree-sap

exudation

Malte Peter University of Augsburg

The study of tree-sap exudation, in which a (leafless) tree generates elevated stem pressure in response to repeated daily freeze-thaw cycles, gives rise to a multiscale problem involving heat and multiphase liquid/gas transport. By assuming a periodic cellular structure based on an appropriate reference cell, we derive a homogenized heat equation governing the global temperature field on the scale of the tree stem, with all the remaining physics relegated to equations defined on the reference cell. The particular form of our homogenized temperature equation is obtained using periodic-homogenization techniques with two-scale convergence, which we apply rigorously in the context of a simpler two-phase Stefan-type problem corresponding to a periodic array of melting cylindrical ice bars, which is prototypical in the sense that it also relates to similar problems such as water uptake beyond capillary suction in concrete structures. Numerical simulations are performed to validate the results and draw conclusions regarding the phenomenon of sap exudation.

This is joint work with Isabell Konrad and John M. Stockie.

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Adaptive finite element method for incompressible

magnetohydrodynamics

Shipeng Mao

Institute of Computational Mathematics, AMSS, CAS, Beijing

Numerical modeling of nonlinear, fully coupled incompressible magnetohydrodynamics problem in three dimensions is usually a challenge work because of its complex features. Accuracy of FEMs for the MHD system is deteriorated by the presence of high Hartmann numbers, interior or boundary layers, shock fronts and complex geometries, which will be frequently encountered in practice. It makes the adaptive mesh refinement indispensable for the approximations by finite element methods. We consider a mixed finite element method for the numerical discretization of a stationary incompressible magnetohydrodynamics problem in three dimensions with its velocity field is discretized using \$H^1\$ conforming elements and the magnetic field is approximated by curl-conforming N & dec elements. Under the assumption that the original model has a unique solution pair, we derive a posteriori error estimates of the incompressible magnetohydrodynamic (MHD) equations with a sharp upper bound. Using these a posteriori error estimates, we construct an adaptive algorithm for computing the solution of 3D magnetohydrodynamics. Numerical experiments are carried out to show the performance of the adaptive finite element method.

Finding 13-Moment System Beyond Grad

Ruo Li Peking University

We point out that the thermodynamic equilibrium is not an interior point of the hyperbolicity region of Grad's 13-moment system. With a compact expansion of the phase density, which is compacter than Grad's expansion, we derived a modified 13-moment system. The new 13-moment system admits the thermodynamic equilibrium as an interior point of its hyperbolicity region. We deduce a concise criterion to ensure the hyperbolicity, thus the hyperbolicity region can be quantitatively depicted.

Two methods for Finding Multiple Solutions of Semilinear

PDEs

Ziqing Xie Hunan Normal University

In this talk, we present two approaches for finding the multiple solutions of semilinear PDEs. The first one is the Normalized Goldstein-type Local Minimax Method (NG-LMM) which is aimed to find multiple minimax-type solutions with variational structures. The second one is the Augmented Partial Newton Method (APNM) which is devoted to find multiple minimax-type solutions of semilinear PDEs no matter whether they are variatioal or not. More significantly, these two approaches are large-scope algorithms. The corresponding theoretical analysis is provided also.

Keywords: Semilinear elliptic PDEs, global convergence, multiple solutions, local minimax method, normalized Goldstein-type search rule, augmented parial Newton method, augmented singular transform.

Numerical homogenization of fault networks

Ralf Kornhuber Free University of Berlin

Numerical homogenization aims at the construction of low-dimensional ansatz spaces for the approximation of solutions of elliptic partial differential equations with fine scale features such as, e.g., strongly oscillating coefficients. Well-known strategies involve the heterogeneous multiscale method [1, 2], the variational multiscale method [4], and multiscale finite elements [3].

A big step forward in the numerical analysis of multiscale finite elements was made in a recent paper by M åqvist and Peterseim [7] based on its reinterpretation in terms of a decomposition into the kernel of a suitable projection to a parent finite element space and its orthogonal complement together with subsequent localization.

We present a novel iterative localization strategy that directly exploits the highfrequency of the kernel of the projection [5]. It allows for adaptive selection of the support of the resulting multiscale basis functions and, in contrast to previous techniques, amounts to the solution of local self-adjoint fine-grid problems instead of local saddle point problems. Optimal discretization error estimates are obtained by basic results from subspace correction. In contrast to this kind of direct numerical homogenization, iterative numerical homogenization techniques [6] provide approximations with optimal discretization error by multiple solutions of a coarse-grid problem and local self-adjoint fine-grid problems.

Our theoretical findings are confirmed by numerical computations for elliptic partial differential equations with strongly oscillating coefficients. As another application we consider elliptic partial differential equations with linear jump conditions on a multiscale network of faults. The jump conditions stand for linear counterparts of rate-and-state-dependent friction [8]. We discuss the selection of appropriate projections and coarse-grid spaces and present numerical experiments with iterative and direct numerical homogenization.

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A continuous DG time stepping method and its adaptive

algorithms for second order evolution problems

Jianguo Huang Shanghai Jiao Tong University

Second order dynamical systems frequently occur In the areas of civil engineering, material science, structural analysis and electrical engineering. The finite difference method is a typical approach for discretization in time. However, such treatment is not convenient to produce adaptive time stepping methods. In this talk, I will first introduce the continuous \$P_2\$ discontinuous Galerkin (DG) method for solving a second order evolution problem. Then, I will introduce an adaptive time stepping method based on the a posteriori error estimator for the previous method. To further increase the computational efficiency, I will introduce a hybrid time stepping method, which is the combination of an adaptive finite element method and the spectral Picard method. This method has the advantage of small amount of computational cost and high accuracy of numerical solution, and is particularly suitable for capturing the solution with rapid change in time. Several numerical experiments are provided to show the computational performance and efficiency of the proposed methods. This is a joint work with Junjiang Lai, Huashan Sheng and Tao Tang.

Finite element approximation of singular solution and singular data of time-harmonic Maxwell equations by Rieszlifting

Huoyuan Duan Wuhan University

A new weak form of the three-dimensional (3D) time-harmonic Maxwell equations in Lipschitz domain is explored, and by mimicking this weak form through the Riesz representation lifting, a new Lagrange finite element method is proposed. With the help of regular-singular decomposition of vector fields, the coercivity, the convergence and the error bounds are established in H(curl;Omega)-norm. The proposed method is suitable for singular solution lying outside $(H^1(Omega))^3$, singular inhomogeneous boundary data in the tangential trace space of H(curl;Omega) and singular right-hand side source data in $(H_0(curl;Omega))'$ (the dual of $H_0(curl;Omega)$). Numerical results are presented to illustrate the performance and the theoretical results of the new method.

A hybrid method for multiscale PDEs

Pingbing Ming The State Key Laboratory of Scientific and Engineering Computing, AMSS, CAS, Beijing

We present a new hybrid numerical method for multiscale partial differential equations, which simultaneously captures both the global macroscopic information and resolves the local microscopic events. The convergence of the proposed method is proved for problems with bounded and measurable coefficient, while the rate of convergence is established for problems with rapidly oscillating periodic or almost-periodic coefficients. Numerical results are reported to show the efficiency and accuracy of the proposed method. This is a joint work with Jianfeng Lu and Yuhuang Huang.

Multilevel domain-decomposition methods for radiation

diffusion and radiation transport

Guido Kanschat Heidelberg University

Radiation diffusion and radiation transport simulations have been an important tool in nuclear reactor design and now are becoming increasingly important in climate modeling. While a detailed computation of radiative energy balance is still challenging due to the fact that we have to consider a six dimensional problem, the increasing memory size of high performance computers has made coupling of radiation and hydrodynamics feasible during the last years. Here, we present numerical methods, which allow the efficient implementation of such models. Both radiation diffusion and radiation transport exhibit features which pose obstacles to the solution of such problems on computers. These are mainly the lack of symmetry of the transport and the energy redistribution operators, as well as extreme parameters in realistic environments. In particular the dominance of scattering, which we find for instance in atmospheric and interstellar clouds, but also in parts of nuclear reactor setups poses a challenge to numerical methods, since the Boltzmann equation modelling transport of radiation in general changes its character from a hyperbolic problem to a diffusive one. We then discuss discontinuous Galerkin methods which are have the same diffusion limit [RGK12], thus overcoming the deficiencies of such methods observed in [Ada01]. The issue at hand is an observed lack of convergence of standard methods if on average photons are scattered more than once while traveling through a mesh cell. We present an optimal domain-decomposition method for the radiation diffusion problem and its analysis, which employs a recently discovered technique [FL13]. Then, we apply the same concept to the harder radiation transport problem and obtain a very fast solver [KR14], which we compare to similar developments for the diamond stencil in [CMMRS07]. Here again, we need a method which can deal with the hyperbolic nature of radiation transport in voids as well as the diffusive nature in dense, scattering clouds. The first aspect is covered by an algorithm which follows rays of radiation in all directions; On standard meshes in three dimensions, this can be covered by eight specially chosen directions and thus at a moderate increase of work. The elliptic nature of the problem is taken into account by solving the whole radiation problem on each subdomain, not just the decoupled transport problem as in previous iterative approaches. We present model applications in astrophysics and nuclear science to show the usefulness of our method, in particular fast convergence independent of the problem parameters.

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Adaptive finite element iterative approximation of optimal

control governed by PDEs

Danping Yang and Zheng Li East China Normal University

There have been extensive researches for adaptive finite element approximations of PDEs. Recently, analysis of adaptive finite element methods for optimal control problems governed by PDEs also were done. In general, optimal control problems governed by PDEs are nonlinear problems. During the procedure of mesh refining, the nonlinear problem must be solved by using iterative algorithm. As result, a lot of computational works are required. In this talk, we will discuss the adaptive finite element iterative algorithms of optimal control governed by PDEs. In this algorithm, we couple iteration step and mesh refining procedure together, i.e., at each iterative step finite element mesh also is refined. Our mathematical analysis and numerical tests show that under some conditions, this algorithm produce the approximating sequences with a geometrically convergent rate.

A Conforming Enriched Finite Element Method for Elliptic

Interface Problems

Hua Wang and Jinru Chen Nanjing Normal University

Let Ω be a convex polygon in \mathbb{R}^2 and separated by a C^2 -continuous interface Γ into two sub-domains Ω_1 and Ω_2 . We consider the following interface problem

$$-\operatorname{div}(\beta \nabla u) = f \text{ in } \Omega_1 \cup \Omega_2,$$
$$u = 0 \text{ on } \partial \Omega,$$

with interface conditions

$$[u] = 0 \text{ on } \Gamma,$$
$$\left[\beta \frac{\partial u}{\partial \mathbf{n}}\right] = 0 \text{ on } \Gamma.$$

And the coefficient function $\beta(x, y)$ is discontinuous across the interface

$$\beta(x, y) = \begin{cases} \beta_1(x, y), & (x, y) \in \Omega_1, \\ \beta_2(x, y), & (x, y) \in \Omega_2, \end{cases}$$

where $\beta_i(x, y) (> 0) \in W^{1,\infty}(\Omega_i)$. The interface problem occurs widely in practical applications, such as fluid mechanics, electromagnetic wave propagations, materials sciences, and biological sciences. There are two major classes of finite element methods (FEM) for interface problems, namely, interface-fitted FEM and interface-unfitted FEM, categorized according to the topological relation between discrete elements and the interface. However, letting the mesh conform to the interfaces requires remeshing as these evolve with time, and leads to significant complications when topological changes such as drop-breakup or coalescence occur. Then interface-unfitted methods have become highly attractive. There are mainly two types of interface-unfitted methods, the extended finite element methods and the immersed finite element methods.

The extended finite element method (XFEM) has been successfully applied to a wide range of engineering problems, e.g., crack-propagation, material modeling, and solid-fluid interactions. XFEM was originally introduced in (Belytschko 1999, Moes 1999) to solve elastic crack problems, and one of its feature is the basis functions can be discontinuous when across the interface. A combination of the extend finite element method and Nitsche scheme is proposed in (Hansbo 2002). Then, an unfitted hp-interface penalty FEM was proposed in (Wu 2010). We refer to (Fries 2010) and the references therein for a historical account of XFEM.

The immersed finite element method (IFEM) was original developed by Z. Li in 1998. And then a lot works based on IFEM were presented (Li 2003, Kwak 2010 and Lin 2015). The key idea of IFEM is to modify basis functions to satisfy the interface conditions such that they can approximate the solutions of interface problems better.

If we use Nitsche-XFEM to solve an interface problem, the variational formulation need to change. And if we use IFEM, the FE space for each component is not independent and the interpolation error estimate remains unproved when it comes to vector field interface problems. It is interesting to construct a conforming approximation space for interface problems with optimal convergence rate. If so, we do not need to change variational formulation and can define the same approximation spaces for each component of vector field spaces.

In this paper, we propose a new conforming FE method for the elliptic interface problem. And it can be used in other interface problems (elasticity or Stokes interface problems) as well. For the sack of simplicity, we take the elliptic interface problem as an example.

Exponential-type time integrators for nonlinear Schrödinger,

Korteweg-de Vries and Klein-Gordon type equations

Katharina Schratz Karlsruhe Institute of Technology

In the context of the numerical time integration of (non)linear partial differential equations splitting methods as well as exponential integrators contribute attractive classes of integration methods. In recent years, they have in particular gained a lot of attention in the context of the numerical time integration of non-linear Schrödinger equations, the Korteweg-de Vries equation, semi-linear wave and Klein-Gordon type equations. In this talk I will present some recent developments in the construction of low-regularity exponential-type integrators for non-linear Schrödinger (NLS) equations as well as the Korteweg-de Vries (KdV) equation. The idea is thereby based on the discretization of Duhamel's formula looking at the "twisted variable" obtained by a rescaling transformation with respect to the leading differential operator. This idea of "twisting" the variable is widely used in the analysis of partial differential equations in low regularity spaces and also well known in numerical analysis in the context of Lawson-type Runge-Kutta methods. Instead of approximating the appearing integrals with a classical Runge-Kutta method we integrate, based on the Fourier decomposition of the exact solution, the dominant stiff parts exactly. This allows us to derive a new class of explicit exponentialtype time integration schemes, which converge under weaker regularity assumptions than classical methods. Similar ideas can be used in the construction of uniformly accurate integration schemes for Klein-Gordon type equations in highly-oscillatory nonrelativistic limit regimes where the speed of light formally tends to infinity. The newly derived exponential-type integrators in particular allow asymptotic converge to classical splitting schemes in the non-linear Schrödinger limit.

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The immersed finite volume method for elliptic interface

problems

Qingsong Zou Sun Yat-sen University

In this talk, we will present immersed FVMs for elliptic interface problems. The stability of the method is shown to be independent of the location of the interface. As a consequence, both the \$H^1\$ and \$L^2\$ norm error of the method have optimal convergence rates. Several numerical examples show the advantages of our method over the classic immersed finite element methods.

Efficient algorithm for nonlocal/time-fractional models

Jiwei Zhang Beijing Computational Science Research Center

This talk has two parts. The first part focuses on the fast evaluation of Caputo fractional derivative and its applications to anomalous diffusion equations. The second part focuses on the design of exact absorbing boundary conditions for nonlocal models, such as nonlocal heat equation, nonlocal Schrödinger equation Some numerical examples are presented to demonstrate the effectiveness of our approach.

Extended WKB analysis for the high-frequency linear wave

equations

Chunxiong Zheng Tsinghua University

WKB analysis is a powerful tool for seeking the asymptotic solutions to the highfrequency wave equations. However, it suffers from the occurrence of caustics, around which the WKB approximation is no longer valid. It turns out that for linear wave equations, the right ansatz to the solution should be the extended WKB functions. In this talk, I will explain the basic idea of extended WKB analysis, formulate the main results, and report its applications to various mathematical physics equations.

Error analysis of a variational multiscale stabilization for

convection-dominated diffusion equations

Mira Schedensack Humboldt University of Berlin

Convection-dominated diffusion equations usually exhibit steep gradients of the solution in boundary layers due to the singularly perturbed nature of the problem. This leads to oscillating approximations, if the boundary layer is not resolved properly by the underlying finite element mesh. This talk formulates a stabilized Petrov-Galerkin method for singularly perturbed convection-diffusion problems based on the variational multiscale method. The stabilization is of Petrov-Galerkin type with a standard finite element trial space and a problem-dependent test space based on precomputed fine-scale correctors. The exponential decay of these correctors and their localisation to local patch problems, which depend on the direction of the velocity field and the singular perturbation parameter, is rigorously justified. Under moderate assumptions, this stabilization guarantees stability and quasi-optimal rate of convergence in 2d for arbitrary mesh Peclet numbers on fairly coarse meshes at the cost of additional inter-element communication. As the discrete solution equals the nodal interpolation of the exact solution up to an exponentially decaying term, also the L² error converges with the optimal rate of convergence. Numerical experiments will provide some insight in the choice of the localisation parameter.

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Convergence of adaptive finite element method for elliptic

optimal control problems

Wei Gong

LSEC, Institute of Computational Mathematics, AMSS, CAS, Beijing

In this talk we present recent advance on the convergence analysis of adaptive finite element method for elliptic optimal control problems with pointwise control constraints. We use variational discretization concept to discretize the control variable and piecewise linear and continuous finite elements to approximate the state variable. Based on the well-established convergence theory of AFEM for elliptic boundary value problems, we rigorously prove the convergence and quasi-optimality of AFEM for optimal control problems with respect to the state and adjoint state variables, by using the so-called perturbation argument. To prove the optimality of AFEM for the control variable, we also study the convergence of L^2-norm based adaptive algorithm. Extensive numerical experiments will be presented to confirm our theoretical analysis.

Numerical simulation of Bose-Einstein-Condensates

Daniel Peterseim University of Augsburg

This talk reviews some numerical methods for the simulation of Bose-Einstein-Condensates modelled by nonlinear Schrödinger equations. We consider both the computation of stationary states as well as the simulation of the dynamics. Among the methodological and mathematical novelties are variational multiscale spatial discretization schemes for the acceleration of non-linear eigenvalue solvers [2,3]. Moreover, the talk addresses the numerical analysis of classical time-stepping schemes in the presence of disorder potentials [3]. Under low regularity assumptions, that are compatible with discontinuous potentials, we prove convergence with rates for the massand energy conserving variant of the Crank-Nicolson time discretization scheme due to Sanz-Serna. While for sufficiently smooth potentials, the rates are optimal without any coupling condition between the time step size and the spatial mesh width, the sharpness of the rates and the necessity of some coupling condition is open in the non-smooth case and will be discussed in a sequence of numerical experiments.

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Decomposition of nonlocal norms and quantitative

dependence analysis for nonlocal diffusion models

Xuying Zhao

Academy of Mathematics and Systems Science, CAS, Beijing

In this talk, several decomposition properties for nonlocal norms of double integrals arising from nonlocal models will be presented. Based on it, how the equivalence between the energy norm and the Sobolev space norm depends on the horizon and other parameters for nonlocal diffusion models will be revealed. More results with quantitative dependence on the horizon and other parameters are further established, such as the nonlocal Poincar\'e inequality, the priori error estimation, and condition numbers of the stiffness matrix. Both the case of integrable kernels and the case of non-integrable kernels are considered herein.

A posteriori error analysis of equations in nondivergence form

with Cordes coefficients

Dietmar Gallistl Karlsruhe Institute of Technology

This talk discusses formulations of some linear and nonlinear second-order elliptic partial differential equations in nondivergence form on convex domains as equivalent variational problems. These formulations enable the use of a class of mixed finite element methods with standard trial spaces. Besides the immediate quasi-optimal a priori error bounds, the variational setting allows for a posteriori error control with explicit constants and adaptive mesh-refinement. The convergence of an adaptive algorithm for linear problems is proved. Numerical results on uniform and adaptive meshes are included.

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A fast numerical method for simulating ion structure near

core-shell dielectric nanoparticle

Manman Ma Tongji University

A generalized image charge formulation is proposed for the Green's function of a core-shell dielectric nanoparticle for which theoretical and simulation investigations are rarely reported due to the difficulty of resolving the dielectric heterogeneity. Based on the formulation, we develop an efficient and accurate algorithm for calculating electrostatic polarization charges of mobile ions. Monte Carlo simulations based on the algorithm show that a fine-tuning of the shell thickness and ion-interface correlation strength can greatly alter electric double-layer structures and capacitances, owning to the complicated interplay between dielectric boundary effects and ion-interface correlations.

Local Information

Accommodation

Kingswell Hotel Tongji 同济君禧大酒店 Address: No. 50, Zhangwu Road, Yangpu District, Shanghai 上海杨浦区彰武路 50 号

Conference Venue

Room 1002, Tongji University Multi-Functional Building 同济大学四平路校区综合楼 1002 室

Transportation

From airports or railway stations to the Hotel:

From Pudong International Airport (PVG)

- 1. By Taxi, about 50 min, RMB 150.
- 2. By Subway:

take Maglev Train to Longyang Road,

transfer to Subway Line 2 (Xujing East direction), to Nanjing East Road Station,

transfer to Subway Line 10 (Xinjiangwancheng direction), to Tongji University Station, walk 5 min to Kingswell Hotel Tongji.

From Hongqiao International Airport / Hongqiao Railway Station

- 1. By Taxi, about 45 min, RMB 100.
- 2. By Subway:

take Subway Line 10 (Xinjiangwancheng direction) to Tongji University Station, walk 5 min to Kingswell Hotel Tongji.

From Shanghai Railway Station

- 1. By Taxi, about 20 min, RMB 25.
- 2. By Subway:

take Subway Line 4 (Baoshan Road direction) to Hailun Road Station,

transfer to Subway Line 10 (Xinjiangwancheng direction), to Tongji University Station, walk 5 min to Kingswell Hotel Tongji.

From hotel to the conference venue:

10 min's walk, about 500 meters, see following maps

Lunch&Dinner

Lunch: October 9-13, at Sanhaowu Restaurant, 2nd Fl. (三好坞餐厅二楼)

Banquet dinner: takes place at 18:50, October 10, at Kingswell Hotel Tongji(同济 君禧大酒店)

Dinner: 18:30, October 8, at Kingswell Hotel Tongji(同济君禧大酒店)

18:50, October 9, 11-13, at Sanhaowu Restaurant, 2nd Fl. (三好坞餐厅二楼)

Maps on the following pages are for participants' reference

Map 1: Pudong International Airport (PVG), Hongqiao International Airport / Hongqiao Railway Station, Kingswell Hotel Tongji



Map 2: Shanghai Railway Station, Kingswell Hotel Tongji



Map 3: Kingswell Hotel Tongji, Conference venue, Sanhaowu Chineses Restaurant

