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Title: A cut-cell Method for the Numerical Solution of flows past obstacles

Abstract: we present a second order cut cell method and applications to the numerical solution of flows around obstacles. The method is based on the MAC-Scheme, but the discretization is adapted close to the obstacle. The second order convergence is observed, simulations at Reynolds Numbers up to 9500 have been performed with a parallel version of the algorithm and using fast solvers.

Weizhu Bao
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Title: Sharp Interface Models for Solid-State Dewetting Problems

Abstract: In this talk, I will present sharp interface models with anisotropic surface energy for simulating solid-state dewetting and the morphological evolution of patterned islands on a substrate. We will show how to derive the sharp interface model via thermovariation dynamics, i.e. variation of the interfacial energy via an open curve with two triple points moving along a fixed substrate. The sharp interface model tracks the moving interface explicitly and it is very easy to be handled in two dimensions via arc-length parametrization. An efficient and accurate parameteric finite element method (PFEM) was proposed for the sharp interface models. It is applied to study numerically different setups of solid-state dewetting including short and long island films, pinch-off, hole dynamics, semi-infinite film, tiny particle migration, etc. Our results agree with experimental results very well. In addition, extension to curved substrate and three dimensions will be discussed. Finally, we also present a reduced variational model via the Onsager's principle for small particle migration in solid-state dewetting. This is joint works with Wei Jiang, David J. Srolovitz, Carl V. Thompson, Yan Wang and Quan Zhao.

Li Cai
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Northwestern Polytechnical University

Title: Immersed boundary method with applications to heart

Abstract: The immersed boundary method is an approach to FSI that uses a Lagrange description of the structural and an Eulerian description of the fluid-structure system. Based on the weak formulation, the standard nodal finite element method is used to calculate the internal force density and the transmission force density. Hence, our

approach uses a finite element discretizations of the structure while using a finite difference scheme for the Eulerian variables. The proposed method is used to study the fluid-structure interaction problems encountered in human cardiovascular system (left ventricle, artery and mitral valve).

Mingchao Cai,
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Title: Fast solvers for models of fluid flow, linear elasticity and poroelasticity

Abstract: Fluid flow model, linear elasticity model, and poroelasticity model have wide applications in geosciences and biomechanics. For example, blood-vessel wall interactions are modeled by using both fluid flow model and elasticity model; brain edema and cancellous bones are usually modeled by using poroelastic models. For incompressible fluid flow model, I will discuss the Cahouet-Chabard preconditioner using exact and inexact Multigrid solvers under the MAC finite difference discretization; particularly, variable-coefficient Stokes solver will be presented. For linear elasticity model under a stable Finite Element discretization, the two-level overlapping Schwarz methods will be presented, robustness of the domain decomposition solvers with respect to coefficient jumps will be discussed. For poroelasticity model, I will show some solvers under the MAC discretization and a stabilized Finite Element discretization.

Shanggui Cai
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Sorbonne Universités/ Université de Technologie de Compiègne, France

Title: Moving Immersed Boundary Method for Fluid-Structure Interaction

Abstract: A new formulation of immersed boundary method, called moving immersed boundary method (MIBM), will be presented for efficient and accurate computation of fluid-structure interaction. The idea of operator splitting is successively used in present work as it decomposes complicated system into simple ones that are easy to be solved. First the pressure, which is usually regarded as a Lagrange multiplier for the continuity condition, is decoupled from the velocity field through a prediction-projection procedure, leading to a Helmholtz type equation for the velocity and a Poisson type equation for the pressure. Similarly, the boundary force, which can be viewed as another Lagrange multiplier for the no-slip wall condition, is formulated into a separated system whose dimension only concerns the discretization of solid surface. Therefore, the fluid is solved sequentially by velocity prediction, boundary forcing and pressure projection. As for the fluid-structure interaction, instead of solving one large system simultaneously (monolithic approach), two solvers are employed for each sub-problem (partitioned approach) which is actually another operator splitting. An implicit scheme is employed for the strong coupling between two physical fields, while a different non-linear Piccard iteration is introduced to reduce the computational time. It

is known that operator splitting may introduce errors in general and can cause added mass instabilities for the fluid-structure interaction computation. Improvements will be presented towards the accuracy and the stability, in order to enjoy the benefits of the operator spitting.

Thierry Coupez
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Title: Implicit Boundary and Anisotropic Mesh Adaptation for Multiphase Flow Simulations

Abstract: A wider use of numerical simulation is still depending on meshing and adaptive meshing capabilities when complex geometry, multi-domain, moving interface and multiphase flow are involved. This task becomes more and more difficult when it is combined with a posteriori adaptive meshing or/and dealing with moving interfaces and boundary layers and also when running on massively parallel computers. In order to overcome the lack of flexibility of the common body fitted method, the alternative proposed here, is based on an implicit representation of the interfaces by a local distance function using a hyperbolic tangent filter. Therefore, the geometries can be interpolated and contribute to the numerical error which is detected by an a posteriori error estimate. This approach favours the full usage of anisotropic adaptive meshing techniques providing an optimal capture of the interfaces within the volume mesh, whatever is the complexity of the geometry involved. From the flow solver side, unstructured meshes with highly distorted elements (however solution aligned) need to rely on a robust solution framework. The interface condition transfer is enforced by following the immersed boundary/volume (IVM) methodologies for fluid/fluid and or fluid/structure interaction. The proposed multiphase flow solver, including the convected local level set technique is based on a stabilized finite element method (VMS) that can afford with anisotropic meshing even with high aspect ratio elements. The general stabilization approach including the interface stabilization term and the dynamic will be introduced with a quasi-optimal calculation of the stabilization parameter for anisotropic finite elements. The multiphase navier stokes error estimation and the associated metric calculation will be discussed and various application examples will be proposed.

Philippe Remy Bernard Devloo1
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Title: On the development of a multiscale reservoir simulator with geomechanics coupling

Abstract: In this contribution the development of a numerical simulator for two phase flow with geomechanics coupling is presented. The simulator uses the Multiscale Hybrid Mixed method to optimize computational costs. The geomechanics coupling

uses a reduced basis approximation, leading to a fully coupled geomechanics simulator with high precision and reduced computational cost. The simulator uses $H(\text{div})$ approximations for approximating the flux function, discontinuous approximations for the pressure variable and saturation and H^1 continuous approximations for the displacement variable. Conservation of mass is ensured by the proper balance of the $H(\text{div})$ approximation space and pressure space. The effectiveness of the proposed simulator is demonstrated by evaluating the error when simulating problems with analytic solution. Finally the simulator is applied to a reservoir simulation of a five spot configuration where the wells are represented with their real geometry.

Robert Dillon

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Title: Immersed interface-immersed boundary methods for AC and DC dielectrophoretic particle interaction in a microchannel.

Abstract: Dielectrophoresis, a nonlinear electrokinetic transport mechanism, has become popular in many engineering applications including manipulation, characterization and actuation of biomaterials, particles and biological cells. Here, we describe a hybrid immersed interface-immersed boundary method to study dielectrophoresis where an algorithm is developed to solve the complex Poisson equation using a real variable formulation. An immersed interface method is employed to obtain the AC electric field in a fluid media with suspended particles and an immersed boundary method is used for the fluid equations and particle transport. In these studies, the Maxwell stress tensor is used to calculate the dielectrophoretic force acting on particles by considering the physical effect of particles in the computational domain. The hybrid method is used to investigate the physics of dielectrophoresis in microfluidic devices using a AC as well as DC electric fields. We present results for dielectrophoretic (DEP) interactions and particle assembly in several scenarios.

Songming Hou

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Title: Some Recent Advances on the Non-traditional Finite Element Method for Interface Problems

Abstract: Interface problems occur in many multi-physics and multi-phase applications in science and engineering. We proposed a non-traditional finite element method for solving elliptic and elasticity interface problems using non-body-fitted mesh. This talk presents an introduction and some recent advances of this method, including multi-domain problems in three dimensions, interface problems with imperfect contact condition, wave equation with interfaces, and some additional topics.

Peiqi Huang
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Title: Some stabilized locking-free nonconforming immersed interface finite element methods for planar elasticity interface problems with non-homogeneous jump conditions

Abstract: In this paper, a class of new nonconforming immersed interface finite element methods are developed to solve elasticity interface problems with non-homogeneous jump conditions in two dimensions. A pair of functions that satisfy the same non-homogeneous jump conditions are constructed using a level-set representation of the interface. With such a pair of functions, the discontinuities across the interface in the solution and flux are removed; and an equivalent elasticity interface problem with homogeneous jump conditions is formulated. Using the stabilized method, we prove the well-posedness of the discrete form. Error analysis are presented to demonstrate that such methods have an optimal convergence rate and are independent of the Lamé constants. Finally, numerical examples are presented to illustrate the theoretical results.

Weihua Geng
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Southern Methodist University

Title: An Regularized Matched Interface and Boundary (rMIB) Method and its Biological Application in Computing Protein pKa Values.

Abstract: The pKa values are important quantities characterizing the ability of protein active sites to give up protons. pKa can be measured using NMR by tracing chemical-shifts of some special atoms, which is however expensive and time-consuming.

Alternatively, pKa can be calculated numerically by electrostatic free energy changes subject to the protonation and deprotonation of titration sites. To this end, the Poisson-Boltzmann (PB) model is an effective approach for the electrostatics.

However, numerically solving PB equation is challenging due to the jump conditions across the dielectric interfaces, irregular geometries of the molecular surface, and charge singularities. Our recently developed matched interface and boundary (MIB) method treats these challenges rigorously, resulting in a solid second order MIBPB solver. Since the MIBPB solver uses Green's function based regularization of charge singularities by decomposing the solution into a singular component and a regularized component, it is particularly efficient in treating the accuracy-sensitive, numerous, and complicated charges distribution from the pKa calculation. Our numerical results demonstrate that accurate electrostatics potentials, forces, energies, and pKa values are achieved at coarse grid rapidly. In addition, the resulting software, which pipelines the entire pKa calculation procedure, is available to all potential users from the greater bioscience community.

Ruchi Guo
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Title: A Fixed Mesh Method With Immersed Finite Elements for Solving Interface Inverse Problems

Abstract: In this talk, we present a new fixed mesh algorithm for solving a class of interface inverse problems for the typical elliptic interface problems. These interface inverse problems are formulated as shape optimization problems whose objective functionals depend on the interface shape. Both the governing partial differential equations and objective functionals are discretized optimally by an immersed finite element (IFE) method on a fixed mesh independent of interface location. The formula for the shape sensitivities of the discretized objective functions is derived within the IFE framework that can be computed accurately and efficiently through the discretized adjoint method. We show its applications to a group of representative interface inverse/design problems.

Kazufumi Ito
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Title: Nonsmooth optimization approach to Free boundary and Interface Problems.

Abstract: Constrained minimization and Variational inequalities are formulated for free boundary problems including fluid-structure interaction. Numerical algorithms are developed and analyzed.

Do Wan Kim
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Inha University

Title: Variational Boundary Integral Method for Finding Free Boundaries on Jet Flow

Abstract: We consider asymmetric impinging jets issuing from an arbitrary nozzle. The flow is assumed to be two-dimensional, inviscid, incompressible and irrotational. The impinging jet from an arbitrary nozzle has a couple of separated infinite free boundaries, which makes the problem hard to solve. We formulate this problem using the stream function represented with a specific single layer potential. This potential can be extended to the surrounding region of the jet flow, and this extension can be proved to be a bounded function. Using this fact, the formulation yields the boundary integral equations on the entire nozzle and free boundary. In addition, a boundary perturbation produces an extraordinary boundary integral equation for the boundary variation. Based on these variational boundary integral equations, we can provide an efficient algorithm that can treat with the asymmetric impinging jets having arbitrarily shaped nozzles. Particularly, the proposed algorithm uses the infinite computational domain instead of

a truncated one. To show the convergence and accuracy of the numerical solution, we compare our solutions with the exact solutions of free jets. Numerical results on diverse impinging jets with nozzles of various shapes are also presented to demonstrate the applicability and reliability of the algorithm.

Do Young Kwak
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Korea Advanced Institute of Science and Technology

Title: A Kouhia Stenberg type immersed finite element method for elasticity problems

Abstract: We develop a new finite element method for solving planar elasticity problems involving heterogeneous materials with a mesh not necessarily aligning with the interface of the materials. This method is based on the Kouhia-Stenberg [CMAME, 1995] method for solving elasticity problem and Crouzeix-Raviart type IFEM scheme developed for scalar interface problems [D.Y. Kwak, K.T. Wee and K.S. Chang, SINUM (2010)]. To ensure the Korn's inequality for the bilinear form for interface problem, we add stabilizing terms as in the discontinuous Galerkin (DG) method in one of the component. The novelty of our method is that we use meshes independent of the interface, so that the interface may cut through the elements. Instead, we modify the basis functions so that they satisfy the traction condition along the interface of each element. We show the uniqueness and existence of IFE satisfying the prove optimal H^1 , L^2 norm error estimates. Numerical experiments are carried out to demonstrate that our method is optimal for various Lam's parameters μ and λ and show the scheme is locking free.

Long Lee

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University of Wyoming

Title: Numerical renormalization group algorithms for self-similar solutions of a modified porous medium equation with discontinuous diffusivity across the interface

Abstract: We systematically study a numerical procedure that reveals the asymptotically self-similar dynamics of solutions of partial differential equations (PDEs). This procedure, based on the renormalization group (RG) theory for PDEs can be applied to a wide range of PDEs to shed lights on new physics, in particular on the asymptotic self-similar solutions of PDEs. We illustrate that this numerical version of RG method, dubbed as the numerical RG algorithm, numerically rescales the temporal and spatial variables in each iteration and drives the solutions to a fixed point exponentially fast, which corresponds to self-similar dynamics of the equations. Using this numerical RG algorithm, we study the time decay rate of the asymptotic self-similarity solution of a nonlinear diffusion equation with absorption. This modified porous medium equation has discontinuous diffusivity across the interface.

Wei Leng
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Title: ALE Method in the Artificial Heart Pump Simulation

Abstract: A dynamic fluid-structure interaction (FSI) problem involving a rotational elastic turbine is studied. The problem is modeled by the incompressible fluid model in the fluid domain with the arbitrary Lagrangian-Eulerian (ALE) description and by the St. Venant-Kirchhoff structure model in the structure domain with the Lagrangian description, and the application to a hemodynamic FSI problem involving an artificial heart pump with a rotating rotor. A linearized rotational and deformable structure model is developed for the rotating rotor and a monolithic mixed ALE finite element method is developed for the hemodynamic FSI system. Numerical simulations are carried out for a hemodynamic FSI model with an artificial heart pump, and are validated by comparing with a commercial CFD package for a simplified artificial heart pump.

Chenliang Li
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Title: Cascadic multigrid method for the interface problems

Abstract: In this talk we present some cascadic multigrid methods for solving the elliptic interface problems based on the linear and bilinear interface elements. Numerical experiments show the efficiency of the new methods.

Xiaofan Li
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Illinois Institute of Technology

Title: Motion of particles in unsteady Stokes and linear viscoelastic fluids

Abstract: Studying effects of moving particles on fluids is of fundamental importance for understanding particle dynamics and binding kinetics. Conventional asymptotic solutions may lead to poor accuracy for neighboring particles. We present an accurate boundary integral method to calculate forces exerted on particles for a given velocity field. The idea is to exploit a correspondence principle between the unsteady Stokes and linear viscoelasticity in the Fourier domain such that a unifying boundary integral formulation can be established for the resulting Brinkman equation.

Ping Lin
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Title: An Energy Law Preserving Finite Element Scheme for a Moving Contact Line Problem

Abstract: In this talk, we consider a phase field model of Cahn-Hilliard type for moving contact line problems governing the motion of isothermal multiphase incompressible fluids. The generalized Navier boundary condition proposed by Qian et al. is adopted. We discretize model equations using a continuous finite element method in space and a modified midpoint scheme in time. A discrete energy law which is a good approximation of the continuous energy law is derived for the scheme. Two kinds of immiscible fluids in a pipe and droplet displacement with a moving contact line under the effect of pressure driven shear flow are computed using a relatively coarse grid. We also derive the discrete energy law for the droplet displacement case, which is a slightly different problem due to the boundary condition. Accuracy and stability of the scheme are validated through some test computations.

Tao Lin
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Virginia Polytechnic Institute and State University (Virginia Tech)

Title: A unified framework for developing and analyzing immersed finite elements

Abstract: We present a unified framework for developing and analyzing immersed finite-element (IFE) spaces for solving typical elliptic interface problems with interface-independent meshes. This framework allows us to construct a group of new IFE spaces with a preferred type of polynomials such as linear or bilinear, or rotated-Q1 polynomials. Shape functions in these IFE spaces are locally piecewise polynomials defined according to the subelements formed by the interface itself instead of its line approximation. The unisolvence for these IFE spaces follows from the invertibility of the Sherman–Morrison matrix. A group of universally valid estimates and identities are established for the interface geometry and IFE shape functions that, together with a unified multipoint Taylor expansion procedure, enable us to prove that these IFE spaces have the expected optimal approximation capability. Extensions to higher degree IFE spaces and other types of interface problems will also be discussed.

Shingyu Leung
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Hong Kong University of Science and Technology

Title: Numerical Methods for Partial Differential Equations on Manifolds and Point Clouds

Abstract: We present recent numerical methods for solving partial differential equations on manifolds and point clouds. In the first part of the talk, we introduce a new and simple discretization, named the Modified Virtual Grid Difference (MVG D), for numerical approximation of the Laplace-Beltrami operator on manifolds sampled by point clouds. We first introduce a local virtual grid with a scale adapted to the sampling density centered at each point. Then we propose a modified finite difference scheme on the virtual grid to discretize the LB operator. The new discretization provides more diagonal dominance to the resulting linear system and improves its conditioning. In the second part, we present a local regularized least squares radial basis function (RLS-RBF) method for solving partial differential equations on irregular domains or on manifolds. The idea extends the standard RBF method by replacing the interpolation in the reconstruction with the least squares fitting approximation. These two are joint work with Prof. Hongkai Zhao, Dr. Meng Wang and Dr. Ningchen Ying.

Hong Luo

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North Carolina State University

Title: A Robust and Efficient Finite Volume Method for Two-phase Flows at All-Speeds on hybrid grids

Abstract: A robust and efficient density-based finite volume method is developed for solving the six-equation single pressure system of two-phase flows based on the stratified flow model at all speeds on hybrid unstructured grids. Unlike conventional approaches where an expensive exact Riemann solver is normally required for computing numerical fluxes at the two-phase interfaces in addition to AUSM-type fluxes for single-phase interfaces in order to maintain stability and robustness in cases involving interactions of strong pressure and void-fraction discontinuities, a volume-fraction coupling term for the AUSM+-up fluxes is introduced in this work to impart the required robustness without the need of the exact Riemann solver. The resulting method is significantly less expensive in regions where otherwise the Riemann solver would be invoked. A transformation from conservative variables to primitive variables is presented and the primitive variables are then solved in the implicit method in order for the current finite volume method to be able to solve, effectively and efficiently, low Mach number flows in traditional multiphase applications, which otherwise is a great challenge for the standard density-based algorithms. A number of benchmark test cases are presented to assess the performance and robustness of the developed finite volume method for both inviscid and viscous two-phase flow problems. The numerical results indicate that the current density-based method has the potential as a true “all-speed” two-phase solution algorithm, which on one hand is able to compute high-speed flows like a conventional density-based method; and on the other, is able to solve low-speed viscous flows with an accuracy comparable to pressure-based methods.

Hailiang Liu
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Iowa State University

Title: On free energy satisfying DG methods for Poisson – Nernst-Planck systems

Abstract: The drift-diffusion (Poisson-Nernst-Planck) model is a mean field approximation of diffusive molecules or ions. Applications of this system are found in electrical engineering and electrokinetics, electrochemistry, and biophysics. We design an arbitrary-order free energy satisfying discontinuous Galerkin (DG) method for solving time-dependent Poisson-Nernst-Planck systems. The schemes are shown to satisfy the corresponding discrete free energy dissipation law and preserve the equilibrium states. Numerical examples are presented to demonstrate the high resolution of the numerical algorithm and illustrate the proven properties of mass conservation, free energy dissipation, as well as the preservation of steady states.

Hayk Mikayelyan
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Title: Regularity of Mumford-Shah minimizers at the crack-tip/crack-front.

Abstract: We consider the Mumford-Shah functional in the plain and study the asymptotics of the solution near the crack-tip. This problem arises in certain models of fracture mechanics. It is well-known that the leading term in the asymptotics at the crack-tip is related to the stress intensity factor. We calculate the higher order terms in the asymptotic expansion, and show that those are related to the curvature of the crack close to the tip. Moreover, we derive a new Euler-Lagrange condition for the minimizers. We also develop a new numerical method to compute the minimizers in 2D and 3D.(joint work with John Andersson, Antoine Lemenant and Zhilin Li)

Peter Mineev
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Title: Splitting schemes for the incompressible fluid-structure interaction problems

Abstract: The presentation will be focussed on a class of recently developed splitting schemes for the Navier-Stokes and linear elasticity equations. They are based on a novel approach that reformulates the equations in terms of a stress variable. It was developed in a recent paper together with P. Vabishchevich (Russian Academy of Sciences). The main advantage of such an approach is that the fluid and the structure equations, when written in terms of a stress variable, become very similar. In particular, it is much easier to impose the boundary condition at the interface. Although at first glance the resulting tensorial problem is more difficult, if it is combined with a proper splitting, it yields locally one-dimensional schemes with attractive properties, that are very competitive

to the the most widely used schemes for the formulation in primitive variables. Several schemes for discretization of this formulation will be presented together with their stability analysis.

Finally, numerical results for a problem with a manufactured solution will be presented.

Sergio Amat Plata

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Universidad Politecnica de Cartagena

Title: A class of nonlinear reconstruction procedures to design high-order accurate shock capturing methods.

Abstract: This paper is devoted to a class of nonlinear reconstruction procedures to design high-order accurate shock capturing methods for hyperbolic conservation laws. The methods are based on numerical fluxes with a total variation diminishing (TVD) Runge-Kutta evolution in time. The methods constructed are upwind conservative schemes that are local in the sense that numerical fluxes are reconstructed without using extrapolation from the data of the smoothest neighboring cell. To design the method, a local smoothing is used to prevent the increasing of total variation of the solution near discontinuities and to achieve high order accuracy.

The methods include: the PPH method, a variant of fifth order monotony preserving method and a new Power-ENO method. We concentrate our attention in the construction of the methods and in their theoretical study. Some preliminary numerical results are also presented.

Weiqing Ren

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National University of Singapore

Title: Modeling and Simulation of Moving Contact Lines in Fluids

Abstract: It is well-known that the no-slip boundary condition leads to an infinite rate of energy dissipation when combined with hydrodynamic equations. To overcome this difficulty, we derive a slip model based on molecular dynamics simulations and thermodynamic principles. We illustrate how this model can be used to analyse the behaviour of the apparent contact angle, hysteresis and other important physical problems for the moving contact line. We also discuss the distinguished limits of the slip model as the slip length tends to zero.

Thomas Richter
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Title: Efficient Finite Elements for Monolithic Fluid-Structure Interactions

Abstract: We describe finite element discretizations for fluid-structure interaction problems that are well suited for stiffly coupled problems as they arise in hemodynamics. To cope with added mass effects we use strictly monolithic formulations coupling fluid-problem, solid-problem and the interface conditions.

Such monolithic formulations pose great challenges in terms of computational - but also in terms of implementational - effort. For an efficient discretization we address several numerical techniques to accelerate the simulation.

First we cover the topic of adaptivity in space and time as a technique for reducing the dimension of the discretized systems. Computable a posteriori error bounds guiding the adaptivity are based on adjoint solutions. Second we discuss the efficient solution of the algebraic equations arising from the finite element discretization. We analyze a Newton scheme with an exact Jacobian and we discuss the multigrid solution of the linear problems.

Hongxing Rui
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Title: Mixed finite element methods for coupled Stokes and Darcy flows with transport

Abstract: Recent years, there is a intense research in building suitable mathematical and numerical models for coupled flows with a porous medium (Darcy) and a free fluid region (Stokes). Many kinds of numerical methods have been studied deeply. But most of them just considered the single component flow problems where just velocity and pressure appear in the models.

The models describing solute transport in the coupled Stokes region and Darcy region appear in a variety of physical phenomena. There are several works to study the existence and stability bounds of the weak solution with the fluid viscosity depending on the concentration.

The purpose of this talk is to present the numerical methods for the coupled Stokes and Darcy problem with solute transport. We present a weak formulation and then construct mixed finite element methods for the coupled flow problem using the nonconforming piecewise linear Crouzeix-Raviart element for the velocity and piecewise constant for pressure, usual mixed element methods, such as R-T or B-D-M element, can also be adapted using the similar weak formulation. And we use classical piecewise linear finite element for concentration. Both same and different time step techniques are used in Stokes and Darcy regions.

Álvarez Juan Ruiz
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Title: A new finite volume algorithm for the solution of hyperbolic conservation laws using the IIM

Abstract: This work is devoted to the construction and analysis of a new finite volume algorithm for the solution of hyperbolic conservation laws. It is inspired by Harten's ENO subcell resolution strategy and on the observation that the cell averages of a discontinuous piecewise smooth function contain information that allows to localize the discontinuity within a cell. The reconstruction of the fluxes is performed using the high order accuracy interpolation based on the IIM introduced in S. Amat, Z. Li, J. Ruiz, *Journal of Scientific Computing* (2014). We use this reconstruction to design a finite volume solver which allows to prevent the smearing of contact discontinuities without using extrapolation. Some experimental results will be presented in order to check the performance of the new algorithm.

Jie Shen
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Purdue University and Xiamen University

Title: Multiple scalar auxiliary variable (MSAV) approach and its application to the phase-field vesicle membrane model

Abstract: We consider the numerical approximation for a phase-field vesicle membrane (PF-VMEM) model whose free energy, in addition to some usual nonlinear terms, has two additional penalty terms to enforce the volume and surface area. These disparate penalty terms in the free energy cannot be efficiently handled with the scalar auxiliary variable (SAV) approach. So we developed the multiple scalar auxiliary variable (MSAV) approach to deal with these cases. The MSAV approach enjoys the same computationally advantages as the SAV approach, but can handle free energies with multiple disparate terms such as the volume and surface area constraints in the PF-VMEM model. The MSAV schemes are unconditional energy stable, second-order accurate in time, and can be decoupled, at each time step, into three linear fourth-order equations with constant coefficients, each can be further reduced to two Poisson type equations. Hence, these schemes are easy to implement and extremely efficient when coupled with an adaptive time stepping. Ample numerical results are presented to validate the stability and accuracy of the MSAV schemes.

Chongmin Song
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University of New South Wales

Title: Recent Advances on the Scaled Boundary Finite-Element Method

Abstract: The scaled boundary finite-element method is a semi-analytical method based on finite element technologies. It not only combines many advantages of the

finite element and boundary element methods but also presents appealing features of its own. This method is particularly attractive in modelling problems with unbounded domains or singularities as it handles infinity analytically. It also offers high flexibility in mesh generation and has great potential in developing a fully automated process of engineering analysis directly from geometrical models.

This talk will start with a brief theoretical background of the scaled boundary finite element method so that the salient features of this method can be appreciated. Some recent advances in the fundamental theory are summarised. Applications in the area of dynamic soil-structure interaction, acoustic fluid-structure interaction, fracture mechanics, elasto-plasticity, piezoelectric composites, Lamb waves, and plate analysis will be presented to demonstrate the accuracy and efficiency of this technique in solving problems challenging to standard numerical methods. The current research activities of the speaker's group on the development of a full automatic procedure for computer simulations directly from CAD models and digital images will be introduced. Challenges and directions of further developments will be discussed.

Pengtao Sun

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University of Nevada, Las Vegas

Title: Numerical Studies for Unsteady Moving Interface problems and Applications to Fluid-Structure Interactions

Abstract: In this talk, I will present our recent numerical methodology studies for unsteady moving interface problems and applications to dynamic fluid-structure interaction (FSI) problems. Our numerical methodologies include the arbitrary Lagrangian–Eulerian (ALE) method, the distributed Lagrange multiplier/fictitious domain (DLM/FD) method and their combinations with the mixed finite element method. A fully coupled (monolithic) mixed finite element approximation is developed for all numerical methodologies to unconditionally stabilize numerical computations for moving–interface and FSI problems. Numerical analyses on the well-posedness, stability and convergence are carried out for the proposed monolithic ALE and DLM/FD methods when they are applied to various moving–interface problems. Convergence theorems conclude those numerical analyses with an optimal convergence in regard to the regularity assumption of real solutions. All theoretical results are validated by numerical experiments as well.

Our applications to FSI problems range from hydrodynamics to hemodynamics, in which the involved structure is either incompressible or compressible and bears a deformable and/or rotational constitutive relation while the surrounding fluid flow is incompressible or nearly incompressible. In particular, our well-developed ALE method has been successfully applied to several realistic dynamic FSI problems. One belongs to the hydrodynamics that involves a deforming and spinning hydro–turbine which is immersed in the fluid flow. Others belong to the hemodynamical applications, e.g., an artificial heart pump is rotating inside the artery to cure the heart–failure patients, and an intravascular stent is installed inside the artery by interacting with the

blood flow as well as the artery to cure the aneurismal patients. Both applications are to improve the human cardiovascular system and to remedy cardiovascular diseases. Some animations will be shown in this talk to illustrate that the proposed and well analyzed numerical methods can produce high fidelity numerical results for realistic FSI problems in an efficient and accurate fashion.

Richard Tsai

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The University of Texas at Austin

Title: The implicit boundary integral method and applications

Abstract: An implicit boundary integral method (IBIM) is derived using a suitable extension of the given integro-differential operator from a smooth hypersurface into the surrounding tubular neighborhood. This formulation enables simple numerical computation of problems involving non-parametrically defined surfaces by a wide class of standard numerical schemes. In this talk, I will demonstrate the IBIM algorithms for solving Poisson-Boltzmann equations for electro-static computation of macromolecules immersed in a solvent and solving a class of surface PDEs. I will also discuss some analysis of the algorithms and computational issues.

Jin Wang

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University of Tennessee at Chattanooga

Title: Computing fluid-structure interaction: from immersed boundaries to immersed domains

Abstract: The interactions between fluid flows and immersed solid structures are nonlinear multi-physics phenomena that have applications to a wide range of scientific and engineering disciplines. There are many numerical techniques currently available for computing fluid-structure interaction (FSI); among these we will focus on methods of the immersed boundary type in this presentation. Starting from the original immersed boundary method, we will discuss several improvements of the method as well as some applications. Following that we will describe an extension of the method to deal with immersed structures that occupy a nonzero volume. Such an extension would allow us to handle more realistic and more sophisticated structures described by detailed constitutive laws. We will demonstrate the application of these methods through several nontrivial numerical examples. We will also mention some challenges and open problems in current FSI computation.

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I will discuss a new second order fully discrete numerical approximation to a thermodynamically consistent quasiincompressible binary fluid model. We employ the energy quadratization technique to arrive at linear schemes. We then show that the linear system resulting from the scheme is uniquely solvable. We then compare the numerical simulation of the new model to that of another model of binary fluid.

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Title: A non-traditional finite element method for solving interface problems

Abstract: Interface problems occur frequently when two or more materials meet. The difficulty of solving interface problems is how to capture complex interface geometry and jump conditions effectively while the PDE is not valid across the interface. I am going to discuss the 2D/3D non-traditional finite element method for solving interface problems. This method can get to second order accuracy for different kinds of PDE with discontinuous matrix coefficients and sharp-edge interfaces on two domains and multiple domains.

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Title: Computational Modeling and Its Limitations-A Few Thoughts on How to Handle Complex Dynamical Systems

Abstract: One of the major challenges in today's Science and Engineering fields is how to handle complex dynamical systems. Fluid-solid interaction systems with complex interfaces are typical examples of such complex dynamical systems. Reductionist principles have helped the scientists and engineers to develop uncanny understanding of universe range from mechanical to electro-magnetic properties and phenomena. Yet, we all have this common sense that world has many uncertainties and in general we do not live in a mechanical universe. The research in chaotic nonlinear systems seems to point us in a direction that even the deterministic nonlinear system can produce unpredictable results. Is it possible that when a large number of factors or entities interact with each other, they eventually yield a completely different system quantifiable with an entirely different set of phenomenological rules? Of course, the intermediate stage is characterized with a so-called positive Lyapunov exponent. It is not difficult to imagine that a large or infinitely large positive Lyapunov exponent will lead us to a stochastic or random system. The accurate description of physical, chemical, and biological phenomena over a wide range of spatial and temporal scales is extremely difficult. The intricate nature of turbulence poses seemingly insurmountable challenges to scientists and engineers. Nevertheless, in practice, various hierarchical modeling techniques have been explored. It appears that various

modeling techniques eventually depend on the singular value decomposition or a similar approach on smooth manifolds, a common method to identify rank, left null space, column space, right null space, and row space for any rectangular matrix representing a tangential plane near the neighborhood of any smooth manifolds. Using the singular value decomposition, it is possible to identify the hidden spatial and temporal correlations and patterns between variables and material properties at that particular instance or spatial point. In this work, we will also show a few examples to illustrate the limitations of traditional computational modeling methods.

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The Hong Kong University of Science and Technology

Title: The threshold dynamics method and applications

Abstract: In this talk, I will review some recent work on the threshold dynamics method for diffusion generated motion of the interface. Applications to wetting on solid surface, image segmentation and topology optimization of thermal fluid systems are also discussed.

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Title: Trace finite element methods for partial differential equations on evolving surfaces

Abstract: Many physical processes and biological phenomena could be modeled by partial differential equations on surfaces or manifolds. Recently, the method to solve surface PDEs has arisen much interests in the community of numerical analysis. In this talk, I will introduce some trace finite element methods for convection-diffusion equations on evolving surfaces. The finite element space is a trace of a standard finite element space defined in the neighboring region of the surface. To deal with the evolving surface, an extension of the solution is done by fast marching method or a stabilization technique. The methods are based on a Eulerian framework and easily treat shape and topology changes of the surface. Numerical experiments and error estimates show the optimal convergence of the methods.

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Title: A Modified Finite Volume WENO Method on 3D Cartesian Grids

Abstract: We present a high-order modified dimension-by-dimension finite volume WENO method for hyperbolic conservation laws on three-dimensional Cartesian grids. Our modification adopts the idea of conversion between face-averaged values and face-centered values due to Buchmüller and Helzel. We propose fourth-order and sixth-order accurate conversion formulas on three-dimensional Cartesian grids, and we use the conversion formulas to compute a high-order accurate face numerical flux at a cell interface as needed by a finite volume method. It is shown that our method is efficient and retains the full order of accuracy when applied to smooth nonlinear problems, and is robust for calculating non-smooth nonlinear problems with shocks.

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Title: Solving Interface Problems on Cartesian Grids in Boundary Integral Formulation

Abstract: I will talk on the boundary integral formulation based Cartesian grid method for interface problems. Boundary integral method has significant advantages for interface problems defined on unbounded domains or time-dependent inter-facial problems due to its dimension reduction and avoiding generation of unstructured volume grids. However, the traditional boundary integral method may encounter nearly singular integrals, which are hard to evaluate, or is not applicable for variable coefficients or nonlinear problems since the fundamental solution or Green's function is unknown then. The Cartesian grid method that I will talk on today is a generalization of the traditional boundary integral method. It can accurately evaluate nearly singular boundary integrals in an efficient way, and is able to solve variable coefficients and nonlinear problems. The method never computes or need to know the fundamental solution of Green's function of the problem. It avoids generation of any unstructured grids for both the domain and the interface in three space dimensions. It represents an interface, a curve or surface, by its intersection points with an underlying Cartesian grid, which brings the method additional advantages. The interface problems to be presented include an interface problem in an unbounded domain around multiple closely packed cells, the nonlinear Poisson-Boltzmann equations, the Hele-Shaw free boundary problem and a Stokes moving interface problem.

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State Key Laboratory of Scientific and Engineering Computing (LSEC)
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Title: The Parallel Adaptive Finite Element Toolbox PHG for Interface Problems

Abstract: Parallel Hierarchical Grid (PHG, http://lsec.cc.ac.cn/phg/index_en.html) is an open source adaptive finite element toolbox which is featured by newest vertex bisection based and fully parallel adaptive mesh refinement/coarsening for unstructured conforming tetrahedral meshes, mesh partitioning based large-scale parallel computing, a flexible and scalable linear solver/preconditioner module, and useful resources for finite element discretization (high order elements, hierarchical elements, high order numerical quadrature, etc.).

This talk is an introduction to the toolbox PHG, with focuses on its support for and application to numerical solution of interface problems with an unfitted interface using finite element methods.

Qinghai Zhang
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Zhejiang University

Title: Interface tracking close to machine precision and the best estimates of interface curvature

Abstract: Most interface tracking IT methods are at best second-order accurate. The most serious disadvantage of explicit IT methods, however, is probably the absence of an analytic framework. Based on the donating region theory [2, 1, 3], and a topological space that models physically meaningful material regions, we resolve this de_cit by proposing a generic framework via Mapping and Adjusting Regular Semialgebraic sets (MARS) [7]. Using MARS, we formally proved the second-order accuracy of Volume-of-Fluid methods, clari_ed many subtle issues such as the accuracy deterioration caused by local C1 discontinuities, and analyzed other explicit IT methods such as moment-of-uid methods and front-tracking methods. Also inspired by MARS, we proposed a new IT method which achieved 4th-, 6th-, and 8th-order accuracy for an arbitrary number of phases [6, 5]. For the classic vortex-shear tests, our new method achieves close to machine precision on a 128-by-128 grid. Finally, we showed under the framework of MARS that there exists a best estimation of curvature at any regular point of the interface, which can be easily obtained by our new eighth-order algorithms [4].

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Title: Modeling and simulation of moving contact line problem for two-phase complex fluids flow

Abstract: We introduce the sharp interface models for moving contact lines with polymeric fluids. A continuous model with the boundary conditions is derived for the dynamics of two immiscible fluids with moving contact lines based on thermodynamic principles. An immersed boundary method is developed to solve the resulting free boundary problem. We also discuss the model reduction of the slip model to the no-slip limit by the technique of asymptotic analysis.

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Nanjing Normal University

Title: An immersed finite volume element method for interface problems and its applications

Abstract: An immersed finite volume element method is developed to solve 2D elliptic interface problems with a variable coefficient that has a finite jump across an interface. The numerical method consists of an immersed finite element method in the physical space and a sparse grid collocation method based on the Smolyak construction in the probability space is proposed for solving elliptic PDEs with both random input and interfaces. At last, an immersed finite element method based on the variational discretization concept is applied to the optimal control problems of elliptic PDEs with interfaces. Numerical experiments demonstrate the convergence rates of the proposed method and confirm the theoretical results.

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The University of Alabama

Title: A spatially second order alternating direction implicit (ADI) method for solving

three dimensional parabolic interface problems

Abstract: In this talk, we will present a novel alternating direction implicit (ADI) method for solving three-dimensional (3D) parabolic interface problems with discontinuous jumps and complex interfaces. The ADI scheme is a powerful finite difference method for solving diffusion equations, due to its stability and efficiency. However, it suffers from a serious accuracy reduction in space for interface problems with different materials and nonsmooth solutions. To restore the second order accuracy, physical interface conditions that describe jumps of the function and its flux have to be enforced in the spatial discretization. To this end, a non-orthogonal local coordinate system is constructed in the proposed matched ADI method, to decouple 3D jump conditions into essentially one-dimensional (1D) ones along the Cartesian directions. These 1D conditions can then be incorporated into the ADI central difference discretization. In time discretization, the matched ADI method is found to be of first order and stable in various experiments. In space discretization, the matched ADI method achieves the second order accuracy based on simple Cartesian grids for various irregularly-shaped surfaces and spatial-temporal dependent jumps. Fast algebraic solvers for perturbed tridiagonal systems are developed so that the matched ADI method is as efficient as the fastest implicit scheme based on the geometrical multigrid for solving 3D parabolic equations, in the sense that its complexity in each time step scales linearly with respect to the spatial degree of freedom N , i.e., $O(N)$. Therefore, the proposed matched ADI method provides a very promising tool for solving 3D parabolic interface problems.

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Title: An Electron-Conservative Mixed Finite Element Method for Inductionless MHD Equations

Abstract: An electron-conservative mixed finite element method is proposed for inductionless and incompressible magnetohydrodynamic (MHD) equations in three dimensions. The divergence-free property of the electric current density, or the conservation of electrons, plays an important role in simulating liquid metals like the lithium-lead experimental blanket of a TOKAMAK. Different from traditional numerical methods which usually realize the divergence-free constraint of discrete current density by post-processing, the discrete current density by our mixed method is divergence-free exactly and globally in the domain. The second objective is to design a robust and quasi-optimal solver for the discrete problem. We propose a block preconditioner for the linearized algebraic system of discrete MHD problem. By extensive numerical examples for both stationary MHD problem and time-dependent MHD problem, we demonstrate the robustness of the preconditioner to Reynolds number and the quasi-optimality to meshes.

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Title: A 3D Immersed Boundary Method for non-Newtonian-Fluid-Structure Interaction with Applications

Abstract: Fluid-structure-interaction (FSI) is complex and challenging to model and simulate, and it is still an area of active research. Motivated by FSI phenomena in life sciences (e.g., motions of sperm and cytoskeleton in complex fluids), we introduce a new immersed boundary method for FSI problems involving non-Newtonian fluids in three dimensions. The non-Newtonian fluids are modelled by the power law or the FENE-P model. The fluid flow is modelled by the lattice Boltzmann equations (the D3Q19 model). The deformable structure and the fluid-structure-interaction are handled by the immersed boundary method. As applications, we consider two toy FSI problems --- an elastic sheet fixed at the midline interacting with a flowing power-law fluid and an elastic sheet being flapped sinusoidally at its leading edge in a still FENE-P fluid in three dimensions.