Workshop on Scientific Computing

Lawson Building Room 1142

Purdue University , West Lafayette

October 8th, 2022

Morning Session

Time	Speaker	Title	Chair
8:30 – 9:00	Check-in and breakfast		
9:00 – 9:40	Andrew Christlieb	Successive convolution, expanding differential operators as convolutional integrals	P. Li
9:40 – 10:00	Lyudmyla Barannyk	Using sharp-interface Stefan models to study the solid-liquid phase change driven by internal heat generation	
10:00 – 10:20	Jiahui Chen	Hodge Laplacians and their biological applications	
10:20 – 10:40	Coffee break and photo		
10:40 – 11:00	Weihua Geng	Modeling and algorithm development for simulating implicitly solvated biomolecules with atomic polarizable multipoles	C. Liu
11:00 – 11:20	Shuwang Li	Modeling and computation of a tumor growth problem	
11:20 – 11:40	Xiaofan Li	Motion of particles in unsteady Stokes and linear viscoelastic fluids	
11:40 – 12:00	Ying Liang	Neural network-assisted methods for inverse random source problems	
Lunch break			

Afternoon Session

Time	Speaker	Title	Chair
2:00 – 2:40	Chun Liu	Dynamic boundary conditions and evolution of grain boundaries	X. Li
2:40 – 3:00	Monika Nitsche	Evaluating near-singular integrals with application to vortex sheet and multi-nested Stokes flow	
3:00 – 3:20	Bill Sands	A particle-in-cell method for plasmas with a generalized momentum formulation	
3:20 – 3:40	Coffee break		
3:40 – 4:00	Lei Wang	Correlated random displacements computed by the spectral Lanczos decomposition method and barycentric Lagrange treecode	S. Li
4:00 – 4:20	Dexuan Xie	Efficient finite element iterative methods for solving Poisson-Nernst-Planck ion channel models	
4:20 – 4:40	Luoding Zhu	Computational studies of osteocyte-fluid interaction	
4:40 – 5:00	Coffee break		
5:00 – 5:30	Discussion		

Abstracts

Successive convolution, expanding differential operators as convolutional integrals

Andrew Christlieb   Michigan State University

In this talk we introduce a noval approach to creating numerical methods that behave unconditionally stable at the cost of an explicit method. The methods are based on the idea of expanding a differential operators as a series of convolutional integrals that are evaluated with fast summation. For this method, unconditional stability can be rigorously established for linear PDEs. The approach has been applied to range of linear and non-linear PDE's. We will review the approach and demonstrate its utility on a range of test problems.

Using sharp-interface Stefan models to study the solid-liquid phase change driven by internal heat generation

Lyudmyla Baranyk   University of Idaho

We study the evolution of the sharp solid-liquid interface during melting and solidification (Stefan problem) of a material with constant internal heat generation and prescribed temperature or heat flux at the boundary in the cylindrical geometry. We consider a weakly nonlinear motion of the interface in the sense that it propagates relatively slowly compared to changes of the temperature in each phase. The equations are solved by splitting them into transient and steady-state components and then using separation of variables. This results in an ordinary differential equation for the interface that involves infinite series. The obtained initial value problem is solved numerically. The results are compared to previously derived quasi-static solutions and numerical simulations generated using the method of catching of the front into a space grid node. The problem is also solved numerically using the commercial software Ansys Fluent, that uses the enthalpy method and allows the formation of a mushy zone. Sharp-interface numerical solutions develop so-called overheated region, whose evolution is compared to the evolution of the mushy zone generated by the enthalpy method.

Hodge Laplacians and their biological applications

Jiahui Chen   Michigan State University

This talk will discuss an evolutionary de Rham-Hodge method by studying Hodge Laplacians to provide a unified paradigm for the multiscale geometric and topological analysis of evolving manifolds constructed from filtration, which induces a family of evolutionary de Rham complexes. While the present method can be easily applied to close manifolds, the emphasis is given to more challenging compact manifolds with 2-manifold boundaries, which require appropriate analysis and treatment of boundary conditions on differential forms to maintain proper topological properties. Three sets of Hodge Laplacians are proposed to generate three sets of topology-preserving singular spectra, for which the multiplicities of zero eigenvalues correspond to exactly topological invariants. This method is applied to study the electrostatics of biomolecules and Cryo-EM molecular data.

Modeling and algorithm development for simulating implicitly solvated biomolecules with atomic polarizable multipoles

Weihua Geng   Southern Methodist University

The Poisson-Boltzmann model is a popular approach for simulating implicit solvated molecules whose charge distribution is modeled by point charges. For highly charged biomolecules, the traditional point charge representation is not accurate enough to characterize electrostatics interaction, which is critical in determining biomolecular structure, function, and dynamics. Instead, the polarizable multipole model provides a better description physically. However, solving the polarizable multipole Poisson-Boltzmann (PMPB) model is numerically challenging due to its sensitivity to the charge distribution represented by singular delta function and its derivatives and computationally demanding due to the iteration needed for satisfying self-consistency of polarization. We attack these difficulties with two approaches. The first approach uses an interface based finite difference discretization with a Green's function based decomposition to analytically regularize the charge singularity associated with point multipole distribution. The second approach uses a boundary elements discretization accelerated by multipole expansion algorithms. The pro and cons of both approaches as well as their connection are investigated with theoretical derivation and numerical results.

Modeling and computation of a tumor growth problem

Shuwang Li   Illinois Institute of Technology

In this talk we investigate the modeling, analysis and computation of tumor growth. The sharp interface model we considered is to incorporate two key factors: (1) the mechanical interaction between the tumor cells and their surroundings; (2) the biochemical reactions in the microenvironment of tumor cells, and understand how they can influence the dynamics of tumor growth. From this general model we give its energy formulation and solve it numerically using the boundary integral methods and the small-scale decomposition under different scenarios.

Motion of particles in unsteady Stokes and linear viscoelastic fluids

Xiaofan Li   Illinois Institute of Technology

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.

Neural network-assisted methods for inverse random source problems

Ying Liang   Purdue University

We propose a data-assisted approach for recovering the statistical properties of the random source in the source scattering problems for acoustic wave propagation, using boundary measurement data of random radiated wave fields. We first implement a regularized Kaczmarz method with the multifrequency scattering data on the boundary to construct approximations of the source profile. Then we compare the performance of different data-driven algorithms to enhance the approximation. This data-assisted approach provides satisfying reconstruction with much fewer realizations than traditional methods. Numerical experiments are presented to compare the performance of different Image-to-Image translation algorithms and demonstrate the efficiency of the proposed framework. The resulting reconstruction is stable with respect to the noise in the observation data.

Dynamic boundary conditions and evolution of grain boundaries

Chun Liu   Illinois Institute of Technology

I will present the dynamic boundary conditions in the general energetic variational approaches and applications in the evolution of grain boundaries. This is a joint work with Yekaterina Epshteyn (University of Utah) and Masashi Mizuno (Nihon University).

Evaluating near-singular integrals with application to vortex sheet and multi-nested Stokes flow

Monika Nitsche   University of New Mexico

Boundary integral formulations yield efficient numerical methods to solve elliptic boundary value problems. They are the method of choice for interfacial fluid flow in either the inviscid vortex sheet limit, or the viscous Stokes limit. The fluid velocity at a target point is given by an integral over all interfaces. However, for target points near, but not on the interface, the integrals are near-singular and standard quadratures lose accuracy. While several accurate methods for near-singular integrals exist in planar geometries, they do not generally apply to the non-analytic case that arises in axisymmetric or 3D geometries. We present a method based on Taylor series expansions of the integrand about basepoints on the interface that accurately resolve a large class of integrals, and apply it to solve the near-interface problem in planar vortex sheet flow, axisymmetric Stokes flow, and Stokes flow in 3D. The application to multi-nested Stokes flow uses a novel representation of the fluid velocity.

A particle-in-cell method for plasmas with a generalized momentum formulation

William Sands   University of Texas at Austin

In this talk, some of our recent work on new particle-in-cell-methods for the Vlasov-Maxwell system will be presented. We propose a formulation in terms of potentials, in which the first-order Maxwell system is cast as a collection of second-order wave equations with the aid of the Lorenz gauge condition. Then, the usual Lorentz force for the particles is expressed in terms of these wave potentials and their spatial derivatives through the use of generalized momentum. A new BDF wave solver is presented for the solution of these equations for the potentials that induces a discrete equivalence between the Lorenz gauge condition and the continuity equation. We also discuss the new methods used to construct the spatial derivatives required in the update for particles, which are inspired by the wave solver used to evolve the potentials. Numerical results will be presented to demonstrate the application of the new method.

Correlated random displacements computed by the spectral Lanczos Ddecomposition method and barycentric Lagrange treecode

Lei Wang   University of Wisconsin at Milwaukee

Brownian Dynamics simulations require correlated random displacements ${\bf g} = \sqrt{D}{\bf z}$ to account for hydrodynamic interactions among solvated biomolecules and polymers, where D is the diffusion matrix based on the Rotne Prager-Yamakawa tensor and ${\bf z}$ is a normal random vector. The Spectral Lanczos Decomposition Method (SLDM) computes a sequence of approximations to ${\bf g}$, but each iteration requires a matrix-vector product $D{\bf q}_k$, where ${\bf q}_k$ is the kth Lanczos vector. The present work applies the barycentric Lagrange treecode (BLTC) to accelerate the matrix-vector product, and numerical results show the performance of the SLDM-BLTC in serial and parallel calculations. This is a joint work with Robert Krasny.

Efficient finite element iterative methods for solving Poisson-Nernst-Planck ion channel models

Dexuan Xie   University of Wisconsin at Milwaukee

A Poisson-Nernst-Planck ion channel (PNPic) model is widely used in the simulation of ion transport across a cell membrane but difficult to solve numerically. In this talk, I will report the recent progresses that we made in the development of PNPic models and finite element solvers. In particular, I will describe how we mimic an infinitely large ion channel membrane and how we deal with membrane charges through introducing novel boundary value conditions and interface conditions. I will then describe the numerical techniques that we developed to overcome the difficulties caused by atomic charge singularity, exponential nonlinearity, and multiple physical domains. Furthermore, I will describe an efficient finite element iterative method for solving a PNPic model and a valuable visualization scheme for displaying the three dimensional functions of electrostatics and ionic concentrations, approximately, as two dimensional curves. This work was partially supported by the National Science Foundation through award number DMS-2153376 and the Simons Foundation through research award 711776.

Computational studies of osteocyte-fluid interaction

Luoding Zhu   Indiana University Purdue University Indianapolis

The osteocyte is a bone cell that is responsible for mechanotransduction and guides bone remodeling. It is encased in a lacunar-canalicular network that permeates the hard bone matrix. The interstices between the cell and the bone matrix are filled with a salt-water-like fluid and pericellular matrix (PCM). When the bone is mechanically loaded, the interstitial fluid is forced to flow through the PCM, generating stresses on the cell. Experiments suggest that those stresses and associated strains are amplified approximately ten-fold compared to the macroscale stress and strain in bone that are induced by normal daily motion. The mechanism of this amplification is not well understood.

We introduce several computational models to investigate the force amplification of the osteocyte -fluid-lacuna-canaliculi system in two and three dimensions. In all the models, the interstitial fluid is modelled as an incompressible viscous fluid and the fluid motion equations (Navier-Stokes) are numerically solved by the lattice Boltzmann approach (D2Q9 and D3Q19 models). The fluid-osteocyte interaction is modelled by the immersed boundary framework and numerically solved by finite difference method. These studies are ongoing research with students and collaborators and I will report our current progress on these efforts in the talk.