Special Session 81: Analysis and Simulation of Multi-Scale Problems

Xiao-Ping Wang, Department of Mathematics, Hong Kong University of Science and Technology, China
Yang Xiang, Department of Mathematics, Hong Kong University of Science and Technology, China

Multiscale phenomena occur in a diverse range of science and engineering problems. Tremendous progress have been made in recent years in analysis, algorithm design and applications for various multi-scale problems. This special session brings together experts in both analysis and numerical methods to report their recent develops in this exciting field.

Numerical simulations of the suspended particle in a shear flow with slipping

Yana Di
Institute of Computational Mathematics, Chinese Academy of Sciences, Peoples Rep of China
yndi@lsec.cc.ac.cn

The talk will study the evolution of an ellipsoid particle in an incompressible, Newtonian shear flow by considering the fluid slipping at solid surface. A continuum hydrodynamic model is constructed, using phase-field diffuse-interface modeling for fluid-solid interface. Fluid slipping at solid particle surface is incorporated into the model by a decrease in the shear viscosity in the interfacial region. Numerical simulations will be given to show the effect of the fluid slipping on the orientational motion of the ellipsoid particle.

Lattice Boltzmann method for Helmholtz equation

Jie Liao
East China University of Science and Technology, Peoples Rep of China
liaojiess@163.com
Radjesvarane Alexandre

Many physical phenomena and engineering problems may have their origins at molecular scales, although they need to interface with the macroscopic scales. The difficulty arises in bridging the results of these models across the span of length and time scales. The lattice Boltzmann method attempts to bridge this gap.

We will present a lattice Boltzmann scheme for solving non homogeneous Helmholtz equation. This massively parallel LB scheme is easy to implement, the computation at each site is determined only by local parameters, and can be easily adapted to solve multiple scattering problem with many scatterers or wave propagation in non homogeneous medium.

A new approach to energy bounds for heterogeneous media

Liping Liu
Rutgers University, USA
liu.liping@rutgers.edu

In this paper we present a new method of deriving microstructure-dependent bounds on the effective properties of general heterogeneous media. We first define and calculate the higher-order polarization tensors for multiphase heterogeneous media, and next derive a differential inequality on the energy with the initial condition given by the polarization tensors. Using the comparison theorem we obtain bounds on the energy induced by the inhomogeneities. These new bounds, taking into account of the average Eshelby tensors for homogeneous problems, are much tighter than the microstructure-independent bounds such as the classic Hashin-Shtrikman bounds on one hand, and on the other hand, recover the classic bounds by minimizing or maximizing the bounds over all possible average Eshelby tensors. Also, these bounds are applicable to non-well-ordered composites and multifunctional composites. It is anticipated that this new approach will be useful for the modeling and optimal design of a variety of heterogeneous media.

Well-posedness of a generalized Peierls-Naborro model

Pingbing Ming
AMSS, Peoples Rep of China
mpb@lsec.cc.ac.cn
Yang Xiang

In this talk, I will present the wellposedness of a generalized Peierls-Nabarromodel recently proposed by us in a natural energy space. The global well-posedness of the classic Peierls-Nabarro model is aby-product of this result.

A seamless multiscale method and its application to complex fluids

Weiqing Ren
New York University
weiqing.ren00@gmail.com

I will present a seamless multiscale method for the study of multiscale problems. The multiscale method captures the macroscale behavior of the system with the help of a microscale model. The macro model provides the necessary constraint for the micro model, and the micro model supplies the missing data (e.g. the constitutive relation or the boundary conditions) for the macro model. The macro and micro models evolve simultaneously using different time steps, and they exchange data at every step. The micro model uses its own appropriate (micro) time step. The macro model uses a macro time step but runs at a slower pace than required by accuracy and stability considerations in order for the micro dynamics to have sufficient time to adapt to the environment provided by the macro state. The method has the advantage that it does not require the reinitialization of the micro model at each macro time step or each macro iteration step. I will discuss the algorithm of the multiscale method, the error analysis, and its application to complex fluids.

$\longrightarrow \infty \diamond \infty \longleftarrow$

Coarse-graining Kohn-Sham density functional theory

Phanish Suryanarayana
Georgia Institute of Technology, USA
phanish.suryanarayana@ce.gatech.edu

Defects, though present in relatively minute concentrations, play a significant role in determining macroscopic properties. Even vacancies, the simplest and most common type of defect, are fundamental to phenomena like creep, spall and radiation ageing. This necessitates an accurate characterization of defects at physically relevant concentrations, which is typically in parts per million. This represents a unique challenge since both the electronic structure of the defect core as well as the long range elastic field need to be resolved simultaneously. Unfortunately, accurate ab-initio electronic structure calculations are limited to a few hundred atoms, which is orders of magnitude smaller than that necessary for a complete description. Thus, defects represent a truly challenging multiscale problem. Density functional theory developed by Hohenberg, Kohn and Sham (DFT) is a widely accepted, reliable ab-initio method for computing a wide range of material properties. Traditional implementations of DFT solve for the wavefunctions, a procedure which has cubic-scaling with respect to the number of atoms. This places serious limitations on the size of the system which can be studied. Further, they are not amenable to coarse-graining since the wavefunctions need to be orthonormal, a global constraint. To overcome this, we have developed a linear-scaling method for DFT where the key idea is to directly evaluate the electron density without solving for the individual wavefunctions. Based on this linear-scaling method, we have developed a numerical scheme to coarse-grain DFT derived solely based on approximation theory, without the introduction of any new equations and resultant spurious physics. This allows us to study defects at a fraction of the original computational cost, without any significant loss of accuracy. We demonstrate the efficiency and efficacy of the proposed methods through examples.

$\longrightarrow \infty \diamond \infty \longleftarrow$

Efficent numerical methods for the phase field simulation of moving contact line problem

Xiaoping Wang
Hong Kong University of Science and Technology, Hong Kong
mawang@ust.hk

In this talk, I will describe a newly developed phase field model for two phase fluid flow based on Cahn Hilliard Navier Stokes equation with generalized Navier boundary condition. Then I will describe some efficeint numerical methods for the model including adaptive mesh methods. Several numerical results will then be presented.

$\longrightarrow \infty \diamond \infty \longleftarrow$

Some uniqueness problems in free boundary problems associated with degeneracy

Peiyong Wang
Wayne State University, USA
pywang@math.wayne.edu

It is known the uniqueness of a solution in a free boundary problem does not always hold (see a manuscript by G.Lu and the author). Degeneracy of a partial differential equation presents another aspect of the uniqueness problem. The author will address this problem and first present the results with degeneracy of the partial differential equation. Then he will turn to the degenerate situation and consider both aspects simultaneously.

$\longrightarrow \infty \diamond \infty \longleftarrow$

A continuum model for the dynamics of dislocation arrays

Yang Xiang
Hong Kong University of Science and Technology, Hong Kong
maxiang@ust.hk
Xiaohong Zhu, Shuyang Dai

We derive a continuum model for the dynamics of a dislocation array that consists of dislocations in different slip planes. In the continuum model, the dislocation array is represented by a continuous surface, of which there are many dislocations in a unit area at the scale of the continuum model. The continuum model is derived rigorously from the discrete model of the dynamics of the constituent dislocations in the array using asymptotic analysis. The obtained continuum model contains an integral over the dislocation array surface representing the long-range interaction of dislocations, and a local term that comes from the line tension effect of dislocations. The size-dependent effect due to dislocation line tension is accurately incorporated in the continuum model. We also present a numerical implementation method based on the level set representation of the surfaces the fast Fourier transform method for the long-range interaction.

$\longrightarrow \infty \diamond \infty \longleftarrow$

Some mathematical analysis for wetting on chemically patterned surfaces

Xianmin Xu
Chinese Academy of Sciences, Peoples Rep of China
xmxu@lsec.cc.ac.cn

Wetting phenomena describe how liquid drops stay and move on solid surfaces. They are common in nature and industrial applications. In this talk, we will introduce our recent analysis for wetting on chemically patterned surfaces using some mathematical models. We mainly concern how the macroscopic properties of wetting, such as apparent contact angles and contact angle hysteresis could be affected by the microscopic information of solid surfaces. We would also like to show the application of our analysis in a two-phase fluid problem.

$\longrightarrow \infty \diamond \infty \longleftarrow$

Minimizers and Meissner states for nonself-dual Chern-Simons-Higgs energy

Xiaodong Yan
University of Connecticut, USA
xiaodong.yan@uconn.edu
Dan Spirn

We prove existence of minimizers of nonself-dual Chern-Simons-Higgs energy. The minimizer is vortexless below the first critical field and vortex appears when h_{ex} exceeds first critical field. We also prove existence of Meissner state solution for h_{ex}

$\longrightarrow \infty \diamond \infty \longleftarrow$