HKUST-SJTU Joint Workshop in Applied math and Computational Science, Apr. 12-13**,** 2013 , HKUST

Apr. 12 (Friday) Room 2404

9:00-9:15 **Opening ceremony**

Session Chair: Xiao-Ping Wang

09:15-09:45 Shi Jin, SJTU

Semiclassical computational methods for quantum dynamics with band-crossing*s*

09:45-10 :15 Xuhui Huang, HKUST

Modeling protein conformational changes using multi-resolution Markov State Models

10 :15-10:45 Coffee Break

Session Chair: Kun Xu

10:45-11:15 David Cai, SJTU

Neuronal Dynamics from Nonlinear Dendritic Integration to Population Responses

11:15-11:45 Zhigang Li, HKUST

Characterization and Applications of Nanoscale Flows

11:45-12:15 Wenjing Ye, HKUST

Numerical and Theoretical Studies of Knudsen Force

Session Chair: David Cai

02:00-02:30 Yaguang Wang, SJTU

Stability of Vortex Sheets in Compressible Flows

02:30-03:00 Jidong Zhao, HKUST

Discrete Modeling of fluid-Particle Interactions in Granular Media

03:00-03:30 Coffee Break

Session Chair: Yang Xiang

03:30-04:00 Lei Zhang, SJTU

Localized bases for numerical homogenization with arbitrary coefficients

04:00-04:30 Xiaoqun Zhang, SJTU

Wavelet Frame Based Multi-Phase Image Segmentation

04:30-05:00 Tim Leung, HKUST

A Splitting Algorithm for Image Segmentation on Manifolds Represented by the Grid based Particle Method

06:30 **Dinner at G-Resturant**

Apr. 13 (Saturday), Room 2404

Session Chair: Yaguang Wang
09:00-09:30 Yachun Li, SJTU
Formation of singularities in solutions to the compressible radiation hydro-dynamics equations with vacuum

09:30-10:00 Tiezheng Qian, HKUST
Hydrodynamics of Leidenfrost Droplets in One-Component Fluids

10:00-10:30 Coffee Break

Session Chair: Tiezheng Qian
10:30-11;00 Dan Hu, SJTU
Optimization, Adaptation, and Initiation of Biological Transport Networks

11:00-11:30 Yang Xiang, HKUST
Continuum models for dislocation structure, energy and dynamics of dislocation arrays and low angle grain boundaries

11:30-12:00 Dongzhuo Zhou, SJTU
Causal and Structural Connectivity of Pulse-coupled Nonlinear Networks

Afternoon Session

Session Chair: Xiao-Ping Wang
02:00-02:30 Chunjing Xie, SJTU
Subsonic Euler flows with large vorticity

02:30-03:00. Shijin Deng, SJTU
Boltzmann equation and Green's function for shock profiles

03:00-03:30 Coffee Break

04:00-06:00 Discussions

Neuronal Dynamics from Nonlinear Dendritic Integration to Population Responses

David Cai
Department of Mathematics, Institute of Natural Sciences,
Shanghai Jiao Tong University

First we will describe our analysis and modeling of a nonlinear dendritic integration rule recently discovered in experiment regarding the summed response in the soma of excitatory and inhibitory inputs present at different locations on a dendrite. We will discuss the origin of the nonlinearity and propose a new integrate-and-fire neuronal model that phenomenologically captures the effect of the integration rule. We will further use a large-scale computational model of the primary visual cortex to study neural population responses as observed in experimental studies of optimal decoding using population responses in the primate visual cortex. Finally we will address interpretation issues arising from data processing of neural population data, which will have strong implications for imaging experimental designs.

Optimization, Adaptation, and Initiation of Biological Transport Networks

Dan Hu
Department of Mathematics, Institute of Natural Sciences,
Shanghai Jiao Tong University

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

Semiclassical computational methods for quantum dynamics with band-crossing

Shi Jin
Department of Mathematics
Shanghai Jiao Tong University

Band-crossing is a quantum dynamical behavior that contributes to important physics and chemistry phenomena such as quantum tunneling, Berry connection, chemical reaction etc. In this talk, we will discuss several recent works in developing semiclassical methods for band-crossing, including examples from surface hopping, Schrodinger equation with periodic potentials, and high frequency solutions of linear hyperbolic systems with polarized waves.

Boltzmann equation and Green's function for shock profiles

Shijin Deng

Department of Mathematics
Shanghai Jiao Tong University

In this talk, we will discuss how to construct the Green's function for shock profiles of viscous conservation law in high dimension based on the Green's function for the Boltzmann equation.

Localized bases for numerical homogenization with arbitrary coefficients

Lei Zhang
Department of Mathematics, Institute of Natural Sciences,
Shanghai Jiao Tong University

We introduce a new method for the numerical homogenization of divergence form elliptic equations with rough ($\L^\infty$) coefficients. Our method does not rely on concepts of ergodicity or scale-separation but on the property that the solution operator is compact from $\L^2$ to $\H^1$. The approximation space is generated as an interpolation basis(over a coarse mesh of resolution H) minimizing the $\L^2$ norm of source terms; its (pre-)computation involves solving $\mathcal{O}(H^{-d})$ bi-harmonic PDEs on localized sub-domains of size $\mathcal{O}(H (\ln H)^2)$; its accuracy ($\mathcal{O}(H)$ in $\H^1$ norm) is established via the introduction of a new classs of higher-order Poincar\'{e} inequalities. The method naturally generalizes to time dependent problems.

Formation of singularities in solutions to the compressible radiation hydrodynamics equations with vacuum

Yachun Li
Department of Mathematics
Shanghai Jiao Tong University

We study the Cauchy problem for multi-dimensional compressible radiation hydrodynamics equations with vacuum. First, we present some sufficient conditions on the blow-up of smooth solutions in multi-dimensional space. Then, we obtain the invariance of the support of density of the smooth solutions with compactly supported initial mass density by the property of the system under the vacuum state. Based on this, we prove that we cannot get a global classical solution no matter how small the initial data are, as long as the initial mass density is compactly supported. Finally, we will see that some of the results that we obtained are still valid for the isentropic flows with degenerate viscosity coefficients as well as for 1-D case.

Subsonic Euler flows with large vorticity

Chunjing Xie
Department of Mathematics, Institute of Natural Sciences,
Shanghai Jiao Tong University

In this talk, we will discuss subsonic Euler flows in a topological half plane where flows may have large vorticity. The result is based on the understanding for subsonic Euler flows in nozzles and some uniform a priori estimate for elliptic equations in unbounded domains.

Causal and Structural Connectivity of Pulse-coupled Nonlinear Networks

Dongzhuo Zhou
Department of Mathematics, Institute of Natural Sciences,
Shanghai Jiao Tong University

We study the reconstruction of structural connectivity for a general class of pulse-coupled nonlinear networks and show that the reconstruction can be successfully achieved through linear Granger Causality (GC) analysis. Using spike-triggered correlation of whitened signals, we obtain a quadratic relationship between GC and the network couplings, thus establishing a direct link between the causal connectivity and the structural connectivity within these networks. Our work may provide insight into the applicability of GC in the study of function of general nonlinear networks.

Wavelet Frame Based Multi-Phase Image Segmentation

Xiaoqun Zhang
Department of Mathematics, Institute of Natural Sciences,
Shanghai Jiao Tong University

Wavelet frames have been successfully applied in various image restoration problems, such as denoising, inpainting, deblurring, etc. However, they are rarely used in geometric applications. Motivated by recently established theoretical connection between wavelet frame based and total variation based image restoration models we pro-pose here a convex multi-phase segmentation model based on wavelet frame transform. The proposed model allows to automatically identify complex tubular structures, including blood vessels, leaf vein system, etc. Numerical results show that our method can extract many more details than existing variational methods especially when the image contains different scales of structures. The proposed method can be parallelized easily and its efficiency is further improved by a GPU implementation.
In addition, we analyze the connection between solutions of the convexied model and the original binary constrained one. This is a joint work with Cheng Tai and Zuowei Shen.

Stability of Vortex Sheets in Compressible Flows

Ya-Guang Wang
Department of Mathematics
Shanghai Jiao Tong University

In this talk, we shall study the linear stability and nonlinear stability of vortex sheets in compressible flows. Both of compressible megneto-hydrodynamical systems and compressible Euler systems in two and three space variables are considered.

Modeling protein conformational changes using multi-resolution Markov State Models

Xuhui Huang
Department of Chemistry, Hong Kong University of Science and Technology

Simulating biologically relevant timescales at atomic resolution is a challenging task since typical atomistic simulations are at least two orders of magnitude shorter. Markov State Models (MSMs) provide one means of overcoming this gap without sacrificing atomic resolution by extracting long time dynamics from short simulations. MSMs coarse grain space by dividing conformational space into long-lived, or metastable, states. This is equivalent to coarse graining time by integrating out fast motions within metastable states. By varying the degree of coarse graining one can vary the resolution of an MSM; therefore, MSMs are inherently multi-resolution. In the talk, I will introduce a new algorithm Super-level-set Hierarchical Clustering (SHC), to our knowledge, the first algorithm focused on constructing MSMs at multiple resolutions. The key insight of this algorithm is to generate a set of super levels covering different density regions of phase space, then cluster each super level separately, and finally recombine this information into a single MSM. SHC is able to produce MSMs at different resolutions using different super density level sets. To demonstrate the power of this algorithm we first apply it to a RNA hairpin, generating MSMs at different resolutions. We validate these MSMs by showing that they are able to reproduce the original simulation data.

A Splitting Algorithm for Image Segmentation on Manifolds Represented by the Grid based Particle Method

Shingyu Leung
HKUST

We discuss a novel numerical approach to solve variational problems on manifolds represented by the Grid Based Particle Method (GBPM). In particular, we propose a splitting algorithm for image segmentation on manifolds represented by unconnected sampling particles. To develop a fast minimization algorithm, we develop a new splitting method by generalizing the augmented Lagrangian method (ALM). To efficiently implement the resulting method, we further incorporate with the local polynomial approximations of the manifold in the GBPM. The resulting method is flexible for segmentation on various manifolds including closed or open or even surfaces which are not orientable.

Characterization and Applications of Nanoscale Flows

Zhigang Li

Department of Mechanical Engineering, HKUST

In nanoscale fluidic systems, the surface area to volume ratio is high and the surface plays important roles in understanding the dynamics of fluids. The surface affects the fluid motion through microparameters, such as fluid-surface binding energy. These microparameters are directly associated with macroparameters, including the temperature and external driving force. The coupling of these parameters at different scales determines the flow regimes in the nanoscale.

In this talk, a general picture of how surfaces affect the motion of fluid molecules is given and a dimensionless number is proposed for characterizing fluid motion in nanochannels. By studying the fluid dynamics of force driven flows between parallel plates, it is shown, through molecular dynamics simulation, that the fluid motion in nanochannels can be classified into different regimes, each of which is associated with a distinct mechanism. The flow regimes indicate that the surface energy of the nanochannel wall is critical in determining the flow direction if the flow is driven by a temperature gradient. In low surface energy channels, the fluid moves from high to low temperature, while the fluid migrates from low to high temperature in high surface energy channels. The possible application of this phenomenon for electronic device cooling is discussed.

Hydrodynamics of Leidenfrost Droplets in One-Component Fluids

Tiezheng Qian

HKUST

Boiling and evaporation of liquids are commonly observed in our daily life. Consider a liquid droplet deposited on a hot solid surface of constant temperature. If the solid temperature is a bit above the boiling point of the liquid, then the droplet will quickly boil and evaporate. However, if the solid temperature is much high than the boiling point, then a thin film of vapor is formed and stabilized between the liquid and the solid. A droplet that levitates over its own vapor is called a Leidenfrost droplet, named after the German physician, Johann Gottlob Leidenfrost, who first reported the phenomena in 1756. The thin vapor film prevents the liquid from directly touching the solid surface. This inhibits the nucleation of vapor bubbles. The vapor film also acts as a thermal insulator that slows down the evaporation process and extends the lifetime of the droplet.

Over the years, the Leidenfrost effect has attracted continuous pure and applied research efforts. This may be partly attributed to a variety of technological applications involving liquid droplets evaporating on hot surfaces. These include quenching of metals, quick-response steam generators, spray drying, spray cooling of nuclear reactor cores, and film cooling of rocket nozzles. Recently, the rich behaviors of the Leidenfrost droplets have become better understood with the help of high speed video imaging, surface coating, and micro-machining.

The Leidenfrost dynamics is characterized by the coupling of mass flow, free interface motion, heat conduction, and phase change (evaporation). This makes it a complicated problem exhibiting rich behaviors. Modeling and simulation efforts made for its understanding are not only of theoretical interest but also necessitated by the rapid advances in experimental study.

Recently, the dynamic van der Waals theory has been presented for one-component fluids, capable of describing two-phase hydrodynamics involving the liquid-vapor phase transition (evaporation/condensation) in inhomogeneous temperature. In addition, the boundary conditions for liquid-vapor hydrodynamics on solid surfaces have been derived by considering the dissipative processes at the fluid-solid interface. Numerical simulations have already been carried out to study the evaporative droplets on solid surfaces. We use the dynamic van der Waals theory, supplemented with the boundary conditions at the fluid-solid interface, to investigate the Leidenfrost effect. This approach will lead to a unified, quantitative and accurate treatment of many aspects of the Leidenfrost effect. In this talk, I will report our numerical results on the steady states of the stable vapor layer which demonstrate different scaling regimes as shown by recent scaling analysis. I will also present results on the take-off of small droplets which invalidates the commonly used lubrication approximation for thin vapor layers.

Continuum models for dislocation structure, energy and dynamics of dislocation arrays and low angle grain boundaries

Yang Xiang
Hong Kong University of Science and Technology

We present continuum models for dislocation structure, energy and dynamics of dislocation arrays and low angle grain boundaries which may be nonplanar and nonequilibrium. In our continuum model, we define a dislocation potential function on the dislocation array surface or grain boundary to describe the orientation dependent continuous distribution of dislocation in a very simple and accurate way. The continuum formulations of energy and dynamics are derived from the discrete dislocation model, and include the long-range interaction of constituent dislocations, local line tension effect of dislocations, and the cooperative motion of dislocations. Applications to low angle grain boundaries are presented.

Numerical and Theoretical Studies of Knudsen Force

Wenjing Ye
Department of Mechanical Engineering
Hong Kong University of Science and Technology

Thermal force created by thermal inhomogeneity in nonequilibrium systems has fascinated scientists since 19th century. As a unique actuation mechanism, mechanical forces can be created devoid of moving parts and physical contact. The early successful application of thermal force was made by Crookes in 1873, who devised the famous radiometer. Another well-known phenomenon induced by this type of force is thermophoresis, in which a small particle migrates in a gas under the influence of the thermophoretic force stemming from the temperature gradient. With the advent of microfabrication techniques, micro/nano devices with integrated heaters have been routinely made and employed for various applications. The small scale of and the large thermal gradient in these devices provide two necessary conditions for the creation of a new type of thermal force, which may benefit or deteriorate the performance of the devices.

Recently Passian *et al.* experimentally demonstrated a mechanical force, entitled as the Knudsen force, acting on a heated micromachined beam embedded in a cold vacuum chamber. The experimental results have shown that this force is proportional to the ambient pressure in low-pressure range, but inversely proportional to the pressure in high-pressure range. In this talk, a numerical and theoretical study on the origin of the Knudsen force and its relationship with the characteristic size will be presented. In particular, the shape effect on the orientation of the Knudsen force will be discussed

Discrete Modeling of fluid-Particle Interactions in Granular Media

Jidong Zhao
Department of Civil and Environmental Engineering
Hong Kong University of Science and Technology

Fluid-particle interaction underpins the performance for a wide range of key engineering infrastructures pertaining to granular media. Typical examples include the sand production in sandstone oil reservoir, internal/surface erosion of embankment dams/slopes, and submerged slope stability relevant to coastal/offshore engineering. Micromechanics-based modeling of fluid-particle interactions in granular media may offer richer information at the particle level and is helpful for reliable scale-up, design and control of different particulate systems and processes. In this talk, we present a coupled Computational Fluid Dynamics and Discrete Element Method (CFD–DEM) approach and its application to the simulation and analysis of fluid–particle interactions relevant to civil and mining engineering. The DEM is employed to model the granular particle system, whilst the CFD is used to simulate the fluid flow by solving the locally averaged Navier–Stokes equation. The particle–fluid interactions are considered with exchange of interaction forces such as drag force, buoyancy force and virtual mass force between the DEM and the CFD computations. The coupled CFD–DEM tool is first benchmarked by two classic geomechanics problems where analytical solutions are available, and is then employed to investigate the characteristics of sand heap formed in water through hopper flow and debris flow falling into a water reservoir along an inclined slope. The influence of fluid–particle interactions on the behavior of granular media is well captured in all the simulated problems. In the sandpiling problem, the sandpile formed in water is more homogeneous in terms of void ratio, contact force and fabric anisotropy. The central pressure dip of vertical stress profile at the base of sandpile is moderately reduced by the presence of water. In the debris flow case, the effect of water presence on the characteristics of granular flow such as Savage number and energy dissipation mechanism is carefully examined and discussed.