Mean-field modeling and multiscale methods for complex physical and biological system

University of California, Santa Barbara
Oct 31 – Nov 3, 2016

Conference location: University Center Santa Barbara Mission room, UCSB Campus

Monday, October 31, 2016

9:00am to 9:20am	Registration and Breakfast
9:20am to 9:30am	Welcome remarks
9:30am to 10:20am	**Pierre-Emmanuel Jabin** *Mean Field limit and Propagation of chaos for stochastic particles' systems*
10:20am to 10:30am	Break
10:30am to 11:30am	**Josselin Garnier** *Stability of mean field model for opinion dynamics and collective motion*
11:30am to 1:00pm	Lunch (on your own)
1:00pm to 1:50pm	**Lin Lin** *Adaptively compressed exchange operator*
1:50pm to 2:30pm	Break
2:30pm to 3:20pm	**Hui Sun** *Multi-scale Modeling and Simulation of the Growth of Bacterial Colony with Cell-Cell Mechanical Interactions*
3:20pm to 3:30pm	Break
3:30pm to 4:20pm	**Kathleen Craig** *From slow diffusion to a hard height constraint: characterizing congested aggregation*

Tuesday, November 1, 2016

9:00am to 9:15am	Breakfast
9:15am to 10:05am	**Bo Li** *Phase-Field Variational Implicit Solvation*
10:05am to 10:15am	Break
10:15am to 11:05pm	**Clemens Heitzinger** *The stochastic drift-diffusion-Poisson system and the Boltzmann-Poisson system*
11:05am to 11:15am	Break
11:15am to 12:05pm	**Kui Ren** *Statistical Physics of Constrained Large Dense Networks*
	Afternoon free

Wednesday, November 2, 2016

9:00am to 9:30am	Breakfast
9:30am to 10:20am	**Yi Sun** *Kinetic Monte Carlo Simulations of Multicellular Aggregate Self-Assembly in Biofabrication*
10:20am to 10:30am	Break
10:30am to 11:30am	**Kieron Burke** *Background and recent developments in density functional theory*
11:30am to 1:00pm	Lunch (on your own)
1:00pm to 1:50pm	**Oliver Pinaud** *Some recent results about wave propagation in random media with long-range dependence*
1:50pm to 2:30pm	Break
2:30pm to 3:20pm	**Emmanuel Lorin** *Nonlinear optics in gases: mathematical and numerical modeling in some nonperturbative regimes*
3:20pm to 3:30pm	Break
3:30pm to 4:20pm	**Lihui Chai** *Frozen Gaussian approximation for 3D seismic wave propagation*

Thursday, November 3, 2016

9:00am to 9:30am	Breakfast
9:30am to 10:20am	**Minh Binh Tran** *The Cauchy problem for the quantum Boltzmann equation for bosons at very low temperature*
10:20am to 10:30am	Break
10:30am to 11:20am	**Yanxiang Zhao** *Crawling and turning in a minimal reaction-diffusion cell motility model*
11:20am to 11:40am	Closing remarks

List of Abstracts

Kieron Burke: I will give an overview of density functional theory, its relation to mean-field theory, and discuss relevant recent developments. Some of my most recent work is available from my website http://dft.uci.edu/.

Lihui Chai: We present a systematic introduction on applying frozen Gaussian approximation (FGA) to compute synthetic seismograms in three-dimensional earth models. In this method, seismic wavefield is decomposed into frozen (fixed-width) Gaussian functions, which propagate along ray paths. Rather than the coherent state solution to the wave equation, this method is rigorously derived by asymptotic expansion on phase plane, with analysis of its accuracy determined by the ratio of short wavelength over large domain size. Similar to other ray-based beam methods (e.g. Gaussian beam methods), one can use relatively small number of Gaussians to get accurate approximations of high-frequency wavefield. The algorithm is embarrassingly parallel, which can drastically speed up the computation with a multicore-processor computer station. The second contribution of this work is that, we incorporate the Snell's law into the FGA formulation, and asymptotically derive reflection, transmission and free surface conditions for FGA to compute high-frequency seismic wave propagation in high contrast media. We numerically test these conditions by computing traveltime kernels of different phases in the 3D crust-over-mantle model. This is joint work with Xu Yang and Ping Tong.

Kathleen Craig: For a range of physical and biological processes—from dynamics of granular media to biological swarming—the evolution of a large number of interacting agents is modeled according to the competing effects of pairwise attraction and (possibly degenerate) diffusion. In the slow diffusion limit, the degenerate diffusion formally becomes a hard height constraint on the density of the population, as arises in models of pedestrian crown motion.

Motivated by these applications, we bring together new results on the Wasserstein gradient flow of nonconvex energies with the theory of free boundaries to study a model of Coulomb interaction with a hard height constraint. Our analysis demonstrates the utility of Wasserstein gradient flow as a tool to construct and approximate solutions, alongside the strength of viscosity solution theory in examining their precise dynamics. By combining these two perspectives, we are able to prove quantitative estimates on convergence to equilibrium, which relates to recent work on asymptotic behavior of the Keller-Segel equation. This is joint work with Inwon Kim and Yao Yao.

Josselin Garnier: In this talk, we consider two models for opinion dynamics (consensus model) and for collective motion (Czirok model). In each model, each agent's opinion or velocity locally interacts with other agents' opinions or velocities in the system. The interaction tends to create consensus convergence or the alignment of collective motion. By analyzing the associated nonlinear Fokker-Planck equation, we obtain the conditions for the existence of stationary states and the conditions for their stabilities. In both cases exogenous noise stabilizes the systems.

Clemens Heitzinger: We consider charge transport in random environments and in a multiscale setting. We use the stochastic drift-diffusion-Poisson system with all random coefficients to describe process variations in nanoscale semiconductor devices and to describe fluctuations in the detection mechanism of nanoscale sensors. We present an existence and uniqueness result and an optimal multi-level randomized quasi Monte-Carlo method, which reduces the computational cost by several orders of magnitude compared to the vanilla Monte-Carlo method. The smaller the given error bound, the more effective this method becomes. Furthermore, we discuss the multiscale setting when a fast oscillating charge concentration at the surface of a nanoscale device is homogenized. Starting from the Boltzmann-Poisson system, an effective drift-diffusion system is obtained in a diffusive scaling. Finally, we present numerical results for the stochastic transport of target molecules through new nanopore sensors. The multiscale problems inherent in these devices (high aspect ratio, two time scales, multiple species) are solved computationally by precomputing the faster transport and then calculating the statistics of the slower transport.

Pierre-Emmanuel Jabin: We consider large systems of stochastic particles interacting through rough but bounded interaction kernels. We are able to control the relative entropy between the N-particles distribution and the expected limit which solvesthe corresponding McKean-Vlasov system. This implies the Mean Field limit tothe McKean-Vlasov system together with Propagation of Chaos through the strong convergence of all the marginals. The method works at the level of the Liouville equation and relies on precise combinatorics results. This is a joint work with Z. Wang.

Bo Li: We construct a phase-field variational model for the solvation of charged molecules with an implicit solvent. The solvation free-energy functional of all phase fields consists of the solute-solvent interfacial energy, solute excluded volume and solute-solvent van der Waals dispersion energy, and electrostatic free energy. The interfacial energy is described by the van der Waals-Cahn-Hilliard functional and the electrostatic free energy is described by the Poisson-Boltzmann theory. Our computational results show that this model captures the multiple hydration states and effect of electrostatics. We prove the the continuity of the electrostatics---its

potential, free energy, and dielectric boundary force---with respect to the perturbation of dielectric boundary. We also prove the convergence of the phase-field free-energy functionals and forces to their sharp-interface limits. In particular, we obtain the force convergence for the van der Waals-Cahn-Hilliard functionals with minimal assumptions.

Lin Lin: The Fock exchange operator plays a central role in modern quantum chemistry, such as in Hartree-Fock calculations and Kohn-Sham density functional theory calculations with hybrid exchange-correlation functionals. The Fock exchange operator significantly increases the computational cost for solving the associated Kohn-Sham eigenvalue problem. We develop the adaptively compressed exchange operator formulation, which greatly reduces the computational cost associated with the Fock exchange operator without loss of accuracy. The ACE formulation does not depend on the size of the band gap, and thus can be applied to insulating, semiconducting as well as metallic systems. Numerical results indicate that the ACE formulation can become advantageous even for small systems with tens of atoms.

Emmanuel Lorin: This talk is dedicated to the mathematical and numerical modeling of nonlinear optics in gases for some nonperturbative regimes. After an overview of the classical perturbative modeling, I will present a multiscale model for short&intense laser-gas interaction. Some mathematical, computational and HPC aspects will be discussed, and some numerical experiments will be presented.

Olivier Pinaud: In a first part, we will present a rigorous derivation of the (fractional) white noise paraxial regime from the random wave equation. This combines two asymptotics: the paraxial approximation, where the wavefield is described by a Schroedinger equation, and the white noise limit, where the random potential becomes a white noise. The latter is actually of fractional type since the original potential has long-range correlations. This leads to great technical difficulties compared to the short-range case since standard diffusion theorems are not available. In a second part, we will consider more general paraxial models and some of their asymptotic regimes, and investigate at which cost a splitting method accurately captures them. This is joint work with C. Gomez (University of Marseille, France).

Kui Ren: We study the asymptotics of large random graphs constrained by the limiting density of edges and the limiting subgraph density of an fixed graph H (for instance two stars and triangles etc). We show numerically and analytically (in some cases) that typical graphs with such constraints have very simple structures: asymptotically in the number of vertices there is a partition of the vertices into $M < \infty$ subsets $V_1, V_2, \ldots, V_M$, and a set of well-defined probabilities g_{ij} of an edge between any $v_i \in V_i$ and $v_j \in V_j$. We discuss briefly some possible applications of this research,

for instance in image processing. This talk is based on joint works with Richard Kenyon (Brown), Charles Radin (Austin) and Lorenzo Sadun (Austin).

Yi Sun: We present a 3D lattice model to study self-assembly of multicellular aggregates by using kinetic Monte Carlo (KMC) simulations. This model is developed to describe and predict the time evolution of postprinting structure formation during tissue or organ maturation in a novel biofabrication technology--bioprinting. Here we simulate the self-assembly and the cell sorting processes within the aggregates of different geometries, which can involve a large number of cells of multiple types.

Hui Sun: The growth of bacterial colony exhibits striking patterns that are determined by the interactions among individual, growing and dividing bacterial cells, and that between cells and the surrounding nutrient and waste. Understanding the principles that underlie such growth has far-reaching consequences in biological and health sciences. In this work, we construct a multi-scale model of the growth of E. coli cells on agar surface. Our model consists of detailed, microscopic descriptions of the cell growth, cell division with fluctuations, and cell movement due to the cell-cell and cell-environment mechanical interactions, and macroscopic diffusion equations for the nutrient and waste. Our large-scale simulations reproduce experimentally observed growth scaling laws, strip patterns, and many other features of an E. coli colony. This work is the first step toward detailed multi-scale computational modeling of three-dimensional bacterial growth with mechanical and chemical interactions. This is joint work with Dr. Mya Warren, Ms. Yue Yan, Dr. Bo Li, and Dr. Terry Hwa.

Minh Binh Tran: This model approximates the evolution of quasiparticles in a dilute gas of bosons at very low temperature by a quadratic Boltzmann problem with a cubic kinetic transition probability kernel. The solution to this equation couples to the a system for the quantum density evolution of the condensate, modeled by a coupled system of Gross-Pitaevskii and quantum Boltzmann equation for bosons.
At this first stage, we prove existence and uniqueness for the quantum Boltzmann model after deriving a priori qualitative properties including propagation and creation of polynomial moments, by means of of ODE's methods in Banach spaces by characterizing an invariant bounded, convex, closed solutions subset of integrable solutions with bounded mass differentiable in time. We also show the propagation and creation of Mittag-Leffler moments that characterize the exponential order of the tails decay.
This is a work in collaboration with Ricardo Alonso and Irene M. Gamba.

Yanxiang Zhao: We study a minimal model of a crawling eukaryotic cell with a chemical polarity controlled by a reaction diffusion mechanism describing Rho

GTPase dynamics. The size, shape and speed of the cell emerge from the combination of the chemical polarity, which controls the locations where act polymerization occurs, and the physical properties of the cell, including its membrane tension. We find in our model both highly persistent trajectories, in which the cell crawls in a straight line, and turning trajectories, where the cell transitions from crawling in a line to crawling in a circle. We discuss the controlling variables for this turning instability, and argue that turning arises from a coupling between the reaction-diffusion mechanism and the shape of the cell. This emphasizes the surprising features that can arise from simple links between cell mechanics and biochemistry. Our result suggest that similar instabilities may be present in a broad class of biochemical descriptions of cell polarity.