Center for Soft Matter and Biological Physics Seminars

Fall 2017

Organizer: *Vinh Nguyen*

Refreshments are served before the seminars *(unless otherwise indicated)*

2017 | August | September | October | November | December |

August 2017	
August 28 Monday 4:00pm 304 Robeson Hall **Joint CM Seminar** (poster)	**Sheng Chen** Department of Physics, Virginia Tech **Computational studies of predator-prey competition models** The two-species stochastic Lotka-Volterra model already displays very interesting non-equilibrium dynamical properties on a two-dimensional square lattice. In order to explore possible origins of biodiversity, we add a second competing predator species, which renders the system even more complex. The individual predators are characterized by randomly distributed predation efficiencies and death rates, to which Darwinian evolutionary adaptation is introduced. We find that direct competition between predator species in combination with so-called character displacement play an important role in stabilizing ecologically diverse communities. **Host: *Uwe Täuber*** **Labor Day. No seminar scheduled.**
September 2017	
September 4 Monday 4:00pm 304 Robeson Hall **Holiday No Meeting** (poster)	
September 11 Monday 4:00pm 304 Robeson Hall (poster)	**Seminar cancelled and rescheduled to a later date.**
September 18 Monday 4:00pm 304 Robeson Hall **Joint CM Seminar** (poster)	**Prof. Lauren Childs** Department of Mathematics, Virginia Tech **Simulating Within-Vector Generation of the Malaria Parasite Diversity** *Plasmodium falciparum*, the malaria parasite causing the most severe disease in humans, undergoes an asexual stage within the human host, and a sexual stage within the vector host, *Anopheles* mosquitoes. Because mosquitoes may be super-infected with parasites of different genotypes, this sexual stage of the parasite life-cycle presents the only opportunity in the full life cycle to generate large genetic differences in parasites through recombination. To investigate the role that mosquitoes' biology plays on the generation of parasite diversity, we constructed a stochastic model of parasite development within-mosquito over its lifespan. We then coupled a model of sequence diversity generation via recombination between genotypes to the stochastic parasite population model. Our two-part model framework shows that bottlenecks entering the oocyst stage decrease diversity from the initial gametocyte population in a mosquito's blood meal, but diversity increases with the possibility for recombination and proliferation in the formation of sporozoites. Furthermore, when we begin with only two distinct parasite genotypes in the initial gametocyte population, the probability of transmitting more than two unique genotypes from mosquito to human is over 50% for

	a wide range of initial gametocyte densities. **Host: *Michel Pleimling***
September 25 Monday 4:00pm 304 Robeson Hall **Joint CM Seminar** (poster)	**Harsh Chaturvedi** Department of Physics, Virginia Tech **Dynamics Of Driven Vortices In Type-II Superconductors** Technical applications of type-II superconductors in external magnetic fields require an effective flux pinning mechanism to reduce Ohmic losses due to flux creep and flow. In addition, driven vortex matter subject to thermal fluctuations and quenched disorder constitutes a system far from equilibrium that yields rich phase diagrams and many novel glassy states. Using numerical and analytical techniques, we have studied in detail, the dynamical relaxation features towards the equilibrium vortex or Bose glass phases following sudden changes in externally applied electric current. Most recently, we have characterized the long-time steady-state behavior of vortices driven perpendicular to a family of parallel planar defects (that model twin boundaries found in superconducting YBCO), revealing in the process, a rich collection of novel dynamical regimes spanning a remarkably broad depinning transition region that separates the pinned and moving-lattice states of vortex matter. **Host: *Uwe Täuber***
October 2017	
October 2 Monday 4:00pm 304 Robeson Hall **Joint CM Seminar** (poster)	**Prof. Xiaowei Wu** Department of Statistics, Virginia Tech **Learning Patterns from Genomics Data through Stochastic Modeling** Next-generation sequencing (NGS) enables a large variety of genomics applications (genome sequencing, transcriptome profiling, DNA-protein interactions, epigenome characterization, etc), and opens up unprecedented opportunities to uncover the genetic architecture and mechanisms of biological processes. However, it still remains challenging to build flexible and robust statistical models for knowledge discovery from the wealth of genomics data generated by NGS. We present several typical applications of state-of-the-art nonparametric methods (e.g., NP-Bayesian clustering, functional mixed model) based on the inhomogeneous Poisson process model of genomic heterogeneity patterns. These methods provide effective solutions to the modeling and analysis of modern omics data. Findings from such applications will help biologists better understand the molecular nature of biological processes such as transcriptional regulation and trait differentiation. **Host: *Uwe Täuber***
October 9 Monday 4:00pm 304 Robeson Hall (poster)	**Condensed Matter seminar. No CSB seminar scheduled.**
October 16 Monday 4:00pm 304 Robeson Hall **Joint CM Seminar** (poster)	**Dr. Charles Reichhardt** Los Alamos National Laboratory **Skyrmion Lattices in Random and Ordered Potential Landscapes** Since the initial discovery of skyrmion lattices in chiral magnets [1], there has been a tremendous growth in this field as an increasing number of compounds are found to have extended regions of stable skyrmion lattices [2] even close to room temperature [3]. These systems have significant promise for applications due to their size scale and the low currents or drives needed to move the skyrmions [4]. Another interesting aspect of skyrmions is that the equations of motion have significant non-dissipative terms or a Magnus effect which makes them unique in terms of collective driven dynamics as compared to other systems such as vortex lattices in type-II superconductors, sliding charge density waves, and frictional systems. We examine the driven dynamics of skyrmions interacting with random and periodic substrate potentials using both continuum based modelling and particle based simulations. In clean systems we examine the range in which skyrmion motion can be explored as a function of the magnetic field and current and show that there can be a current-induced creation or destruction of skyrmions. In systems with random pinning we find that there is a finite depinning threshold and that the Hall angle shows a strong dependence on the disorder strength. We also show that features in the transport curves correlate with different types of skyrmion flow regimes including a skyrmion glass depinning/skyrmion plastic flow region as well as a transition to a dynamically reordered skyrmioncrystal at higher drives. We find that increasing the Magnus term produces a low depinning threshold which is due to a combination of skyrmions forming complex orbits within the pinning sites and skyrmion-skyrmion scattering effects. If the skyrmions are moving over a periodic substrate, with increasing drive the Hall angle changes in quantized steps which correspond to periodic trajectories of the skyrmion that lock to symmetry directions of the substrate potential. [1] S. Muhlbauer et al Science 323 915 (2009). [2] X. Z. Yu et al. Nature 465, 901-904 (2010). [3] X.Z. Yu et al Nature Materials, 10, 106 (2011). [4] A. Fert, V. Cros, and J. Sampaio Nature Nanotechnology 8, 152 (2013). **Host: *Michel Pleimling***

October 17 Tuesday 2:00pm 304 Robeson Hall **Special CSB Seminar** (poster)	**Dr. Charles Reichhardt** Los Alamos National Laboratory **Jamming and Clogging of Passive and Active Particles in Disordered Media** There has been tremendous growth in studying nonequilibrium systems of particle assemblies which can exhibit jamming effects. In general jamming has been studied in the absence of quenched disorder. Here we examine the dynamics of active and passive matter systems interacting with random or periodic substrates and obstacle arrays, and show that it is possible to make a clear distinction between jammed systems and clogged systems. For non-active systems of particles flowing through random obstacle arrays, when the particle density is well below that at which an obstacle free system would jam, we find that the system can reach a clogged state. The clogged states can be distinguished from jammed states in that they are spatially heterogeneous, are fragile, and have a pronounced memory effect. In contrast, jammed states are much more homogeneous, robust, and have much weaker memory effects. We outline a possible scenario in which jamming is dominated by a diverging length scale associated with a critical density at point J, while clogging is associated with the coarsening of a dense area across the sample. We have also investigated clogging and jamming in active matter or self-motile particle systems. Such dynamics can effectively describe certain biological systems such as run-and-tumble bacteria or crawling cells, as well as non-biological systems such as self-driven colloids or artificial swimmers. For active matter systems driven over random disorder we find that for intermediate amounts of self-motility the system does not clog; however, for increasing self-propulsion of the particles there is a strong reduction of the mobility due to a self-clogging or self-clustering in the system that resembles the "faster is slower" effect found in certain pedestrian panic models. **Host: *Michel Pleimling*** **No seminar scheduled.**
October 23 Monday 4:00pm 304 Robeson Hall (poster)	
October 30 Monday 4:00pm 304 Robeson Hall **Joint CM Seminar** (poster)	**Madhurima Nath** Virginia Tech Biocomplexity Institute **Statistical Mechanical Applications of Graph Dynamical Systems** Moore and Shannon's reliability polynomial can be used as a global statistic to explore the behaviour of a diffusive process on a network that represents a finite sized interacting system. It depends on both the network topology and the dynamics of the process and gives the probability that the system has a particular desired property. Due to the complexity to evaluate the exact network reliability, it has been classified as a NP-hard problem. The estimation of the reliability polynomials for large graphs is feasible using Monte-Carlo simulation. Depending on the description of the functionality, network reliability can be utilized for a number of applications ranging from epidemiology to statistical physics. For example, it serves as a measure to study the sensitivity of the outbreak of an infectious disease on a network to the structure of the network. Further, it is analogous to the partition function of a statistical mechanical system which provides insights to the interpolation between the low and high temperature limits. **Host: *Uwe Täuber***
November 2017	
November 6 Monday 4:00pm 304 Robeson Hall (poster)	**Condensed Matter seminar. No CSB seminar scheduled.**
November 9 Thursday 4:00pm 304 Robeson Hall **Special CSB Seminar** (poster)	**Professor Srividya Iyer-Biswas** (Department of Physics, Purdue University) **Making the right noise** In this talk I will introduce a theoretical framework that serves as the natural representation for biochemical dynamics, and illustrate its utility in a variety of contexts. **Host: *Uwe Täuber***

November 13 Monday 4:00pm 304 Robeson Hall (poster)	**Condensed Matter seminar. No CSB seminar scheduled.**
November 20 Monday 4:00pm 304 Robeson Hall **Holiday No Meeting** (poster)	**Thanksgiving Break. No seminar scheduled.**
November 27 Monday 4:00pm 304 Robeson Hall **Joint CM Seminar** (poster)	**Prof. Jiangtao Cheng** Department of Mechanical Engineering, Virginia Tech **Mechanism and Universal Scaling Law for Contact Line Friction of Cassie-State Droplets on Nano-Structured Ultrahydrophobic Surfaces** The design and optimization of micro/nano-fluidic devices or wetting-related applications necessitate the knowledge of the physical mechanisms underlying the moving contact line, which is beyond the predictive capability of the continuum theory. Here we use the molecular dynamics (MD) simulations to explore the Cassie-state wetting dynamics on nano-structured surfaces with an emphasis on the contact line friction (CLF). We find that CLF emerges as a result of the solid-liquid interactions and liquid-liquid interactions, which are termed as solid-liquid retarding and viscous damping respectively. Solid-liquid retarding is ascribed to the work of adhesion and viscous damping is related to the depletion of liquid density near the solid-liquid interface. With gradually decreased solid-liquid contact fraction (larger apparent contact angle), solid-liquid retarding remains unchanged while viscous damping is increased. A universal scaling law is derived to describe the CLF on ultrahydrophobic surfaces before the Cassie-to-Wenzel transition. It is suggested that the non-sticking feature (smaller CLF) of nanostructured ultrahydrophobic surfaces is indeed caused by the lowered fraction of the solid-liquid contact. Our results have revealed the genesis of CLF from an ab initio perspective and have demonstrated the effects of surface structures on dynamic wetting by justifing the dominant role of solid fraction in lowering CLF. **Host: *Shengfeng Cheng*** 
December 2017	
December 4 Monday 4:00pm 304 Robeson Hall **Joint CM Seminar** (poster)	**Yanfei Tang** Department of Physics, Virginia Tech **Molecular Dynamics Simulations of Drying Colloidal Films** Evaporating solvent out of a colloidal suspension is an important technology to fabricate thin-film materials. The structure of the deposited film highly depends on the drying process. For example, when the solvent evaporates fast the colloidal particles can accumulate near the receding liquid-vapor interface, a phenomenon known as skin-layer formation. In this talk, I will discuss our recent molecular dynamics simulations of a drying suspension containing a binary mixture of colloidal nanoparticles. A distinguishing feature of our work is that the solvent is modelled explicitly as a Lennard-Jones liquid, which allows us to explore the effects of solvent on the structure of the drying film. We have confirmed a recently-found "small-on-top" stratification phenomenon in which the smaller nanoparticles form a layer closer to the liquid-vapor interface and on top of the layer of the larger nanoparticles. However, our results show that density and temperature gradients can develop in the solvent during drying and these gradients have profound effects on stratification that are not revealed in previous work based on an implicit solvent model. I will also talk about theory and simulations of a nanoparticle at a liquid-vapor interface, which clarifies the physical foundation of the implicit solvent model used in literature in which the liquid-vapor interface is modeled as a potential barrier or well. **Host: *Shengfeng Cheng***
December 11 Monday 4:00pm 304 Robeson Hall **Joint CM Seminar**	**Prof. Robert S. Hoy** University of South Florida **Thermalized soft glassy rheology** As far back as the work of Ree and Eyring in the 1950s, plastic deformation of solids has been modeled as being controlled by multiple relaxation processes with different characteristic rates. The energy landscape picture of Stillinger et. al. allows it to be

(poster)	simultaneously viewed as being controlled by energy minima of broadly distributed depths and statistical weights. Modern theories of plasticity such as soft glassy rheology (SGR) and shear transformation zones (STZ) connect these two ideas, viewing amorphous solids as being composed of spatially localized "plastic zones": basins in systems' energy landscapes with characteristic relaxation rates determined by the depths of their associated energy barriers. Recent studies have shown that the STZ and SGR theories are thermodynamically consistent and therefore amenable to rigorous nonequilibrium- thermodynamic treatment. However, a particularly important open problem is determining the degree to which plastic flow is thermalized, i.e. the degree to which the "slow" degrees of freedom corresponding to plastic zone configurations are in equilibrium with the "fast" degrees of freedom corresponding to localized motions of systems' constituent atoms and molecules. I will describe a recently developed continuous formulation of SGR theory corresponding to the infinite-system-size limit and including fully thermalized strain degrees of freedom, and show that it enables prediction of many physical properties that cannot be straightforwardly accessed within the standard, discrete-zone formulation. Most notably, it allows direct calculation of systems' nonequilibrium, strain-history-dependent positions on their energy landscapes, which in turn allows standard statistical mechanics to be employed for followup calculations. These in turn allow straightforward quantitative analyses of model amorphous systems' heterogeneous yielding dynamics and nonequilibrium deformation thermodynamics. As a demonstration of the method, I will illustrate the very different characters of fully-thermal and nearly-athermal plasticity by comparing results for thermalized vs. nonthermalized strain degrees of freedom and plastic flow rules. **Host: *Shengfeng Cheng***