Short Talk Schedule

SESSION A – *Monday Morning*

A1: N. Giovambattista, CUNY

Coauthor: Thomas Loerting, Boris R. Lukanov, Francis W. Starr
Interplay of the Glass Transition and the Liquid-Liquid Phase Transition in Water
Abstract: Most liquids can form a single glass or amorphous state when cooled sufficiently fast (in order to prevent crystallization). However, there are a few substances that are relevant to scientific and technological applications which can exist in at least two different amorphous states, a property known as polyamorphism. Examples include silicon, silica, and in particular, water. In the case of water, experiments show the existence of a low-density (LDA) and high-density (HDA) amorphous ice that are separated by a dramatic, first-order like phase transition. It has been argued that the LDA-HDA transformation evolves into a first-order liquid-liquid phase transition (LLPT) at temperatures above the glass transition temperature Tg. However, obtaining direct experimental evidence of the LLPT has been challenging since the LLPT occurs at conditions where water rapidly crystallizes. In this talk, I will explore the effects of a LLPT on the pressure dependence of Tg(P) for LDA and HDA. Our study is based on computer simulations of two water models -- one with a LLPT (ST2 model), and one without (SPC/E model). In the absence of a LLPT, Tg(P) for all glasses nearly coincide. Instead, when there is a LLPT, different glasses exhibit dramatically different Tg(P) loci which are directly linked with the LLPT. Available experimental data for Tg(P) are only consistent with the scenario that includes a LLPT (ST2 model) and hence, our results support the view that a LLPT may exist for the case of water.

A2: S. Fortin, Rutgers University

Coauthor: S. Ji
First Law of Transcriptomics: Transcriptosomes and Degradosomes are Molecular Machines that 'Curve' RNA Concentration Space
Abstract: Transcriptomics is the study of the metabolism of RNA molecules in living cells, including their synthesis and degradation catalyzed by molecular machines known as transcriptosomes and degradosomes, respectively. Transcriptomics is analogous to classical mechanics in that the former studies the time-dependent changes in (or the trajectories of) RNA molecules inside the living cell whereas the latter studies the trajectories of moving objects in space and time. Just as physicists can determine the forces acting on a moving object by examining its trajectory, so biophysicists can infer the forces acting on individual RNA molecules inside the cell by examining their trajectories in the concentration space. Go to: http://www.math.rutgers.edu/events/smm/ to view the entire abstract.

A3: V. Tkachenko, Ben Gurion University of the Negev

Gaps in spectra of 1d periodic differential operators of order $n > 2$
Abstract: It is well known that the spectra of 1d Hill operators, i.e., of differential operators with periodic potentials, have a band structure [1]. It is less known that generically all virtual spectral gaps are open, {\it cf}., [2]. We discuss the same phenomena for 1d periodic dfferential operators of order $n > 2$.
References
[1] E.C.Titchmarsh, {\it Eigenfunction expansions associated with second-order differential equations}, Claredon Press, Oxford (1946).
[2] V.Marchenko, and I.Ostrovskii, {\it Characterization of the spectrum of Hill's operator}, Mathem. Sborn., 97, 4 (1975), 540-606; English transl. in Math. USSR-Sb. 26 (175).

A4: J.-J. Dong, Bucknell University
Coauthors: Stefan Klumpp, Royce K.P. Zia
"Novel Phases in Accelerated Exclusion Process"
Abstract: We introduce a class of distance-dependent interactions in an accelerated exclusion process (AEP) inspired by the cooperative speed-up observed in transcribing RNA polymerases. On a ring, a particle hops to the neighboring site if it is vacant and, if reaching another cluster of particles, can kick up the frontmost particle in that cluster. The steady state of AEP shows a discontinuous transition, from being homogeneous (with augmented currents) to phase-segregated. More surprisingly, the current-density relation in the phase-segregated state is simply $J=1-\rho$, indicating the particles (or holes) are moving at unit velocity despite the inclusion of long-range interactions.

A5: Y-Y. Liu, Northeastern University
Coauthors: Yang-Yu Liu*, Endre Csóka, Haijun Zhou, and Márton Pósfai
Core percolation on complex networks
Abstract: As a fundamental structural transition in complex networks, core percolation is related to a wide range of important problems, including combinatorial optimizations and network controllability. Yet, previous theoretical studies of core percolation have been focusing on the classical Erdő-Rényi random networks with Poisson degree distribution, which are quite unlike many real-world networks with scale-free or fat-tailed degree distributions. Here we analytically solve the core percolation problem for complex networks with arbitrary degree distributions. We find that purely scale-free networks have no core for any degree exponents. We show that for undirected networks if core percolation occurs then it is continuous while for directed networks it is discontinuous (and hybrid) if the in- and out-degree distributions differ. We also find that core percolation on undirected and directed networks have completely different critical exponents associated with their critical singularities.

A6: L. Colwell, IAS
Coauthor: Yu Qin, Michael Brenner (Harvard University)
Detecting correlations in large, undersampled datasets
Abstract: We use Random Matrix Theory (RMT) to study the behaviors of eigenvalues and eigenvectors of the Pearson correlation matrix of multivariate datasets. By both numerical and analytical methods, we discover that when the signal and noise are mixed, the imprint of the signal tends to equally spread over several eigenvectors rather than mostly concentrate in one eigenvector. Accordingly, we develop an algorithm that uses eigenvector pairs to extract clusters of co-varied variables.

A7: B. Miller, Texas Christian University
Coauthor: A. Hartl and B. Miller*
Dynamics of a Real World Billiard
Abstract: The seminal model for investigating formulations of nonlinear dynamics is the billiard. We introduce a mathematical model for describing the motion of a realistic billiard for arbitrary boundaries, where we include rotational effects and additional forms of energy dissipation. Simulations of the model are applied to parabolic, wedge and hyperbolic billiards that are driven sinusoidally. The simulations demonstrate that the parabola has stable, periodic motion, while the wedge and hyperbola (at high driving frequencies) appear chaotic. The hyperbola, at low driving frequencies, behaves similarly to the parabola; i.e., has regular motion. Comparisons are made between the model's predictions and previously published experimental data. The representation of the coefficient of restitution employed in the model resulted in approximate agreement with the experimental data for all of the considered boundary shapes. We investigate how the apparent coefficient of restitution varies under different model

assumptions. It is shown that the data can be successfully modeled with a simple set of parameters.

A8: S. Rahi, The Rockefeller University
Optimal cell cycle checkpoint decisions
Abstract: Cells replicate in a stereotyped process called the cell cycle. At specific points, called checkpoints, the sequence of cell cycle events halts if errors are detected or prior events are not complete. Motivated by experiments which show that the cell cycle ignores unrepaired damage after arresting for some time, we postulate that unicellular organisms have evolved to balance the likelihood of lethality of errors and the time needed for correcting them. We calculate the decision function which maximizes the expected size of the population for a stochastic repair process. Our results provide testable, system-level predictions and show how the textbook picture of (absolute) checkpoints may need to be refined.

A9: N. Mangan, Harvard University
Coauthor: M. Brenner
Organizing biochemical reactions: Lessons from cyanobacteria
Abstract: Cyanobacteria are model organisms for photosynthesis and are of interest for bio-fuel production and carbon dioxide sequestration. I present a mathematical model of the carbon concentrating mechanism (CCM) in cyanobacteria. The CCM is a combination of transporters and enzymes distinctively organized in the cell, which increase the internal concentration of carbon dioxide, and improve the efficiency of converting carbon dioxide to sugar. I find that the internal carbon concentration can be completely described by solutions in two parameter regimes of the model. These solutions correspond to varying transporter and enzymatic activity, which can be directly connected to experimental measurements. I also find a dependence of the carbon concentration on the spatial organization of the reactions within the cell. Understanding the CCM in cyanobacteria gives us insight into design principles for the cellular organization of biological reactions.

A10: I. Segota, Cornell University
Coauthor(s): Igor Segota*, Carl Franck
Signal processing in eukaryotic chemotaxis Abstract: Unlike inanimate condensed matter, living cells depend upon the detection of chemical signals for their existence. First, we experimentally determined the chemotaxis response of eukaryotic Dictyostelium cells to static folic acid gradients and show that they can respond to gradients as shallow as 0.2% across the cell body. Second, using Shannon's information theory, we showed that the information cells receive about the gradient exceeds the theoretically predicted information at the receptor-ligand binding step, resulting in the violation of the data processing inequality. Finally, we analyzed how eukaryotic cells can affect the gradient signals by secreting enzymes that degrade the signal. We analyzed this effect with a focus on a well described Dictyostelium cAMP chemotaxis system where cAMP signals are affected by an extracellular cAMP phosphodiesterase (PDE) and its inhibitor (PDI). Using a reaction-diffusion model of this set of interactions in the extracellular space, we show that cells can effectively sense much steeper chemical gradients than naively expected (up to a factor of 12). We also found that the rough estimates of experimental PDE and PDI secretion rates are close to the optimal values for gradient sensing as predicted by our model.

A11: C. Franck, Cornell University

Coauthors: Igor Segota, Ariana Strandburg-Peshkin, Xiao-Qiao S. Zhou, Archana Rachakonda, Benjamin Yavitt, Catherine J. Lussenhop, Sungsu Lee, Kevin Tharratt, Amrish Deshmukh, Elisabeth Sebesta, Myron Zhang, Sharon Lau, Sarah Bennedsen, David Franck*, Junseok Oh, Anthony Hazel and Viyath Fernando
Experimental Insights into Collective Effects for Eukaryotic Cell Proliferation in Dilute Suspensions
Abstract: Physicists can look to dilute suspensions of apparently solitary cells in stirred suspension for elegant realizations of multicellular behavior. In contrast to our earlier work (Phys. Rev. E v. 77, 041905 (2008)) with the amoeba Dictyostelium discoideum we are discovering that the vital intercellular communications responsible for the well-known but poorly understood slow to fast transition in a growing culture as a function of time might be due to the passage of chemical messages between transient cell clusters or throughout the entire system rather than because of binary collisions. In considering the observed significant variation in proliferation rates we feel that a possible explanation is provided by our recent discovery that for best growth cultures are surprisingly dependent on incubator geometry.

A12: N. Giovambattista, CUNY
Coauthors: Thomas Loerting, Boris R. Lukanov, Francis W. Starr
Interplay of the Glass Transition and the Liquid-Liquid Phase Transition in Water
Abstract: Most liquids can form a single glass or amorphous state when cooled sufficiently fast (in order to prevent crystallization). However, there are a few substances that are relevant to scientific and technological applications which can exist in at least two different amorphous states, a property known as polyamorphism. Examples include silicon, silica, and in particular, water. In the case of water, experiments show the existence of a low-density (LDA) and high-density (HDA) amorphous ice that are separated by a dramatic, first-order like phase transition. It has been argued that the LDA-HDA transformation evolves into a first-order liquid-liquid phase transition (LLPT) at temperatures above the glass transition temperature Tg. However, obtaining direct experimental evidence of the LLPT has been challenging since the LLPT occurs at conditions where water rapidly crystallizes. In this talk, I will explore the effects of a LLPT on the pressure dependence of Tg(P) for LDA and HDA. Our study is based on computer simulations of two water models -- one with a LLPT (ST2 model), and one without (SPC/E model). In the absence of a LLPT, Tg(P) for all glasses nearly coincide. Instead, when there is a LLPT, different glasses exhibit dramatically different Tg(P) loci which are directly linked with the LLPT. Available experimental data for Tg(P) are only consistent with the scenario that includes a LLPT (ST2 model) and hence, our results support the view that a LLPT may exist for the case of water.

SESSION B – *Tuesday morning*

B1: S. Ji, Rutgers University
The Metabolic Tetractys: The Four Forces that Determine the whole-Cell RNA Kinetic Patterns (RNA Dissipatons)
Abstract: The cell force can be operationally defined as any physical agent or entity that can cause changes in cell metabolism. For example, switching the nutrient from glucose to galactose [1] or shifting the environmental temperature from 25° to 37° [2] in cell suspensions of budding yeast constitute cell forces since they cause rapid changes in the intracellular levels of millions of RNA molecules in individual cells, each RNA molecule being encoded by one of the 6,300 genes in the yeast genome. When these forces are applied to yeast cells, the intracellular RNA levels exhibit two kinds of changes as revealed by the microarray technique the RNA-specific and RNA-non-specific kinetic patterns [3]. The former patterns account for about 15% and the latter 85 % of the whole intracellular RNA population. Go to: http://www.math.rutgers.edu/events/smm/ to view full abstract.

B2: D. Yao, Rutgers University
Coauthor: David Yao* and Sungchul Ji
Non-Exponential Distributions of 'Homeodynamic' RNA Dissipative Structures (Dissipatons) in 20 Breast Cancer Patients
Abstract: I. Prigogine (1917-2003) divided all the material structures in the Universe into dissipative and equilibrium structures, depending on whether or not energy dissipation is required for their maintenance. The dynamic patterns of the changes in the RNA levels in living cells are examples of dissipative structures (or dissipatons for convenience) because they disappear when energy supply to the cell is blocked. The term "homeodynamic" is adopted here to refer to the maintenance (`homeo-') of dynamic patterns (`dynamic') in contrast to `homeostasis' which refers to the maintenance of static or steady states. Please go to: http://www.math.rutgers.edu/events/smm to view the entire abstract.

B3: R. Fisch
Evidence of Long Range Order in the Riemann Zeta Function
Abstract: We have done a statistical analysis of some properties of the contourlines Im$(\zeta (s))$ = 0 of the Riemann zeta function. We find that this function is broken up into strips whose average width on the critical line does not appear to vary with height. We also compute the position of the primary zero for the lowest 200 strips, and find that this probability distribution also appears to be scale invariant.

B4: E. DeGiuli, UBC
The stress-geometry equation for granular materials
Abstract: Using discrete calculus, we derive the missing stress-geometry equation for isostatic granular materials in two dimensions, in the mean-field approximation. We show that (a) the equation imposes granularity in a literal sense; (b) we recover anisotropic elasticity, without reference to strain, and (c) stress anisotropy arises from fabric anisotropy.

B5: B. Brinkman,University of Illinois at Urbana-Champaign
Coathors: Michael LeBlanc, Yehuda Ben-Zion, J. T. Uhl and Karin A. Dahmen
Predicting large quakes using small-quake tidal correlations
Abstract: Recent earthquake analyses indicate correlations between tidal stresses and small earthquakes preceding large earthquakes in Indonesia and Japan. This suggests correlations between small quakes and external periodic stresses may be viable indicators of impending large earthquakes, in contrast to previous expectations. In this talk I discuss a simple probabilistic model of earthquake statistics developed in order to better understand the behavior of earthquake faults subjected to external periodic stresses and how we can use such observations to perhaps one day predict large earthquake events.

B6: J. Ellowitz, James Franck Institute/University of Chicago
Coauthor(s): Jake Ellowitz*, Nicholas Guttenberg, Wendy Zhang
Collimated ejecta and perfect-fluid flow from colliding granular jets Abstract: We show that the collision of two densely packed granular jets containing rigid particles supports a simple continuum description when the particle diameter is much smaller than the jet diameter. Comparisons between discrete-particle simulations and exact solutions demonstrate that the averaged velocity- and pressure-fields produced in this regime are described by perfect-fluid flow. One, highly visible, consequence of this limiting behavior is that the particles ejected away from the center of the collision are highly collimated. The thin sheet of ejecta produced in this perfect-fluid flow regime contrasts sharply with the wide scatter produced by the collision of granular jets containing larger particles and/or particles at lower volume fraction. Finally, we show that this simplifying behavior is robust: dissipative processes such as inelasticity and/or friction

during grain-grain collisions yield only small perturbations to the averaged velocity- and pressure fields.

B7: A. Kabakcioglu, Koc University, Istanbul
Coauthors: A. Bar and D. Mukamel
Macroscopic loop formation during thermal denaturation of DNA with a fixed linking number
Abstract: Statistical mechanics of DNA denaturation under fixed linking number (LK) - a topological constraint imposed by the boundary conditions - is qualitatively different from that of the unconstrained DNA. The phase transition is continuous irrespective of whether LK conservation is maintained through plectoneme formation or overtwisting, or both. We recently showed that, a macroscopic loop accompanies the high-temperature phase through a mechanism similar to Bose-Einstein condensation. While the macroscopic loop grows with T>Tc, the total mass of microscopic loops decreases with a cusp at Tc.

B8: F. Gasparini, University at Buffalo, SUNY
Coauthor: J. K. Perron
Weal-link coupling in a critical system: 4He at the superfluid transition
Abstract: Recent experiments with helium confined in an array of boxes, and linked through a 33 nm film have shown that both the specific heat and the superfluid density show significant enhancements relative to control experiments where these links are not present. The behavior of the data can be understood in terms of the expected temperature dependence of the 3D correlation length [1]. However, surprisingly, the coupling extends to distances as large as 30-50 times the correlation length. We believe these are the first measurements of coupling in a controlled geometry for a critical system. [1] J. K. Perron and F. M. Gasparini, Phys. Rev. Lett. 109,035302, 2012

B9: M. Fedele, New York University
Coauthors: Cecilia Vernia, Pierluigi Contucci
Inverse problem robustness for multi-species mean field models
Abstract: In recent years there has been an increasing interest in studying the inverse problem in statistical mechanics mostly due to the fact that the thermodynamic formalism on a macroscopic base has proved to be effective in a variety of scientific applications. We handle this problem for a particular class of models that have naturally emerged within the application of the statistical mechanics formalism to socio-economical sciences. We show how to reconstruct the parameter values and test the robustness of the method for different values of such parameters.

B10: A. Toom, Universidade Federal de Pernambuco
Coauthors: A. D. Ramos, F. Sinatra, C. S. Souza
Variable-Length Analog of Stavskaya Process: A New Example of Misleading Simulation
Abstract: Let M denote the sigma-algebra generated by cylinder subsets of the set of bi-infinite sequences of two letters called "minus" and "plus". We study ergodicity of an operator from M to M, which is a variable-length version of the well-known Stavskaya operator. We prove that this operator is ergodic, in fact tends to "all pluses" from all initial conditions except a few extreme cases. Also we perform the Monte Carlo and Chaos approximation of the same operator and to our astonishment these approximation behave as if our operator were ergodic only for some values of parameters and non-ergodic for others with a sharp boundary between the two cases.

B11: V. Geyko, Princeton University
Coauthor: N.J. Fisch
Negative Compressibility and Inverse Problem for Spinning Gas

Abstract: A spinning ideal gas in a cylinder with a smooth surface is shown to have unusual properties. First, under compression parallel to the axis of rotation, the spinning gas exhibits negative compressibility because energy can be stored in the rotation. Second, the spinning breaks the symmetry under which partial pressures of a mixture of gases simply add. Thus, remarkably, in a mixture of spinning gases, an inverse problem can be formulated such that the gas constituents can be determined through external measurements only.

B12: R. Vaidyanathan, Georgia Institute of Technology
Coauthor(s): Federico Bonetto, Michael Loss, Ranjini Vaidyanathan*
Thermostat-coupled Kac Model
Abstract: We consider the Kac model coupled to a thermostat. Propagation of chaos holds for this system as well and a Boltzmann equation can be written down in the limit. We extended the following results that hold for the Kac model: convergence to equilibrium in L^2 (existence of a spectral gap) and convergence in entropy. In this case, however, the rate of convergence turns out to be independent of the number of particles. In addition, this system was found to obey Newton's Law of Cooling.

B12: M. Zyskin, Rutgers University
Coauthor: K. Martirosyan
Fast oxidation and pressure wave generation in nanoscaled thermite mixtures
Abstract: We model fast oxidation of aluminum nanosized particles using Cabrera- Mott oxidation model. We also model pressure shock wave generated as a result. Results are in good agreement with recent experiments.

B13: S. Neihsial, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore
Coauthors: S. Neihsial,* G. Periyasamya, P. K. Samantaa and S. K. Pati
"Understanding the Binding Mechanism of Various Chiral SWCNTs and ssDNA: A Computational Study"
Abstract: Molecular Dynamics (MD) simulations have been carried out to understand the binding mechanism of various chiral single-walled carbon nanotubes (SWCNTs) and single-stranded deoxyribonucleic acid (ssDNA) of four different nucleobase sequences (i. e. ssdA14, ssdT14, ssdG14 and ssdC14, where, A, T, G and C are Adenine, Thymine, Guanine and Cytosine respectively) in aqueous media at room temperature (300 K) and atmospheric pressure (1 atm). The simulations studies reveal that ssDNA undergoes rapid structural changes and wrap around the SWCNTs via π-stacking interactions between SWCNT's wall and the nucleobases of ssDNA. Our computations demonstrate that the length of the ssDNA plays important role during the wrapping process. Moreover, it suggests that the length of the sequence should be proportional to the diameter of the SWCNT, in order to overcome the intra-locked π-stacking interactions between the nucleobases of an ssDNA. In addition, simulations provide the evidence that there is no correlation between the diameter of SWCNT and the sequence of ssDNA. However, in the MD simulation, we find the correlation between electronic nature and sequence selectivity. In order to understand that, quantum calculations have been performed at Hartree-Fock level. The quantum chemical calculations provide evidence that the sequence selectivity is correlated with the HOMO-LUMO gap of the ssDNA@SWCNT hybrid. For a single chiral SWCNT, the ssDNA sequence which results larger HOMO-LUMO gap forms chemically more stable ssDNA@SWCNT hybrid.

B14: Y. Subasi, University of Maryland
Coauthors: Y. Subasi*, C. H. Fleming, J. M. Taylor, B. L. Hu
The equilibrium states of open quantum systems in the strong coupling regime
Abstract: In this talk I will report on our work on the late-time stationary states of open quantum systems coupled to a thermal reservoir in the strong coupling regime. In general such systems do not necessarily

relax to a Boltzmann distribution if the coupling to the thermal reservoir is non-vanishing or equivalently if the relaxation timescales are finite. We show that starting from a product state of the closed system = system + environment, with the environment in its thermal state, the open system which results from coarse graining the environment will evolve towards an equilibrium state at late-times. This state can be expressed as the reduced state of the closed system thermal state at the temperature of the environment. For a linear (harmonic) system and environment, which is exactly solvable, we are able to show in a rigorous way that all multi-time correlations of the open system evolve towards those of the closed system thermal state. Multi-time correlations are especially relevant in the non-Markovian regime, since they cannot be generated by the dynamics of the single-time correlations. For more general systems, which cannot be exactly solved, we are able to provide a general proof that all single-time correlations of the open system evolve to those of the closed system thermal state, to first order in the relaxation rates.

B15: K. Sytwu, Rutgers University
Coauthors: Diego Alcala, Shane Squires, Michelle Girvan, Edward Ott, Thomas Antonsen
Explosive Percolation in Directed Networks
Abstract: Complex networks arise in various areas of interest: power grids, gene regulation, information networks, etc. One important characteristic of complex networks is their ability to percolate, or form a giant component that connects a macroscopic fraction of the total network. Past research has shown that if connections are competitively added in undirected complex networks, the formation of a giant connected component can be delayed, resulting in a first-order transition known as explosive percolation. Generalizing that concept onto directed networks, we found that the giant out component also undergoes explosive percolation. Furthermore, we compare our findings with the corresponding undirected case.

B16: S. Mandre, Brown University
Coauthors: A. He and K. Nguyen
The Short-range Capillary Force on Floating Objects
Abstract: We develop a general method to study the capillary force between objects of arbitrary shape which float close to each other on an interface, a regime in which multipole expansion is not useful. The force is represented as a power series in the small distance between the objects, of which the leading-order is finite. For objects with size a much larger than the capillary length l_c, the force scales as $\sqrt{a/l_c}$ and the prefactor depends on the mean radius of curvature R at the closest points. After contact the objects roll and/or slide with respect to each other to locally maximize R. For smaller objects ($a\ll l_c)$, the force scales as $(a/l_c)^{-1}\log(a/l_c)^{-2}$, and the prefactor depends only weakly on the shape and relative orientation of the objects.

B17: B. Liebchen, University of Hamburg, Germany
Interaction-induced current-reversals in driven lattices
Coauthors: F.K. Diakonos & P. Schmelcher
Abstract: A key topic concerning the ratchet mechanism are current-reversals, i.e. the tunability of the orientation of directed currents via system parameters, without changing the symmetry of the system. We demonstrate that long-range interactions can cause, as time evolves, consecutive reversals of directed currents for dilute ensembles of particles in driven lattices, without requiring modulations of external parameters. We analyze these surprising self-driven reversals to be expressions of a more general mechanism based on an interaction-induced accumulation of particles in the regular regions of the underlying single-particle phase space and leading to synchronized single-particle motion as well as an enhanced efficiency of Hamiltonian ratchets.

B18: J. Kominiarczuk, University of California, Berkeley
Coauthor(s): A. Chorin
Acyclic Monte Carlo sampling of Markov fields with applications to spin glasses
Abstract: We present a method for sampling high-dimensional probability spaces, applicable to Markov fields with both discrete and continuous variables, based on an approximate acyclic representation of the probability density. Our method generalizes and places in a common framework some recent work on computing renormalized Hamiltonians and stochastic multigrid sampling.

An acyclic representation of a probability distribution function (PDF) is obtained when one chooses an ordering of the variables and writes the PDF as a product of conditional probabilities, so that the probability of any variable is conditional only on the variables that precede it in the ordering. An acyclic representation makes the sampling efficient, because it uses the sparsity present in the model. We derive an approximate acyclic representation for general graphs by finding marginals through a fast marginalization scheme. The partial derivatives of the logarithm of the marginal probability are computed approximately through stochastic linear projection onto a polynomial basis, followed by reconstruction of the marginal through integration. The projection is based on an optimized inner product, making possible the use of Gaussian quadrature. Probability distributions involving discrete variables are handled by embedding the PDFs in differentiable extensions. Our algorithm can be extended to the evaluation of renormalized Hamiltonians formed using general renormalization schemes.

The approximate acyclic representation of the PDF is then used for sampling. The variables are sampled in a fixed order, producing independent samples together with their sampling weights. We present an optimized sampling strategy that uses a maximum amount of information to choose individual variable values. The samples are further improved using techniques from particle filtering. We also introduce a block Markov chain Monte Carlo scheme based on the sampling weights. Finally, we present applications of our methodology to lattice models: the Ising model and the Edwards-Anderson spin glass.

B19: L. Cheng, Rutgers University
Differential Poisson distributions of beneficial and harmful RNA dissipative structures (dissipatons) in breast cancer patients
Abstract: There are two kinds of structures in the living cell-equilibrium structures that do not require any energy dissipation to exist (e.g., DNA sequences) and dissipative structures that disappear upon blocking energy supply to the cell (e.g., mRNA gradients inside the cell; see Figure 15.1 in [1])). Since cells cannot survive without energy, it follows that what distinguishes life and death on the cellular level is dissipative structures or dissipatons for brevity [2]. It would also follow that to understand how living cells function, either normally or pathologically, it is necessary to study cellular dissipatons [3]. There are two kinds of dissipatons - the time-dependent and the sample-dependent. The former is alternatively referred to as RNA trajectories and the latter as RNA expression profiles, the latter of which is the focus of this presentation. Go to: http://www.math.rutgers.edu/events/smm/ to view the entire abstract.

B20: R. Chereji, Rutgers University
Coauthors: Razvan Chereji*, Alexandre Morozov
New insights into nucleosome unwrapping
Abstract: We present a statistical mechanics model for the nucleosome unwrapping [1-3], which is able to take into account sequence-dependent binding energies, sequence-independent potential barriers and wells, effective two-body interactions between the nucleosomes, competition between different

species, cooperative-binding, and other important factors which dictate the nucleosome distribution along the DNA. We are able to reproduce the distribution of the internucleosomal distances, which cannot be explained if there is no nucleosome unwrapping. The nucleosome unwrapping model can explain also the variable DNA accessibility and the nucleosome-induced cooperativity, which were observed experimentally.

1. R. V. Chereji et al. - Statistical mechanics of nucleosome ordering by chromatin-structure-induced two-body interactions, Phys. Rev. E 83, 050903 (2011)
2. R. V. Chereji and A. V. Morozov - Statistical Mechanics of Nucleosomes Constrained by Higher-Order Chromatin Structure, J. Stat. Phys. 144, 379 (2011)
3. R. V. Chereji and A. V. Morozov - New insights into nucleosome unwrapping, in preparation (draft available on request)

B21: M. Manhart, Rutgers University

Coauthor: A. Morozov

An Algorithm to Compute Statistics of Stochastic Paths on Complex Landscapes

Abstract: Many systems in physics, chemistry, and biology can be modeled as a random walk on a network subject to a potential landscape. There is great interest in understanding the statistical properties of pathways on these landscapes, especially their times, lengths, and distributions in space. The complexity of the networks and landscapes arising in many models makes them difficult to solve by traditional analytical and computational tools. Moreover, standard methods do not always provide the most relevant information for characterizing these pathways. We develop an explicitly path-based formalism for studying these problems, which we implement using a numerical dynamic programming algorithm. It is especially well-suited to studying first-passage problems and rare transitions between metastable states. This method is valid for arbitrary networks and landscapes, as well as semi-Markovian processes with non-exponential waiting-time distributions. We explore this method on a variety of simple models including regular lattices, fractals, and protein sequence evolution.

B22: V. Golyk, MIT

Coauthor: V. Golyk*, M. Kruger, G. Bimonte and M. Kardar

The Proximity Approximation and heat transfer between rough or modulated curved objects

Abstract: The Proximity Approximation (PA) is a well known tool for computing the net force between objects of arbitrary shape at close separations. We use this approximation to probe the interplay of roughness/modulation at short scale, and curvature at large scale, with emphasis on heat transfer at small separations. We find that surface modulation/roughness can modify the asymptotic scaling of diverging quantities at proximity. For example, our results indicate that for a rough sphere in front of a plate heat transfer approaches a constant value with decreasing separation, in contrast to diverging as the inverse separation for a smooth sphere in front of a plate.

B23: M. Maghrebi, MIT

Coauthor: Ramin Golestinian, Mehran Kardar

Quantum friction on a particle moving parallel to a surface

Abstract: Quantum zero point fluctuations of the electromagnetic field can lead to macroscopic phenomena such as non-contact friction. For example an accelerating mirror in vacuum will experience dissipation and radiate photons. I will reexamine the uniform motion of a small spherical particle parallel to a surface, and argue that a frictional force arises only if the particle has internal loss mechanisms.