THE RAYMOND AND BEVERLY SACKLER CENTER
FOR COMPUTATIONAL MOLECULAR AND MATERIALS SCIENCE

Classical and Quantum Non-Equilibrium Dynamics

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Presentation Abstracts

Non-equilibrium Methods for Equilibrium Free Energy Computations

Christoph Dellago, University of Vienna, Austria

As shown by Jarzynski, free energy differences between equilibrium states can be expressed in terms of the statistics of work carried out on a system during non-equilibrium transformations. This exact result, as well as the related Crooks fluctuation theorem, provide the basis for the computation of free energy differences from fast switching molecular dynamics simulations, in which an external parameter is changed at a finite rate driving the system away from equilibrium. In my lecture, I will first briefly review the Jarzynski identity and the Crooks fluctuation theorem and then survey various algorithms building on these relations, briefly touching also on the application of these ideas for the analysis of non-equilibrium experiments. I will pay particular attention to the statistical efficiency of these methods and discuss practical issues arising in their implementation

Percolation and the Glass Transition - Crash Course on Kinetically-Constrained Models

Yair Shokef, Tel Aviv University, Israel

Kinetically-constrained models provide a promising framework for describing the cooperatively slow relaxation dynamics in diverse systems such as glass-forming liquids, colloidal suspensions and granular materials. These models are defined with non-interacting binary state variables 0,1 on each site of a periodic lattice, either such that a site can flip its state (0 <-> 1 , like in an Ising model) or such that two neighboring sites can exchange their states (10 <-> 01 , like motion of a particle to a neighboring vacant site in a lattice gas), but that such transitions require a certain local kinetic constraint to hold.
Certain sets of kinetic rules map to bootstrap percolation, thus these kinetically-constrained models become jammed, or nonergodic only either at the limit of zero temperature (Ising spins) / full occupation (lattice gas), or when considering finite-sized, confined systems. An interesting exception is the spiral model, which by mapping to directed percolation was proven to undergo an ergodicity-breaking transition at a finite density (or temperature). Finally, the self-diffusivity of particles in such lattice gases depends on the percolation properties of the accessible region in space. Thus there are at least three different percolation problems related to jamming and glassiness in kinetically-constrained models. This talk will introduce such models and the approaches to analyze their dynamics, mainly from the percolation perspective.

.*A Short Course on Rare Events and Large Deviations*

Yariv Kafri, Technion - Israel Institute of Technology, Israel

In recent years that has been much progress in our understanding of large derivations in out of equilibrium systems. These are analogs of free energies in equilibrium systems display out of equilibrium behavior that is very different than free energies in equilibrium. The talk will give an introduction to what large deviation are. The methods for calculating them will be outlined and an overview of some recent results will be given.

Non-equilibrium Continuum Physics

Eran Bouchbinder, Weizmann Institute of Science, Israel

The aim of this lecture is to introduce the attendees to basic concepts and tools in non-equilibrium continuum physics, such as dissipation inequalities, configurational forces, internal variables, moving boundary problems and spatiotemporal instabilities. Applications of these concepts and tools in various problems at the forefront of diverse fields, such as dynamic fracture, glass physics, dynamics of living systems and interfacial physics, will be demonstrated. Whenever possible, the interplay between theory and cutting-edge computational approaches will be highlighted, and open challenges will be discussed

Flow in Disordered Systems: From Simple Fluids to Athermal Solids

Mark O. Robbins, Johns Hopkins University, USA

The talk will start by describing non-equilibrium molecular dynamics (MD) simulation methods and how quantities of interest are measured. Next, coarse-graining methods and the challenges to extending them to far-from-equilibrium conditions will be discussed. The methods will be illustrated with simulations of flow in disordered systems, following the evolution of stress strain-rate curves, conformational changes, and spatial correlations as systems are quenched from simple fluids through the glass transition and to athermal solids. The shear thinning response of simple binary Lennard Jones fluids, small molecules and the lubricant squalane are followed over more than 6 orders of magnitude in strain rate while the system is driven through the glass transition by varying temperature, pressure or confinement. The implications for fundamental theories of the glass transition and practical models of elastohydrodynamic lubrication will be discussed. Then the extreme athermal limit appropriate to sand piles, foams and earthquakes will be discussed. Here the system evolves through mechanical instability rather than thermal activation. Inthe thermodynamic limit, there is a yield stress followed by a power law rise in shear stress with strain rate. The power law is related to critical exponents describing a diverging correlation length and a power lawdistribution of avalanches as the system approaches the quasistatic limit.

Simulation of Nonequilibrium Quantum Dynamics Using Multiconfiguration Wave-function Methods

Michael Thoss, University of Erlangen-Nuremberg, Germany

The accurate theoretical treatment and simulation of quantum dynamical processes in many-body systems is a central goal in chemical and condensed matter physics. In this talk, the multilayer multiconfiguration time-dependent Hartree (ML-MCTDH) method [1] is discussed as an example of an approach that allows an accurate description of quantum dynamics and transport in systems with many degrees of freedom. The ML-MCTDH method is a variational basis-set approach, which uses a multiconfiguration expansion of the wave function employing a multilayer representation and time-dependent basis functions. It extends the original MCTDH method [2] to significantly larger and more complex systems. Employing the second quantization representation of Fock space, the ML-MCTDH method can also be used to treat the dynamics of indistinguishable particles [3,4]. Illustrative applications of the methodology to models for charge and heat transport are discussed, including electron transport in molecular junctions.

[1] H. Wang and M. Thoss, J. Chem. Phys. 119, 1289 (2003).
[2] H.-D. Meyer, U. Manthe, L.S. Cederbaum, Chem. Phys. Lett. 165 , 73 (1990); H.-D. Meyer, F. Gatti, G.A. Worth (Eds.), Multidimensional Quantum Dynamics: MCTDH Theory and Applications, Wiley-VCH, Weilheim, 2009.
[3] H. Wang and M. Thoss, J. Chem. Phys. 131, 024114 (2009)); 138, 134704 (2013).
[4] E. Wilner, H. Wang, G. Cohen, M. Thoss, E. Rabani, Phys. Rev. B 88, 045137 (2013); 89, 205129 (2014).

Open Quantum System's Approach to Charge and Heat Transport in Nano-scale Systems

Yonatan Dubi, Ben-Gurion University, Israel

In recent years, new approaches to study heat and charge transport in nano-scale systems have been proposed, based on thinking of the electronic system as an open quantum system. In this tutorial I will review some of these developments, going from the basic formalism to physical insight. Specific attention will be given to problems in which these approaches have clear advantages over common approaches, such as local temperature and the onset of Fourier's law, local dephasing, and combined Fermion-Boson systems.

Quantum and Classical Simulations of Enzymatic Reactions – Approaches

Dan Major, Bar-Ilan University, Israel

Enzymes are fascinating biological macromolecules which catalyze chemical reactions at rates which approach the encounter rate between the enzyme and substrate. Studying the nature of enzyme catalysis is of great importance in order to appreciate Nature's achievement, develop synthetic catalysts, and design new inhibitors. Our current understanding of enzyme catalysis dates back to the early days of Linus Pauling who introduced the concept of a pre-organized active site, which provides preferential stabilization of the transition state. Although this concept remains the pillar of enzyme catalysis, there are numerous cases where other effects are at play. In the current talk, I will focus on several current challenges relating to statistical and non-statistical behavior in enzyme catalysis, which we have addressed using multi-scale simulation approaches in our group. In particular, I will discuss specific approaches for studying such effects, including hybrid quantum mechanical-molecular mechanical (QM/MM) approaches to quantize electrons, various simulation approaches including activated dynamics and transition path sampling, and free energy methods. Finally, I will discuss strategies to quantize nuclear motion, via path-integral and wavefunction methods.

How do cells move? Non-Equilibrium Models of Active Polymer-based Motility

Herbert Levine, Rice University, Texas, USA

Cell motility is essential for many biological processes including wound healing, immune response, and cancer metastasis. For cells crawling on surfaces, motility involves a complex interplay between acto-myosin based force generation, adhesion to the substrate and chemical-based polarization to determine a direction. Here, we discuss our work aimed at developing integrative computational models of cell motility, ranging in complexity from simple geometrical models to complex phase-field approaches coupled to cytoskeletal mechanics. We also discuss initial efforts at using single cell models to understand the collective behavior of motile cells when they interact.