Nonequilibrium Statistical Mechanics: Mathematical Understanding and Numerical Simulation
12-16 November 2012

MEALS

*Breakfast (Buffet): 7:00–9:30 am, Sally Borden Building, Monday–Friday
*Lunch (Buffet): 11:30 am–1:30 pm, Sally Borden Building, Monday–Friday
*Dinner (Buffet): 5:30–7:30 pm, Sally Borden Building, Sunday–Thursday
Coffee Breaks: As per daily schedule, in the foyer of the TransCanada Pipeline Pavilion (TCPL)
***Please remember to scan your meal card at the host/hostess station in the dining room for each meal.**

MEETING ROOMS

All lectures will be held in the new lecture theater in the TransCanada Pipelines Pavilion (TCPL). LCD projector and blackboards are available for presentations.

SCIENTIFIC PROGRAM

Sunday

16:00	Check-in begins (Front Desk - Professional Development Centre - open 24 hours)
17:30–19:30	Buffet Dinner, Sally Borden Building
20:00	Informal gathering in 2nd floor lounge, Corbett Hall (if desired) Beverages and a small assortment of snacks are available on a cash honor system.

Monday

7:00–8:45	Breakfast
8:45–9:00	Introduction and Welcome by BIRS Station Manager, TCPL
9:00–9h40	Herbert Spohn, *The Hubbard-Boltzmann equation - general properties and 1D simulations*
9:40–10h20	Stefano Lepri, *The nonequilibrium discrete nonlinear Schrödinger equation*
10:20–10h50	Coffee break
10:50–11h30	Roberto Livi, *Breathers and metastable states in the discrete nonlinear Schrödinger Equation*
11:30–13:40	Lunch
13:40–14:20	David Sanders, *Efficient algorithm for dynamics in a random environment*
14:20–15:00	Yannis Pantazis, *Measuring the irreversibility of numerical schemes*
15:00–15h30	Coffee break
15:30–16:10	Tony Lelièvre, *Numerical methods to accelerate metastable dynamics*
16:10	Joel Lebowitz, “Concerned Scientist session”
17:30–19:30	Dinner

Tuesday

7:00–9:00	Breakfast
9:00–9h40	Joel Lebowitz, *Fourier's law, where do we stand?*
9:40–10h20	Jani Lukkarinen, *Nonequilibrium stationary states of harmonic chains with bulk noises*
10:20–10h50	Coffee break
10:50–11h30	Chanwoo Kim, *Fourier Law and Non-Isothermal Boundary in the Boltzmann Theory*
11:30–12:30	Lunch
12:30–13:30	Guided Tour of The Banff Centre; meet in the 2nd floor lounge, Corbett Hall
13:30	Group Photo; meet in foyer of TCPL (photograph will be taken outdoors so a jacket might be required).
13:40–14:20	David Mukamel, *Long-Range correlations in driven systems*
14:20–15:00	Christian Maes, *Clausius heat theorem for driven systems*
15:00–15h30	Coffee break
15:30–16:10	Johannes Zimmer, *Scale-bridging from particles to diffusional gradient flows*
16:10–16:50	Frédéric Legoll, *Derivation of Langevin dynamics in a nonzero background flow field*
16:50–17:30	Rémi Joubaud, *Langevin dynamics for shear viscosity computations*
17:30–19:30	Dinner

Wednesday

7:00–9:00	Breakfast
9:00–9h40	Federico Bonetto, *Non equilibrium steady state for a simple model of electric conduction*
9:40–10h20	Martin Evans, *Explosive Condensation in one-dimensional particle systems*
10:20–10h50	Coffee break
10:50–11h30	Marielle Simon, *Hydrodynamic limits for the velocity-flip model*
11:30–12h10	Makiko Sasada, *Mixing rates of stochastic energy exchange models with degenerate rate functions*
12:10–13:30	Lunch
	Free Afternoon
17:30–19:30	Dinner

Thursday

7:00–9:00	Breakfast
9:00–9h40	Abhishek Dhar, *Levy walk description of anomalous heat transport*
9:40–10h20	Alessandra Iacobucci, *Negative thermal conductivity of chains of rotors with mechanical forcing*
10:20–10h50	Coffee break
10:50–11h30	Gary Morriss, *Heat Conduction in quasi-one-dimensional Hard Disks*
11:30–13:40	Lunch
13:40–14:20	Carsten Hartmann, *How to mimic equilibrium by optimal nonequilibrium protocols—some ideas from risk-sensitive optimal control*
14:20–15:00	Mathias Rousset, *Langevin dynamics, constraints, and free energy calculations*
15:00–15h30	Coffee break
15:30–16:10	Francois Huveneers, *Asymptotic localization of energy in some Hamiltonian chains*
16:10–16:50	Carlangelo Liverani, *Fast-slow systems and statistical mechanics*
17:30–19:30	Dinner

Friday

7:00–9:00	Breakfast
9:00–9h40	Cédric Bernardin, *Anomalous diffusion in Hamiltonian systems perturbed by a conservative noise*
9:40–10h20	Milton Jara, *Fluctuations of one-dimensional, weakly asymmetric, conservative systems*
10:20–10h50	Coffee break
10:50–11h30	Informal discussion
11:30–13:30	Lunch

Checkout by 12 noon.

** 5-day workshop participants are welcome to use BIRS facilities (BIRS Coffee Lounge, TCPL and Reading Room) until 3 pm on Friday, although participants are still required to checkout of the guest rooms by 12 noon. **

Nonequilibrium Statistical Mechanics: Mathematical Understanding and Numerical Simulation 12-16 November 2012

ABSTRACTS
(in alphabetic order by speaker surname)

Speaker: **Cédric Bernardin** (Ecole Normale Supérieure de Lyon)
Title: *Anomalous diffusion in Hamiltonian systems perturbed by a conservative noise.*
Abstract: I will discuss a class of Hamiltonian systems perturbed by a conservative noise in the spirit of models considered in Basile-Bernardin-Olla'06-'09. For exponential interactions we will show that the system is super diffusive.

Speaker: **Federico Bonetto** (Georgia Institute of Technology)
Title: *Non equilibrium steady state for a simple model of electric conduction*
Abstract: A very simple model for electric conduction consists of N particles moving in a periodic array of scatterers under the influence of an electric field and of a Gaussian thermostat that keeps their energy fixed. I will present analytic result for the behaviour of the steady state of the system at small electric field, where the velocity distribution becomes independent of the geometry of the scatterers, and at large N, where the system can be described by a linear Boltzmann type equation.

Speaker: **Wojciech De Roeck** (Universität Heidelberg)

Speaker: **Abhishek Dhar** (Raman Research Institute)
Title: *Levy walk description of anomalous heat transport*
Abstract: Anomalous heat transport refers to heat conduction in low-dimensional systems where Fourier's law is found to be not valid. Some recent work suggests that a good description of heat transport in such systems is obtained by considering the heat carriers to be Levy walkers rather than simple random walkers. I will discuss this and present some exact results obtained for this model.

Speaker: **Martin Evans** (University of Edinburgh)
Title: *Explosive Condensation in one-dimensional particle systems*
Abstract: We study a far-from-equilibrium system of interacting particles, hopping between sites of a 1d lattice with a rate which increases with the number of particles at interacting sites. We find that clusters of particles, which initially spontaneously form in the system, begin to move at increasing speed as they gain particles. Ultimately, they produce a moving condensate which comprises a finite fraction of the mass in the system. We show that, in contrast with previously studied models of condensation, the relaxation time to steady state decreases as an inverse power of $\ln L$ with system size L and that condensation is instantenous for $L \to \infty$. This provides a first example of instantaneous gelation (known so far only from mean-field models of coagulation) in a spatially extended system.

Speaker: **Carsten Hartmann** (Freie Universität Berlin)
Title: *How to mimic equilibrium by optimal nonequilibrium protocols—some ideas from risk-sensitive optimal control*

Speaker: **Francois Huveneers** (Université Paris-Dauphine)
Title: *Asymptotic localization of energy in some Hamiltonian chains*

Abstract: It is known that energy transfer in close to integrable Hamiltonian systems can sometimes be much slowed down or even suppressed. Anderson localization, breathers, KAM tori or Nekhoroshev estimates can in some cases be invoked to justify this claim. However, given a chain at positive temperature in the infinite volume limit, it is generally hard to infer any clear picture on heat transfer out of such mathematical results. In this talk I will consider a class of nearly integrable Hamiltonian chains in a weak coupling regime (that sometimes translates into a high or small temperature regime). I will present some rigorous asymptotic results, suggesting a very rapid fall-off of the thermal conductivity with the coupling strength. We will see that both disorder and strong anharmonicity play a similar role in the considered regime. Comparison with numerical results will be discussed (joint work with Wojciech De Roeck).

Speaker: **Alessandra Iacobucci** (Université Paris-Dauphine)
Title: *Negative thermal conductivity of chains of rotors with mechanical forcing*
Abstract: We consider chains of rotors subjected to both thermal and mechanical forcings, in a nonequilibrium steady-state. Unusual nonlinear profiles of temperature and velocities are observed in the system. In particular, the temperature is maximal in the center, which is an indication of the nonlocal behavior of the system. Despite this uncommon behavior, local equilibrium holds for long enough chains. Our numerical results also show that, when the mechanical forcing is strong enough, the energy current can be increased by an inverse temperature gradient. This counterintuitive result again reveals the complexity of nonequilibrium states.

Speaker: **Milton Jara** (IMPA)
Title: *Fluctuations of one-dimensional, weakly asymmetric, conservative systems*
Abstract: We consider a system of oscillators perturbed by a noise that conserves the energy and momentum of the system, like the one introduced by Basile, Bernardin, Olla or Bernardin, Stoltz. When the strength of the noise is tuned properly (the so-called weakly asymmetric scaling), we show that the scaling limit of the fluctuations of the conserved quatities is given by a system of stochastic Burgers equations. This system corresponds to a generalization of the celebrated KPZ equation. Joint work with Cédric Bernardin and Patricia Goncalves.

Speaker: **Rémi Joubaud** (Imperial College London)
Title: *Langevin dynamics for shear viscosity computations.*
Abstract: Determining transport properties of fluids using molecular dynamics is still a very challenging problem. We focus here on non-equilibrium shear viscosity computations. Shear computations are most often performed using deterministic dynamics, typically with Nose-Hoover like thermostats or isokinetic dynamics. Many formal proof of theoretical results can be performed for these dynamics, but rigorous mathematical results (such as the well posedness of the linear response) cannot be obtained without further assumptions on the ergodic properties of the dynamic. We present a dynamics for shear computation which is a linear perturbation of the standard Langevin dynamics. We prove the existence and the uniqueness of the invariant measure of the dynamics and state rigorously the linear response result. This allows us to obtain a conservation equation satisfied by the local angular momentum depending on the longitudinal friction coefficient of the Langevin dynamics, following the seminal work of Irving and Kirkwood. Then we expose some new results on the asymptotic behavior of the shear viscosity coefficient as a function of the frictions, based on the study of some Poisson equation. These theoretical results are illustrated by numerical simulations of a bi-dimensional Lennard-Jones system. We also present links with the Green-Kubo formalism.

Speaker: **Chanwoo Kim** (Cambridge University)
Title: *Fourier Law and Non-Isothermal Boundary in the Boltzmann Theory*
Abstract: In the study of the heat transfer in the Boltzmann theory, the basic problem is to construct solutions to the steady problem for the Boltzmann equation in a general bounded domain with diffuse reflection boundary conditions corresponding to a non-isothermal temperature of the wall. Denoting by δ

the size of the temperature oscillations on the boundary, we develop a theory to characterize such a solution mathematically. We construct a unique solution F_s to the Boltzmann equation, which is dynamically asymptotically stable with an exponential decay rate. We remark that this solution differs from a local equilibrium Maxwellian, hence it is a genuine non-equilibrium stationary solution. A natural question in this setup is to determine if the general Fourier law, stating that the heat conduction vector q is proportional to the temperature gradient, is valid. As an application of our result we establish an expansion in δ for F_s whose first order term F_1 satisfies a linear, parameter free equation. Consequently, we discover that if the Fourier law were valid for F_s, then the temperature of F_1 must be linear in a slab. Such a necessary condition contradicts available numerical simulations, leading to the prediction of break-down of the Fourier law in the kinetic regime. This talk is based on the joint work with Esposito, Guo, Marra.

Speaker: **Joel Lebowitz** (Rutgers University)
Title: *Fourier's law, where do we stand?*
Abstract: Informal presentation with audience participation.

Speaker: **Frédéric Legoll** (Ecole des Ponts)
Title: *Derivation of Langevin dynamics in a nonzero background flow field*
Abstract: We propose a derivation of a nonequilibrium Langevin dynamics for a large particle immersed in a background flow field. Motivation stems from multiscale simulations of liquids, where molecular dynamics models are coupled with continuum descriptions, using e.g. the Navier-Stokes equation. In such computations, one has to simulate a system at the atomistic scale, with a background flow field imposed by the continuum part of the simulation. The question arises on how to exactly do this. In our work, we consider a single large particle, placed in an ideal gas heat bath composed of point particles that are distributed consistently with the background flow field and that interact with the large particle through elastic collisions. In the limit of small bath atom mass, the large particle dynamics converges to a Langevin-type stochastic dynamics, which is parameterized by the background flow field. This derivation follows the ideas of D. Durr, S. Goldstein and J. Lebowitz. The limiting dynamics is found to be similar to the g-SLLOD dynamics. Some numerical experiments illustrate the use of the obtained dynamic to simulate homogeneous liquid materials under flow. Joint work with Matthew Dobson, Tony Lelievre and Gabriel Stoltz.

Speaker: **Tony Lelièvre** (Ecole des Ponts)
Title: *Numerical methods to accelerate metastable dynamics*
Abstract: For many applications, molecular dynamics simulations are still of limited predictability. Among the many reasons, one is the timescale problem: the typical timescale at the microscopic level is much smaller than the macroscopic timescales of interest. This is related to the metastability of the trajectories: the system remains for very longtime in a so-called metastable state before hopping to another one.

We will present two recent works to overcome such difficulties. First, we would like to discuss (equilibrium preserving) non-reversible perturbations of metastable reversible dynamics, which may be used to accelerate the convergence to the stationary state. Second, we will present the numerical analysis of accelerated dynamics techniques which have been introduced by A. Voter (LANL) in the nineties to generate efficiently state to state dynamics. The notion of quasi-stationary distribution is pivotal to understand these algorithms.

Speaker: **Stefano Lepri** (Istituto dei Sistemi Complessi)
Title: *The nonequilibrium discrete nonlinear Schrödinger equation*
Abstract: We study nonequilibrium steady states of the one-dimensional discrete nonlinear Schrödinger equation. This system can be regarded as a minimal model for stationary transport of bosonic particles like photons in layered media or cold atoms in deep optical traps. Due to the presence of two conserved quantities, energy and norm (or number of particles), the model displays coupled transport in the sense of linear irreversible thermodynamics. Monte Carlo thermostats are implemented to impose a given temperature and chemical potential at the chain ends. As a result, we find that the Onsager coefficients are finite

in the thermodynamic limit, i.e. transport is normal. Depending on the position in the parameter space, the "Seebeck coefficient" may be either positive or negative. For large differences between the thermostat parameters, density and temperature profiles may display an unusual nonmonotonic shape. This is due to the strong dependence of the Onsager coefficients on the state variables.

Speaker: **Carlangelo Liverani** (Universita Roma Tor Vergata)
Title: *Fast-slow systems and statistical mechanics*
Abstract: I will discuss the statistical properties of a very simple fast-slow deterministic system and will explain the motivations for considering such a problem. Motivations stemming out of the (premature) attempt of rigorously deriving hydrodynamics from a weakly interacting microscopic Hamiltonian system.

Speaker: **Roberto Livi** (Universita di Firenze)
Title: *Breathers and metastable states in the Discrete Nonlinear Schrödinger Equation*
Abstract: We discuss how the interaction with thermal baths may yield unusual transport properties and fluctuations in the Discrete Nonlinear Schrödinger Equation. The origin of such peculiar behavior can be traced back to the spontaneous formation of nonlinear excitations in the form of breathers. Such excitations are also responsible for the appearance of metastable states living over exceedingly long time scales, thus inhibiting any appreciable signal of relaxation to equilibrium, while yielding the formation of "negative" temperature conditions.

Speaker: **Jani Lukkarinen** (University of Helsinki)
Title: *Nonequilibrium stationary states of harmonic chains with bulk noises*
Abstract: In a joint work with C. Bernardin, J.L. Lebowitz, and V. Kannan, we consider a chain composed of N coupled harmonic oscillators in contact with heat baths at its end points. The oscillators are also subjected to non-momentum conserving bulk stochastic noises; these make the heat conductivity satisfy Fourier's law. We describe some new results about the hydrodynamical equations for typical macroscopic energy and displacement profiles, as well as their fluctuations and large deviations, in two simple models of this type.

Speaker: **Christian Maes** (University of Leuven)
Title: *Clausius heat theorem for driven systems*
Abstract: Heat divided by temperature is an exact differential for reversible processes. We give extensions of that thermodynamic fact to simple systems of nonequilibrium statistical mechanics. There appears a relation with dynamical large deviations. Joint work with Karel Netocny.

Speaker: **Gary Morriss** (University of New South Wales)
Title: *Heat Conduction in quasi-one-dimensional Hard Disks*
Abstract: This study is based on the model introduced by Taniguchi & Morriss in *Comptes Rendus Physique*, **8**, 625 (2007).

Speaker: **David Mukamel** (Weizmann Institute)
Title: *Long-Range correlations in driven systems*
Abstract: Systems driven out of thermal equilibrium often reach a steady state which under generic conditions exhibits long-range correlations. As a result these systems sometimes share some common features with equilibrium systems with long-range interactions, such as the existence of long range-order and spontaneous symmetry breaking in one dimension, non-local response to local perturbations and other properties. Some models of driven systems will be presented, and features resulting from the existence of long-range correlations will be discussed.

Speaker: **Yannis Pantazis** (University of Massachussetts)
Title: *Measuring the irreversibility of numerical schemes*
Abstract: For a Markov process the detailed balance condition is equivalent to the time-reversibility of

the process. For stochastic differential equations (SDE's) time discretization numerical schemes usually destroy the property of time-reversibility. Despite an extensive literature on the numerical analysis for SDE's, their stability properties, strong and/or weak error estimates, large deviations and infinite-time estimates, no quantitative results are known on the lack of reversibility of the discrete-time approximation process. In this paper we provide such quantitative estimates by using the concept of entropy production rate, inspired by ideas from non-equilibrium statistical mechanics. By construction the entropy production rate is nonnegative and it vanishes if and only if the process is reversible. Crucially, from a numerical point of view, the entropy production rate is an *a posteriori* quantity, hence it can be computed in the course of a simulation as the ergodic average of a certain functional of the process (the so-called Gallavotti-Cohen (GC) action functional). We compute the entropy production for various numerical schemes such as explicit Euler-Maruyama and explicit Milstein's for reversible SDEs with additive or multiplicative noise. Additionally, we analyze the entropy production for the BBK integrator of the Langevin processes. We show that entropy production is an observable that distinguishes between different numerical schemes in terms of their discretization-induced irreversibility. Furthermore, our results show that the type of the noise critically affects the behavior of the entropy production rate.

Speaker: **Mathias Rousset** (INRIA Rocquencourt)
Title: *Langevin dynamics, constraints, and free energy calculations*
Abstract: In this talk, I will present the mathematical formalism of Langevin processes with constraints that can be used in molecular dynamics for free energy calculations. The emphasis will be laid on Jarzynski-Crooks fluctuation identities.

Speaker: **David Sanders** (National University of Mexico)
Title: *Efficient algorithm for dynamics in a random environment*
Abstract: I will discuss algorithms for simulating deterministic dynamics in a quenched (fixed) random environment of obstacles on a lattice, and present an efficient algorithm that we have developed for the case of low density. The main application is to a Lorentz lattice gas or mirror model. This is joint work with Tom LaGatta, Courant Institute of Mathematical Sciences, New York University

Speaker: **Makiko Sasada** (Keio University)
Title: *Mixing rates of stochastic energy exchange models with degenerate rate functions*
Abstract: In recent years, stochastic energy exchange systems of locally confined particles in interaction have been studied intensively, as accessible models for the rigorous study of the derivation of Fourier's law from microscopic dynamics of mechanical origin. As a generalization of them, Grigo et al. introduced a class of pure jump Markov processes of energies and studied the spectral gap of them under the assumption that the rate function of the energy exchange is uniformly positive. In this talk, I will consider the case where the rate function does not have a uniform lower bound, and give a lower bound estimate of the spectral gap. The hydrodynamic behavior of these systems will be also discussed.

Speaker: **Marielle Simon** (Ecole Normale Supérieure de Lyon)
Title: *Hydrodynamic limits for the velocity-flip model*
Abstract: We will study the diffusive scaling limit for a chain of N coupled oscillators. In order to provide the system with good ergodic properties, we perturb the Hamiltonian dynamics with random flips of velocities, in such a way as to conserve the energy of particles, and such that momentum conservation is no longer valid. We derive the hydrodynamic equations by estimating the relative entropy with respect to the local equilibrium state modified by a second order correction term. To perform the relative entropy method, we need to control the energy moments.

Speaker: **Herbert Spohn** (Technische Universität München)
Title: *The Hubbard-Boltzmann equation - general properties and 1D simulations*
Abstract: The Hubbard hamiltonian describes electrons on a lattice with on-site interaction. For small interactions the dynamics is well approximated by a kinetic equation, the matrix-valued Hubbard-Boltzmann

equation. We discuss general features of this equation. For 1D with nearest neighbor hopping we simulate the spatially homogeneous equation and study the approach to the steady state. This is joint work with Fuerst, Lukkarinen, Mei, and Mendl.

Speaker: **Johannes Zimmer** (University of Bath)
Title: *Scale-bridging from particles to diffusional gradient flows*
Abstract: The diffusion equation is the scaling limit of Brownian motion, and can be reformulated as gradient flow of the entropy in the Wasserstein metric. The latter formulation is physically very appealing, since it reveals in a mathematically rigorous the entropy as driving force out of equilibrium. How can we directly obtain the entropic gradient flow as a scaling limit of particles undergoing Brownian motion? One way to see this is by relying on work by Dawson-Gärtner or Kipnis-Olla and apply the Otto calculus to rephrase the rate functional in terms of entropy flows. However, we will describe a different limit passage which directly reveals the entropy as the driving force. The method combines a Large Deviation principle from probability and Gamma-convergence from analysis. Time permitting, some related scale-bridging results leading to stochastic models or Kramers'equation will be sketched.