Special Session 4: Effective Stochastic and Statistical Modeling of Multiscale Systems

Ilya Timofeyev, University of Houston, USA
Gregor Kovacic, Rensselaer Polytechnic Institute, USA

Linear fluctuation-dissipation for a model of the barotropic climate

Rafail Abramov
University of Illinois at Chicago, USA
abramov@math.uic.edu
Andrew J. Majda

The response of climate dynamics on the planetary scale to changes of various global physical parameters is an area which is being extensively studied in the contemporary atmosphere/ocean science. Recently, we developed and tested new computational algorithms for predicting the mean linear response of a chaotic dynamical system to small changes in external forcing via the fluctuation-dissipation theorem (FDT). The new methods yield greater accuracy than classical FDT methods for the linear response of a chaotic dynamical system. Here we present new results of the linear fluctuation-dissipation climate response for a more realistic model of the barotropic atmosphere on the sphere over the Earth topography. We demonstrate that the apparent lack of structural stability does not seem to pose a significant problem in practice.

⟶ ∞ ⋄ ∞ ⟵

Parameterization for mesoscale ocean transport through random flow models

Banu Baydil
Rensselaer Polytechnic Institute, USA
baydib@rpi.edu
Peter R. Kramer and Shafer Smith

We describe a mathematical approach based on homogenization theory toward representing the effects of mesoscale coherent structures, waves, and turbulence on large-scale transport in the ocean. We are developing a systematic parameterization strategy by building up deterministic and random subgrid-scale flow models in an increasing hierarchy of complexity, coupling the results from numerical simulations of cell problems with asymptotic analysis with respect to key nondimensional physical parameters such as Peclét and Strouhal numbers.

⟶ ∞ ⋄ ∞ ⟵

Regularity and synchrony for motor proteins

Lee Deville
University of Illinois, USA
rdeville@math.uiuc.edu
Eric Vanden-Eijnden

The majority of intracellular transport is performed by nanometer-scale proteins, known as "molecular motors", or "motor proteins". These motors convert chemical energy to mechanical work, but, unlike macroscopic motors, the energy is typically transferred by a single ATP molecule. Because of this, one expects the dynamics of the motor to be quite random; however, it has been observed that populations of such motors act regularly in certain situations. We present a family of models for the dynamics of motor proteins and show that there are generic organizing principles which lead to regular behavior in a motor's dynamics during interaction with its environment. This analysis is able to explain observations made in the literature of regularity for myosin V during vesicle transport and myosin II during muscle contraction.

⟶ ∞ ⋄ ∞ ⟵

Mathematical strategies for filtering turbulent signals in complex systems

John Harlim
New York University, USA
jharlim@cims.nyu.edu
A. J. Majda

An important emerging scientific issue in many practical problems ranging from climate and weather prediction to biological science involves the real time filtering and prediction through partial observations of noisy turbulent signals for complex dynamical systems with many degrees of freedom as well as the statistical accuracy of various strategies in this context. Our strategies blend classical stability analysis for partial differential equations and their finite difference approximations, suitable versions of Kalman filtering, and stochastic models from turbulence theory to deal with the large model errors in realistic systems.

⟶ ∞ ⋄ ∞ ⟵

Drift diffusion parameterization for solvent molecules around a solute

Adnan Khan
Lahore University of Management Sciences, Pakistan
adnan.khan@lums.edu.pk
Peter Kramer

The dynamic functioning of proteins is very hard to visualize experimentally as it is difficult to make protein movies with the current technology. Because of these experimental limitations Molecular Dynamics (MD) simulations play a vital role in determining the functioning of a protein once its structure is known. A major obstacle in accelerating MD simulations is the fact that the solvent molecules surrounding the proteins play a vital role in the dynamics and hence a large number of these solvent molecules must be included in the simulation. One would like to represent the effects of water molecules on the protein dynamics without explicitly resolving the water dynamics. We consider stochastic models that capture the behavior of the solvent molecules without explicitly resolving their motion. We study a parameterization for the dynamics of water around a simple solute molecule. We consider two models, where we seek to parameterize the state of water near the solute through the drift and diffusion of water molecules parallel and perpendicular to the protein surface. We calculate a measure of diffusivity, commonly used in the literature, from our models. We then compare the results from the two parameterizations to those from MD.

$\longrightarrow \infty \diamond \infty \longleftarrow$

Applications of kinetic theory to neuronal network dynamics

Gregor Kovacic
Rensselaer Polytechnic Institute, USA
kovacg@rpi.edu
David Cai and Aaditya Rangan

Using kinetic theory is a common coarse-graining technique for integrate-and-fire neuronal networks. After revieweing the basics of this theory, this talk will concentrate on the kinetic theory for networks with fast and slow conductances driven by the same spike trains, and the Fokker-Planck limit of the kinetic equations. In the former, correlations due to the two types of conductances sharing some of the same input spikes will be discussed. In the latter, neuronal gain curves will be presented, and the limit of small fluctuations will be described.

$\longrightarrow \infty \diamond \infty \longleftarrow$

Homogenization-based approach for coarse-graining molecular motor models

Peter Kramer
Rensselaer Polytechnic Institute, USA
kramep@rpi.edu
Juan Latorre and Grigorios Pavliotis

Homogenization theory provides a framework for computing effective properties of stochastic (Brownian) molecular motor models in terms of their design parameters. We develop a spectral numerical scheme for solving these equations and compare its performance relative to that derived from an alternative framework of Wang, Peskin, and Elston. Particular themes we consider include continuous-in-time modulation of a flashing ratchet and the validity of approximating continuous motor models by simpler discrete random walk models.

$\longrightarrow \infty \diamond \infty \longleftarrow$

Coding in neuronal networks, event-chains, and functional connectivity

Aaditya Rangan
Courant Institute, USA
rangan@cims.nyu.edu
David Cai

Networks of neurons respond to different stimuli in different ways, namely, distinct inputs generate reproducibly distinct activity profiles within the network. The talk will discuss certain coding properties of these systems, and illustrate these properties with numerical examples.

$\longrightarrow \infty \diamond \infty \longleftarrow$

Rare events in information transmission

Maxim Shkarayev
Rensselaer Polytechnic Institute, USA
shkarm@rpi.edu

Using methods borrowed from statistical physics, we carry out analytical, numerical and experimental study of error statistics in optical communication systems in the presence of additive and multiplicative noise. In the slowly varying envelope approximation light propagation through optical fiber is described by Schrödinger equation. Signal transmission is impeded by the spacial disorder (birefringence) of the optical fibers as well as short correlated noise from the optical amplifiers. This results in signal distortion that may lead to erroneous interpretation of the signal. System performance is characterized by the probability of error occurrence. Fluctuation of spacial disorder due to changing external factors (temperature, vibrations, etc) leads to fluctuations of error rates. Commonly the distribution of error rates is assumed to be Gaussian. Using optimal fluctuation method we show that this distribution is in fact lognormal. Such distribution has "fat" tails implying that the likelihood of system failure is much higher than it would be in the Gaussian approximation. Our theory provides excellent agreement with experiment.

⟶ ∞ ⋄ ∞ ⟵

Stochastic mode–reduction in large deterministic systems

Ilya Timofeyev
University of Houston, USA
ilya@math.uh.edu
A. Majda and E. Vanden-Eijnden

In this talk we will discuss a novel application of the stochastic mode-reduction (adiabatic elimination of fast variables) for a class of deterministic systems. Under assumptions of mixing and ergodicity, the procedure gives closed-form stochastic models for the slow variables in the limit of infinite separation of time-scales. We show that under these assumptions coefficients in the reduced model can be computed numerically as averages from a single micro-canonical realization on the energy surface E=1, and then extrapolated to other energy levels. The procedure is applied to the truncated Burgers-Hopf (TBH) system as a test case where the separation of timescale is only approximate. It is shown that the stochastic models reproduce the statistical behavior of the slow modes in TBH when the fast modes are artificially accelerated to enforce the separation of time-scales. It is shown that this operation of acceleration only has a moderate impact on the bulk statistical properties of the slow modes in TBH. As a result, the reduced stochastic models are sound for the original TBH system.

⟶ ∞ ⋄ ∞ ⟵

A numerical scheme for stationary statistical properties of the infinite Prandtl number model

Xiaoming Wang
Florida State University, USA
wxm@math.fsu.edu
Wendy Cheng

We propose a semi-discrete in time semi-implicit numerical scheme for the infinite Prandtl model for convection. Besides the usual finite time convergence, this scheme enjoys the additional highly desirable feature that the stationary statistical properties of the scheme converge to those of the infinite Prandtl number model at vanishing time step. One of the key characteristics of the scheme is that it preserves the dissipativity of the infinite Prandtl number model uniformly in terms of the time step. So far as we know, this is the first rigorous result on convergence of stationary statistical properties of numerical schemes for infinite dimensional dissipative complex systems.

⟶ ∞ ⋄ ∞ ⟵