MATHEMATICAL SCIENCES RESEARCH INSTITUTE

1000 Centennial Drive, Berkeley, CA 94720

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MESOSCOPIC MODELING OF NONEQUILIBRIUM SYSTEMS

Workshop: 23-27 May 1994

FINAL REPORT

31 May 1994

Recent years have seen important advances in the mathematical modeling of nonequilibrium phenomena. Probabilistic, kinetic and asymptotic approaches have been proved particularly fruitful in gaining insight into the complexity of nonequilibrium dynamics. Over the week of May 23-27, the MSRI hosted a workshop entitled "Mesoscopic Modeling of Nonequilibrium Systems", which was supported by the U.S. Department of Energy and the MSRI. This workshop brought together experts in these areas from the fields of Mathematics and Physics in order to exchange viewpoints and discuss future directions. In addition to the fourteen speakers there were thirty-three other registered participants, including nine junior people who were subsidized from the DOE grant and nine junior people who were part of the MSRI program. There were also many other people who attended at least one talk, but did not register.

Macroscopic systems displaying complex nonequilibrium dynamics are characterized by interactions between a wide range of excited spatial and temporal scales. Mesoscopic phenomena are characterized by the importance of fluctuations in determining the dynamics of macroscopic variables. Such systems arise in problems involving high Reynolds number fluid turbulence, or the breakdown of fluid or mean-field approximations. Indeed, understanding the shortcomings of these classical approximations is critical to efforts to make advances in ultra-small scale semiconductor fabrication, hypersonic craft, biomechanical micromachines, and other advanced technologies. A full description of all the excited scales in such systems appears mathematically formidable and sometimes necessary for describing the essence of large scale dynamics in real applications. A combination of asymptotic, stochastic and kinetic tools are used to develop mesoscale models that are both computationally and analytically tractable.

The presentations at the workshop, which we briefly summarize below, naturally fell into four categories:

1. Modeling and Analysis of Far-From-Equilibrium Systems

- Kurt Wiesenfeld gave a broad introduction to the concept of self-organized criticality. He described who is interested in it, why they are interested, what are the open questions; and how we might go about resolving these questions.
- Sidney Redner discussed the kinetics of transport-limited reaction processes. He described new phenomena associated with discrete velocity distributions and with mixed ballistic and diffusive reactant motion.
- Charles Doering presented some exactly soluble systems of interacting particles that illustrate some features of far-from-equilibrium dynamics, including the breakdown of mean-field approximations and the failure of conventional descriptions based on differential equations.
- Vladimir Privman described models of irreversible surface deposition on planar substrates that lead to the formation of amorphous layers due to jamming: incoming particles cannot fit in between the previously deposited particles. Diffusive relaxation rearranges the empty space and allows the deposition process to reach saturation. In this context he showed how to quantitatively evaluate the consistency of mean-field approximations in nonequilibrium situations.
- George Oster proposed a class of mechanical models for subcellular transport processes. These models fall within the class of so-called "Brownian ratchets" because they rectify Brownian fluctuations. He laid out the challenge to devise experimental approaches to test the mechanical principles underlying their operation.

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2. Mathematical Analysis of Closure Approximations

- David Levermore presented a systematic nonperturbative derivation of a hierarchy of closed systems of moment equations corresponding to any classical kinetic theory. Unlike previous closures, every member of the hierarchy is a hyperbolic system with relaxation terms and entropy that is formally well-posed.
- Marco Avellaneda analyzed the Burgers equation with random initial data, which was proposed by Burgers and Hopf as a "cartoon" model for understanding turbulence in fluid flow. He presented a new method for characterizing rigorously the probability distribution functions (PDFs) for the velocity, shocks and rarefaction action intervals.
- Kirill Vaninsky showed that the invariant Gibbs states for classical completely integrable systems can be written as product measures in global action-angle coordinates. He indicated how to construct such coordinates for the nonlinear Schrödinger equation.
- Andrew Majda described simple models for turbulent diffusion involving random shear layers with arbitrarily many spatio-temporal scales. The renormalization theory for scalar and higher order statistics was discussed and explicit examples exhibiting a variety of non-Gaussian probability distributions were presented.

3. Fluid Turbulence Modeling

- Gregory Eyink examined closure hypotheses for Large-Eddy Simulation (LES) turbulence models. He used the LES technique to establish basic properties of weak solutions of the inviscid Navier-Stokes equations relevant to inertial-range turbulence.
- Zhen-Su She proposed a new approach to deriving scaling laws of turbulence based possible singularities of the Euler equation. He showed that the resulting process describing the inertial range must have log-Poisson statistics and he predicted scaling laws that are in very good agreement with recent experimental measurements.
- Vladimir Zakharov illustrated the derivation of a kinetic equation to describe weak turbulence in the context of uniformly rotating incompressible fluid. He also presented a criterion for the applicability of the theory.

4. Large-Scale Numerical Simulations

- Shiyi Chen summarized some recent direct numerical simulations of isotropic turbulence. Inertial-range and far-dissipation range statistics were discussed and scaling dynamics in high-order structure functions of a passive scalar were presented and compared with recent theoretical predictions.
- Anthony Ladd gave an overview of direct simulations of molecular liquids and other particle systems which have contributed to our understanding of the molecular basis of macroscopic properties. He summarized some key historical applications of molecular dynamics and indicated some important future trends and prospects.

In addition to the scheduled talks, the early afternoons saw the participants break up into many small informal groups, often pairing junior with senior researchers, to air ideas further. The workshop concluded with a lively round table session where techniques, paradigms, and themes were discussed and debated, and especially promising directions for future research were suggested. The organizers were especially pleased to witness the fruitful exchange of ideas amongst the collection of experts and young researchers from the different disciplines that were brought together for this workshop.

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Workshop on Mesoscopic Modeling of Nonequilibrium Systems

May 23-27, 1994

Name	University
Marco Avellaneda	Courant Institute, New York University
Jared C. Bronski	Princeton University
Annalisa Calini	University of Arizona
Daniel Carati	Center for Turbulence Research
Shiyi Chen	Los Alamos National Laboratory
Peter Constantin	University of Chicago
Annalisa Crannell	Franklin and Marshall College
Gustavo Cruz-Pacheco	University of Arizona
Rudi De Koker	Stanford University
Anne De Wit	Stanford University
Gianne Derks	University of California Santa Cruz
Charles Doering	Clarkson University
Boris Dubrovin	International School for Advanced Studies
Weinan E	Institute for Advanced Study
Nick Ercolani	University of California Los Angeles
Gregory Eyink	University of Illinois at Urbana-Champaign
Wilfrid Gangbo	Carnegie Mellon University
Karla Horsch	University of Arizona
Markos Katsoulakis	Michigan State University
Allan Kaufman	University of California, Berkeley
Peter Kramer	Princeton University
Tony Ladd	Lawrence Livermore National Laboratories
David Levermore	University of Arizona
Andrew Majda	Princeton University
Daryl McCallister	University of Colorado Boulder
Richard McLaughlin	Princeton University
Robert McOwen	Northeastern University
William Morokoff	University of Arizona
Sergey Nazarenko	University of Arizona
Vladimir Privman	Clarkson University
Sidney Redner	Boston University
Fraydoun Rezakhanlou	University of California, Berkeley
Luis San Martín	University of Illinois at Urbana-Champaign

Name	University
Harvey Segur	University of Colorado Boulder
Zhen-Su She	University of Arizona
Peter Smereka	University of California Los Angeles
Nils Svanstedt	University of California at Santa Barbara
Esteban G. Tabak	Princeton University
Enrique Thomann	Oregon State University
Cristina Turner	Ciudad Universitaria
Kirill Vaninsky	New York University, Courant Institute
Edward Waymire	Oregon State University
Gene Wayne	Pennsylvania State University
Tony Werkman	University of Colorado Boulder
Kurt Wiesenfeld	Georgia Tech
Akira Yabe	University of California, Berkeley
Vladimir Zakharov	University of Arizona

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Workshop: 23-27 May 1994

General Information

The workshop is open to the scientific public; there is no registration fee. The Mathematical Sciences Research Institute (MSRI) is located at 1000 Centennial Drive in the hills above the UC Berkeley campus and just above the Lawrence Hall of Science. Parking is available in the lot down the hill from MSRI. Please ask the MSRI receptionist for a Temporary Parking Permit. For more information please call: 510-642-0143.

Activities will begin with registration at 9:00 a.m. on Monday, May 23, 1994. The sessions will be held in the Institute Lecture Hall with the first talk at 9:30 a.m. each day. Refreshments will be served in the MSRI lobby during the 10:30 a.m. breaks and the 3:15 p.m. MSRI Teas. There will be a special reception in the MSRI lobby at 3:30 p.m. on Monday. The Workshop Dinner will be at 6:30 p.m. on Thursday at the Mandarin Garden Restaurant located at 2025 Shattuck Avenue in Berkeley, which is two blocks west of the campus. The Dinner costs \$15.00, which you must pay to the MSRI receptionist by noon on Wednesday in order to reserve a place.

Tentative Schedule (as of 16 May)

all talks in the MSRI Lecture Hall

Monday, 23 May

- 9:00 Registration begins
- 9:15- 9:30 Welcoming Remarks
- 9:30-10:30 Kurt A. Wiesenfeld, Georgia Tech
Self-Organized Criticality: Who, What, How, and Why — But Mostly What
- 10:30-11:00 break
- 11:00-12:00 Gregory Eyink, University of Illinois at Urbana-Champaign
Mathematical Analysis of Subgrid Energy Transfer in LES Modeling of Turbulent Flows
- 12:00- 2:00 lunch
- 2:00- 3:00 C. David Levermore, University of Arizona and MSRI
Moment Closure Hierarchies for Kinetic Theories
- 3:30- 5:00 Workshop Reception at MSRI

Tuesday, 24 May

- 9:30-10:30 Sidney Redner, Boston University
Kinetics of Heterogeneous Reactions
- 10:30-11:00 break
- 11:00-12:00 Zhen-Su She, University of Arizona and MSRI
Scaling Solutions of the 3-D Incompressible Navier-Stokes Equations
- 12:00- 3:15 lunch and informal discussions
- 3:15- 3:45 MSRI Tea
- 3:45- 4:45 Marco Avellaneda, New York University
Probabilistic Methods in Burgers' Turbulence

Wednesday, 25 May

- 9:30-10:30 Charles R. Doering, Clarkson University and MSRI
Nonequilibrium Dynamics of a Diffusion-Limited Reaction Process
- 10:30-11:00 break
- 11:00-12:00 Shiyi Chen, Los Alamos National Laboratory
New Understanding of Turbulence Resulting from High Resolution Simulations
- 12:00- 3:15 lunch and informal discussions
- 3:15- 3:45 MSRI Tea
- 3:45- 4:45 Kirill Vaninsky, MSRI
On the Structure of Invariant Gibbs States in Classical Completely Integrable Systems

Thursday, 26 May

- 9:30-10:30 Vladimir Privman, Clarkson University
Diffusional Relaxation in Surface Deposition
- 10:30-11:00 break
- 11:00-12:00 Vladimir E. Zakharov, University of Arizona
Deriving Kinetic Equations for Weak Turbulence
- 12:00- 3:15 lunch and informal discussions
- 3:15- 3:45 MSRI Tea
- 3:45- 4:45 Andrew J. Majda, Princeton University
Random Shearing Direction Models for Turbulent Diffusion with Many Scales
- 6:30 Workshop Dinner at the Mandarin Garden, 2025 Shattuck Avenue, Berkeley

Friday, 27 May

- 9:30-10:30 George Oster, University of California at Berkeley
Brownian Motors and Cell Motions
- 10:30-11:00 break
- 11:00-12:00 Anthony J. Ladd, Lawrence Livermore National Laboratory
Simulations of Particle Systems by Molecular Dynamics
- 12:00- 1:30 lunch
- 1:30- 3:15 Round Table Discussion
- 3:15- 3:45 MSRI Tea
- 3:45 Workshop ends