Nonequilibrium Statistical Mechanics and Molecular Dynamics

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Overview

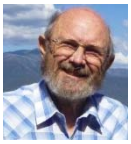
Statistical mechanics seeks to explain the behaviour of macroscopic systems through a statistical treatment of the mechanics of their constituent atoms and molecules. Statistical mechanics can be classified broadly as equilibrium and nonequilibrium, depending upon whether the system of interest is in an equilibrium state or not. While the properties of equilibrium systems are well understood, and there are various techniques of handling those in near-equilibrium conditions, the scientific community has just begun to understand some of the nuances of far-from-equilibrium systems. Nonequilibrium statistical mechanics, aided by the computational tool of nonequilibrium molecular dynamics, has been successfully applied in solving some of the open problems in physics and material science.

These lectures will start with the fundamentals of equilibrium statistical mechanics and thermodynamics, introduce molecular dynamics simulations along with their applications, and then discuss advanced topics in non-equilibrium statistical mechanics. The lectures will provide exposure to classical problems and their solutions, using state-of-the-art techniques along with some of the open problems in physics.The course is intended for advanced undergraduates, post graduates and researchers. The course is organized in two modules that should be taken together. The topics in Module A will cover classical thermodynamics, classical molecular dynamics and computer programming techniques. In Module B fundamentals of nonequilibrium statistical mechanics, nonequilibrium molecular dynamics and fluctuation theorems will be discussed along with some exciting discoveries made in the last two decades.

Course participants will learn these topics through lectures and computer programs. There will be regular assignments to stimulate research motivation of participants.

Modules	**A: Equilibrium statistical mechanics and molecular dynamics :Dec5 - Dec9,2016** **B: Nonequilibrium statistical mechanics and molecular dynamics : Dec11–Dec 16,2016** **Number of participants for the course will be limited to 25**
You Should Attend If…	▪ You are a physics/chemistry/biology graduate interested in understanding the physics of small-scale equilibrium/nonequilibrium systems. ▪ You are a chemical/civil/mechanical/aerospace/metallurgical engineer interested in developing new materials and understanding the behavior of systems in real environments. ▪ You are a student or faculty from academic institution interested in learning the state-of-the-art in the field of nonequilibrium statistical mechanics, molecular dynamics and utilizing advanced computational techniques to understand physical phenomena.
Fees	The course fess are as follows(in INR for participants from India/ USD for participants from abroad): **Industry/Research Organizations: Rs. 30000 / US $500** **Academic Institutions (Faculty) : Rs. 12000 / US $200** **Academic Institutions (Students) : Rs. 2000 /US $50** The above fees include all instructional materials, computer use for tutorials and assignments, 24 hr free internet facility.Boarding and lodging charges are not included and will be charged on actuals.

The Faculty



Prof.William Graham Hooveris an Emeritus Professor of Engineering in the Department of Applied Science at the University of California Davis.He worked for more than forty years at the Lawrence Livermore National Laboratory with a joint appointment as University Professor at the Davis campus.His main research interests include nonequilibrium statistical mechanics, chaos and dynamical systems, atomistic and continuum mechanics, smooth-particle mechanics, and computational physics. Professor Hoover is a pioneer in the development of nonequilibrium molecular dynamics simulations for simulating far-from-equilibrium flows along with the calculation of the underlying equilibrium and nonequilibrium properties of manybody systems. He has developed a wide variety of time-reversible deterministic algorithms and approaches including the Gaussian isokinetic thermostat, several isobaric-isothermal algorithms, as well as the widely-adopted Nosé-Hoover algorithm – the mainstay of most temperature-controlled molecular dynamics simulations. He is the author of more than 300 research papers and has written six books. Professor Hoover is a Fellow and Outstanding Referee of the American Physical Society.

Dr. Carol Griswold Hooverobtainedher PhD in Applied Science from University of California at Davis. Shejoined the Lawrence Livermore Laboratory in 1972 where she served as a Project Leader developingparallel methods for finite element algorithms and in management positions at theNational MagneticFusion Energy Computer Center and in the Methods DevelopmentGroup. She retired from the laboratory in 2005.She has coauthored two books on chaotic nonequilibrium systems, and has published more than 50 research papers.

Prof. AbhishekDharworks at the International Center for Theoretical Sciences of the Tata Institute of Fundamental Research.His research interest is in nonequilibrium statistical mechanics, particularly heat transport problems. He has authored more than 65 research papers. He holds the prestigious Shanti SwarupBhatnagar prize for making significant contributionsin understanding transport properties in low dimensional systems and non-equilibrium fluctuation theorems.

Prof. Baidurya Bhattacharya works at the Indian Institute of Technology Kharagpur. He has authored more than 70 research papers. His research interest is in probablisitic mechanics and computational materials science. His research group is actively involved in understanding the mechanics of small scale systems and determining how defects affect the behaviour of structural/mechanical components.

Course Co-ordinator

Prof. Baidurya Bhattacharya
Phone: 03222-283422
E-mail: baidurya@civil.iitkgp.ernet.in

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