Center for Scientific Computation And Mathematical Modeling

University of Maryland, College Park

A Program on
"Nonequilibrium Interface Dynamics: Theory and Simulation from Atomistic to Continuum Scales"

October 13 - 31, 2003

Organizers: T. Einstein, B. Li, J-G. Liu, E. Tadmor, J. Warren, J. Weeks & E. Williams

Invited Participants

Jacques Amar
William Boettinger
Russel E. Caflisch
John W. Cahn (*)
Weinan E
Theodore L. Einstein
Ken Elder
Bjorn Engquist
James W. Evans
J. William Gadzuk
George Gilmer
László Gránásy
Jonathan Guyer
Richard D. James
Alain Karma
Yannis G. Kevrekidis
David Kinderlehrer
Robert V. Kohn
David P. Landau
Stephen A. Langer
John Lowengrub
Mitchell B. Luskin
Chaouqu Misbah
Ray Mountain
Ricardo H. Nochetto
Dimitris Papaconstantopoulos
Robert L. Pego
Alberto Pimpinelli
Paolo Politi (*)
Karin Rabe
Talat S. Rahman
Mark O. Robbins
Alexander L. Roytburd
Vivek B. Shenoy
Peter Smereka
David Srolovitz
Francis Sullivan
Shlomo Ta'asan
Jerry Tersoff
Makio Uwaha
Eric Vanden-Eijnden
Peter Voorhees
James A. Warren
John D. Weeks
Ellen D. Williams
Dieter Wolf
Zhenyu Zhang
Royce Zia

(*) To be confirmed

A limited number of openings are available.
To apply please RSVP at:
http://www.cscamm.umd.edu/programs/nid03/rsvp.htm

ADDITIONAL INFORMATION is posted at
http://www.cscamm.umd.edu/programs/nid03/
email: nid03@cscamm.umd.edu

SCIENTIFIC CONTENT: The rapid development in materials science and nanotechnology have added importance to the challenges of understanding non-equilibrium interface dynamics. Technologically, assemblies with highly-ordered quantum dots or quantum wires have shown remarkable optoelectronic, magnetic, and mechanical properties but must be fabricated on a surface through processes that are often far from equilibrium. Scientifically, as sizes decrease, interfacial properties become essential and even dominant, and theories for surfaces and interfaces of bulk materials must be revisited. Existing analytical approaches to the study of complex interfacial systems characterized by multiscale, fluctuation, and singularities range from first-principles calculations to kinetic Monte Carlo simulations to coarse-grained continuum modeling. Applied mathematics makes important contributions in bridging these descriptions by developing rigorous mathematical theories and innovative simulation techniques.

This program brings together leading physicists, materials scientists, computational scientists, and applied mathematicians to review recent research developments, identify critical scientific issues, and accelerate the interaction of mathematics with physics and materials science, in the research of non-equilibrium interface dynamics.

TUTORIALS (October 13 - 17): Introductory lectures on a variety of topics ranging from atomic step dynamics and phase field modeling to mathematical description of internal layers and coarsening, and to first-principles and kinetic Monte Carlo simulations.
Speakers: **T. Einstein, K. Rabe, R. Pego, F. Sullivan, J. Warren, E. Williams**

WORKSHOP 1 (October 20 - 24): ***FUNDAMENTAL PHYSICAL ISSUES IN NONEQUILIBRIUM INTERFACE DYNAMICS***. Participants from statistical mechanics, surface physics, materials science, and applied mathematics communities discuss new issues and possible approaches to attack new problems related to growing surfaces and evolving interfaces. Topics include thermal fluctuation, nonlinear instabilities, nucleation, kinetic roughening, coarsening, surface reconstruction, impurities, surface magnetism, spin transport across interface, stress effects, nanoscale pattern formation, etc.

WORKSHOP 2 (October 27 - 31): ***HIERARCHICAL MODELING AND MULTISCALE SIMULATION OF MATERIALS INTERFACES***. Extending the discussion in Workshop 1, this workshop covers more mathematical and computational aspects of the development of hierarchical models and multiscale algorithms. Topics include stress-driven and noise-driven interface dynamics; grain-boundary motion; plate and shell theories for nanostructures; and martensitic, ferromagnetic, and ferroelectric interfaces. Calculations ranging from first-principles to molecular dynamics to kinetic Monte Carlo and to continuum equations are examined.

The Center for Scientific Computation
And Mathematical Modeling (CSCAMM)
CSIC Building #406, Paint Branch Drive
University of Maryland, College Park

CSCAMM is part of the College of Computer, Mathematical and Physical Sciences

UNIVERSITY OF MARYLAND

Partial funding is provided by the NIST Center for Theoretical and Computational Materials Science (CTCMS) and by the Materials Research Science and Engineering Center (MRSEC) at the University of Maryland.
Additional support is provided by the Institute for Physical Science & Technology (IPST) and by the Department of Mathematics at the University of Maryland.