Center for Scientific Computation And Mathematical Modeling

University of Maryland, College Park

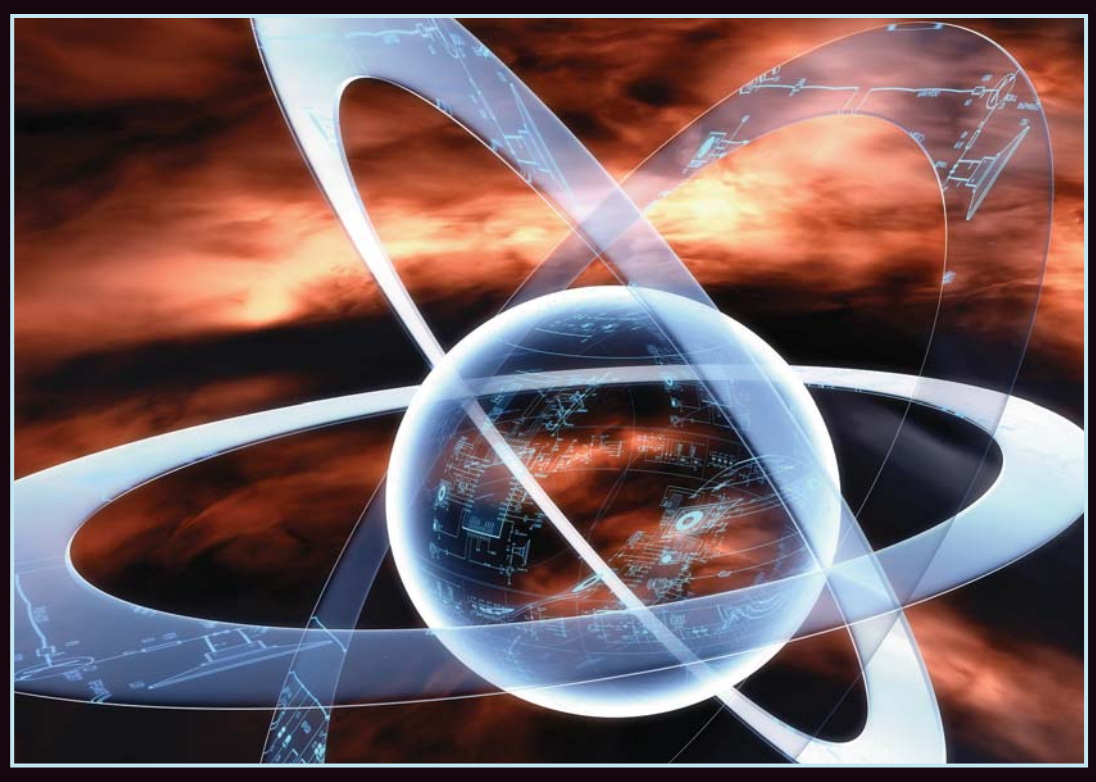
Workshop Announcement

Quantum-Classical Modeling of Chemical Phenomena

March 8-11, 2010

Organizers

Victor Batista	Yale University
Shi Jin	University of Wisconsin
Millard Alexander	University of Maryland
Eitan Tadmor	University of Maryland



Confirmed Participants

Millard Alexander University of Maryland
Victor Batista Yale University
Wei Cai University of North Carolina, Charlotte
Roberto Car Princeton University
Weinan E Princeton University
Carlos Garcia-Cervera UC, Santa Barbara
George Hagedorn Virginia Tech
Sharon Hammes-Schiffer Penn State University
Michael Herman Tulane University
Shi Jin University of Wisconsin
Caroline Lasser Free University, Berlin
Claude Le Bris CERMICS - ENPC
Christian Lubich Universitat Tubingen
Nancy Makri University of Illinois
David Manolopolous Oxford University
William Miller UC, Berkley
Kyle Novak Air Force Institute of Technology
Oleg Prezhdo University of Washington
Tamar Schlick New York University
Jing Shi Wayne State University
Eitan Tadmor University of Maryland
Mark Tuckerman New York University
Haobin Wang New Mexico State University
Weitao Yang Duke University

Scientific Background

This workshop will focus on deterministic and stochastic methods for sparse representations and simulations of quantum transport and quantum reaction dynamics. The aim is to bring together a group of experts in Applied Mathematics, Physics and Theoretical Chemistry to examine the current state of development of numerical techniques and foster interdisciplinary research in the development of computational methods at the interface of quantum and classical dynamics. Fundamental challenges in simulations of quantum dynamics will be addressed within the context of molecular dynamics, including wave-packet propagation methods, density functional theory methods (Car-Parrinello molecular dynamics CPMD), and hybridization of computational schemes linking classical and quantum theories such as quantum-classical coupling, surface-hopping and semiclassical methods.

A limited number of openings are available.
To apply, please RSVP at:
www.cscamm.umd.edu/programs/qcp10/rsvp.htm

For more information:
Website: **www.cscamm.umd.edu/programs/qcp10**
Email: **qcp10@cscamm.umd.edu**

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