



Institute for Pure and Applied Mathematics
University of California, Los Angeles presents

Bridging Time and Length Scales in Materials Science and Bio-Physics

Workshop I: Multiscale Modeling in Soft Matter and Bio-Physics

September 26 - 30, 2005

Organizing Committee: **Cecilia Clementi**, Chair (Rice University) and **Joel Ireta** (FHI Berlin)

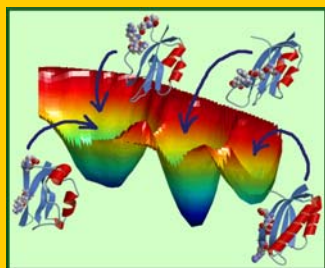


Image courtesy of Cecilia Clementi research group (Rice University)

Scientific Overview: This workshop will focus on current problems in computational and theoretical biophysics, in particular problems that can only be addressed within a **multiscale approach**. An important example is the characterization of protein folding and assembly processes over the broad range of time scales that are biologically relevant. Molecular Dynamics (MD) or Monte Carlo (MC) simulations that include every atom give the most detailed information and are often used, but are limited to the nanosecond time scale. An important issue in detailed simulation is the development of reliable and effective potentials and force fields. Coarse-graining procedures and simplified models are oftentimes used to reduce the problem to fewer (larger) building blocks (such as groups of atoms, or peptide units), so that simulations can be performed more efficiently and on larger time scale. Critical issues in this context are the definition of coarse-graining procedures, the theoretical validation of the approximations used, and the quantitative comparison of the results with experimental data and detailed atomistic simulations. Another approach is to employ continuum models, where the parameters are obtained from the microscopic approaches, and the time evolution of proteins can be tracked with state-of-the-art methods for moving fronts and boundaries. This is also relevant for

problems like DNA stretching, where one needs to understand the extent to which continuum elasticity theory can be used to describe the mechanical response of nano-objects measured using e.g. atomic force microscopes.

The definition and application of a combination of models and methods addressing different resolutions is emerging as a common issue in many different biophysical problems. It is the goal of this workshop to bring together researchers from different communities with expertise in different modeling techniques to understand how to address multiscale problems in computational biophysics.

Confirmed Speakers:

- Nathan Baker (Washington University, St. Louis)
- Charlie Brooks (The Scripps Research Institute)
- Robijn Bruinsma (UCLA)
- Ken Dill (UCSF)
- Angel Garcia (Rensselaer Polytechnic Institute)
- Alexander Grosberg (University of Minnesota)
- Anatoly Kolomeisky (Rice University)
- Kurt Kremer (Max-Planck Institut für Polymerforschung)
- Alexander Lyubartsev (Stockholm University)
- John Maddocks (École Polytechnique Fédérale de Lausanne)
- Jose Onuchic (UCSD)
- Vijay Pande (Stanford University)
- Monte Pettitt (University of Houston)
- Rob Phillips (Caltech)
- Philip Pincus (UCSB)
- Steve Plotkin (University of British Columbia)
- Jeff Saven (University of Pennsylvania)
- Klaus Schulten (University of Illinois)
- Mike Thorpe (Arizona State University)
- Mark Tuckerman (New York University)
- Michele Vendruscolo (Cambridge University)
- David Wales (Cambridge University)
- Arieh Warshel (University of Southern California)

Semester Program Schedule:

- Tutorials. September 13 - 16, 2005
- ▶ Workshop I: Multiscale Modeling in Soft Matter and Bio-Physics. September 26 - 30, 2005
- Workshop II: Multiscale Modeling in Condensed Matter and Materials Sciences. October 17 - 20, 2005
- Mini-Workshop: Time Acceleration Methods in Atomistic Simulations. October 21 - 22, 2005
- Workshop III: Density-Functional Theory Calculations for Modeling Materials and Bio-Molecular Properties and Functions – A Hands-on Computer Course. October 30 - November 5, 2005
- Workshop IV: Multiscale Analysis and Computation. November 14 - 16, 2005
- CIMMS Satellite Workshop at Caltech: Multiscale Modeling and Computation – Basic Theory and the Geosciences. November 17 - 18, 2005



Participation: Financial support for this workshop is available for participants at all academic levels, and recent PhD's, graduate students, and researchers in the early stages of their career are especially encouraged to apply. An online application for support is available at <http://www.ipam.ucla.edu/programs/maws1>. Encouraging the careers of women and minority mathematicians and scientists is an important component of IPAM's mission and we welcome their applications. Applicants who are interested in becoming core participants and participating in the semester program (September 12 – December 16, 2005) should apply at <http://www.ipam.ucla.edu/programs/ma2005>.

<http://www.ipam.ucla.edu/programs/maws1>

or email questions to maws1@ipam.ucla.edu