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

Monday September 26, 2005

8:00–8:30 *From atomistic detail to (macro) molecular motion*

8:00–8:50 *Check-In/Light Breakfast (Hosted by IPAM)*

8:50–9:00 *Welcome and Opening Remarks*

9:00–9:50 **Klaus Schulten** (University of Illinois at Urbana-Champaign)
Multiscale simulations of DNA-protein, and protein-lipid complexes

9:50–10:20 *Break*

10:20–11:10 **Joel Ireta** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
IInfinite polypeptides: An approach to study the secondary structure of proteins

11:10–12:00 **Joan-Emma Shea** (UC Santa Barbara)
Design of Inhibitors of Alzheimer Amyloid-ß Peptide Aggregation

12:00–2:00 *Lunch (on your own)*

2:00–2:30 *The coarse-graining approach: new methods and perspectives*

2:00–2:50 **William Gelbart** (UCLA)
Chain translocation in a biological context

2:50–3:40 **John Maddocks** (École Polytechnique Fédérale de Lausanne (EPFL))
Parametrizations of Coarse-Grain Sequence-Dependent Models of DNA Mechanics

3:40–4:10 *Break*

4:10–5:00 **Alexander Lyubartsev** (University of Stockholm)
Invese Monte Carlo method for determination of effective potentials for coarse-grained models

5:00–7:00 *Wine & Cheese Reception and Poster Session*

Tuesday September 27, 2005

8:00–8:30 *Multiscaling and collective behaviors: insights from analytical theories*

8:30–8:50 *Continental Breakfast*

9:00–9:50 **Michael Schick** (University of Washington)
A comparison of two routes to membrane fusion

9:50–10:20 *Break*

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10:20–11:10 **Anatoly Kolomeisky** (Rice University)
Growth Dynamics of Cytoskeleton Proteins: Multiscale Theoretical Analysis

11:10–12:00 **Steve Plotkin** (University of British Columbia)
How do many-body interactions and transition state structure determine how a protein folds?

12:00–2:00 *Lunch (on your own)*

2:00–2:30 *Water interactions and hydrophobic effect: an intrinsically multiscale problem*

2:00–2:50 **Monte Pettitt** (University of Houston)
Hydrophobicity at different length scales

2:50–3:40 **Philip Pincus** (UC Santa Barbara)
Multi-Scale Views of the Hydrophobic Interaction

3:40–4:10 *Break*

4:10–4:20 *Emerging techniques to combine multiple resolutions*

4:10–5:00 **Daniel Zuckerman** (University of Pittsburgh)
Exploring Algorithm Space: Resolution Exchange Simulation and Other Exchange Variants

5:00–5:50 **Zan Luthey-Schulten** (University of Illinois at Urbana-Champaign)
Using Evolutionary Concepts to Study the Function and Folding of Proteins

Wednesday September 28, 2005

8:00–8:30 *From atomistic detail to (macro) molecular motion*

8:30–9:00 *Continental Breakfast*

9:00–9:50 **Angel Garcia** (Rensselaer Polytechnic Institute)
Theoretical Studies of Pressure effects on folding/unfolding of proteins

9:50–10:20 *Break*

10:20–11:10 **Mark Tuckerman** (New York University)
Enhanced conformational sampling via novel variable transformation and very large time-step molecular dynamics

11:10–12:00
TBA

12:00–6:00 *Excursion to the Getty Center: lunch and afternoon visit*

Thursday September 29, 2005

8:00–8:30 *Water interactions and hydrophobic effect: an intrinsically multiscale problem*

8:30–8:50 *Continental Breakfast*

9:00–9:50 **Jeffery Saven** (University of Pennsylvania)
Solvation and the design and engineering of folding molecules

9:50–10:20 *Break*

10:20–11:10 **Ken Dill** (University of California, San Francisco)
Statistical mechanical models of water and aqueous solvation

11:10–12:00 **Nathan Baker** (Washington University in St. Louis)
Multiscale methods for biomolecular electrostatics and diffusion

12:00–2:00 *Lunch (on your own)*

2:00–2:30 *Multiscaling and collective behaviors: insights from analytical theories*

2:00–2:50 **Alexander Grosberg** (University of Minnesota, Twin Cities)
How proteins find their target on DNA? Delbruck model revisited

2:50–3:40 **Peter Wolynes** (University of California, San Diego)
Recent Successes of Energy Landscape Theory of Protein Folding

3:40–4:10 *Break*

4:10–5:00 **David Wales** (University of Cambridge)
Navigating the Energy Landscape: Pathways and Rates

5:00–5:50 **Mrs. Bruinsma** (UCLA)
Physical Models of Viruses

Friday September 30, 2005

8:00–8:30 *Emerging techniques to combine multiple resolutions*

8:30–8:50 *Continental Breakfast*

9:00–9:50 **Steve Nielsen** (University of Texas at Dallas)
Coarse grained to atomistic mapping algorithm: a tool for multiscale simulations

9:50–10:20 *Break*

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10:20–11:10 **Mike Thorpe** (Arizona State University)
Flexibility in Biomolecules: Beyond Molecular Dynamics

11:10–12:00 **Kurt Kremer** (Max Planck Institute for Polymer Research)
Linking Structure and Properties: Multiscale Simulations of Macromolecules

12:00–2:00 *Lunch (on your own)*

2:00–2:50 **Arieh Warshel** (University of Southern California)
Multiscale Modeling of Biological Functions

2:50–3:40 *Panel Discussion*

3:40–4:10 *Break*

4:10–5:50 *Panel Discussion*