Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules

07/23/2010 - 07/27/2010

Telluride Science Research Center

Address: Telluride Intermediate School
725 West Colorado Avenue, Telluride CO, 81435

Monday (July 23)

7:30 – 8:30 Breakfast at TSRC

Morning session
Session chair: Robert L. Jernigan

8:30 – 9:10, **Bert de Groot - Max Planck Institute for Biophysical Chemistry:** Coarse graining at atomic detail

9:10 – 9:50, **Shoji Takada - Kyoto University:** Coarse-Grained simulations of proteins, nucleic acids, and their complexes.

9:50 - 10:30, **Xavier Salvatella - Barcelona Institute of Biomedical Research**: Towards an experimental characterization of concerted motions in proteins

15 min coffee break

Session chair: Michael Feig

10:45 – 11:25, **Ilya Vakser – University of Kansas**: Comparative docking
11:25 – 12:05, **Gregory Chirikjian - Johns Hopkins University:** Multiscale Modeling of Double-Helical DNA: A Reconciliation

Hiking in the afternoon

Tuesday (July 24)

7:30 – 8:30 Breakfast at TSRC

Morning session
Session chair: Xavier Salvatella

8:30 – 9:10, **Modesto Orozco - Barcelona Institute of Biomedical Research:** DNA from electron to the chromosome

9:10 – 9:50, **Robert L. Jernigan – Iowa State University**: TBA

9:50 - 10:30, **Karissa Sanbonmatsu – Los Alamos National Laboratory:** Quantifying energy landscapes of the ribosome: translocation and accommodation

15 min coffee break

Session chair: Modesto Orozco

10:45 – 11:25, **Xiaoqin Zou - University of Missouri-Columbia:** Predicting protein-ligand interactions:

Scoring and benchmark

11:25 – 12:05, **Daisuke Kihara – Purdue University**: Prediction of structures of protein interactions

12:10-1:10 Group lunch at TSRC

Hiking in the afternoon

6:00 - 7:15, Town Talk:
Location: Palm Theater, 721 West Colorado Avenue

Wednesday (July 25)

7:30 – 8:30 Breakfast at TSRC

Morning session
Session chair: Bert de Groot

8:30 – 9:10, **Michael Feig - Michigan State University:** Coarse-grained models for cellular scales

9:10 – 9:50, **John Hunt – Columbia University:** Experimental studies of the role of protein dynamics in controlling complex catalytic processes

9:50 - 10:30, **Wenjun Zheng – University of Buffalo:** Recent Developments on Coarse-Grained Modeling of Protein Structures and Dynamics Using Modified Elastic Network Model And Low-Resolution Structural Data

15 min coffee break

Session chair: John Hunt

10:45 – 11:25, **Shi-Jie Chen – University of Missouri:** RNA Folding: Insights from coarse-grained modeling

11:25 – 12:05, **Osamu Miyashita - University of Arizona:** Adding Dynamic Insight to Protein X-ray Images by Solution and Crystal Molecular Dynamics Simulation

Hiking in the afternoon

Thursday (July 26)

7:30 – 8:30 Breakfast at TSRC

Morning session
Session chair: Cristian Micheletti

8:30 – 9:10, **Ruxandra Dima – University of Cincinnati:** Development of coarse-grained models for probing the nanomechanics of biomolecules

9:10 – 9:50, **George Stan – University of Cincinnati:** Coarse-grained models of substrate protein unfolding and translocation by AAA+ biological nanomachines

9:50 - 10:30, **Donghan Lee - Max Planck Institute for Biophysical Chemistry:** Exceeding the limit of dynamics studies and direct observation of correlated motions

15 min coffee break

Session chair: Ilya Vakser

10:45 – 11:25, **Cristian Micheletti - International School for Advanced Studies, Trieste**: DNA knotting inside viral capsids: a computational approach

11:25 - 11:55, **Esai Selvan Myvizhi (postdoc at Schrödinger Inc:** Technological issues and workarounds in the force matching algorithm: Application to POPC membranes

12:00-1:00 Group lunch at TSRC

Hiking in the afternoon

6:00, Group picnic provided by TSRC, family and TSRC guests welcome free of charge

Friday (July 27),

7:30 – 8:30 Breakfast at TSRC

Morning session
Session chair: Florence Tama

8:30 – 9:10, **Sanzo Miyazawa - Gunma University**: Prediction of Contact Residue Pairs Based on Concurrent and Compensatory Substitutions between Sites in Protein Evolution

9:10 – 9:50, **Andrzej Kloczkowski – The Ohio State University:** New Approaches to Improve Protein Structure Prediction and Refinement

9:50 – 10:30, **Florence Tama – University of Arizona**: Flexible Fitting Approaches for Low-Resolution Structural Data with Quality Assessments

Hiking in the afternoon and leaving