# Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules

07/05/2010 - 07/09/2010

**Telluride Science Research Center**

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

## Monday (July 5)

7:30 – 8:30 Breakfast at TSRC

***Morning session***
*Session chair: Robert L. Jernigan*

8:30 – 9:10, **Ivet Bahar – University of Pittsburgh:** Intrinsic Dynamics of Proteins: Learning from Structural Data and Normal Mode Analyses

9:10 – 9:50, **Shoji Takada - Kyoto University:** CG modeling of biomolecular machines: Specificity, non-linearity, and function

9:50 - 10:30, **Qiang Cui - University of Wisconsin**: Protein dynamics from coarse-grained models in "solution" and crystals

15 min coffee break

*Session chair: Michael Feig*

10:45 – 11:25, **Joanna Trylska - Warsaw University:** One-bead coarse-grained models of biomolecules in molecular dynamics simulations

11:25 – 12:05, **Bernard R. Brooks NHLBI, NIH**: Multiscale modeling efforts involving CHARMM

Hiking in the afternoon

***Evening session***
*Session chair: Florence Tama*

7:00 – 7:40, **Wenjun Zheng - University at Buffalo**: Toward multiscale modeling of protein conformational dynamics (with application to myosin motor)

7:40 – 8:20, **Robert L. Jernigan – Iowa State University:** Functional Motions of Proteins with Elastic Network Models

8:20 – 8:50, **Adam de Graff (Mike Thorpe group) - Arizona State University**: Flexibility, mobility and unfolding of proteins: A constraint-based approach

## Tuesday (July 6)

7:30 – 8:30 Breakfast at TSRC

***Morning session***
*Session chair: Pemra Doruker*

8:30 – 9:10, **Gregory Chirikjian - Johns Hopkins University:** Group-Theoretic Methods in Protein Structure Determination

9:10 – 9:50, **Ilya Vakser – University of Kansas:** Modeling of protein-protein interactions in structural genomics

9:50 - 10:30, **Sandor Vajda - Boston University**: Multi-scale models in protein-protein docking

15 min coffee break

*Session chair: Gregory Chirikjian*

10:45 – 11:25, **Xiaoqin Zou - University of Missouri-Columbia:** Structure-based predictions of protein-protein interactions and CAPRI applications

11:25 – 12:05, **Daisuke Kihara – Purdue University**: Protein surface representation for structure-based function prediction and docking

Hiking in the afternoon

6:00 - 7:15, Town Talk: **Mark Cohen, SUNY University Distinguished Professor of Anthropology**
The Decline of Human Health and the Rise of Civilization: A surprising relationship
*Location: Palm Theater, 721 West Colorado Avenue*

***Evening session***
*Session chair: Ivet Bahar*

7:30 – 8:10, **Saraswathi Vishveshwara - Indian Institute of Science, Bangalore:** Allosteric communication in tRNA synthetases elucidated through simulations and network analysis

8:10 – 8:50, **Florence Tama - University of Arizona:** Modeling conformational changes from low-resolution data with coarse-grained models

8:50 – 9:30, **Hamid R. Eghbalnia – University of Cincinnati:** Using data to confine the conformational space of proteins

# Wednesday (July 7)

7:30 – 8:30 Breakfast at TSRC

***Morning session***
*Session chair: Bernard R. Brooks*

8:30 – 9:10, **Michael Feig - Michigan State University:** PRIMO: Coarse-graining with quasi-atomistic accuracy

9:10 – 9:50, **Yaoqi Zhou - Indiana University:** Conformational space sampling with predicted torsion angles as restraints

9:50 - 10:30, **Jie Liang - University of Illinois at Chicago:** Perturbative Markovian Transmission model for predicting allosteric effects, signaling pathway, and sequence of enzymatic reaction events

15 min coffee break

*Session chair: Sandor Vajda*

10:45 – 11:25, **Karissa Sanbonmatsu - Los Alamos National Laboratory:** Linking Simulation and Experiment: All-atom Go-like simulations of Riboswitches and Ribosome

11:25 – 12:05, **Osamu Miyashita - University of Arizona:** Effect of Crystal Packing on Protein Conformations and Dynamics

Hiking in the afternoon

6:00 – 8:00, Group dinner in a restaurant New Sheridan Chop House *233 West Colorado Avenue* (attendees share the cost $48 per person for a three course meal with choices all the way)

# Thursday (July 8)

7:30 – 8:30 Breakfast at TSRC

***Morning session***
*Session chair: Wenjun Zheng*

8:30 – 9:10, **Pemra Doruker - Bogazici University**: Exploration of protein conformational transitions by Monte Carlo simulations integrated with collective modes

9:10 – 9:50, **Guang Song - Iowa State University**: Mapping of Ligand Migration Channel Network in Dynamic Proteins

9:50 - 10:30, **Shi-Jie Chen- University of Missouri**: Effect of Ion correlation in RNA folding

15 min coffee break

*Session chair: Ilya Vakser*

10:45 – 11:25, **Cristian Micheletti - International School for Advanced Studies, Trieste**: Dynamics-based alignment: detecting low-energy modes correspondences in enzymes with different folds

11:25 – 11:55, **Joanna Sulkowska (Jose N. Onuchic group) – UCSD:** Dodging the crisis in protein folding with knots

11:55 – 12:25, **Barry Grant (J. Andrew McCammon group) - UCSD**: Electrostatically biased binding in kinesin-microtubule association

Hiking in the afternoon

6:00, Group picnic provided by TSRC

# Friday (July 9),

7:30 – 8:30 Breakfast at TSRC

***Morning session***
*Session chair: Guang Song*

8:30 – 9:10, **Sanzo Miyazawa - Gunma University**: On an ideal pairwise contact potential of proteins

9:10 – 9:50, **Andrzej Kloczkowski – Iowa State University:** Statistical multibody potentials in protein structure prediction

9:50 - 10:20, **Srayanta Mukherjee (Yang Zhang group) – University of Michigan:** Template-based modeling of protein-protein complex structures from sequences: An I-TASSER based approach

15 min coffee break

*Session chair: Andrzej Kloczkowski*

10:35 – 11:05, **Anatoly Ruvinsky (Ilya Vakser group) - University of Kansas**: Residue fluctuations in proteins and protein complexes: Sequence composition and environment effects

11:05 – 11:45, **Dima Kozakov – Boston University:** Spherical FFT based docking methods

Hiking in the afternoon and leaving