Challenges in Large-Scale Biomolecular Simulations

 Dates:     June 14-18, 2015

 Location:  Telluride Elementary School, 447 West Columbia Ave,
            Telluride, CO 81435

      NOTE: This is a separate location from the Telluride Intermediate
      School where past conferences were held.

 Organizers: Tamar Schlick:  schlick@nyu.edu (917-592-9979)
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 TSRC Hosts: Mark Kozak <mark@telluridescience.org>, Executive Director
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     Telluride Science Research Center (TSRC)
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     <http://www.telluridescience.org>

                       Preliminary Program

NOTE: All talks are 30min + 5min discussion

  ~~~~~~   Sunday, June 14   ~~~~~~

  8:15 - 9:15  Breakfast at TSRC

  9:15 -  9:30  Welcome and introduction

  Session I:  Approaches for Long-Time, Large-Scale Simulations
  Chair: Tamar Schlick

1  9:30 - 10:00

Klaus Schulten: Mechanism of substrate translocation by a ring-shaped ATPase motor at millisecond resolution

2  10:05 - 10:35

Albert Pan: Using long-timescale molecular dynamics simulations to benchmark enhanced sampling methods

 10:40 - 11:00  Coffee break

3 11:00 - 11:30

Alfredo Cardenas: Membrane simulations with Milestoning

4  11:35 - 12:05

Ana Damjanovic: Constant pH Molecular Dynamics in Explicit Solvent with Enveloping Distribution Sampling and Hamiltonian Exchange

 12:10 - 12:30  Open Discussion (meeting goals, agenda, etc.)

 Lunch on your own, free afternoon

 3:30 - 6:30    Group Hike: Jud Weibe Trail
                meet at breakfast area

 ~~~~~~ Monday, June 15 ~~~~~~

  8:15 - 9:15  Breakfast at TSRC

  Session II: Coarse-graining and multiscale approaches
  Chair: Klaus Schulten

5  9:15 -  9:45

Cecilia Clementi:  Multiscale modeling of macromolecular dynamics

6  9:50 - 10:20

Ivan Coluzza: Transferable coarse-grained potential for **\*de novo\*** protein folding and design

 10:25 - 10:45  Coffee break

7 10:45 - 11:15

Tamar Schlick: Coarse-graining and multiscaling studies of the chromatin fiber's higher-order structures

8 11:20 - 11:50

Ruihan Zhang: The role of histone tails in intra-/inter-nucleosome interaction

9 11:55 - 12:25

Samuela Pasquali: Predicting and exploring complex nucleic acids architectures through a coarse-grained model

 12:30 - 6:00    Free Time

 ~~~~~~ Tuesday, June 16 ~~~~~~

 8:15- 9:15 Breakfast at TSRC

 Session III: Applications to Macromolecular Complexes
 Chair:

10  9:15 - 9:45

Zan-Luthy Schulten:

11  9:50 - 10:20

JC Gumbart: Simulating the periplasmic space of Gram-negative bacteria

 10:25 - 10:45  Coffee break

12  10:45 - 11:15

Peter Freddolino: Understanding regulatory networks from the atom up

13  11:20 - 11:50

Peter Tieleman: Modeling lateral structure in membranes

14 11:55 - 12:25

Loukas Petridis: High Performance MD Simulation in Bioenergy

 12:30 -    Free Time

 6:00 - 7:15 "Science Town Talk"

             Telluride Conference Center in Mountain Lodge

 ~~~~~~ Wednesday, June 17 ~~~~~~

   8:15 - 9:15  Breakfast at TSRC

 Session IV: Methods and Applications in Biomolecular Simulations
 Chair:

15   9:15 - 9:45

Rommie Amaro:

16  9:50 - 10:20

Monte Pettitt:  DNA in confinement

 10:25 - 10:45  Coffee break

17  10:45 - 11:15

Alex Mackerel: Role of explicit polarizability in the conformational heterogeneity of peptides and DNA studied using the classical Drude oscillator force field

18 11:20 - 11:50

TBA

 Lunch on your own and free time

 Session V: Perspectives

  4:00 - 5:30  Open discussion:
               Open challenges
               Conference report?
               Goals for next meeting (TSRC, June 2017 ?)

  6:00 - 9:00 TSRC Picnic under the tent at the Elementary School
             (Family and guests welcome free of charge)

 ~~~~~~ Thursday, June 18 ~~~~~~~

 8:15 - 9:15 Breakfast at TSRC

 Session VII:  Summary

  9:15 - 11:00 Writeups and summary