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](mailto:schlick@nyu.edu) (917-592-9979)   
             Klaus Schulten: [kschulte@ks.uiuc.edu](mailto:kschulte@ks.uiuc.edu)   
  
 TSRC Hosts: Mark Kozak [<mark@telluridescience.org>](mailto:mark@telluridescience.org), Executive Director   
     (970-708-4426)   
     Telluride Science Research Center (TSRC)   
     PO Box 2429 Telluride, CO 81435   
     <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