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 Challenges in Large-Scale Biomolecular Simulations  
  
 Dates:     June 17-21, 2018  
  
Location:   Telluride Intermediate School,  
            [725 W. Colorado Avenue, Telluride, CO](https://maps.google.com/?q=725+W.+Colorado+Avenue,+Telluride,+CO&entry=gmail&source=g)  
  
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               Final Program  
  
NOTE: All talks are 30min + 10min discussion  
  
  
 ~~~~~~   Sunday, June 17   ~~~~~~  
  
  8:30 - 9:00  Breakfast at TSRC  
  
  Session I:  Membrane, rare events, and confined domain challenges  
  Chair: Tamar Schlick  
  
  9:00 -  9:10  Welcome and introduction  
  
  9:10 -  9:40  Ron Elber: Simulating heterogeneous membranes  
  9:40 -  9:50  Discussion  
  
  9:50 - 10:20  Peter Tielman: Challenges in simulations of more realistic membrane models  
 10:20 - 10:30  Discussion  
  
 10:30 - 11:00  Coffee break  
  
 11:00 - 11:30  Rebecca Wade: Towards simulation tools for studying macromolecular  
                binding in crowded and confined environments  
 11:30 - 11:40  Discussion  
  
 11:40 - 12:20  Frank Noe: Reliable calculation of protein kinetics with  
                very rare events  
 12:20 - 12:30  Discussion  
  
 12:30 - 1:00   Open Discussion (meeting goals: working group, etc.)  
  
  
 Lunch on your own  
  
  
 Session II: From bacteria to genomes and the environment  
 Chair: Rommie Amaro  
  
 3:30 - 4:00  Jeremy Smith: Large-Scale Simulations of Lignocellulosic Biomass  
 4:00 - 4:10  Discussion  
  
 4:10 - 4:40  Syma Khalid: Zooming in and out: the challenges of simulating  
              bacterial cell envelopes  
 4:40 - 4:50 Discussion  
  
 4:50 - 5:10 Coffee break  
  
 5:10 - 5:40  Tamar Schlick: Multiscale modeling of the chromatin fiber  
 5:40 - 5:50  Discussion  
  
 5:50 - 6:20 Ivan Coluzza: General principles for protein design reveal  
             fundamental aspects of protein evolution  
 6:20 - 6:30 Discussion  
  
  
 ~~~~~~ Monday, June 18 ~~~~~~  
  
  8:30 - 9:00  Breakfast at TSRC  
  
  Free time (hiking, water rafting, working...)  
  
 Session III:  Macromolecular system challenges  
 Chair: Sarah Harris  
  
 3:15 - 3:45 Albert Pan: Atomic-level characterization of protein-protein  
             association  
 3:45 - 3:55 Discussion  
  
 3:55 - 4:25 Peter Freddolino: New insights into cellular behavior and evolution  
             through genomic-scale molecular modeling  
 4:25 - 4:35 Discussion  
  
 4:35 - 4:45 Afternoon Break  
  
 4:45 - 5:15 Rommie Amaro: Molecular Simulation at the Mesoscale  
 5:15 - 5:25 Discussion  
  
 5:25 - 5:55 Cecilia Clementi: Incorporating experimental data into long timescale  
             simulation of macromolecular dynamics  
 5:55 - 6:05 Discussion  
  
 ~~~~~~ Tuesday, June 19 ~~~~~~  
  
 8:30 - 9:00 Breakfast at TSRC  
  
 Session IV:  Nucleic Acid Complex Challenges  
 Chair: Rebecca Wade  
  
 9:00 -  9:30  Tom Bishop: What lies beyond the Standard Model in Biomolecular  
               Modeling  
 9:30 -  9:40  Discussion  
  
 9:40 - 10:20  Angelo Rosa: Ring polymers, the physics of crumpling and  
               chromosome territories  
10:20 - 10:30  Discussion  
  
10:30 - 11:00  Coffee Break / Group photo  
  
11:00 - 11:30  Helmut Grubmuller: Towards a mechanistic understanding of ribosomal  
               function 11:30 - 11:40  Discussion  
  
11:40 - 12:20  Sarah Harris:  Exploring the new physics needed to describe the  
               biological mesoscale with Fluctuating Finite Element Analysis".  
12:20 - 12:30  Discussion  
  
  
 3:00 - 5:30    Group Hike: Jed Wiebe Trail  
                meet:  Aspen St. at Colorado Ave.  
  
  
 6:30           Town Talk:  Nancy Levinger: Suspended Animation: Exploring  
                            Secrets of Cryopreservation  
                Telluride Conference Center in Mountain Lodge  
  
 7:45           Group Pizza  Dinner at Bear Creek Lodge  
                (take shuttle from bus stop near Conference Center or walk  
                to Bear Creek)  
  
 ~~~~~~ Wednesday, June 20 ~~~~~~  
  
 8:30 - 9:00 Breakfast at TSRC  
  
  
 Free time for hiking, etc.  
  
 6:00 -     Picnic in Tent outside the Telluride Intermediate School  
  
             Friends and family welcome!  
  
 ~~~~~~ Thursday, June 21 ~~~~~~~  
  
  
  8:00 - 9:00 Breakfast  
  
  Departure