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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)

 Organizers: Tamar Schlick: schlick@nyu.edu (917-592-9979)
             Rommie Amaro:  ramaro@ucsd.edu (858-534-9629)

 TSRC Hosts: Mark Kozak <mark@telluridescience.org>, Executive Director
                        (970-708-4426)
             Kristen Redd <kristen@telluridescience.org>, Lodging Director
                        (970-708-0827, office 970-729-8375)

             Cindy Fusting <cindy@telluridescience.org> , Managing Director
                        (970-708-5069)
Participants:

    Rommie Amaro <ramaro@ucsd edu>                  Univ. California San Diego
    Thomas C. Bishop <bishop@latech.edu>            Louisina Tech Univ.
    Cecilia Clementi <cecilia@rice.edu>,            Rice Univ.
    Ivan Coluzza <ivan.coluzza@univie.ac.at>        Center for Cooperative Res.
                                                    Biomaterials, San Sebastian
    Ron Elber <ron@ices.utexas.edu>                 Univ. Texas Austin
    Peter Freddolino <petefred@umich.edu>           Univ. Michigan
    Helmut Grubmueller <hgrubmu@gwdg.de>            Max Planck Inst. Biol. Chem.
    Sarah Harris <S.A.Harris@leeds.ac.uk>           Univ. Leeds
    Syma Khalid <S.Khalid@soton.ac.uk>              Univ. Southampton
    Frank Noe <frank.noe@fu-berlin.de>              Free Univ. Berlin
    Albert Pan <Albert.Pan@DEShawResearch.com>      DE Shaw
    Angelo Rosa <anrosa76@gmail.com>                SISSA
    Tamar Schlick  <schlick@nyu.edu>                New York Univ.
    Jeremy C. Smith <smithjc@ornl.gov>              Univ. Tennessee, ORNL
    Peter Tieleman <tieleman@ucalgary.ca>           Univ. Calgary
    Rebecca Wade <rebecca.wade@h-its.org>           Inst. Theoretical Studies,
                                                    Heidelberg

               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