Development and Deployment of Chemical Software for Advanced Potential Energy Surfaces

June 14-18, 2015

Telluride Research Science Center

Attendees:

Teresa Head-Gordon, UC Berkeley, Chair
Jonathan Essex, U. Southampton, Co-Chair
Jay Ponder, Washington U, Co-Chair
Alex Albaugh, UC Berkeley
Henry Boateng, STFC Daresbury Laboratory
Richard Bradshaw, University of Southampton
Bernard Brooks, National Institutes of Health
David Case, Rutgers University
Omar Demerdash, UC Berkeley
Jacek Dziedzic, University of Southampton
Peter Eastman, Stanford University
Chao Lu, Washington University
Alex MacKerell, U. Maryland
Daniel Margul, New York University
Mahmoud Moradi University of Illinois
Paul Nerenberg, Caltech
Frank Pickard, NIH, NHLBI
Jean-Philip Piquemal, Sorbonne Universités, Université pierre et Marie C
Joshua Rackers, Washington University
Young Min Rhee,POSTECH
Steve Rick, University of New Orleans
Michael Schnieders, University of Iowa
Klaus Schulten, University Illinois-Urbana
Yihan Shao, Q-Chem
Andrew Simmonett, National Institutes of Health
Chris Skylaris, University of Southampton
Jason Swails, Rutgers University
Ilian Todorov, STFC Daresbury Laboratory
Mark Tuckerman, New York University
Lee-Ping Wang, Stanford University
Qiantao Wang, University of Texas at Austin
Wei Yang, Florida State University

WORKSHOP SCHEDULE

Sunday June 14, 2015

6:30-8:30	***Informal reception in Telluride*** ***Arroyo located at 220 East Colorado Avenue***

Monday June 15, 2015

7:30-8:30	***Breakfast***
8:30—8:45	***Opening remarks***
	Advanced Force Fields, Applications and Methods (Teresa Head-Gordon, Chair)
8:45-9:15	*Jay Ponder, Washington U* TBA
9:15-9:45	*Jonathan Essex, U. Southampton* Applying AMOEBA in a Biomolecular Context
9:45-10:15	*Richard Bradshaw, U. Southampton* Ambitions with AMOEBA - Where do we go from here?
10:15-10:30	***Coffee***
	Algorithms and Software Implementations for Permanent Multipole Electrostatics (Ilian Todorov, Chair)
10:30-11:00	*Frank Pickard, NIH* Rapid evaluation of static multipoles using spherical harmonics and an intermediate frame of reference
11:00-11:30	*Henry Boateng, Daresbury Labs* Advanced Potential Energy Surfaces in DL_POLY
11:30-12:00	*Peter Eastman, Stanford* Permanent Multipoles in OpenMM
12:00-1:15	***Code Discussion (Frank Pickard)***
1:15-7:30	***Free Time***
	Obstacles for Advanced Models, Applications and Methods in Community Codes (Paul Nerenberg, Chair)
7:30-8:00	*Klaus Schulten, Illinois-Urbana* Ongoing and future developments and applications of the Illinois molecular modeling codes NAMD, VMD, MDFF for simulation, physical analysis and structure analysis
8:00-8:30	*David Case, Rutgers* Amber: Advanced and not-so-advanced force fields: lessons from crystal simulations
8:30-9:00	*Bernie Brooks, NIH* Charmm: Exploring the need for Advanced Potential Energy Surfaces: Constant pH, Free energies, and QM/MM

Tuesday June 16, 2015

7:30-8:30	***Breakfast***
	Algorithms and Software Implementations for Polarization (Jay Ponder, Chair)
8:30-9:00	*Andrew Simmonett, NIH* An accurate, analytical potential energy method for Induced dipoles
9:00-9:30	*Omar Demerdash, UC Berkeley* Importance of permanent electrostatic contributions to the 3-body approximation of polarization: Initial results and implementation considerations
9:30-10:00	*Michael Schnieders, U. Iowa* Can Polarizable AMOEBA Thermodynamics Approach the Speed of Fixed Charge Force Fields?
10:00-10:15	***Coffee***
10:15-10:45	*Alex Albaugh, UC Berkeley* Novel Methods and Models for AMOEBA Polarization
10:45-11:15	*Jean-Philip Piquemal, Paris* Scalable polarizable molecular dynamics simulations with Tinker-HP: development and perspectives
11:15-12:30	***Code Discussion (Peter Eastman)***
1:00-7:30	***Free Time***
	New Molecular Interactions for Force Fields (Omar Demerdash, Chair)
7:30-8:00	*Steve Rick, U. New Orleans* Charge transfer and polarization interactions
8:00-8:30	*Josh Rackers, Washington St Louis* Screened Short-range Electrostatics in AMOEBA
8:30-9:00	*Alex MacKerell, U. Maryland* Explicit treatment of polarization using the classical Drude oscillator

Wednesday June 17, 2015

7:30-9:00	***Breakfast***
	Algorithms and Software Implementations using QM (Lee-Ping Wang, Chair)
9:00-9:30	*Chris Skylaris, Southampton* QM/MM in ONETEP with the polarisable AMOEBA force field
9:30-10:00	*Yihan Shao, Q-Chem* Towards DFT/polarizable MM Calculations
10:00-10:30	*Young-Min Rhee, Postech* Interpolation of intramolecular interactions: Getting the accuracy of quantum chemistry at the speed of molecular mechanics
10:30-10:45	***Coffee Break***
10:45-12:00	***Code Discussion (Jacek Dziedzic)***
12:00-1:30	***Lunch***
	Algorithms and Software Implementations for Sampling and Approximate Models (Steve Rick, Chair)
1:30-2:00	*Wei Yang, Florida State* Free Energy Simulation: Orthogonal Space Sampling of Slow Environment Responses
2:00-2:30	*Jason Swails, Rutgers* A General MPI-Based Replica Exchange Framework
2:30-3:00	*Mark Tuckerman, NYU* Resonance free multiple time-stepping in constant-volume and constant-pressure ensembles for polarizable models
3:00-3:15	***Coffee***
3:15-3:45	*Mahmoud Moradi University of Illinois* An iterative approach to combine free energy calculation methods and path-finding algorithms
3:45-4:15	*Lee-Ping Wang, Stanford* A software framework for force field optimization and application to a protein force field
4:15-5:30	***Code Discussion (Jason Swails)***

Thursday June 18, 2015

8:00-9:00	***Breakfast***
	Takeaways and action items
9:00-11:00	*Essex, Head-Gordon, Ponder*
11:00	Departures