5th Tinker Software Developer Workshop

Washington University in St. Louis, Saint Louis, MO
Thursday June 15th through Saturday June 17th, 2023

Thursday, June 15th — *Morning Session*

Bauer Hall, BH330, Active Learning Lab, 9:00am - Noon

9:00 - 9:10	Welcome to WashU! & Workshop Announcements	Jay Ponder
9:10 - 9:35	CpHMD and Crystal Polymorph Algorithms for AMOEBA	Mike Schnieders
9:35 - 10:00	A Comparison of Methods for Computing Relative Anhydrous–Hydrate Stability with Molecular Simulation	Eric Dybeck
10:00 - 10:25	Scalable Electrostatics via Spherical Grids and Treecode Summation	Bernie Brooks
10:25 - 10:45	***Break***	
10:45 - 11:10	Computational Protein Design with Multisite Lambda Dynamics	Ryan Hayes
11:10 - 11:35	Lambda-ABF: An Efficient and Robust Strategy for Alchemical Free Energy Computations	Louis Lagardère
11:35 - 12:00	Improving Precision and Accuracy in Alchemical Free Energy Simulations for Drug Discovery	Darrin York
12:00 - 1:00	***Lunch***	

Thursday, June 15th — *Afternoon Session*

Bauer Hall, BH330, Active Learning Lab, 1:00pm - 4:40pm

1:00 - 1:25	Constant Pressure Implementation and Orthogonal Space Sampling	Wei Yang
1:25 - 1:50	Accelerated CRISPR-Cas9 Enzyme Simulations:	Yihan Shao

	Progress and Challenges	
1:50 - 2:15	Mechanisms of SARS-CoV-2 Evolution and Transmission	Guowei Wei
2:15 - 2:40	Exact Reaction Coordinates for Flap Opening and Ligand Dissociation in HIV Protease	Ao Ma
2:40 - 3:00	***Break***	
3:00 - 3:25	From Small Molecules to Proteins: Progress in ML Potentials	Hatice Gokan
3:25 - 3:50	Toward General, Reliable and Reactive Machine Learning Potentials using Force Field-enhanced Neural Networks	Thomas Plé
3:50 - 4:15	ML Force Fields for Chemical Reactivity	Teresa Head-Gordon
4:15 - 4:40	Accelerating *ab Initio* QM / AMOEBA MD	Filippo Lipparini

■ *Thursday, June 15th* *Evening Session*

Whittemore House (WashU Faculty Club), 5:00pm - 8:00pm

5:00 - 6:30	Poster Session & Open Bar Reception
6:30 - 8:00	Seated Buffet Dinner

■ *Friday, June 16th* *Morning Session*

Bauer Hall, BH330, Active Learning Lab, 9:00am - Noon

9:00 - 9:10	Welcome Back! & Workshop Announcements	Jay Ponder
9:10 - 9:35	STORMM: High-Performance Studies in Small Molecules	Dave Cerutti
9:35 - 10:00	NAMD 3.0 Leveraging GPUs	Dave Hardy
10:00 - 10:25	The SPICE Dataset for Training Machine Learning Potentials	Peter Eastman
10:25 - 10:45	***Break***	
10:45 - 11:10	The *apo*Charmm GPU Code & Bridge-EDS Free	Felix Aviat

	Energy Method	
11:10 - 11:35	Recent Development in the Tinker-HP Software	J-P Piquemal
11:35 - 12:00	Psi4 for Interoperable and High-Throughput Quantum Chemistry	David Sherrill
12:00 - 1:00	***Lunch***	

■ *Friday, June 16th* *Afternoon Session*

Bauer Hall, BH330, Active Learning Lab, 1:00pm - 4:40pm

1:00 - 1:25	Generalizing Drude Polarizable Force Field to Drug-like molecules	Anmol Kumar
1:25 - 1:50	AMOEBA+ / Poltype Development and Milestoning	Chengwen Liu
1:50 - 2:15	HIPPO Force Field Parameters for Organic Molecules	Rose Silva
2:15 - 2:40	AMOEBA for Ionic Liquids: The AMOEBA-IL Force Field	Andrés Cisneros
2:40 - 3:00	***Break***	
3:00 - 3:25	Polarizable Force Fields for Modeling Cation Binding to Proteins and Nucleotides	Samar Varma
3:25 - 3:50	Force Field Development for Large Chemical Space Coverage of Drug-like Molecules	Chuanjie Wu
3:50 - 4:15	Thermodynamics of Lipid Phase Separation from Molecular Simulations	Alan Grossfield
4:15 - 4:40	Polarizable Embedding of Multireference Electronic Structure Methods in AMOEBA for Rigorous Simulation of Nonadiabatic Molecular Dynamics	Lee-Ping Wang

■ *Saturday, June 17th* *Morning Session*

Bauer Hall, BH330, Active Learning Lab, 9:00am - Noon

9:00 - 9:10	Welcome Back! & Workshop Announcements	Jay Ponder
9:10 - 9:35	Quantifying Cooperativity and Anti-Cooperativity	Nohad Gresh

	in Multimolecular Complexes. Polarizable Molecular Mechanics and QC DFT-D Computations	
9:35 - 10:00	Developments for GK Implicit Solvation in AMOEBA	Rae Corrigan
10:00 - 10:25	Coarse-Grained Cavity for Large-Scale ddCOSMO	Filippo Lipparini
10:25 - 10:45	***Break***	
10:45 - 11:15	Panel Discussion: Advanced Sampling Methods	Wei Yang Louis Lagardère Alan Grossfield Bernie Brooks
11:15 - 11:45	Panel Discussion: Databases for ML and Beyond	Darrin York Peter Eastman Teresa Head-Gordon
11:45 - 12:15	Panel Discussion: The Future for Simulation Software	Dave Hardy J-P Piquemal Felix Aviat Dave Cerutti
12:15 - 1:30	***Informal Discussions***	