Agenda

Workshop on Atomistic Simulations for Industrial Needs
August 13-14, 2013
National Institute of Standards and Technology, Gaithersburg, Maryland with VTC to other locations
Organizers: Chandler Becker, Fred Phelan and Dan Siderius (NIST)

Tuesday, Aug. 13

Time	Session	Speaker
09:00 AM	Welcome	Jim Warren
09:15 AM	Introduction	Becker, Phelan, Siderius
09:30 AM	Prediction and Validation of Diffusion Constants in a Model Drug Delivery System	Christopher Forrey, FDA
10:00 AM	Experimental validation of MD simulations	Matthew Kramer, Ames Lab.
10:30 AM	*Break / Discussion*	
11:00 AM	The ground state elemental crystals as a guideline for the assessment of solid state DFT accuracy	Kurt Lejaeghere, U. Ghent
11:30 AM	Validation in statistical mechanical simulations	Michael Shirts, U. Virginia
12:00 PM	Validation of Atomistic Simulation Under Aleatory and Epistemic Uncertainties	Wan Yang, Ga. Tech.
12:30 PM	*Lunch*	
02:00 PM	Hierarchical Atom-type Definitions and Force Field Automation	Huai Sun, Shanghai Jiao Tong U.
02:30 PM	The Knowledgbase of Interatomic Models (KIM): An online resource for standardized testing and long-term warehousing of interatomic models and data	Ryan Elliott, U. Minnesota
03:00 PM	Automation for Atomistic Simulation	Zachary Trautt, NIST
03:30 PM	*Break / Discussion*	
04:00 PM	A Materials Simulation Challenge – how it would work, what challenges would be, how it they would be judged	Siderius / All
05:00 PM	*Adjourn for day*	
06:00 PM	*Dinner*	

Wednesday, Aug. 14

Time	Session	Speaker
09:00 AM	Response Embedded Atom Method for Interatomic Potentials	Hanchen Huang, U. Connecticut
09:30 AM	Using Liquid Structure Data to Validate Interatomic Potentials	Mikhail Mendelev, Ames Lab.
10:00 AM	Compatibility of force fields for different materials classes and validation of interfacial properties: The Interface force field as an integrated approach	Hendrik Heinz, U. Akron
10:30 AM	Application of Third-Generation Charge Optimization Many-Body Potentials in LAMMPS	Tao Liang, U. Florida
11:00 AM	*Break / Discussion*	
11:30 AM	Testing and generation of accurate MEAM potentials through coupling to an evolutionary structure prediction algorithm	Will Tipton, Cornell Univ.
12:00 PM	Adapting Thermodynamic Perturbation Theory to Expedite Force Field Characterization	J. Richard Elliott, U. Akron
12:30 PM	Improving simple potentials with statistical corrections	Jason Gruber, Bechtel Marine Propulsion Corp.
01:00 PM	*Lunch*	
02:00 PM	Discussion: Formulate a list of recommendations for using interatomic potentials and force fields	All
03:00 PM	*Adjourn*	