NIST Workshop on Atomistic Simulations for Industrial Needs

National Cybersecurity Center of Excellence — August 1-3, 2018
9700 Great Seneca Highway, Rockville, MD 20850

Wednesday, August 1st, 2018

8:30 AM	Arrive at NCCoE building, security check	
	MORNING: POTENTIALS DEVELOPMENT	
9:00 AM	Welcome and Introductions	Hale, Campbell
9:30 AM	State-of-the-art semi-empirical potentials for simulation of Fe and steel properties	Mendelev
10:00 AM	Some Current Interatomic Potential Applications at Sandia	Zhou
10:30 AM	*Break/Discussion*	
10:45 AM	Atomistic simulations with applications to Si and Ge systems	Hickman
11:15 AM	Machine Learning Based Atomistic Force Fields	Batra
11:45 AM	NIST DFT-related databases for solids: a high-throughput way to investigate material properties	Tavazza
12:15 PM	*Lunch Break*	
	AFTERNOON: MACHINE LEARNING AND ANALYSIS	
2:00 PM	High Performance Computing in Atomistic Simulations	Yamakov
2:30 PM	Searching chemical compound space: Where novelty lies	Rinderspacher
3:00 PM	*Break/Discussion*	
3:15 PM	Multipole coarse-graining of rigid-body molecular dynamics: Exact and approximate solutions to the transferability and representability problems	Patrone
3:45 PM	Multiscale Approach and Workflow Development for Enhanced Understanding of Manufacturing Materials	Thomas
4:15 PM	*Adjourn for day*	

Thursday, August 2nd, 2018

	MORNING: ATOMISTIC APPLICATIONS	
9:00 AM	Introductions, NIST Materials Resource Registry	Becker
9:30 AM	The role of entropy in high-entropy alloys: an insight from atomistic computer simulation	Sheng
10:00 AM	Coupled atomistic-continuum coupling for crack propagation	Ghosh
10:30 AM	*Break/Discussion*	
10:45 AM	Discussion: How do we better engage industry? What is needed of atomistics?	All
11:15 AM	Building more physical microstructures for atomistic simulations	Gupta
11:45 AM	Challenges in Atomistic Simulations of Interface Structures	Patala
12:15 PM	*Lunch Break*	

Thursday, August 2nd, 2018, continued

AFTERNOON: WORKFLOW TOOLS AND DATA MANAGEMENT

2:00 PM	Analyzing MD simulations with virtual diffraction	Coleman
2:30 PM	Facilitating finding and selecting potentials from the Interatomic Potentials Repository	Hale
3:00 PM	The MolSSI Framework for Atomistic Simulations and Workflows	Saxe
3:30 PM	*Break/Discussion*	
3:45 PM	OpenKIM: Tested, portable interatomic models for molecular and multiscale simulations	Karls
4:15 PM	Building Infrastructure for Materials Data Science: Where does Atomistic Simulation Fit In?	Elbert
4:45 PM	*Adjourn for day*	

Friday, August 3rd, 2018

MORNING: ROOM A

9:00 AM	Hands-on/discussion: cross-project data curation	Hale
9:30 AM	Discussion: formats and schemas for data and how to share (transform) the data between projects	Coleman
10:30 AM	Discussion: Opinions on the current state of atomistics and the future of the field	
11:30 AM	Hands-on: materials data science infrastructure	Elbert
12:30 PM	*Lunch Break*	

MORNING: ROOM B

9:30 AM	Hands-on: optimized Monte Carlo code	Yamakov
10:30 AM	Hands-on: iprPy and atomman calculations	Hale
11:30 AM	Hands-on: getting started with openKIM	Karls
12:30 PM	*Lunch Break*	

AFTERNOON: ROOM A

2:00 PM	Discussion: final thoughts, future plans	
3:00 PM	*Adjourn*	