Agenda for the 2008 NIST Workshop on Atomistic Simulations for Industrial Needs
Building 223 Room B307 (MSEL Conference Room)

April 28

08:30 AM	Clear Security and the front gate	
09:00 AM	Introduction and Welcome (Chandler Becker and Frank Gayle)	
09:30 AM	Baskes	“Semi-empirical atomistic modeling: a perspective of the past and gateway to the future”
10:00 AM	Mishin	“Methodological aspects of potential development for metallic systems”
10:30 AM	DISCUSSION/BREAK	
11:00 AM	Mendelev	“Development of Semi-Empirical Interatomic Potentials Appropriate for Simulation of Solid and Liquid Metallic Alloys.”
11:30 AM	Widom	“Quick and dirty pair potentials for multicomponent alloys”
12:00 PM	LUNCH (NIST Cafeteria)	
01:30 PM	Goddard	“Advances in applications of atomistic simulations to industrial applications in catalysis, fuel cells, and nanoelectronics and future needs.”
02:00 PM	Siegel	“An industrial perspective on atomistic simulations”
02:15 PM	Chandran	“Challenges in abinitio modeling of thermo-physical properties of materials"
02:45 PM	DISCUSSION/BREAK	
03:15 PM	Foiles	“Atomistic Simulations of Interfaces: Opportunities and Pitfalls”
03:45 PM	Qi	“Multiscale modeling for metal forming and a wish list of alloying elements”
04:15 PM	DISCUSSION/BREAK	
05:30 PM	DAILY WRAP-UP	
07:00 PM	DINNER at Cafe Mileto Cloppers Mill Village 18056 Mateny Road Germantown, MD 20874	

April 29

08:30 AM	Schweiger	“Industrial materials R&D using the MedeA software platform”
09:00 AM	Kattner	“The need and use of atomistic simulations in Calphad methods”
09:30 AM	Johnson	“NIST Computational Chemistry Comparison and Benchmark Database”
10:00 AM	Elliott	“A Knowledge-base of Interatomic Models (KIM): A platform for the integrated development, testing and application of atomistic models.”
10:30 AM	BREAK	
10:45 AM	DISCUSSION/CLOSING	
12:30 PM	LUNCH (NIST Cafeteria)	

Participant	Affiliation
Baskes, Michael	Los Alamos National Laboratory and University of California, San Diego
Becker, Chandler	NIST Metallurgy Division
Chandran, Mahesh	GE Global Research
Elliott, Ryan	Department of Aerospace Engineering and Mechanics, University of Minnesota
Foiles, Stephen	Sandia National Laboratories
Frolov, Timofey	Department of Physics, George Mason University
Goddard III, William A.	Materials and Process Simulation Center, California Institute of Technology
Ivanov, Vladimir	Department of Physics, George Mason University
Johnson, Russell	NIST Physical and Chemical Properties Division
Kattner, Ursula	NIST Metallurgy Division
Lill, James	Air Force Research Laboratory
Mendelev, Mikhail	Ames Laboratory
Miller, Ronald	Mechanical and Aerospace Engineering, Carleton University
Mishin, Yuri	Department of Physics, George Mason University
Pun, Ganga P Purja	Department of Physics, George Mason University
Qi, Yue	General Motors
Schweiger, Hannes	Materials Design
Siegel, Donald	Ford Motor Company
Tadmor, Ellad	Department of Aerospace Engineering and Mechanics, University of Minnesota
Tulyani, Sonia	United Technologies Research Center
Widom, Michael	Department of Physics, Carnegie Mellon University
Woodward, Christopher	Air Force Research Laboratory

Additional NIST participants for all or part of the workshop:

Boettinger, William	NIST Metallurgy Division
Burton, Benjamin	NIST Ceramics Division
Campbell, Carelyn	NIST Metallurgy Division
Cockayne, Eric	NIST Ceramics Division
Guyer, Jonathan	NIST Metallurgy Division
Levine, Lyle	NIST Metallurgy Division
Mountain, Raymond	NIST Physical and Chemical Properties Division
Tavazza, Francesca	NIST Metallurgy Division
Tsang, Wing	NIST Physical and Chemical Properties Division
Wagner, Richard	NIST Metallurgy Division
Warren, James	NIST Metallurgy Division