Welcome to the

NIST Workshop on Atomistic Simulations for Industrial Needs

July 27-28, 2010

Introduction

- Atomic-scale simulations are increasingly common
  - insight into nanoscale phenomena (e.g. catalysis, defects and segregation, ordering in solids and liquids, ...)
  - input for higher-level models (e.g. FEA, phase-field, or Calphad)
- Fits into the ICME paradigm:
  - NRC report:" Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security," 2008.

- These methods can ultimately reduce costs -- faster R&D cycles, fewer expensive / difficult / impossible experiments.
- BUT, there are still many issues to address, including
  - accuracy, software availability and standardization, transferability, system sizes, methods, the number of components and phases, data, ...

NIST Interatomic Potentials Project overview

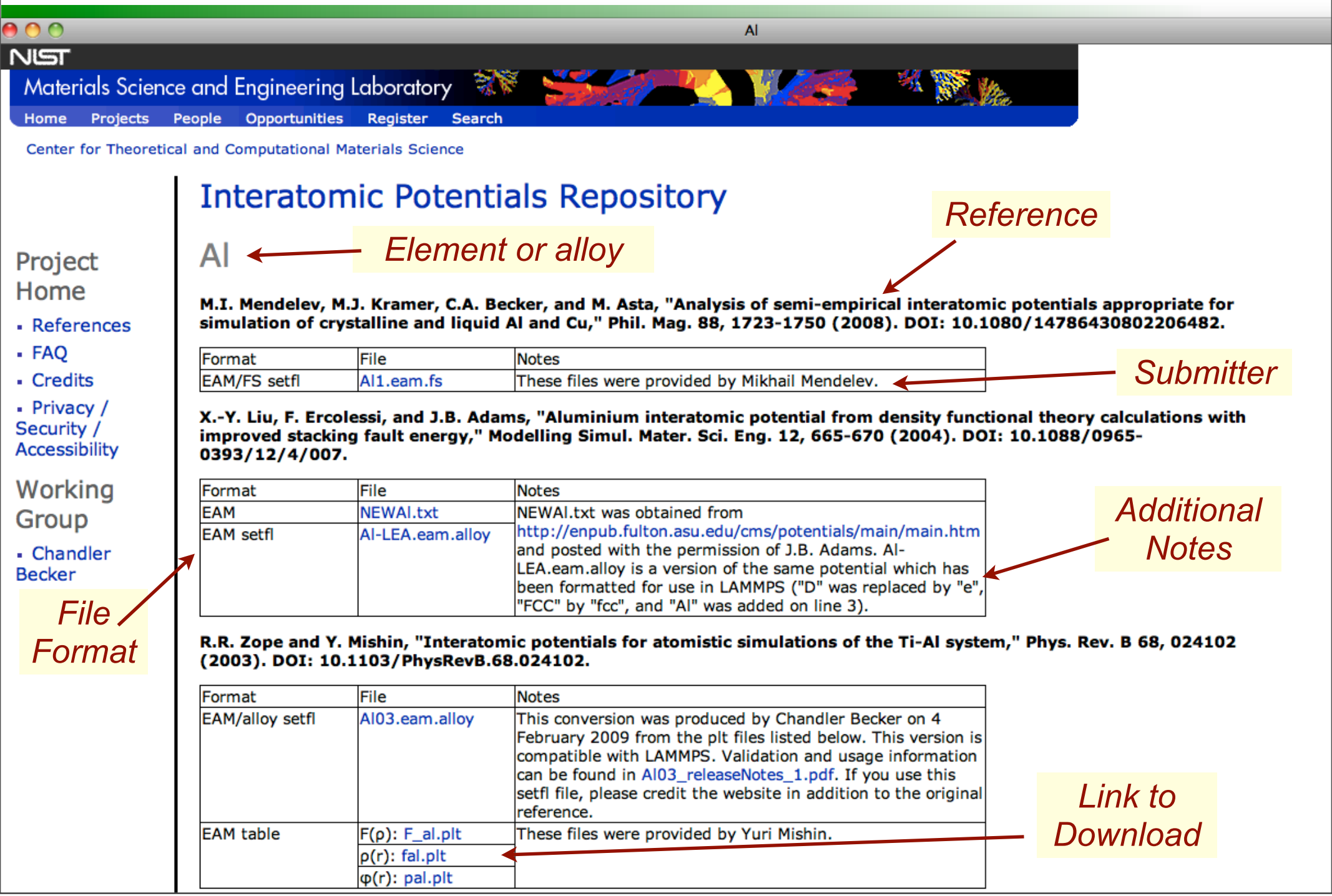
- NIST-sponsored **workshops** to facilitate interactions between industrial and academic researchers, identify and address specific topics.
- **Public repository of interatomic potentials** (models of interactions between atoms) from *known sources with references*.
  - Not to declare "The Best" since that depends on application
  - work with developers to make files available
  - no particular formats are required, but documentation is
- Conversions between file formats
- **Standardization efforts** (formats, automated property evaluations) with KIM collaboration
- **Property comparisons** with experiment and/or first-principles
  - e.g., C. A. Becker and M. J. Kramer, "Atomistic comparison of volume-dependent melt properties from four models of aluminum," MSMSE, in press (2010).

Available potentials

- www.ctcms.nist.gov/potentials/
- **Approximately 75 element and alloy potentials are available for download.**
- Most are compatible with readily-available molecular simulation packages such as LAMMPS and iMD.
- Approved by submitters, but ...
- *It is the user's responsibility to ensure the potentials give expected results.*

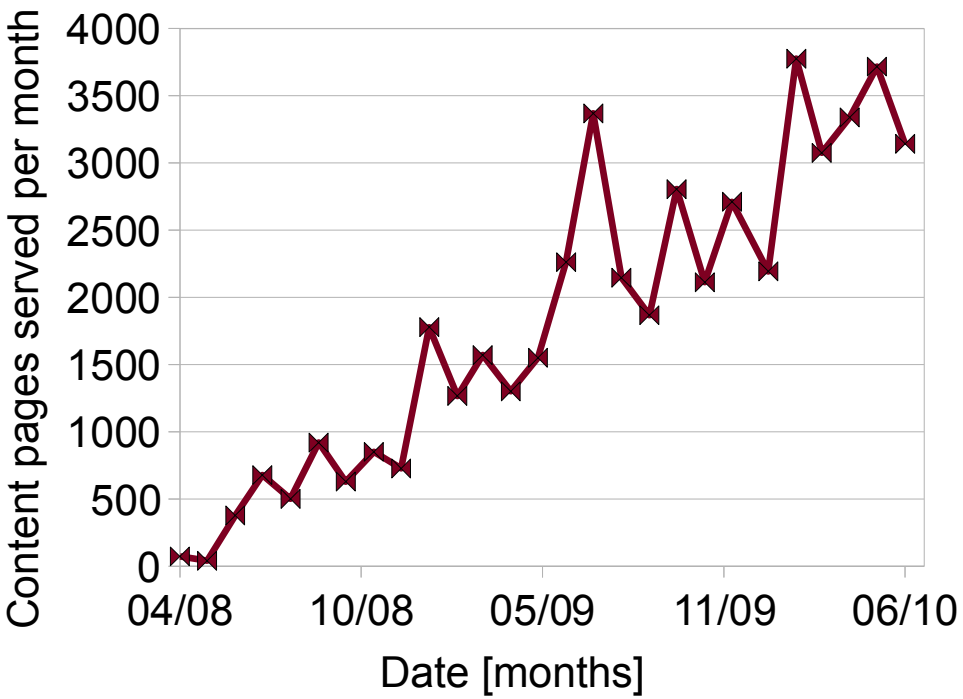
Elements	Multi-component
Ag	Ag-Cu
Al	Al-Cu Al-Fe Al-Mg Al-Ni Al-Ti
Au	
	C-Fe
	C-H-O
Cs	
Cu	Cu-Ag Cu-Al Cu-Fe Cu-Ni Cu-Pb Cu-Ta Cu-Zr
Fe	Fe-Al Fe-C Fe-Cu Fe-Cu-Ni Fe-Ni Fe-P Fe-V
K	
Li	
Mg	Mg-Al
Mo	
Na	
Nb	
Ni	Ni-Al Ni-Al-H Ni-Cu Ni-Fe
	P-Fe
	Pb-Cu
Pd	
Pt	
Rb	
Ru	
Si	
Ta	Ta-Cu
Ti	Ti-Al
V	V-Fe
W	
Zr	Zr-Cu
Fictional	

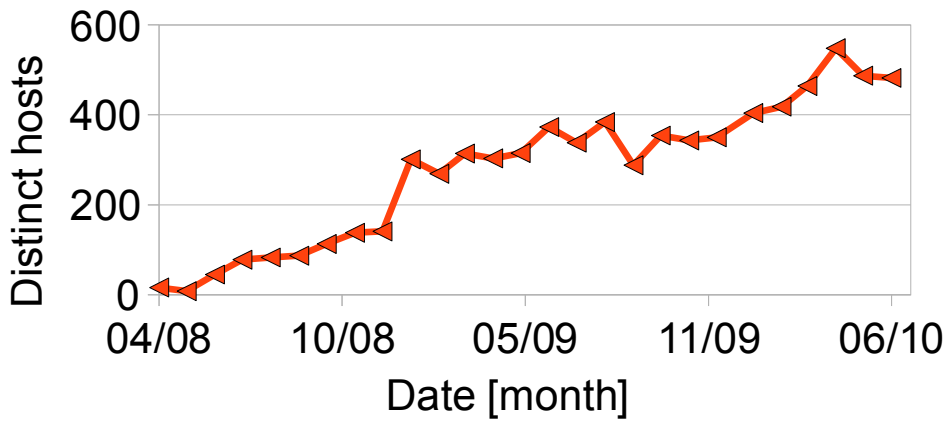
Potentials Download Pages

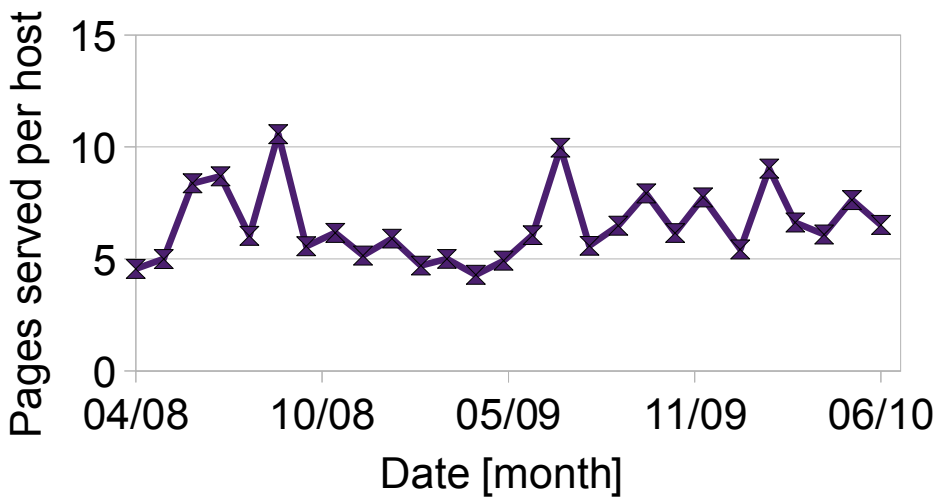


Repository Usage

- Per month: ~ 3400 content pages to ~500 hosts
- 2010 TMS tutorial on "Nanoscale Computational Materials Science"
- Word of mouth: Professors sending students, mailing lists







No bots, web crawlers, or nist.gov.
Requests for style sheets and images are also ignored.
All of these artificially inflate hit counts.

2010 Workshop Questions

- What can we do to make atomistic simulations more accepted as an industrial tool?
- Which interatomic potentials are available? Which are most needed?
- Can we create standards for software interoperability (e.g. MD + first-principles, MD + FEA)? What would they look like?
- Common formats for interatomic potentials? What would they look like?
- Are there mechanisms for "pairing" what experiments are being done with those that would be useful for validating potentials?
- Other topics for discussion?

Agenda (Tuesday)

Tuesday, July 27, 2010

08:30 AM	Clear security and the front gate	
09:00 AM	Introduction and Welcome	
09:30 AM	Robust Quantum-Based Interatomic Potentials for Transition Metals	John Moriarty, LLNL
10:00 AM	Limitations of Atomic Modeling for Nanomaterial Applications	Sadasivan Shankar, Intel
10:30 AM	Discussion / break	
11:00 AM	Development and applications of ReaxFF reactive force fields for combustion, catalysis and material failure	Adri Van Duin, Penn. State U.
11:30 AM	Applications of ReaxFF reactive force fields in hydrogen storage	Julius Ojwang, CIW
12:00 PM	lunch (NIST cafeteria)	
01:30 PM	Interatomic potentials for complex systems: recent development	Yuri Mishin, George Mason U.
02:00 PM	Ideas from Multi-state MEAM Applied to the Pu-Ga System	Mike Baskes, LANL
02:30 PM	Molecular dynamics simulations of multicomponent oxide glasses	Jincheng Du, U. North Texas
03:00 PM	Discussion / break	
03:30 PM	Integrating atomic potentials across the interfaces	Yue Qi, GM
04:00 PM	MEAM Interatomic Potential Generation: Coupling MATLAB with Atomistic Codes	Mark Tschopp, MS State U.
04:30 PM	Discussion and daily wrap-up	

07:00 PM Dinner at The Fontina Grille
801 Pleasant Drive, Rockville, MD 20850
301-947-5400

Agenda (Wednesday)

Wednesday, July 28, 2010

09:00 AM	Forcefield parameter determination in and from atomistic scale for non-covalent interactions	Jian-jie Liang, Accelrys
09:30 AM	A comprehensive environment for property prediction and forcefield development	Hannes Schweiger, Materials Design
10:00 AM	Open Knowledgebase of Interatomic Models (OpenKIM.org): an online platform for testing and archiving empirical potentials.	Ellad Tadmor, U. Minnesota
10:30 AM	Towards an API standard for the Knowledgebase of Interatomic Models (KIM)	Valeriu Smiricinschi, U. Minnesota
11:00 AM	Discussion	
12:00 PM	lunch (NIST cafeteria)	
01:00 PM	Role of precipitates in commercial Al and Mg alloys	Bita Ghaffari, Ford
01:30 PM	Development of Interatomic Potentials Appropriate for Simulation of Solid-Liquid Interface Properties in Al-Mg Alloys	Mikhail Mendelev, Ames Nat. Lab.
02:00 PM	Role of Sr in the Atomic Structure of Liquid Al-Si Hypoeutectic Alloys Using High Energy X-Ray Diffraction	Matthew Kramer, Ames Nat. Lab
02:30 PM	Finding long-range orientational order in a metallic glass	Howard Sheng, George Mason U.
03:00 PM	Discussion and workshop wrap-up	

Items of interest

- TMS First World Congress on Integrated Computational Materials Engineering
  - July 10-14, 2011; abstracts due 11/1/2010
- Virtual Vault for Pseudopotentials
  - Derek Stewart, Cornell Nanoscale Facility
  - http://www.nnin.org/nnin_comp_psp_vault.html