

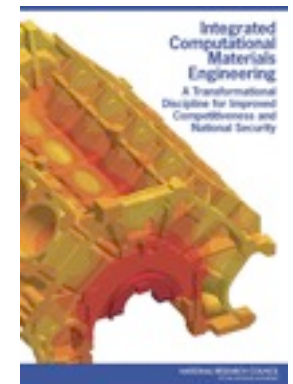
Welcome to the

**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-Ni	Al-Fe Al-Ti	Al-Mg
Au			
	C-Fe		
	C-H-O		
Cs			
Cu	Cu-Ag Cu-Ni Cu-Zr	Cu-Al Cu-Pb	Cu-Fe Cu-Ta
Fe	Fe-Al Fe-Cu-Ni Fe-V	Fe-C Fe-Ni	Fe-Cu Fe-P
K			
Li			
Mg	Mg-Al		
Mo			
Na			
Nb			
Ni	Ni-Al Ni-Fe	Ni-Al-H	Ni-Cu
	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

NIST
Materials Science and Engineering Laboratory
Home Projects People Opportunities Register Search
Center for Theoretical and Computational Materials Science

Interatomic Potentials Repository

Al ← *Element or alloy*

Reference →

M.I. Mendeleev, M.J. Kramer, C.A. Becker, and M. Asta, "Analysis of semi-empirical interatomic potentials appropriate for simulation of crystalline and liquid Al and Cu," Phil. Mag. 88, 1723-1750 (2008). DOI: 10.1080/14786430802206482.

Format	File	Notes
EAM/FS setfl	Al1.eam.fs	These files were provided by Mikhail Mendeleev. ← <i>Submitter</i>

X.-Y. Liu, F. Ercolessi, and J.B. Adams, "Aluminium interatomic potential from density functional theory calculations with improved stacking fault energy," Modelling Simul. Mater. Sci. Eng. 12, 665-670 (2004). DOI: 10.1088/0965-0393/12/4/007.

Format	File	Notes
EAM	NEWAl.txt	NEWAl.txt was obtained from
EAM setfl	Al-LEA.eam.alloy	http://enpub.fulton.asu.edu/cms/potentials/main/main.htm and posted with the permission of J.B. Adams. Al-LEA.eam.alloy is a version of the same potential which has been formatted for use in LAMMPS ("D" was replaced by "e", "FCC" by "fcc", and "Al" was added on line 3). ← <i>Additional Notes</i>

File Format →

R.R. Zope and Y. Mishin, "Interatomic potentials for atomistic simulations of the Ti-Al system," Phys. Rev. B 68, 024102 (2003). DOI: 10.1103/PhysRevB.68.024102.

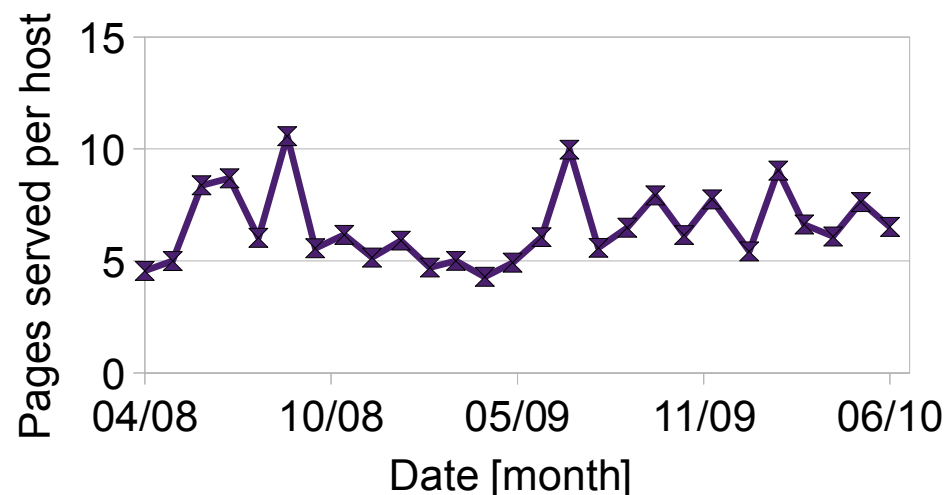
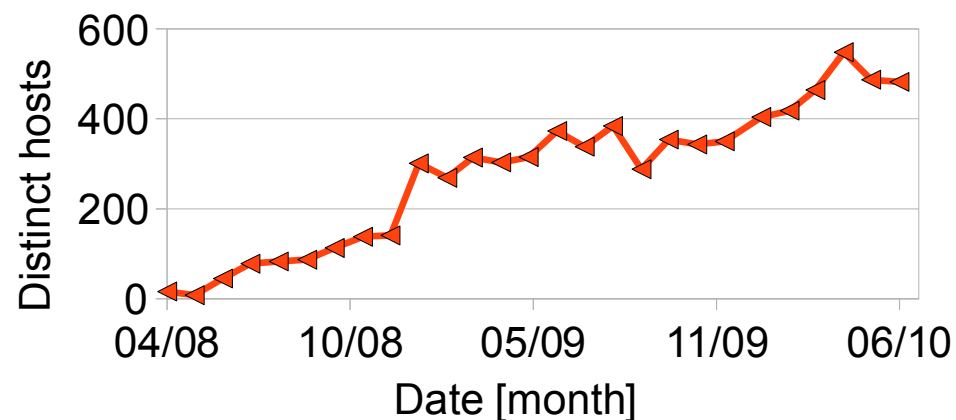
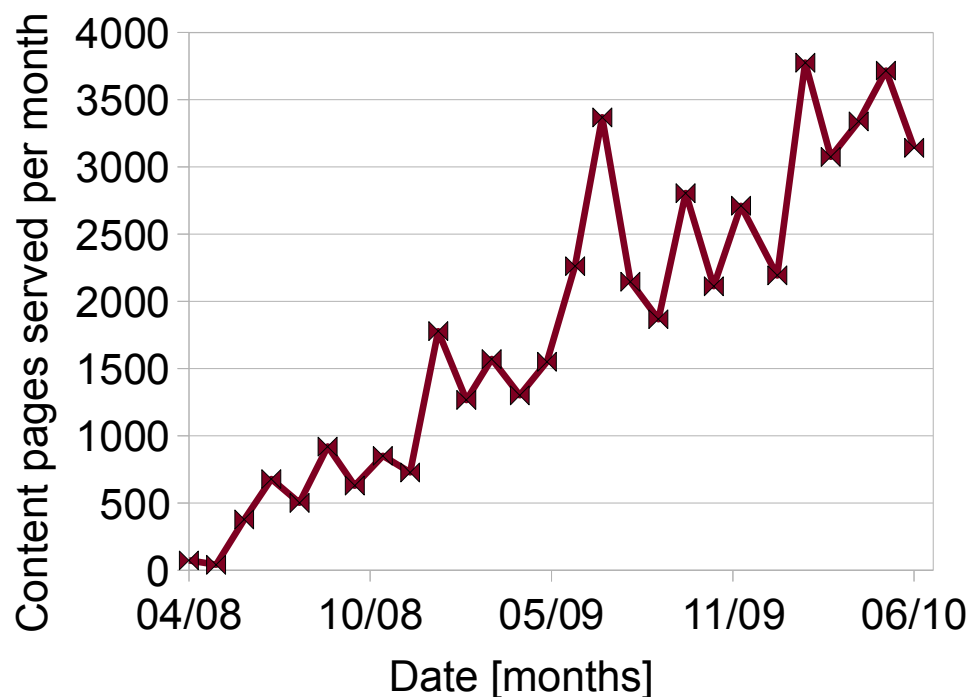
Format	File	Notes
EAM/alloy setfl	Al03.eam.alloy	This conversion was produced by Chandler Becker on 4 February 2009 from the plt files listed below. This version is compatible with LAMMPS. Validation and usage information can be found in Al03_releaseNotes_1.pdf . If you use this setfl file, please credit the website in addition to the original reference.
EAM table	F(ρ): F_al.plt ρ (r): fal.plt ϕ (r): pal.plt	These files were provided by Yuri Mishin. ← <i>Link to Download</i>

Project Home
• References
• FAQ
• Credits
• Privacy / Security / Accessibility

Working Group
• Chandler Becker

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 Smircinschi, U. Minnesota
11:00 AM	Discussion	
12:00 PM	lunch (NIST cafeteria)	
01:00 PM	Role of precipitates in commercial Al and Mg alloys	Bitra Ghaffari, Ford
01:30 PM	Development of Interatomic Potentials Appropriate for Simulation of Solid-Liquid Interface Properties in Al-Mg Alloys	Mikhail Mendeleev, 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