The NIST Interatomic Potentials Repository

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What is an interatomic potential?

- Description of the interactions between atoms
- aka "forcefields"
- Can be analytical or non-analytical
- Models can include different physics (e.g. metallic vs. covalent bonds, charge)
- Files can be various formats

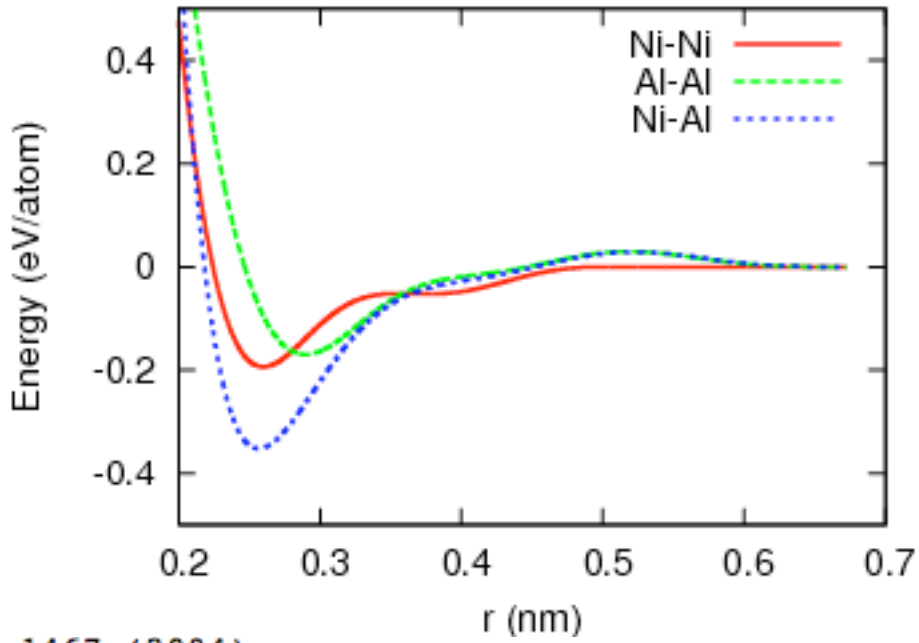
Pair interactions

Embedding energy

$$E_{tot} = \frac{1}{2}\sum_{ij}\phi(r_{ij}) + \sum_{i}F(\overline{\rho}_i)$$

$$\overline{\rho}_i = \sum_{j\neq i}\rho(r_{ij})$$

Host electron density

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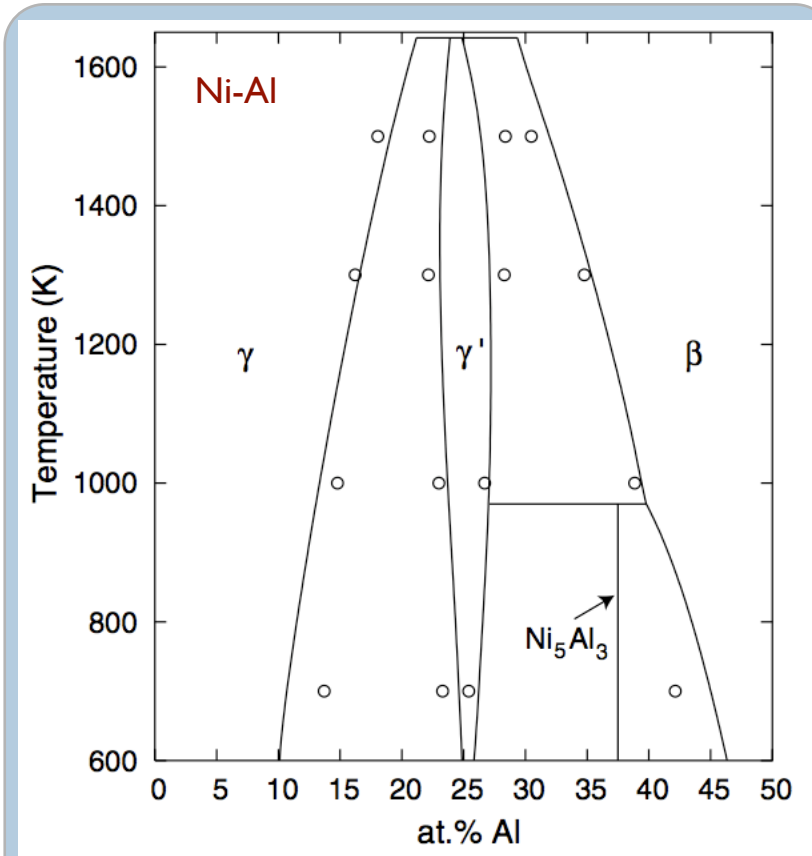
NiAl (L12) EAM from Y. Mishin, Acta Mat. 52, 1451-1467 (2004).
LAMMPS setfl format.  Conversion by C. A. Becker from Y. Mishin files.
7 January 2009.  http://www.ctcms.nist.gov/potentials
           2 Ni  Al
10000   0.6995103513405870E-03   10000  0.6724883999724820E-03  0.6724883999724820E+01
   28    0.5871000000E+02    0.3520000000E+01      fcc
  -0.2254965015409191E-01
  -0.4608461404747549E-01
  -0.6722644273232049E-01
  -0.8623912617422493E-01
```

Why isn't everyone using them?

- accuracy of interatomic models
- multicomponent systems
- transferability - behavior outside the fitted region
- calculation speed, tractable system sizes
- finding, evaluating, and comparing models
- incompatible file formats for software
- version control: files may be corrupt, incorrect user implementation, multiple versions, websites out of date



Mishin, Acta Mat. (2004)

reference?

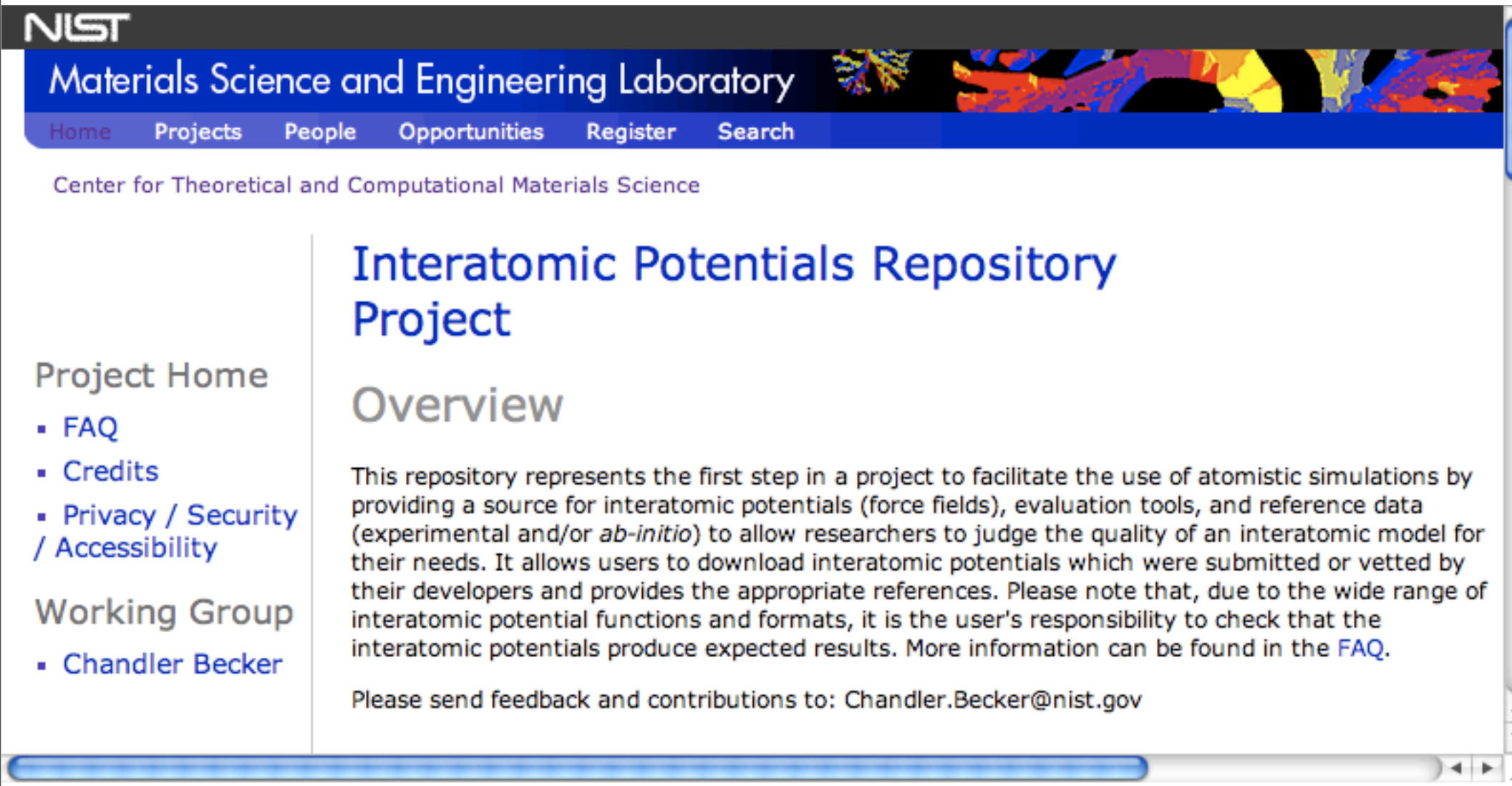
```
Ag functions (universal 3)
   47     107.87          4.0900    FCC
  500  5.0100200400801306e-04  500  1.1212121212121229e-02  5.550000
  0.                     -5.3437496524125194e-01 -7.9903970176950523
 -1.3414582590500288e+00 -1.4853604249917538e+00 -1.6189116822476493
 -1.9760965580129337e+00 -2.0844912853647344e+00 -2.1888075291300311
 -2.4820202718935036e+00 -2.5743582262663978e+00 -2.6644475069132341
 -2.9231988641276132e+00 -3.0061444187879260e+00 -3.0876567146272297
```

Project overview and goals

- Provide a **public repository of interatomic potentials** from *known sources* with *reference data and tools* to facilitate comparison.
- Not to declare "The Best" since that depends on application
- One-stop shop for interatomic potentials with references
  - work with developers to make potentials available
  - find out references and version information of existing files
  - multiple formats and materials
- Conversions between formats. Standardization.
- Develop standard property evaluation metrics and methods
- Reference data from experiment and/or first-principles

NIST Interatomic Potentials Repository

www.ctcms.nist.gov/potentials/



NIST Interatomic Potentials Repository

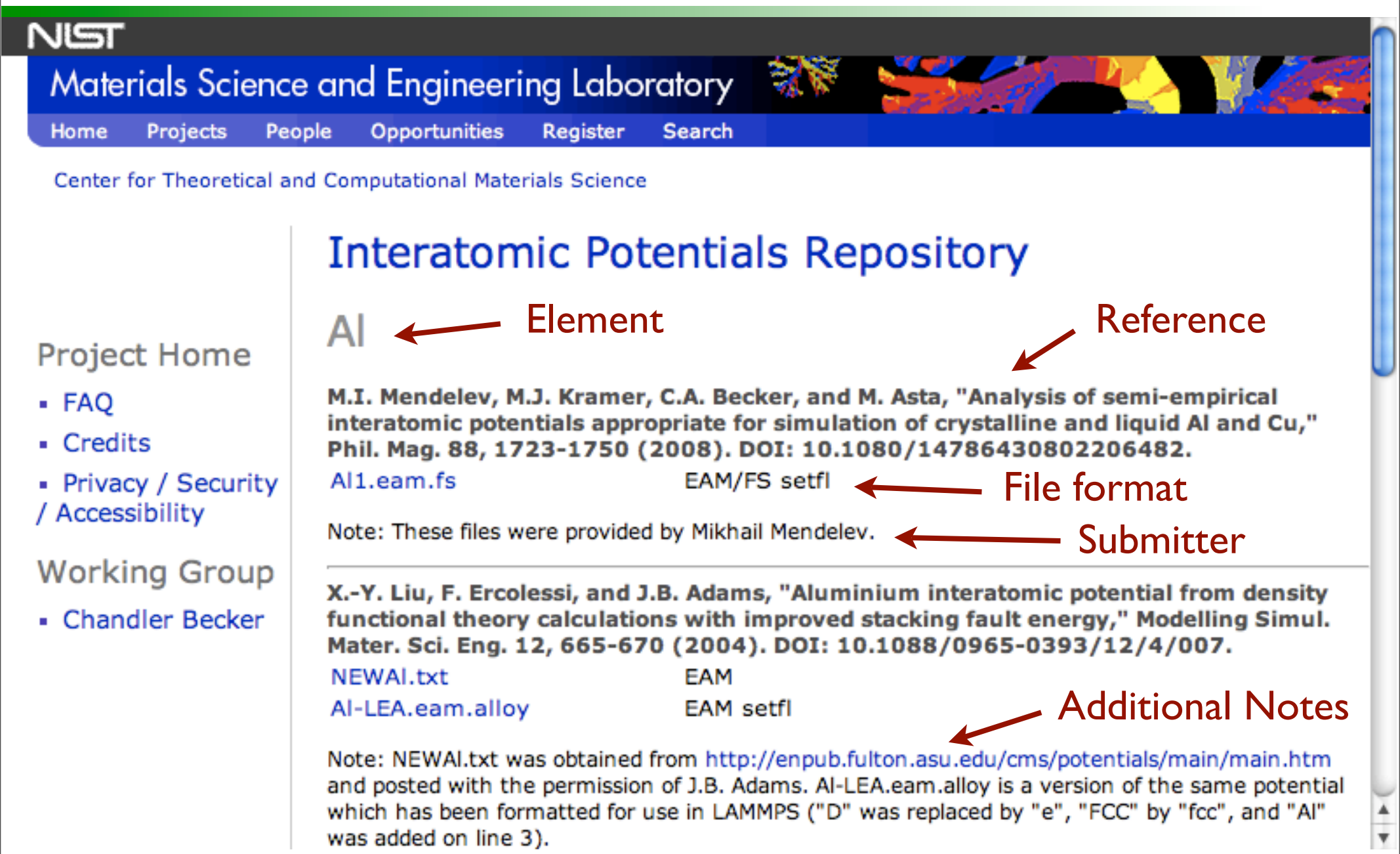
Interatomic Potentials

Elements	Multi-component
Ag	Ag-Cu
	Al-Cu
Al	Al-Fe
	Al-Mg
	Al-Ni
Au	
	Cu-Ag
	Cu-Al
Cu	Cu-Ni
	Cu-Pb
	Cu-Zr
	Fe-Al
	Fe-Ni
Fe	Fe-P
	Fe-V
Mg	Mg-Al
Mo	
	Ni-Al
Ni	Ni-Cu
	Ni-Fe
P	P-Fe
Pb	Pb-Cu
Pd	
Pt	
Ru	
V	V-Fe
Zr	Zr-Cu

www.ctcms.nist.gov/potentials/

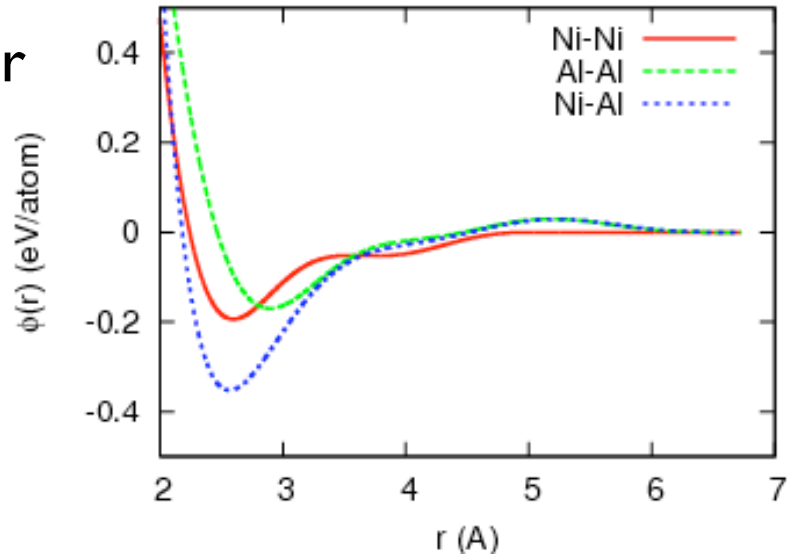
- Various elements and alloys are available for download.
- All have been vetted by their developers (authors of the files).
- Many are compatible with the LAMMPS MD package (lammps.sandia.gov) and other open source software.
- No particular format is required, but formatting information is.
- We are expanding to include more potentials and different types.

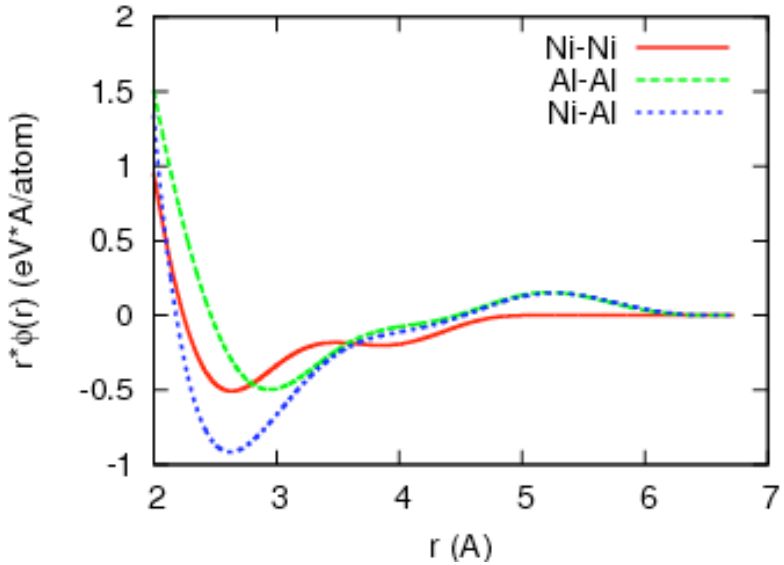
Download Potentials



FAQ

- Project information, including instructions for submitting potentials and crediting the site
- Descriptions of file formats
- "Why doesn't it look like the figure in the paper?"
  - Different file formats
  - Different functions
  - Invariant transformations
  - Interatomic potentials which look very similar (different) may have properties that are very different (similar).
- Links to other software (e.g. LAMMPS)





Format Conversion

- Conversion from the *plt* (x,y) format to the *EAM/alloy setfl* format:

Pair interactions

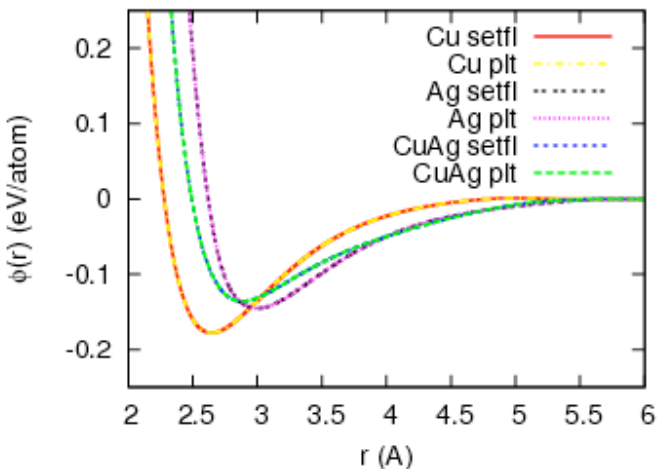
Embedding energy

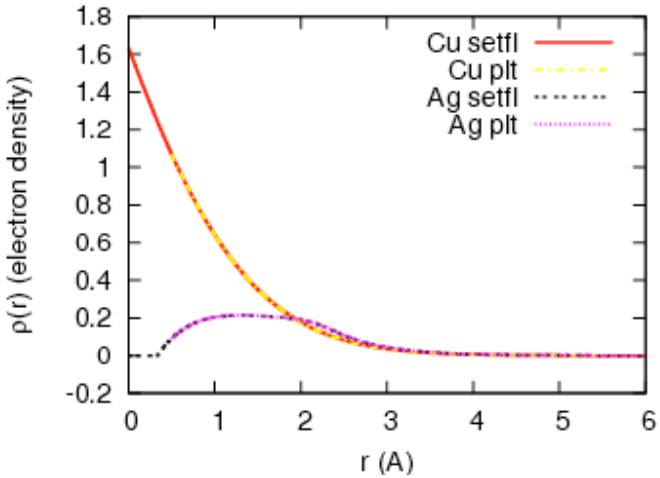
$$E_{tot} = \frac{1}{2}\sum_{ij}\phi(r_{ij}) + \sum_{i}F(\overline{\rho}_i)$$

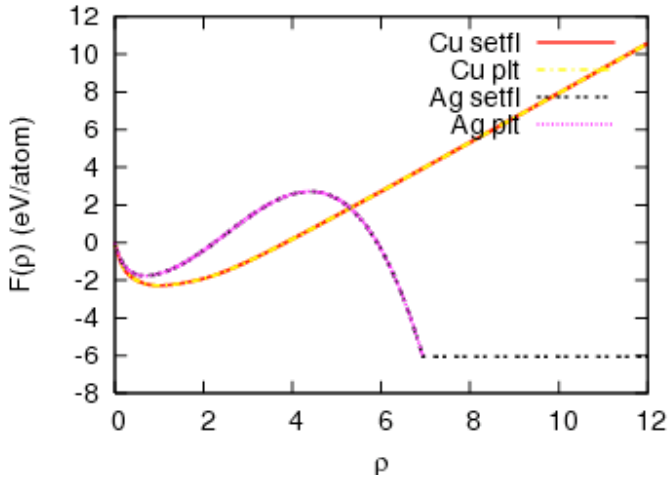
$$\overline{\rho}_i = \sum_{j\neq i}\rho(r_{ij})$$

Host electron density

- Issues:
  - splines
  - need a common scale
  - upper/lower bounds
    - r_{min}=0, r_{min}=dr, r_{min}=0.5 A
  - different order of functions
  - Φ(r) vs r*Φ(r)







Conversion testing

- Calculated E_0 and EAM functions for *setfl* (LAMMPS) and *plt* (SOLD) for atoms in ideal fcc positions

Pair interactions

Embedding energy

$$E_{tot} = \frac{1}{2}\sum_{ij}\phi(r_{ij}) + \sum_{i}F(\overline{\rho}_i)$$

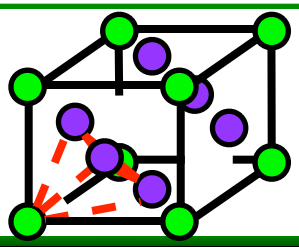
$$\overline{\rho}_i = \sum_{j\neq i}\rho(r_{ij})$$

Host electron density

- Differences between results are highlighted:

Comparison of minimum energies from SOLD and LAMMPS

Alloy	a (A)	E_min(SOLD,eV)	E_min(LAMMPS,eV)	Notes
fcc Ag	4.085	-0.113996999978E+02	-11.3996999978	
	4.09	-0.113999998989E+02	-11.3999998989	= -2.849999974725 eV/atom
	4.095	-0.113997024609E+02	-11.3997024609	
fcc Cu	3.614	-0.141599858176E+02	-14.1599858176	
	3.615	-0.141599998746E+02	-14.159999874 7	= -3.539999968675 eV/atom
	3.616	-0.141599858326E+02	-14.1599858326	
L12 Ag3Cu	3.9834	-0.117565455676E+02	-11.7565455676	
	3.9835	-0.117565455929E+02	-11.7565455929	= -2.939136398225 eV/atom
	3.9836	-0.117565453583E+02	-11.7565453583	
L10 CuAg	3.880	-0.123070560947E+02	-12.3070560948	
	3.881	-0.123070804962E+02	-12.3070804962	= -3.07677012405 eV/atom
	3.882	-0.123070738275E+02	-12.3070738275	
L12 Cu3Ag	3.757	-0.130877673407E+02	-13.0877673407	
	3.758	-0.130877880950E+02	-13.087788095	= -3.27194702375 eV/atom
	3.759	-0.130877780304E+02	-13.0877780304	



$L1_2$

SOLD was kindly provided by Yuri Mishin

EAM function values from SOLD and LAMMPS

Cu3Ag a=3.758 A

r^2	rho(SOLD)	rho(LAMMPS)
7.061282	0.062852970138718	0.062852970138713
7.061282	0.080422918188860	0.080422918188852
14.122564	0.007884125490181	0.007884125490182
14.122564	0.011022393370322	0.011022393370319
21.183846	0.001113794054072	0.001113794054071
21.183846	0.002301934021530	0.002301934021529
28.245128	0.000004416130543	0.000004416130543
28.245128	0.000444063188335	0.000444063188335
35.306410	0.000000017231091	0.000000017231090

r^2	phi(SOLD)	phi(LAMMPS)
7.061282	-0.051746694850591	-0.051746694850604
7.061282	-0.088898522362072	-0.088898522362017
14.122564	-0.019108034575602	-0.019108034575602
14.122564	-0.035264699809090	-0.035264699809092
21.183846	-0.001446381632289	-0.001446381632290
21.183846	-0.010516854510566	-0.010516854510556
28.245128	0.000052252751389	0.000052252751390
28.245128	-0.002236685226569	-0.002236685226569
35.306410	-0.000000042896298	-0.000000042896298

rho(SOLD)	F(SOLD)
0.852429817444297	-1.730440623420056
0.908109495258908	-2.2757109732261 81
0.908109495258909	-2.2757109732261 81
rho(LAMMPS)	F(LAMMPS)
0.852429817444197	-1.730440623413965
0.90810949525 8811	-2.275710973226475

User community

- Working with users and developers
  - helping people use potentials; answering questions about formats, etc.
  - helping developers convert potentials, ensure they run, distribute the files
- Informal interactions with individuals in academia, government, and industry (what do you need? what can you provide?)
  - radiation potentials
- these workshops
- LAMMPS mailing list - users refer each other to the website
- word of mouth

Summary and Future

- NIST Interatomic Potentials Repository to provide a resource for obtaining and evaluating interatomic potentials (with references): www.ctcms.nist.gov/potentials
- Conversions of interatomic potentials to common formats.
- Begun developing tools and methods to help users evaluate the suitability of an interatomic potential.
- Future directions:
  - Other elements, multicomponent alloys, and other forms of interatomic interactions, e.g. those used in polymers and ceramics
  - Standardization (with the help of the community); user forum
  - Collecting reference data for properties
  - Property evaluations -- systematically examine the significance of parameters like system size, relaxation times, run lengths, timesteps,....