Comparing Property Predictions Across Interatomic Potentials

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LAMMPS Users Workshop
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NIST
National Institute of Standards and Technology
U.S. Department of Commerce

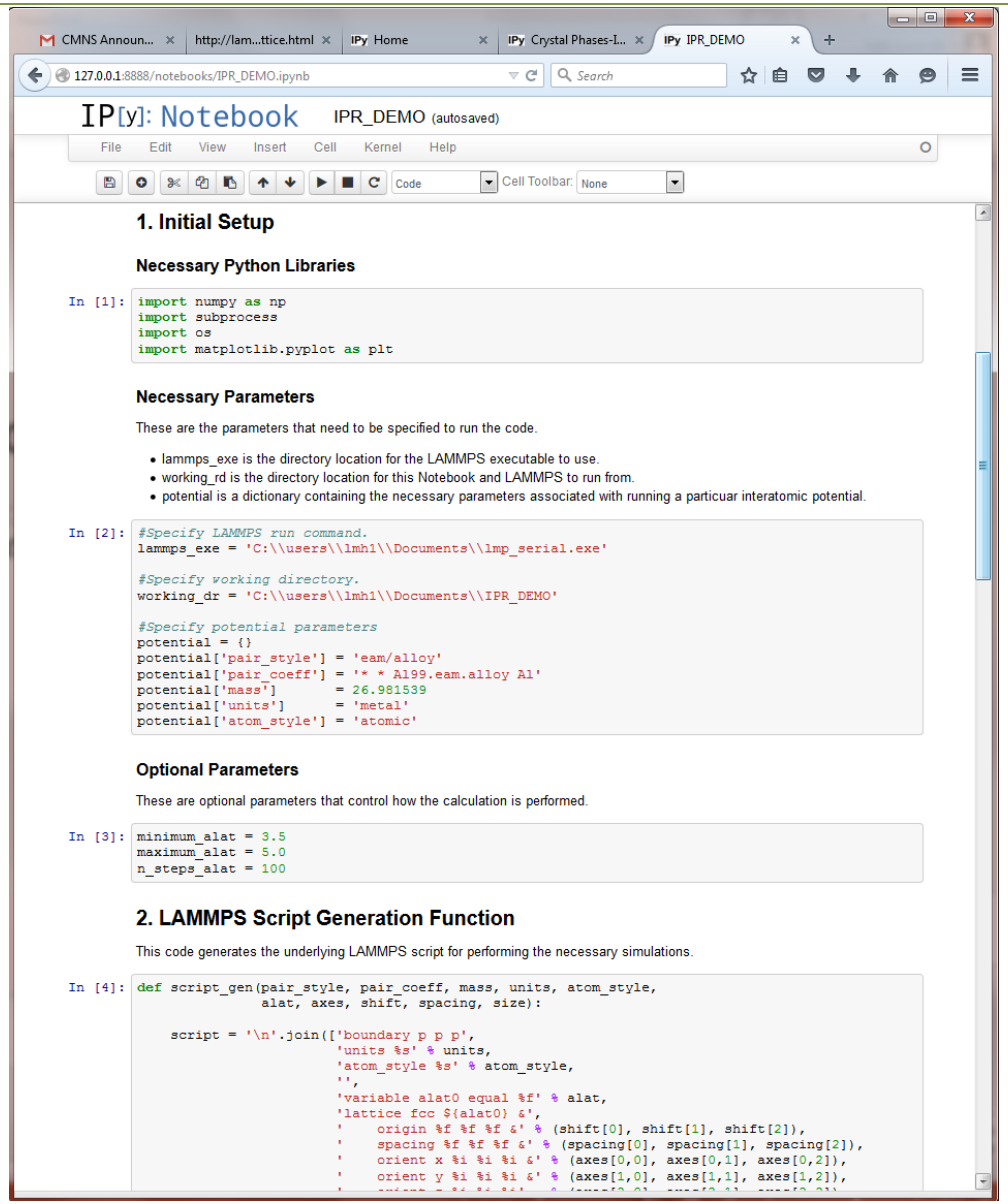
Python-Based Calculation Framework

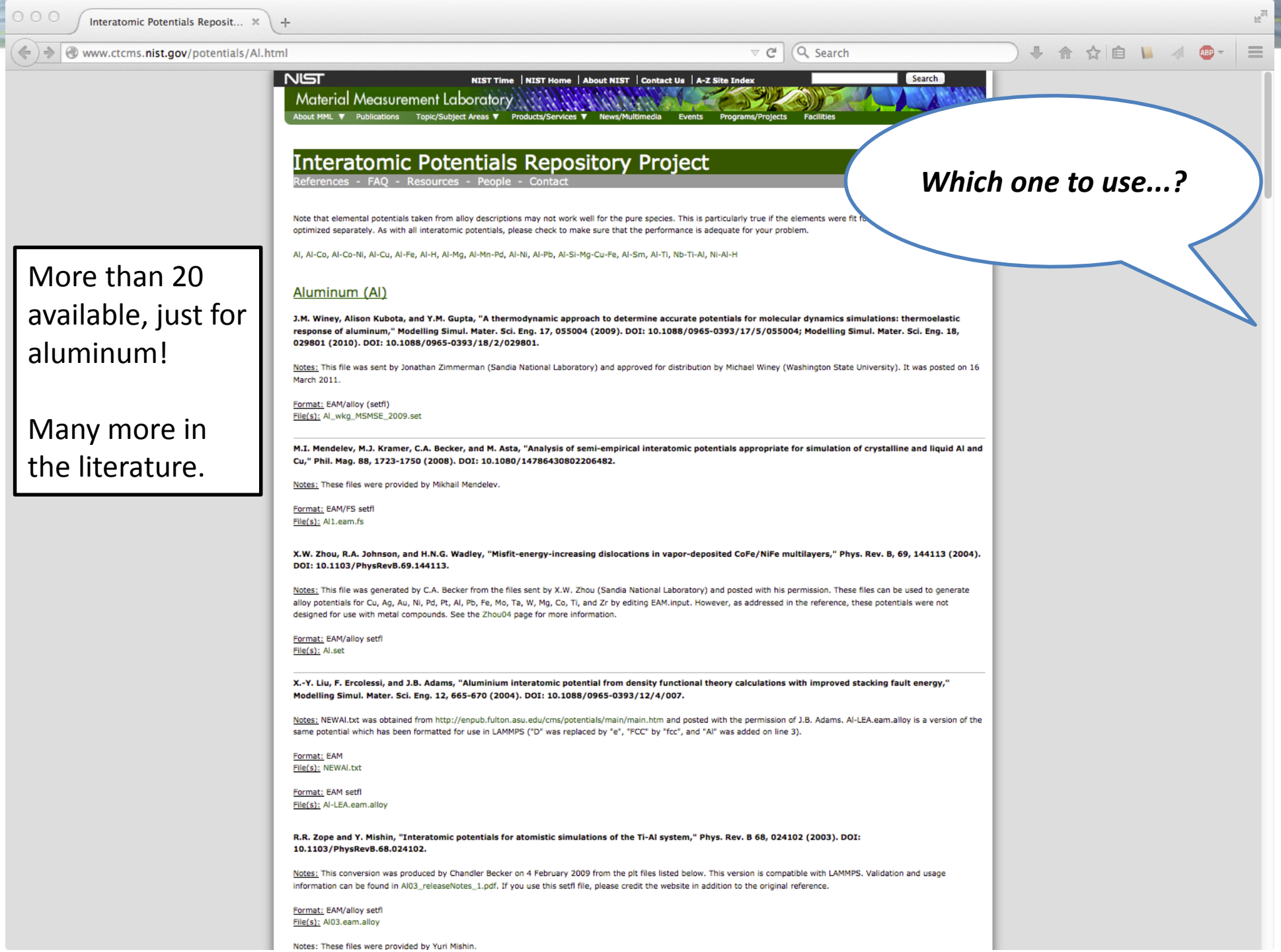
Forthcoming extension of the NIST Interatomic Potentials Repository Project

Property predictions for all available interatomic potentials

Allows measurements to be:

- Reproducible
- Well documented
- Transparent
- Iterable (automation)
- Comparable
- Archived




Interatomic Potentials Reposit...
www.ctcms.nist.gov/potentials/Al.html
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Interatomic Potentials Repository Project
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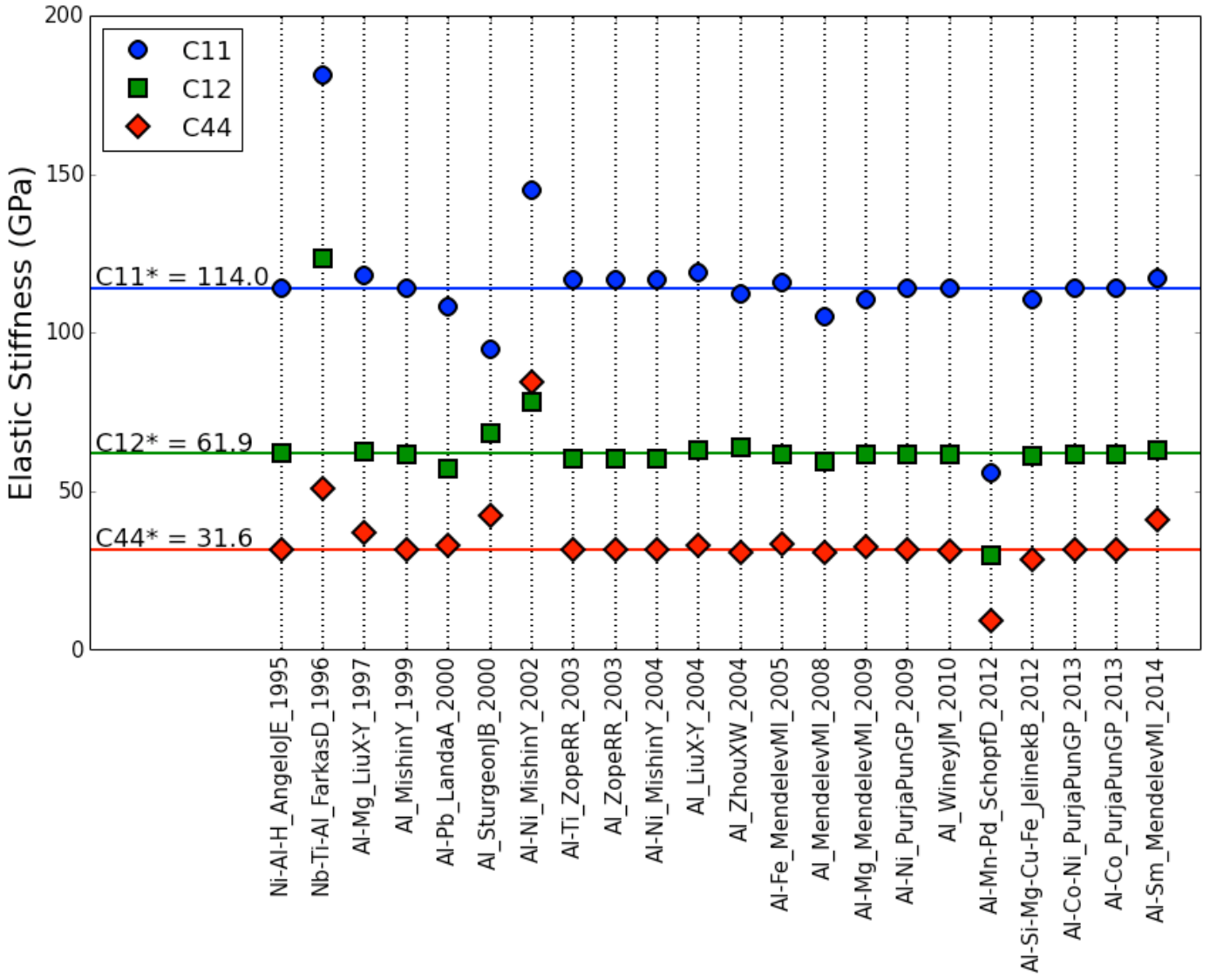
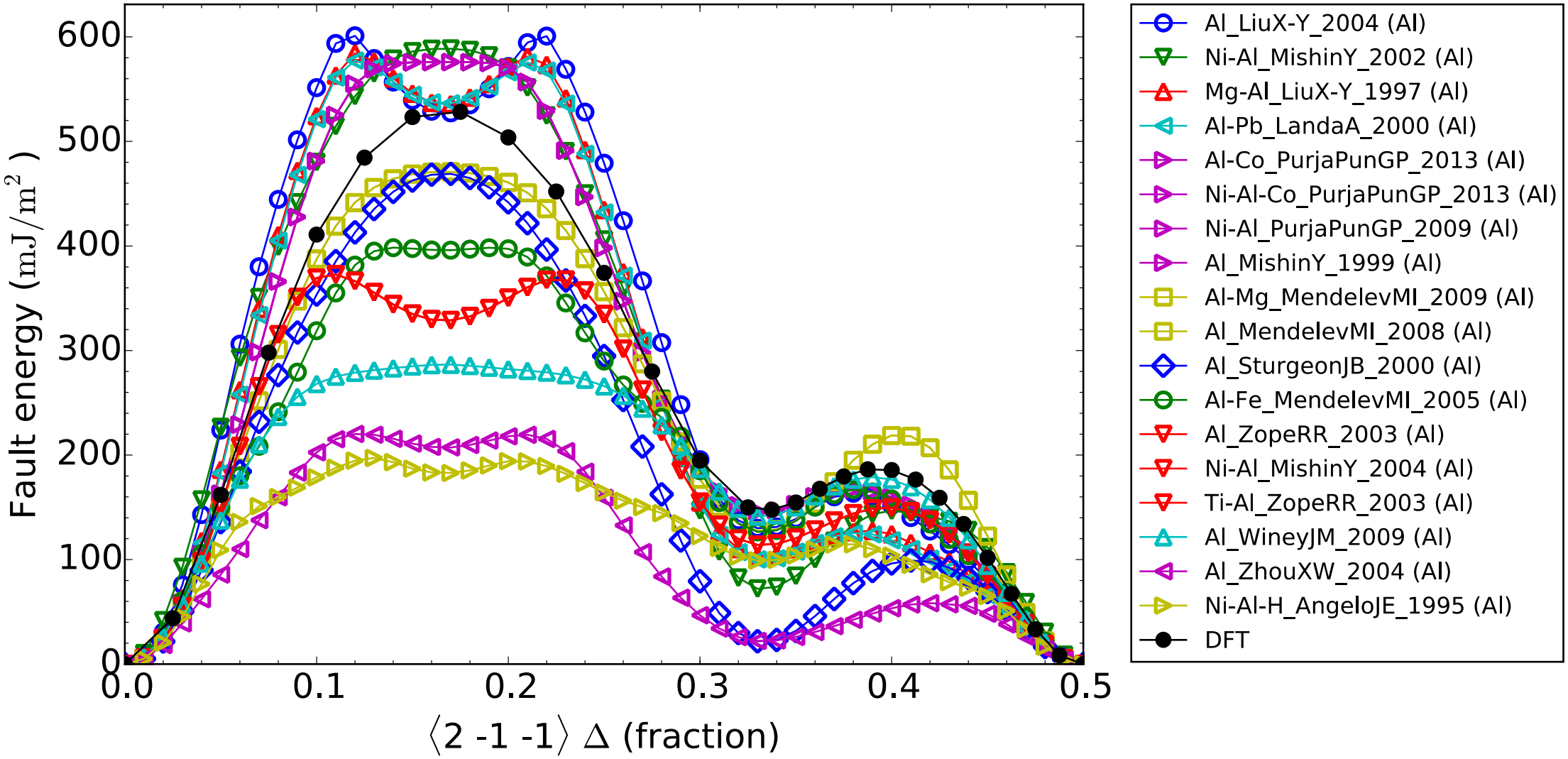
Note that elemental potentials taken from alloy descriptions may not work well for the pure species. This is particularly true if the elements were fit fo
optimized separately. As with all interatomic potentials, please check to make sure that the performance is adequate for your problem.
Al, Al-Co, Al-Co-Ni, Al-Cu, Al-Fe, Al-H, Al-Mg, Al-Mn-Pd, Al-Ni, Al-Pb, Al-Si-Mg-Cu-Fe, Al-Sm, Al-Ti, Nb-Ti-Al, Ni-Al-H
Aluminum (Al)
J.M. Winey, Alison Kubota, and Y.M. Gupta, "A thermodynamic approach to determine accurate potentials for molecular dynamics simulations: thermoelastic response of aluminum," Modelling Simul. Mater. Sci. Eng. 17, 055004 (2009). DOI: 10.1088/0965-0393/17/5/055004; Modelling Simul. Mater. Sci. Eng. 18, 029801 (2010). DOI: 10.1088/0965-0393/18/2/029801.
Notes: This file was sent by Jonathan Zimmerman (Sandia National Laboratory) and approved for distribution by Michael Winey (Washington State University). It was posted on 16 March 2011.
Format: EAM/alloy (setfl)
File(s): Al_wkg_MSMSE_2009.set
M.I. Mendelev, 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.
Notes: These files were provided by Mikhail Mendelev.
Format: EAM/FS setfl
File(s): Al1.eam.fs
X.W. Zhou, R.A. Johnson, and H.N.G. Wadley, "Misfit-energy-increasing dislocations in vapor-deposited CoFe/NiFe multilayers," Phys. Rev. B, 69, 144113 (2004). DOI: 10.1103/PhysRevB.69.144113.
Notes: This file was generated by C.A. Becker from the files sent by X.W. Zhou (Sandia National Laboratory) and posted with his permission. These files can be used to generate alloy potentials for Cu, Ag, Au, Ni, Pd, Pt, Al, Pb, Fe, Mo, Ta, W, Mg, Co, Ti, and Zr by editing EAM.input. However, as addressed in the reference, these potentials were not designed for use with metal compounds. See the Zhou04 page for more information.
Format: EAM/alloy setfl
File(s): Al.set
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.
Notes: NEWAl.txt was obtained from 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).
Format: EAM
File(s): NEWAl.txt
Format: EAM setfl
File(s): Al-LEA.eam.alloy
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.
Notes: 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.
Format: EAM/alloy setfl
File(s): Al03.eam.alloy
Notes: These files were provided by Yuri Mishin.
Which one to use...?
More than 20 available, just for aluminum!
Many more in the literature.

Property Comparison

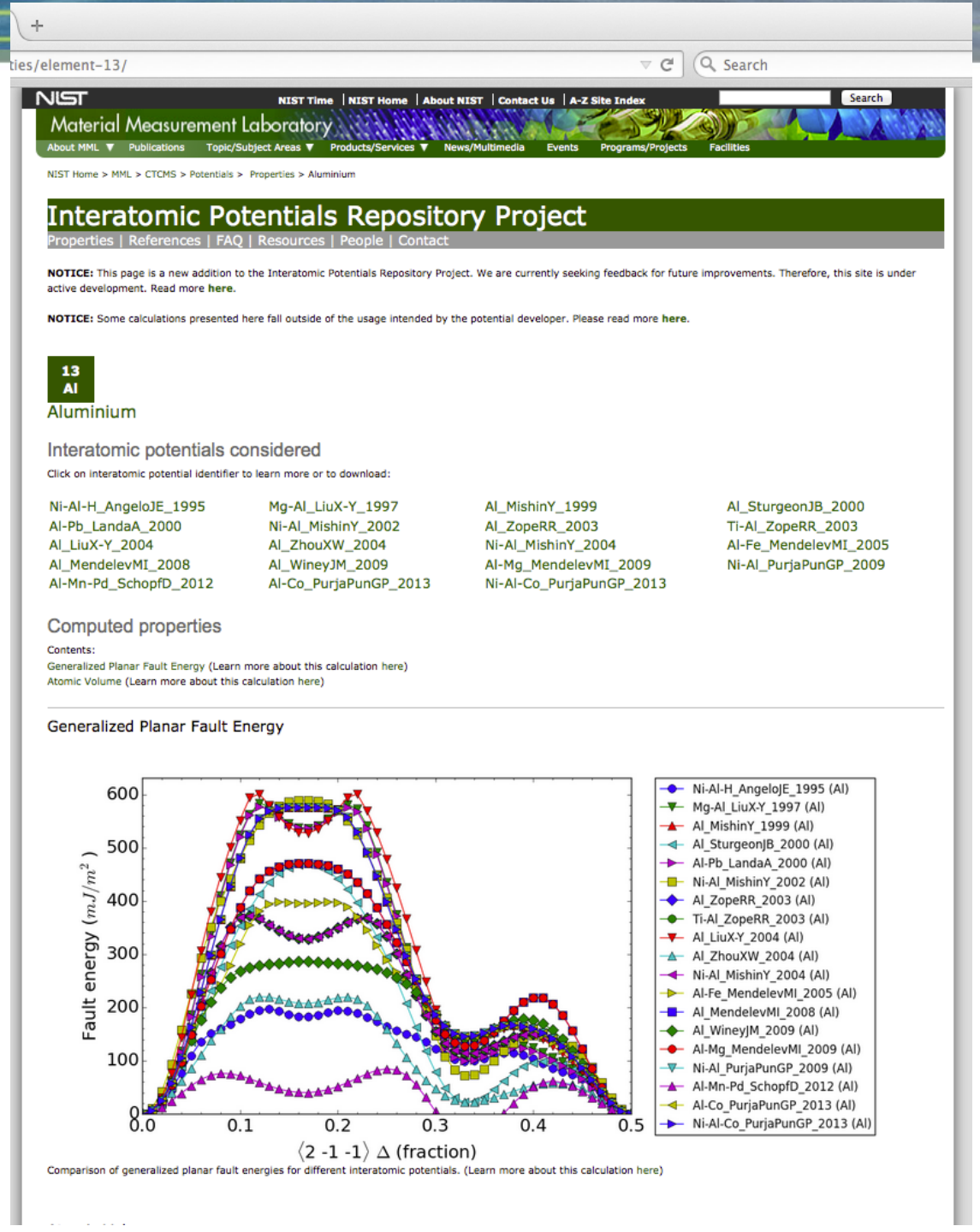


Property Comparison



Updated Website Coming Soon!

- Element-wise comparison pages
- Potential specific breakdowns
- Dynamically searchable results
- All calculation tools used



LAMMPS Input script

Compute energy of fcc system for different sizes and orientations

```
boundary p p p
units metal
atom_style atomic

variable alat0 equal 3.25
lattice fcc ${alat0} &
    origin 0.0 0.0 0.0 &
    spacing 1.0 1.0 1.0 &
    orient x 1 0 0 &
    orient y 0 1 0 &
    orient z 0 0 1

region box block 0 3 0 3 0 3
create_box 1 box
create_atoms 1 box

thermo_style custom step pe

mass 1 26.981539
pair_style eam/alloy
pair_coeff * * Al99.eam.alloy Al

run 0
```

Potential Specific Parameters

Simulation Design Parameters

Potential Specific Parameters

Python script_gen()

```
def script_gen(pair_style, pair_coeff, mass, units, atom_style,
               alat, axes, shift, spacing, size):

    script = '\n'.join(['boundary p p p',
                        'units %s' % units,
                        'atom_style %s' % atom_style,
                        '',
                        'variable alat0 equal %f' % alat,
                        'lattice fcc ${alat0} &',
                        '    origin %f %f %f &' % (shift[0], shift[1], shift[2]),
                        '    spacing %f %f %f &' % (spacing[0], spacing[1], spacing[2]),
                        '    orient x %i %i %i &' % (axes[0,0], axes[0,1], axes[0,2]),
                        '    orient y %i %i %i &' % (axes[1,0], axes[1,1], axes[1,2]),
                        '    orient z %i %i %i'   % (axes[2,0], axes[2,1], axes[2,2]),
                        '',
                        'region box block %i %i %i %i %i %i' % (size[0,0], size[0,1],
                                                               size[1,0], size[1,1],
                                                               size[2,0], size[2,1]),
                        'create_box 1 box',
                        'create_atoms 1 box',
                        '',
                        'thermo_style custom step pe',
                        '',
                        'mass 1 %f' % mass,
                        'pair_style %s' % pair_style,
                        'pair_coeff %s' % pair_coeff,
                        '',
                        'run 0'])
    return script
```

Python Calculation Function

```
def e_vs_a(lammps_exe, potential, amin, amax, asteps):
    avals = []
    evals = []

    #Read potential specific information
    pair_style = potential['pair_style']
    pair_coeff = potential['pair_coeff']
    mass =       potential['mass']
    units =      potential['units']
    atom_style = potential['atom_style']

    #Set constant simulation information
    axes = np.array([ [1, 0, 0], [0, 1, 0], [0, 0, 1] ])
    shift = np.array([0.0, 0.0, 0.0])
    spacing = np.array([1.0, 1.0, 1.0])
    size = np.array([ [0, 3], [0, 3], [0, 3] ])

    #Loop over range of lattice parameters
    for i in xrange(asteps):
        alat = amin + i * (amax - amin) / (asteps - 1)

        #Generate LAMMPS script
        with open('alat.in','w') as script:
            script.write(script_gen(pair_style, pair_coeff, mass, units, atom_style,
                                    alat, axes, shift, spacing, size))

        #Run LAMMPS
        output = subprocess.check_output(lammps_exe+' < alat.in',shell=True)

        #Distil results
        energy = extract_results(output)
        avals.append(alat)
        evals.append(energy)

    return avals, evals
```

Parameter Setup

Run simulation(s)

Process results

Demonstration IPython Notebooks

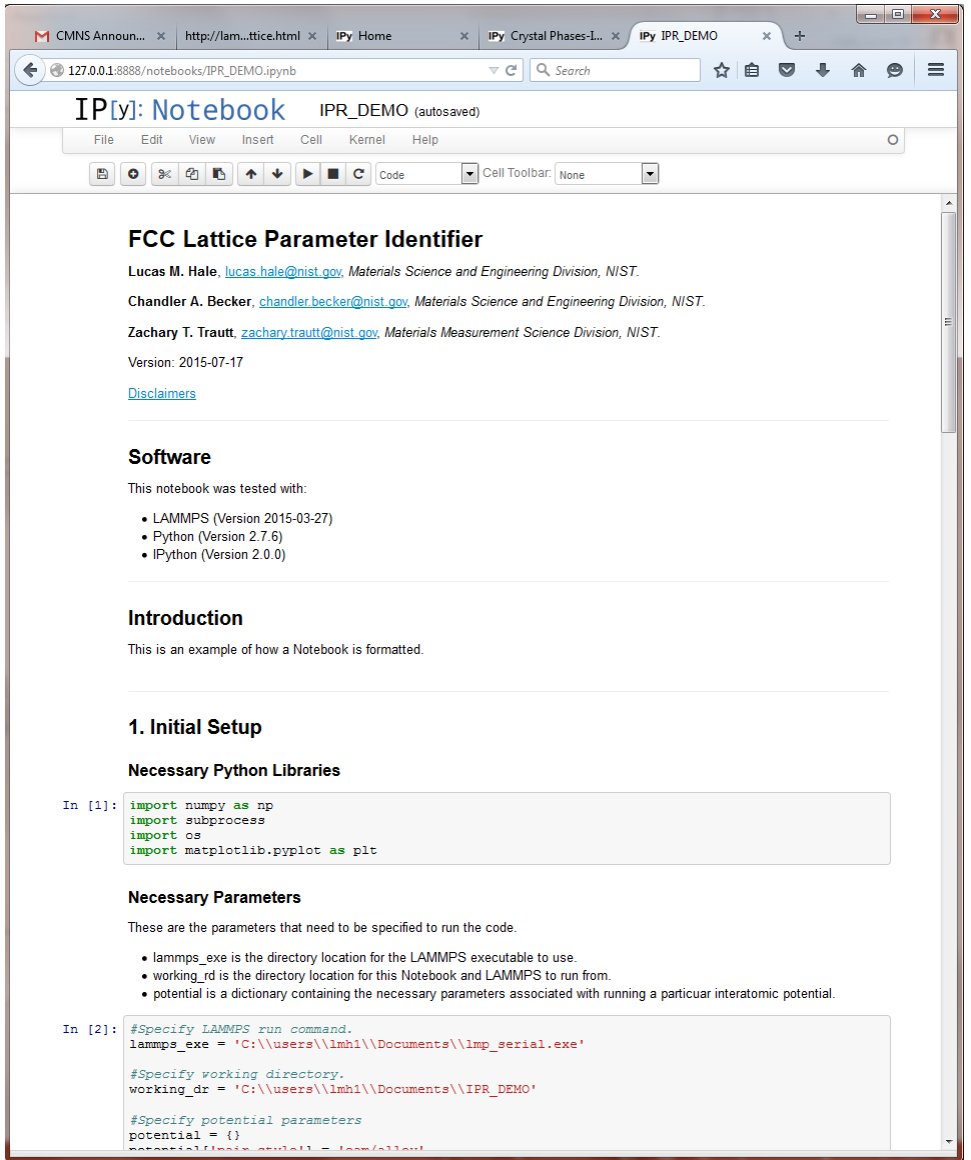
Mimics Mathematica Notebooks

Runs Python

Allows for complete documentation

- Comments describing calculation method
- Input parameters used
- Underlying LAMMPS script
- Code for calculation
- Results

Easy to learn, reproduce, and adapt



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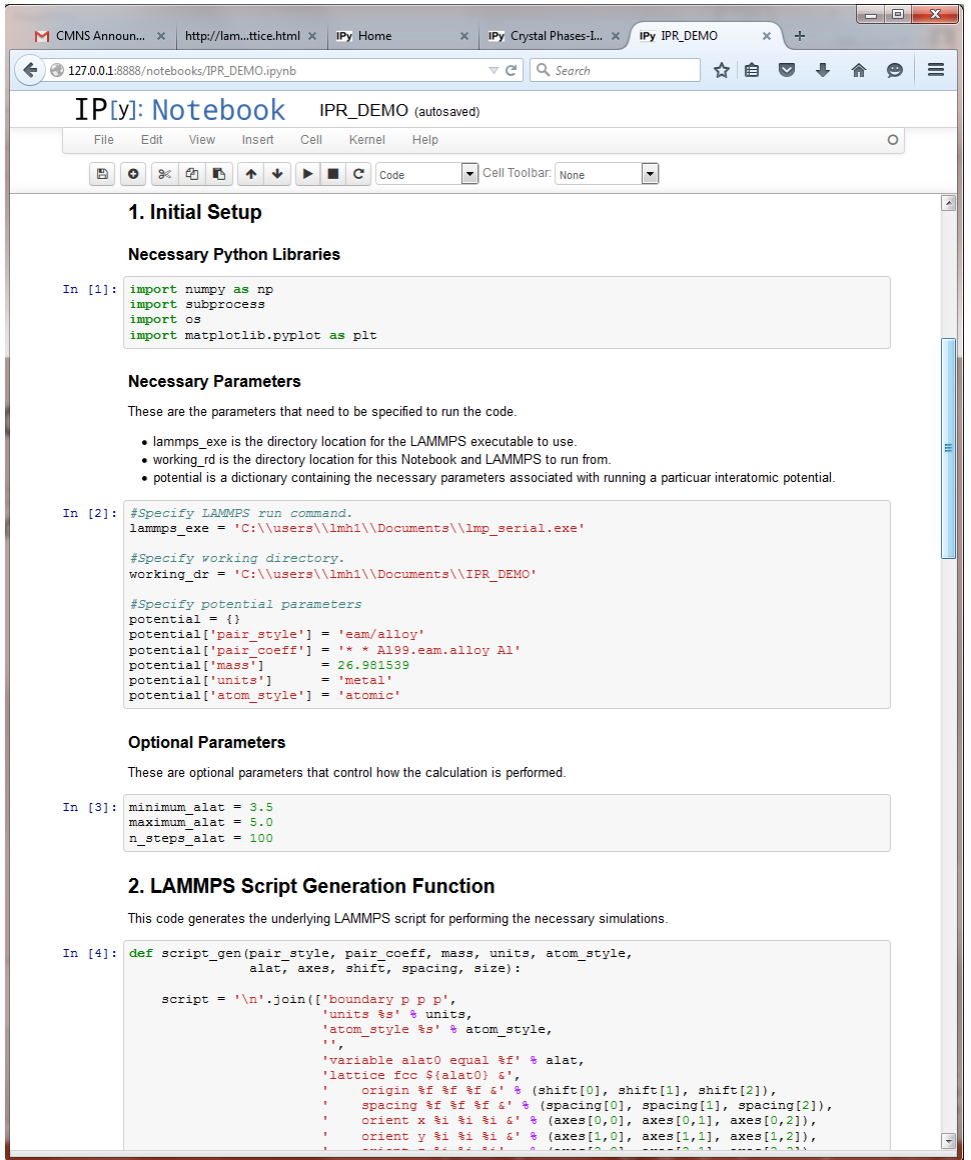

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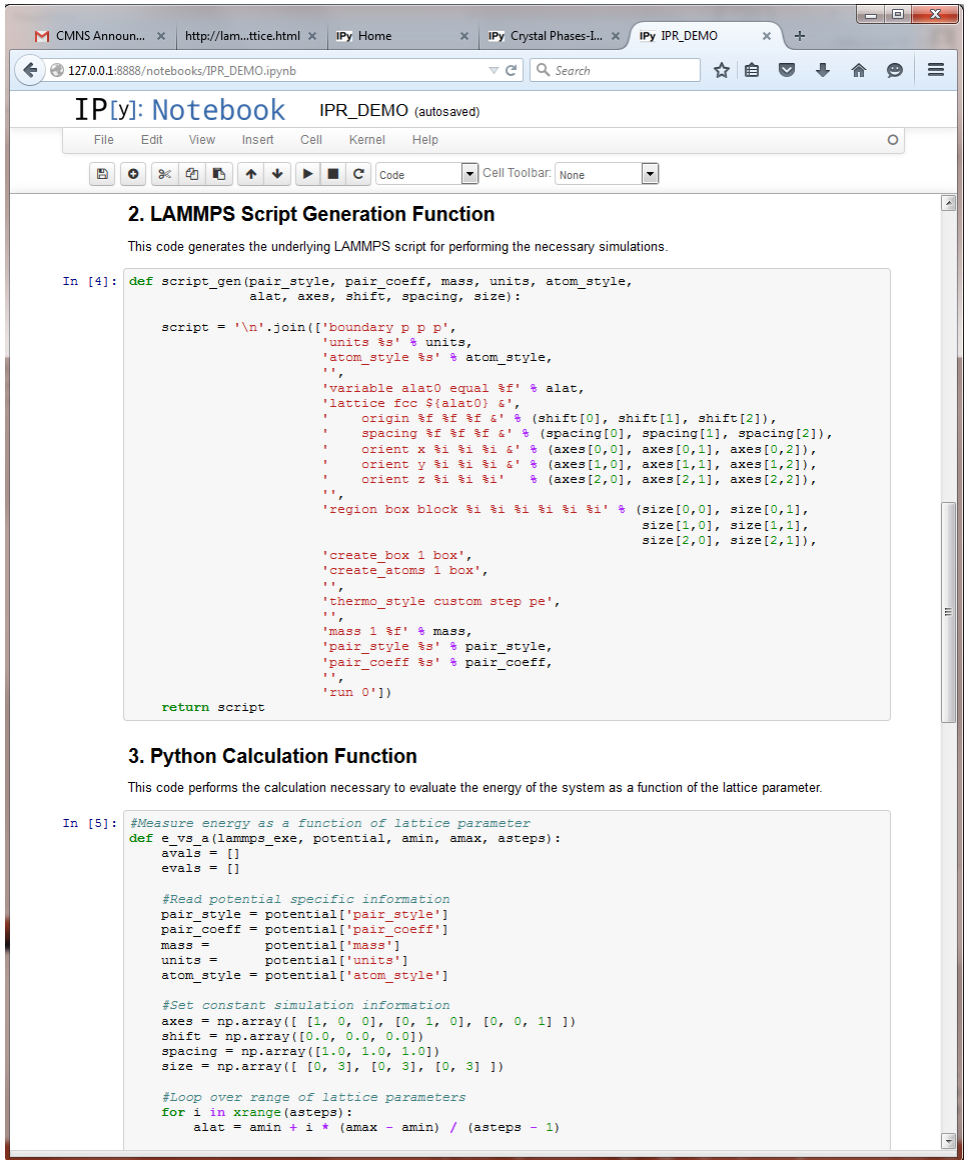

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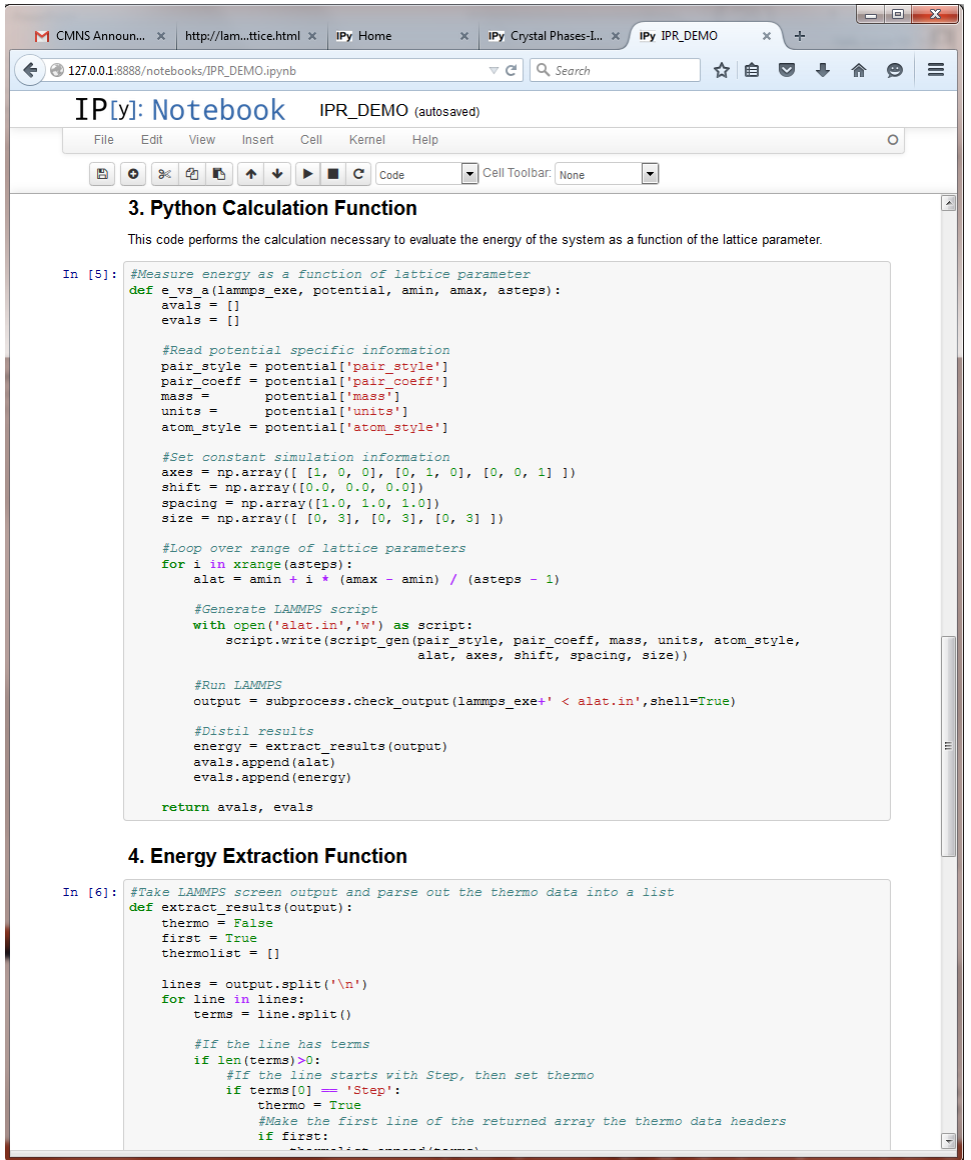

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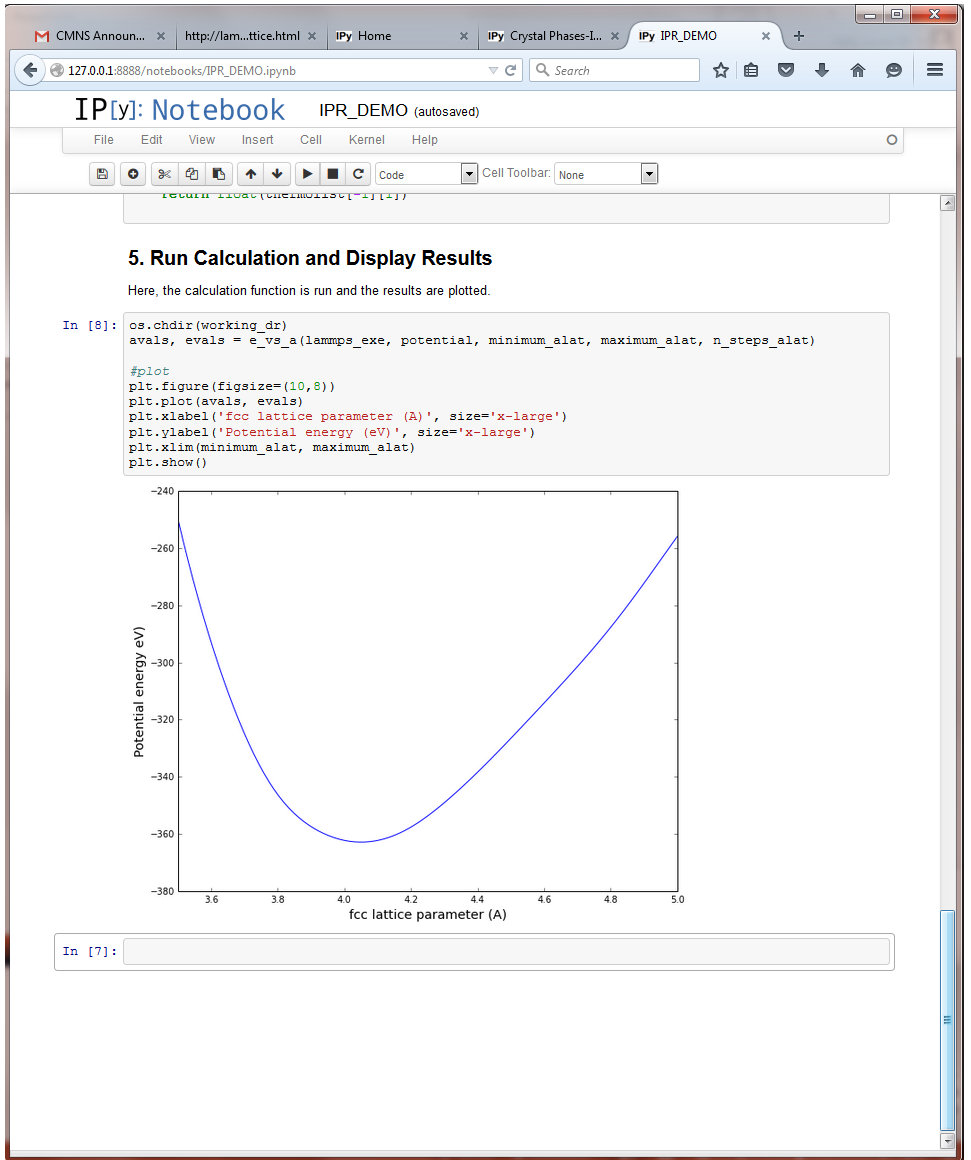


High-Throughput Scripts

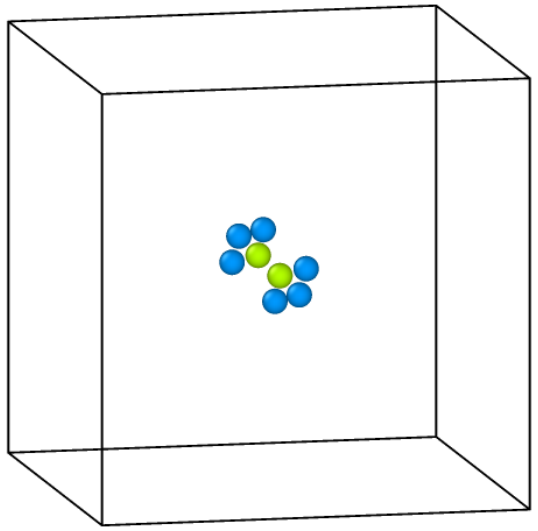
1. Each calculation function should be independent and isolated
   - Serial and parallel looping
   - Cluster distribution

2. Python tools for easy creation and manipulation of atomic systems

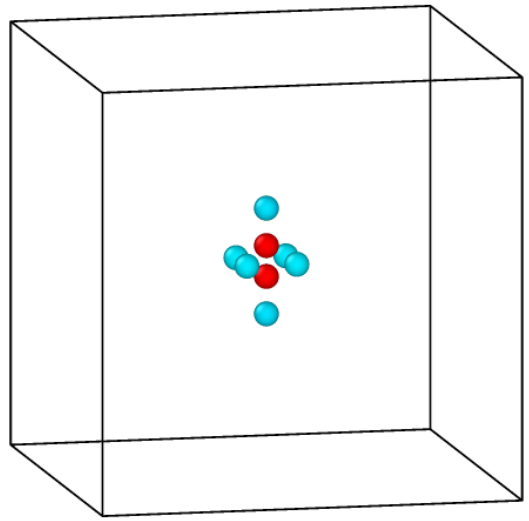
3. Data models for handling, representing, and archiving the input and output data

IPRP Python Package

- Main iprp
  - Classes representing atoms, atom types and systems
  - Functions for manipulating systems (i.e. add defects)
- Submodule iprp.lammps
  - Converters for LAMMPS <-> Python system information
  - Basic LAMMPS script generators
- Submodule iprp.models
  - XML <-> json <-> Python conversions
  - Classes associated with specific input data models



[111] interstitial



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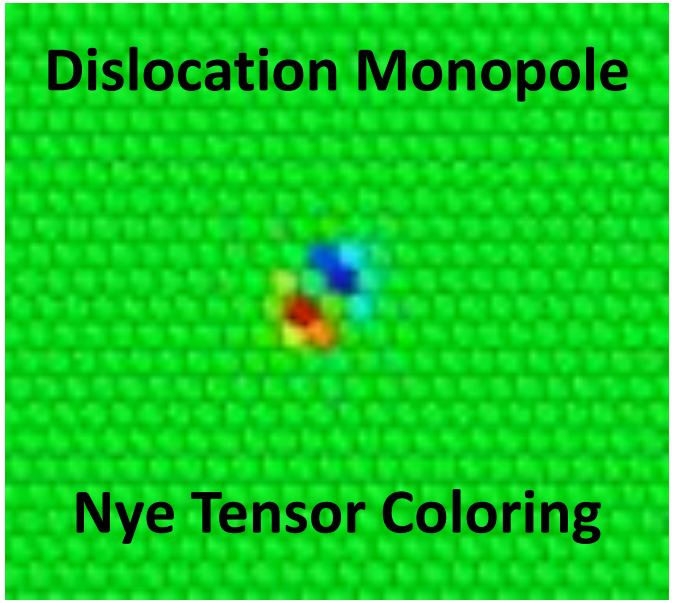


LAMMPS Implementation Data Model

- Read file
- Supply elements list
- Get run parameters
- Seamlessly switch potentials!
- Why pick only one potential?

```
In [1]: import iprp

In [2]: import iprp.lammps

In [3]: pot = iprp.lammps.Potential('C:/lmp-U-Mo-Xe_SmirnovaD_2013.json')

In [4]: print pot.coeff(['U','U','Xe'])
pair_style eam/alloy
pair_coeff * * U_Mo_Xe.2013.eam.alloy U U Xe


In [5]:
```


```
{
    "interatomicPotentialImplementationLAMMPS": {
        "potentialID": {
            "descriptionIdentifier": "U-Mo-Xe_SmirnovaD_2013"
        },
        "units": "metal",
        "atom_style": "atomic",
        "atom": [
            {
                "element": "U",
                "mass": "238.02891"
            },
            {
                "element": "Mo",
                "mass": "95.96"
            },
            {
                "element": "Xe",
                "mass": "131.293"
            }
        ],
        "pair_style": {
            "type": "eam/alloy"
        },
        "pair_coeff": [
            {
                "term": [
                    {
                        "file": "U_Mo_Xe.2013.eam.alloy"
                    },
                    {
                        "symbols": "True"
                    }
                ]
            }
        ]
    }
}
```

LAMMPS Implementation Data Model

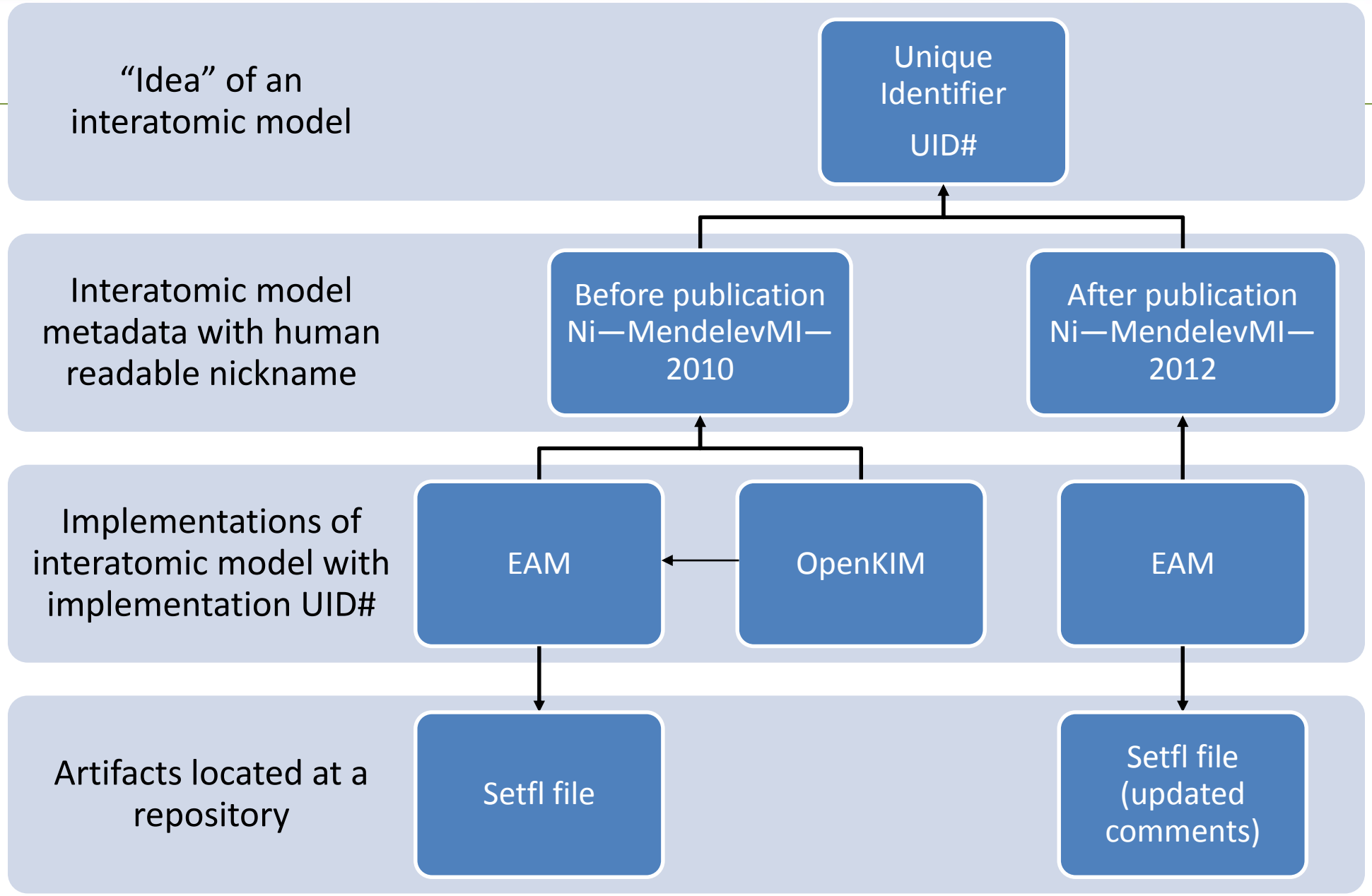
```
{"interatomicPotentialImplementationLAMMPS": {
    "potentialID":
      {"descriptionIdentifier": "Al-Si-Mg-Cu-Fe_JelinekB_2012"},
    "units": "metal",
    "atom_style": "atomic",
    "atom": [
      {"element": "Al", "symbol": "AlS"},
      {"element": "Si", "symbol": "SiS"},
      {"element": "Mg", "symbol": "MgS"},
      {"element": "Cu", "symbol": "CuS"},
      {"element": "Fe", "symbol": "FeS"}
    ],
    "pair_style": {"type": "meam"},
    "pair_coeff": {
      "term": [
        {"file": "Jelinek_2012_meamf"},
        {"symbolsList": True},
        {"file": "Jelinek_2012_meam.alsimgcufe"},
        {"symbols": True}]}}
}
```

LAMMPS Implementation Data Model

```
{"interatomicPotentialImplementationLAMMPS": {
    "potentialID":
      {"descriptionIdentifier": "MO_751354403791_001"},
    "units": "metal",
    "atom_style": "atomic",
    "atom": [
      {"element": "Al"},
      {"element": "Ni"}
    ],
    "pair_style": {
      "type": "kim",
      "term":
        {"option": "KIMvirial MO_751354403791_001"}
    },
    "pair_coeff": {"term": {"symbols": "True"}}
  }
}
```

LAMMPS Implementation Data Model


```
{"interatomicPotentialImplementationLAMMPS": {
    "potentialID": {
    "descriptionIdentifier": "O-Cu-N-C-H-Ti-Zn_LiangT_2013"},
    "units": "metal",
    "atom_style": "charge",
    "atom": [
      {"element": "O"}, {"element": "Cu"},
      {"element": "N"}, {"element": "C"},
      {"element": "H"}, {"element": "Ti"},
      {"element": "Zn"}
    ],
    "pair_style": {"type": "comb"},
    "pair_coeff": {
      "term": [{"file": "ffield.comb"}, {"symbols": "True"}]
    },
    "supplement":{
    "term":{"option": "fix qeq all qeq/comb 1 0.0001"}
    }
  }
}
```


"Idea" of an interatomic model
Unique Identifier
UID#
Interatomic model metadata with human readable nickname
Before publication Ni—MendelevMI—2010
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Implementations of interatomic model with implementation UID#
EAM
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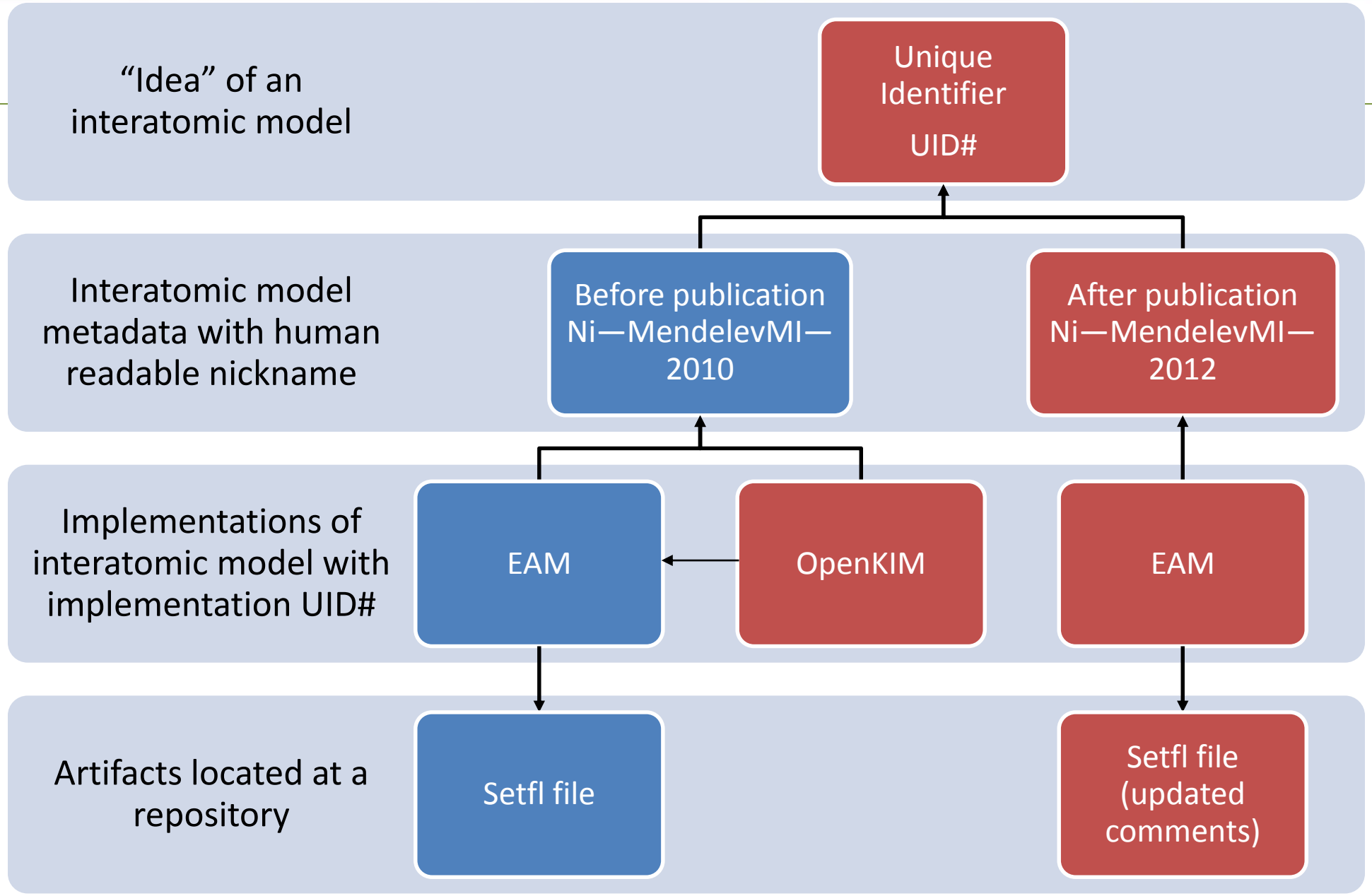
Setfl file
Setfl file (updated comments)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Want To Help?

- Scripts for basic materials properties
- Beta testers for iprp package and Python scripts
- Community involvement for standardized interatomic model metadata and citations
- lucas.hale@nist.gov