The OpenKIM testing framework for interatomic potentials

Ellad B. Tadmor and Ryan S. Elliott
Department of Aerospace Engineering and Mechanics
University of Minnesota

Collaborators: James Sethna, Daniel Karls, Matthew Bierbaum, John Hooper.

NSF CDI and CDS&E programs

LAMMPS Users’ Workshop, Albuquerque, NM, August 1-3, 2017
Open Knowledgebase of Interatomic Models (OpenKIM)

Project Objectives

- Development of an online open resource for standardized testing long-term warehousing of interatomic models (potentials and force fields) and data.

- Development of an application programming interface (API) standard for atomistic simulations, which will allow any interatomic model to work seamlessly with any atomistic simulation code.

- Development of a quantitative theory of transferability of interatomic models to provide guidance for selecting application-appropriate models based on rigorous criteria, and error bounds on results.

**PIs:** Ellad Tadmor (U. Minn), Ryan Elliott (U. Minn), James Sethna (Cornell)

**Funding:** NSF CDI (2009-2014); NSF CDS&E (2014-)
KIM Overview

Repository: A user-extendible database of
- interatomic Models
- standardized Tests (simulation codes)
- Predictions (results from Model-Test couplings)
- Reference Data (obtained from experiments and first principles calculations)

Web portal: A web interface that facilitates:
- user upload and download of Tests, Models, and Reference Data
- searching and querying the repository
- comparing and visualizing Predictions and Reference Data
- recording user feedback

Processing pipeline: An automatic system for generating Predictions by mating Tests and Models in the KIM Repository.
- puts the “knowledge” in “knowledgebase”
- employs virtual machines and cloud-based computing
An interatomic model (IM) can be understood to mean different things.

Consider the following views of the Lennard-Jones (LJ) potential:

I. The functional form of LJ:

\[ \phi(r) = 4\varepsilon \left( \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right) \]

II. The LJ parameter set for a given material:

- **Argon**
  - \( \epsilon = 0.0104 \text{ eV} \)
  - \( \sigma = 3.40 \text{ Å} \)

This is common in EAM potentials where the parameter file is considered to be the potential.

III. A computer implementation of the LJ potential:

```fortran
subroutine ljpotential(r,sig,eps,func,dfunc,d2func)
implicit none

!-- Transferred variables
double precision, intent(in) :: r, sig, eps
double precision, intent(out) :: func, dfunc, d2func

!-- Local variables
double precision rm,rm2,rm6,eos24

rm = sig/r ! sig/r
rm2 = rm*rm ! (sig/r)^2
rm6 = rm2*rm2*rm2 ! (sig/r)^6
eos24 = 24.0*eps/sig

func = 4.0*eps*rm6*(rm6-1.0)
dfunc = eos24*rm*rm6*(-2.0*rm6+1.0)
d2func = (eos24/sig)*rm2*rm6*(26.0*rm6-7.0)

end subroutine ljpotential
```
Why a is a Parameter Set not enough?

- Interatomic models are often stored as a table of discrete data points that are interpolated by the simulation code:

\[
\begin{array}{|c|c|}
\hline
r_1 & \phi(r_1) \\
\hline
r_2 & \phi(r_2) \\
\hline
r_3 & \phi(r_3) \\
\hline
\ldots & \ldots \\
\hline
\end{array}
\]

- The interpolation choice (e.g. spline order) affects some results, e.g. Quasi-harmonic estimate of the elastic constant for a 1D chain of atoms interacting via a nearest-neighbor Morse pair potential:

\[
c = a \left[ \phi''(a) + \frac{k_B T}{2} \frac{\phi^{(4)}(a) \phi''(a) - (\phi''(a))^2}{(\phi''(a))^2} \right]
\]

\[c [\text{nN}] \quad T [\text{K}]\]

![Graph showing stress-free spatial elastic constant as a function of temperature computed using the QH approximation with different splines](image)

Wen et al., MSMSE, 23:074008 (2015)
The KIM framework defines an interatomic model as follows.

- **A KIM Model** is an **autonomous** computational entity:
  - Atomic configuration → KIM Model → Energy and its derivatives

- KIM Models can have two forms:
  1. **Stand-alone Model** for a particular functional form and parameters.
  2. **Parameterized Model** that is read in by a **Model Driver**; for example:

    - **Lennard-Jones Model Driver**:
      \[
      \phi(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right]
      \]
      (Computer implementation including any interpolations or other data processing.)

    - **Material specific LJ Models**:
      - Argon: \( \epsilon_{\text{Ar}} = 10.4 \text{ meV}, \sigma_{\text{Ar}} = 0.340 \text{ nm} \)
      - Krypton: \( \epsilon_{\text{Kr}} = 14.0 \text{ meV}, \sigma_{\text{Kr}} = 0.365 \text{ nm} \)
      - (Each Model is a parameter file read in by its Model Driver.)
In order to maximize the portability of KIM Models, an Application Programming Interface (API) standards has been defined for exchanging information between simulators and models.

- Stand-alone simulation computer program (MD, lattice dynamics, etc.)
- Can be written in any language supported by the API (Fortran 77, Fortran 90, Fortran 2003, C, C++, ...)

Currently working on support for electrostatics and charge equilibration.
Efficiency of the KIM API

- The KIM API is a lightweight efficient interface.

LAMMPS benchmark results (scaled size with 32,000 atoms per core)
KIM-Compliant Codes

Asap
ASE
DL_POLY
GULP
IMD
libAtoms + QUIP
nanoHUB
potfit
QuasiContinuum Method
LAMMPS
MDStressLab
Using KIM Models with LAMMPS is straightforward:

- Install the KIM API from source or using binary packages (packages available for Ubuntu, CentOS, Fedora, OpenSUSE, others in development).

- Precede LAMMPS installation with “make yes-kim”

- Add the KIM Models that you want to use. (Binary packages have option to add all models.)

- Replace native potential with pair style KIM and KIM ID

```plaintext
pair_style     eam/alloy
pair_coeff     * * Al_ercolessiAdams.alloy Al

pair_style     kim LAMMPSvirial EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_001
pair_coeff     * * Al
mass            1 26.98
```

- Run as usual

MDStressLab is a program for computing stress fields from MD simulation results.

**INPUT**
- Particle coordinates, velocities, and species
- Model KIM ID
- Grid information
- Weighting function

**COMPUTE:**
- Calculated Cauchy and first PK versions of Hardy, Tsai and virial stress
- Decompose stress field into unique and non-unique parts

Reference:
N. C. Admal and E. B. Tadmor,
*J. Elast.*, 100:63, 2010

Available at
[http://mdstresslab.org](http://mdstresslab.org)
All KIM Models are subjected to Verification Checks when uploaded to openkim.org.

**Mandatory**
- Species supported as stated;
- Unit conversion handled correctly;
- Domain decomposition handled correctly;
- ...

**Consistency**
- Numerical derivative check of forces, virial, hessian, ...
- Translational and rotational invariance;
- ...

**Informational**
- Smooth energy, forces, etc. at cutoff;
- Inversion symmetry;
- Coding issues: Dependence on optimization, memory leaks, etc.
- ...
The predictive capability of an atomistic simulation is dependent on the fidelity of the interatomic model.

Example: Projectile impacting silicon plate

- Tersoff
- Stillinger-Weber
**KIM Tests**

**Test:** A computer program that when coupled with a suitable Model generates one or more Predictions, each of which is associated with a specific KIM Property.

- **Test Types**
  - **Test** (stand-alone test limited to a single case, or a parameter set to a driver)
  - **Test Driver + Parameter Set** (can work with multiple conditions)

A Test can be a program or an input file to an installed Simulator (e.g. LAMMPS)

- **What constitutes a KIM Property?**
  - An “ideal” physical property without reference to the algorithmic details of how it is computed (e.g. “melting temperature” as opposed to a specific approach for getting it).
  - A “canonical property”, i.e. a basic atomistic property to which Models are often fitted and from which larger-scale behavior might be inferred.

<table>
<thead>
<tr>
<th>Bulk</th>
<th>Wall</th>
</tr>
</thead>
<tbody>
<tr>
<td>- lattice constants</td>
<td>- surface energy</td>
</tr>
<tr>
<td>- cohesive energy</td>
<td>- surface structure</td>
</tr>
<tr>
<td>- elastic constants</td>
<td>- gamma surface</td>
</tr>
<tr>
<td>- phonon spectrum</td>
<td>- grain boundary structure</td>
</tr>
<tr>
<td>- ...</td>
<td>- dislocation core structure</td>
</tr>
<tr>
<td><strong>Line</strong></td>
<td></td>
</tr>
<tr>
<td>- dislocation core energy</td>
<td>- Peierls barrier</td>
</tr>
<tr>
<td></td>
<td>- ...</td>
</tr>
</tbody>
</table>

**Point**
- vacancy formation energy
- vacancy migration barrier
- ...
Interacting with KIM

Uploading new KIM Test to the OpenKIM Repository

Couple Test $T$ with all valid Models and store resulting Predictions in Repository.

- Model 1
- Model 2
- Model 3
- Model 4
- ...

... Model Predictions ...
KIM Visualizers are designed to display/analyze Test results (i.e. Property Instances) and are displayed on Model pages.

KIM Visualizers work by
- querying openkim.org to obtain desired Test results (see https://query.openkim.org/)
- plotting the results using Javascript libraries and templates developed in KIM

Follow the tutorials to adapt a visualizer to your own needs
KIM Models (https://openkim.org)

- KIM Models are archived on the OpenKIM website https://openkim.org:
KIM Models (https://openkim.org)
# KIM Models (https://openkim.org)

<table>
<thead>
<tr>
<th>Extended KIM ID</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>EAM_Dynamo_Ackland_Tichy_Cu_MO_179025960738_001</td>
<td>Finnis Sinclair potential for Cu</td>
</tr>
<tr>
<td>EAM_Dynamo_Bonny_Pasiannot_FeCuNi_MO_469343973171_001</td>
<td>FeCuNi potential to model reactor pressure vessel steels</td>
</tr>
<tr>
<td>EAM_Dynamo_Cai_Ye_ALCu_MO_942551040047_001</td>
<td>EAM potential for Al-Cu binary system</td>
</tr>
<tr>
<td>EAM_Dynamo_Foiles_Baskes_Universal3_Cu_MO_666348409573_000</td>
<td>Third universal Cu potential of Foiles, Baskes, and Daw; obtained from LAMMPS</td>
</tr>
<tr>
<td>EAM_Dynamo_Hoyt_Garvin_PbCu_MO_119135752160_001</td>
<td>Embedded Atom Method parametrization of the Pb-Cu system</td>
</tr>
<tr>
<td>EAM_Dynamo_Mendelev_King_Cu_MO_748636486270_001</td>
<td>FS potential for Cu</td>
</tr>
<tr>
<td>EAM_Dynamo_Mendelev_Kramer_Cu_MO_945691923444_001</td>
<td>FS/EAM potential for Cu</td>
</tr>
<tr>
<td>EAM_Dynamo_Mendelev_Kramer_CuZr_MO_60002160456_001</td>
<td>FS potential for Cu-Zr</td>
</tr>
<tr>
<td>EAM_Dynamo_Mendelev_Soodaei_Cu-Zr_MO_12959890178_001</td>
<td>FS potential for Cu-Zr</td>
</tr>
<tr>
<td><strong>EAM_Dynamo_Mishin_Mehi_Cu_MO_346334655118_001</strong></td>
<td><strong>EAM Cu Potential</strong></td>
</tr>
<tr>
<td>EMT_Aspal_MetalGlass_CuMgZr_MO_655725647552_002</td>
<td>Effective Medium Theory potential for CuMg and CuZr alloys, in particular metallic glasses.</td>
</tr>
<tr>
<td>EMT_Aspal_Standard_Jacobsen_Stoltze_Norskov_ALAgCuNPt_MO_118428466217_002</td>
<td>Standard Effective Medium Theory potential for face-centered cubic metals as implemented in ASE/Asp.</td>
</tr>
<tr>
<td>MEAM_2NN_Fe_to_Ga_MO_145522277939_001</td>
<td>Model parameterization of 2NN MEAM model</td>
</tr>
<tr>
<td>Pair_Morse_Modified_MacDonald_MacDonald_Cu_MO_03482374811_001</td>
<td>Modified Morse pair potential for copper due to MacDonald and MacDonald</td>
</tr>
<tr>
<td>Pair_Morse_Shifted_GirifalcoWeizer_HighCutoff_Cu_MO_1510023996060_001</td>
<td>This is a Cu Morse Model Parameterization by Girifalco and Weizer using a high accuracy cutoff distance.</td>
</tr>
<tr>
<td>Pair_Morse_Shifted_GirifalcoWeizer_LowCutoff_Cu_MO_67377079812_001</td>
<td>This is a Cu Morse Model Parameterization by Girifalco and Weizer using a low accuracy cutoff distance.</td>
</tr>
<tr>
<td>Pair_Morse_Shifted_GirifalcoWeizer_MedCutoff_Cu_MO_173878283511_001</td>
<td>This is a Cu Morse Model Parameterization by Girifalco and Weizer using a medium accuracy cutoff distance.</td>
</tr>
</tbody>
</table>
### KIM Models (https://openkim.org)

<table>
<thead>
<tr>
<th>Title</th>
<th>EAM Cu Potential</th>
</tr>
</thead>
<tbody>
<tr>
<td>Short KIM ID</td>
<td>MO_346334655118_002</td>
</tr>
<tr>
<td>Extended KIM ID</td>
<td>EAM_Dynamo_Mishin_Mehl_Cu__MO_346334655118_002</td>
</tr>
<tr>
<td>KIM Item Type</td>
<td>Parameterized Model using Model Driver EAM_Dynamo__MD_120291908751_002</td>
</tr>
<tr>
<td>Contributor</td>
<td>ymishin</td>
</tr>
<tr>
<td>Maintainer</td>
<td>ymishin</td>
</tr>
<tr>
<td>Author</td>
<td>Yuri Mishin</td>
</tr>
<tr>
<td>Publication Year</td>
<td>2016</td>
</tr>
<tr>
<td>Species</td>
<td>Cu</td>
</tr>
<tr>
<td>Description</td>
<td>EAM Cu potential fit to experimental and first-principles data</td>
</tr>
<tr>
<td>Disclaimer</td>
<td></td>
</tr>
<tr>
<td>Programming Language(s)</td>
<td>N/A</td>
</tr>
<tr>
<td>Link to NIST</td>
<td><a href="http://www.ctcms.nist.gov/potentials/Cu.html">http://www.ctcms.nist.gov/potentials/Cu.html</a></td>
</tr>
<tr>
<td>Item Citation</td>
<td>Click here to download a citation in BibTeX format.</td>
</tr>
<tr>
<td>Previous Version</td>
<td>EAM_Dynamo_Mishin_Mehl_Cu__MO_346334655118_001</td>
</tr>
</tbody>
</table>

- **Unique archival KIM ID for citation in papers**
- **Scientific reference for the potential.**
Further down the model page for
EAM_Dynamo_Mishin_Mehl_Cu__MO_346334655118_002

Tests

<table>
<thead>
<tr>
<th>Test</th>
<th>Test Results</th>
<th>Link to Test Results page</th>
<th>Benchmark time</th>
</tr>
</thead>
<tbody>
<tr>
<td>ElasticConstantsCubic_fcc_Cu__TE_188557531340_002</td>
<td>✔️ expand</td>
<td>Q view</td>
<td>1674</td>
</tr>
<tr>
<td>ElasticConstantsCubic_sc_Cu__TE_319353354686_002</td>
<td>✔️ expand</td>
<td>Q view</td>
<td>1635</td>
</tr>
</tbody>
</table>

Usertime multiplied by the Whetstone Benchmark. This number can be used (approximately) to compare the performance of different models independently of the architecture on which the test was run.
Elastic constants (note that c44 is negative indicating the sc structure is unstable).
Visualizers (in-page)

Cohesive Energy Graph
This graph shows the cohesive energy versus volume-per-atom for the current mode for four mono-atomic cubic phases (body-centered cubic (bcc), face-centered cubic (fcc), simple cubic (sc), and diamond). The curve with the lowest minimum is the ground state of the crystal if stable. (The crystal structure is enforced in these calculations, so the phase may not be stable.) Graphs are generated for each species supported by the model.

FCC Lattice Constant
This bar chart plot shows the mono-atomic face-centered cubic (fcc) lattice constant predicted by the current model (shown in red) compared with the predictions for all other models in the OpenKIM Repository that support the species. The vertical bars show the average and standard deviation (one sigma) bounds for all model predictions. Graphs are generated for each species supported by the model.
KIM Models (https://openkim.org)

Model: EAM_Dynamo_Mishin_Mehl_Cu_MO_346334655118_001
Species: Cu

This graph shows the cohesive energy versus volume-per-atom for the current model for four mono-atomic cubic phases (body-centered cubic (bcc), face-centered cubic (fcc), simple cubic (sc), and diamond). The curve with the lowest minimum is the ground state of the crystal if stable. (The crystal structure is enforced in these calculations, so the phase may not be stable.) The curves below are for the species specified above.
Current Status (August 1, 2017)

- Web portal
- Repository
- Processing pipeline

- 189 Models
- 2612 Tests
- 53 property definitions
- 9 visualizers

- Interface to explore content
- Content upload by members
- Forums and Wikis for member input
- Online bootcamp w/lectures

- Automatic VM-based computations
- Downloadable KIM VM
- Handling of dependencies

**Software supporting KIM API:**

ASAP, ASE, DL_POLY, GULP, IMD, LAMMPS, libAtoms/QUIP, nanoHUB, Potfit, Quasicontinuum, VirtualFab, MDStressLab
Summary

KIM provides **archival** permanent storage of interatomic models, tests, and reference data with known provenance.

All KIM content is **citable** with unique permanent identifiers. This makes it possible to reproduce simulation results in the future.

Models stored in the OpenKIM Repository are **portable** as they conform to an API that allows them to run seamlessly with any KIM-compliant simulation code.

Models are **tested** against a user-extendible set of calculations for well-defined material properties using an automated processing pipeline.

**Transferability** is quantified by estimating the energy error of a new configuration by using Gaussian process regression to interpolate between errors of known configurations.
Welcome to the Knowledgebase of Interatomic Models!

OpenKIM is an online suite of open source tools for molecular simulation of materials. These tools help to make molecular simulations more accessible and more reliable. Within OpenKIM, you will find an online resource for standardized data, and an application programming interface (API) standard for coupling atomic simulation codes with first principles and experimental reference data.

- Start here if you are new to KIM
- Become a member to get updates and vote on KIM policy
- Get interatomic potentials
- Get model predictions
- Get property simulators
- Get involved

https://openkim.org