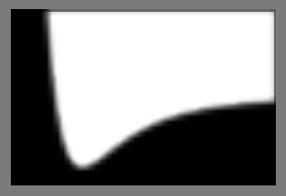


The OpenKIM testing framework for interatomic potentials

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

OpenKIM

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.

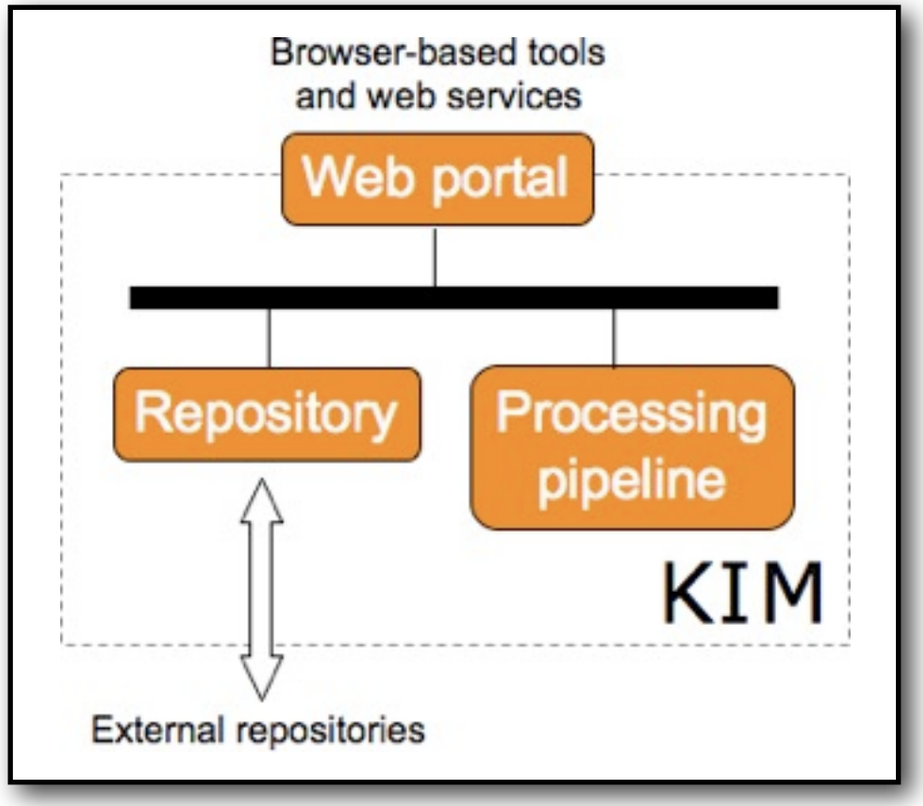
- Development of a quantitative *theory of transferability* of interatomic models to provide *guidance for selecting* application-appropriate models based on rigorous criteria, and *error bounds* on results.

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

KIM Philosophy on an Interatomic Model

- 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:

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

II. The LJ parameter set for a given material:

Argon

$\epsilon = 0.0104$ eV

$\sigma = 3.40$ Å

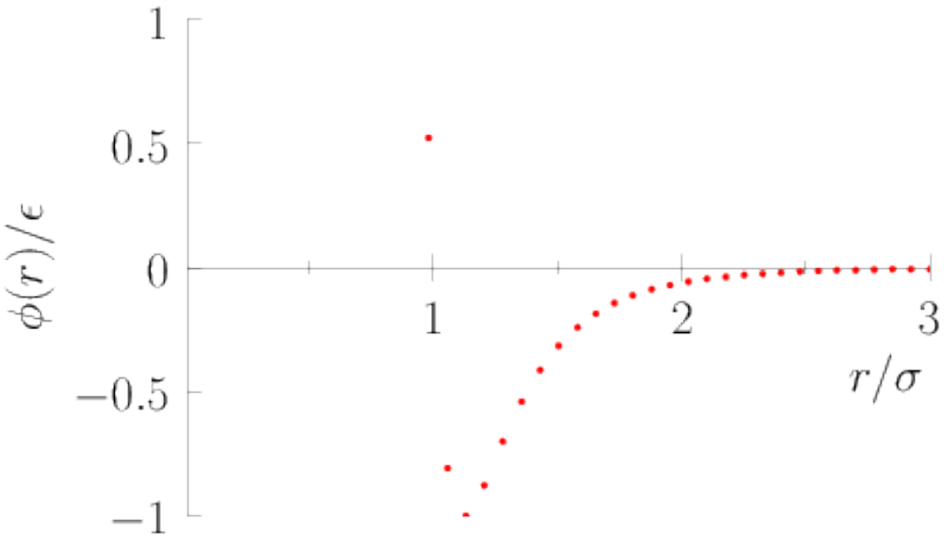
This is common in EAM potentials where the parameter file is considered to be *the* potential.

III. A computer implementation of the LJ potential:

```
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:

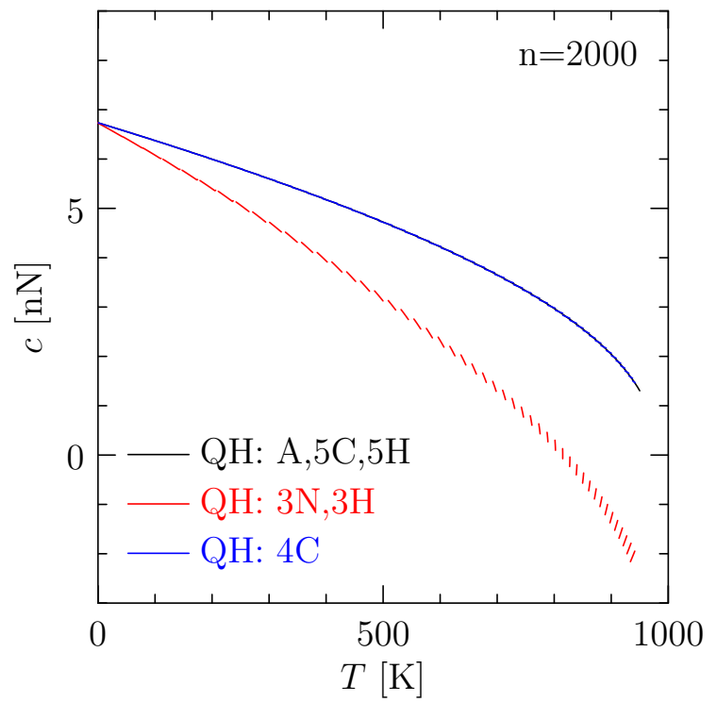


r_1	$\phi(r_1)$
r_2	$\phi(r_2)$
r_3	$\phi(r_3)$
...	...

- 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:

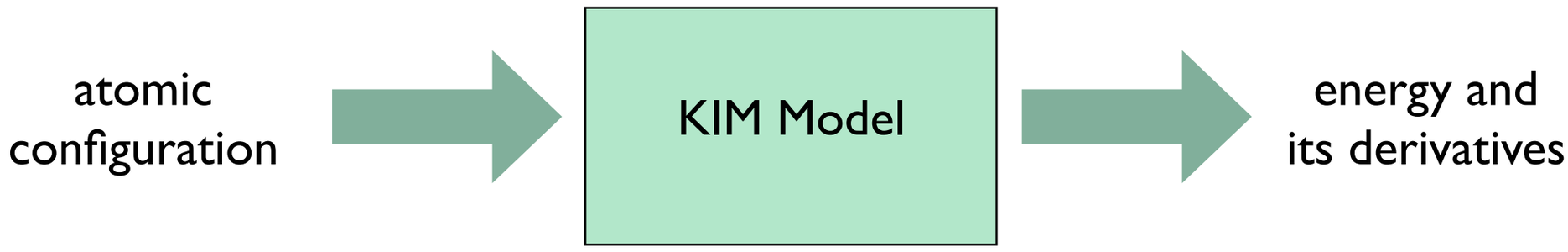
$$c = a\left[\phi''(a) + \frac{k_B T}{2}\frac{\phi^{(4)}(a)\phi''(a) - (\phi''(a))^2}{(\phi''(a))^2}\right]$$



Wen et al., *MSMSE*, 23:074008 (2015)

KIM Models

- The KIM framework defines an interatomic model as follows.
  - A KIM Model is an <u>autonomous</u> computational entity:



  - 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:

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

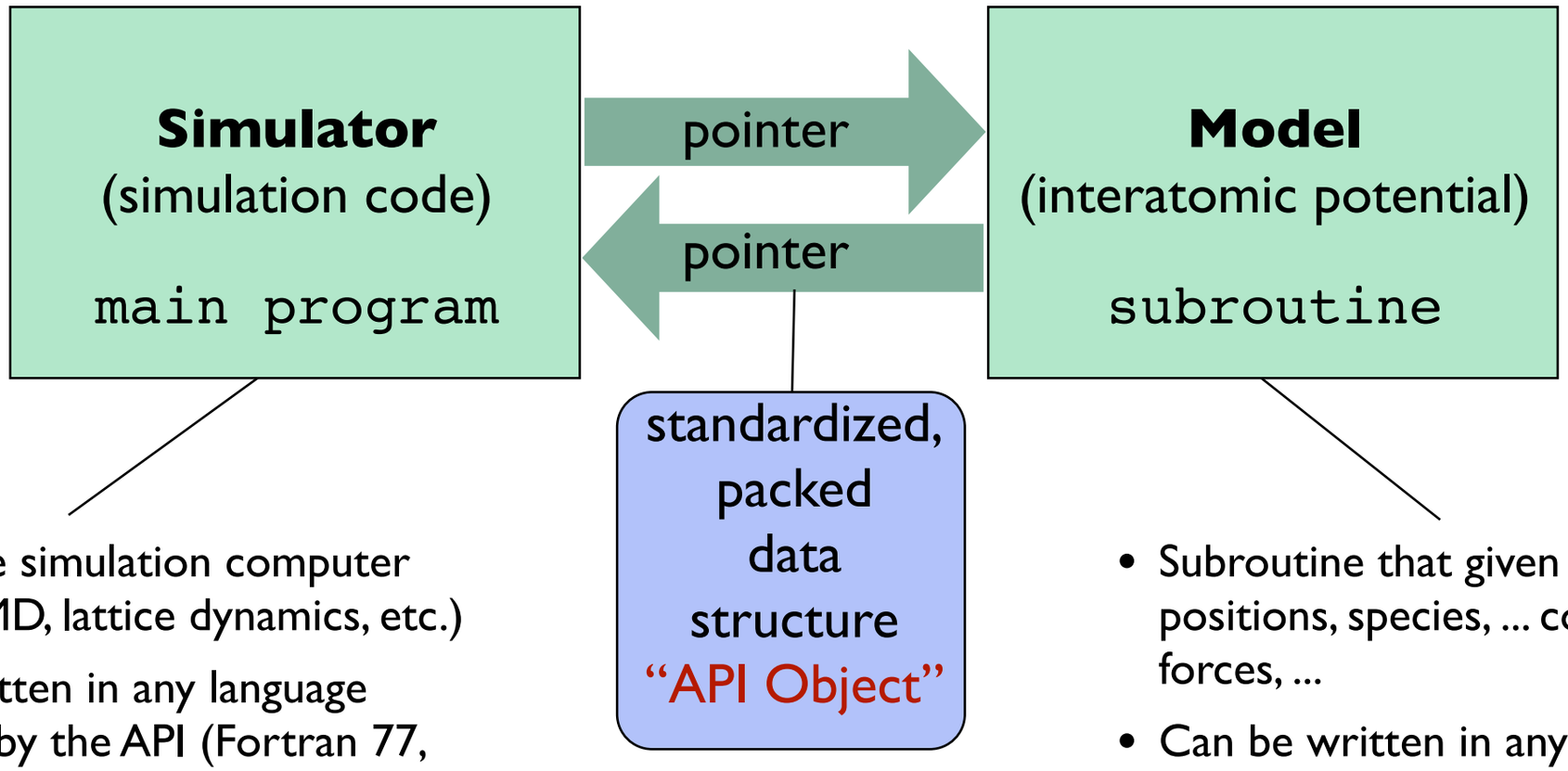
(Computer implementation including any interpolations or other data processing.)

Material specific LJ Models:

Argon; ϵ_{Ar}=10.4 meV, σ_{Ar}=0.340 nm
Krypton; ϵ_{Kr}=14.0 meV, σ_{Kr}=0.365 nm
...
(Each Model is a parameter file read in by its Model Driver.)

Portability and the KIM API Standard

- 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++, ...)

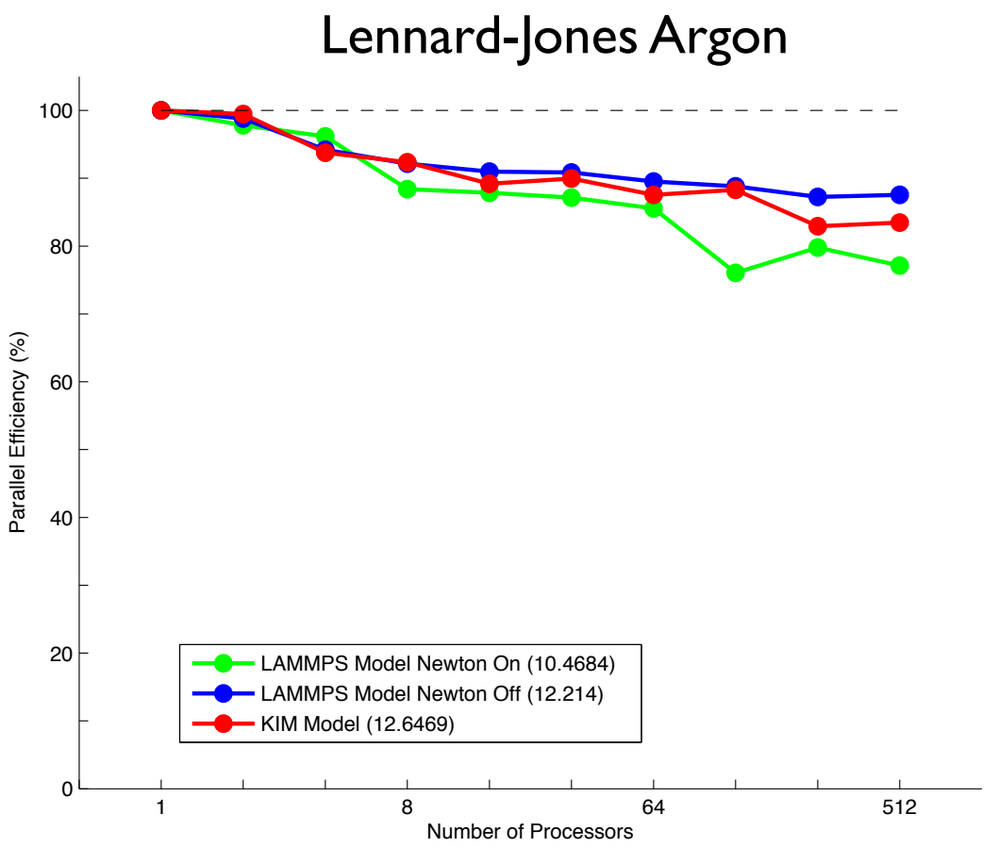
- Subroutine that given a set of atomic positions, species, ... computes energy, forces, ...
- Can be written in any language (Fortran 77, Fortran 90, Fortran 2003, C, C++, ...)

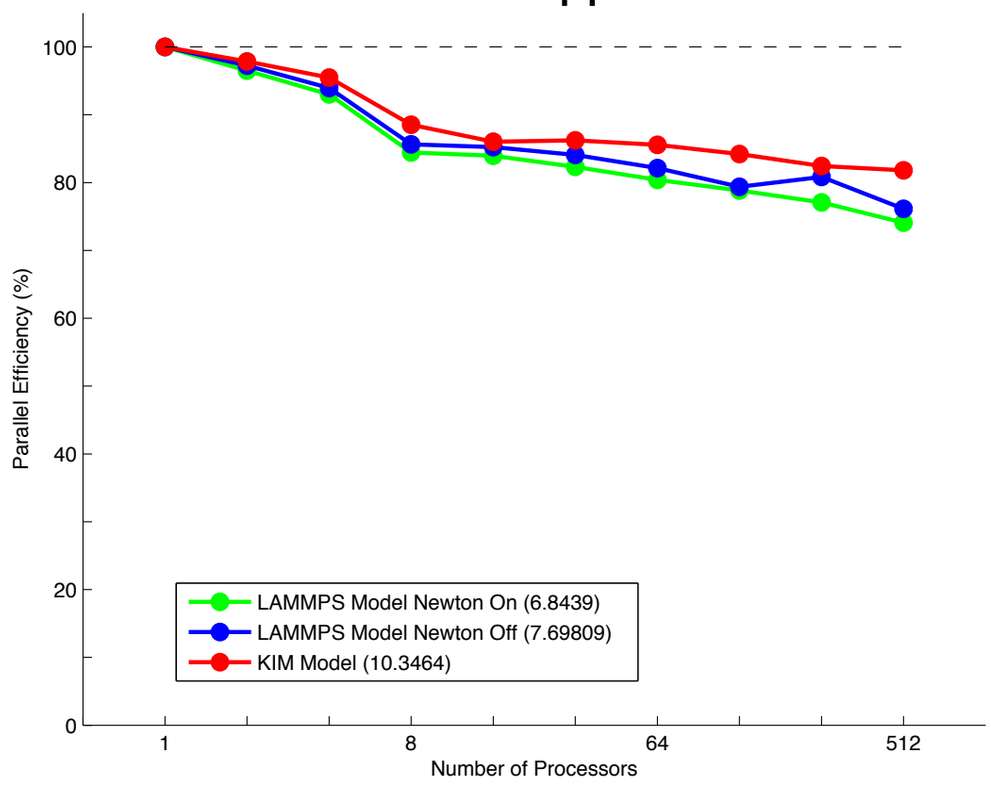
- Currently working on support for electrostatics and charge equilibration.

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

libAtoms + QUIP

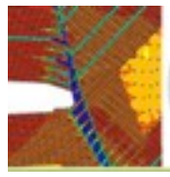
nanoHUB

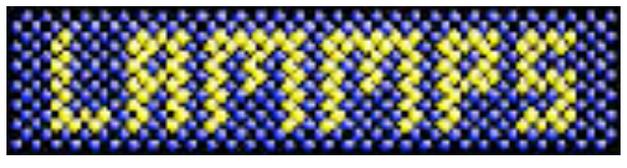
DL_POLY

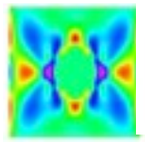
potfit

GULP

IMD







MDStressLab

Example: Using KIM Models with LAMMPS

- 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

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

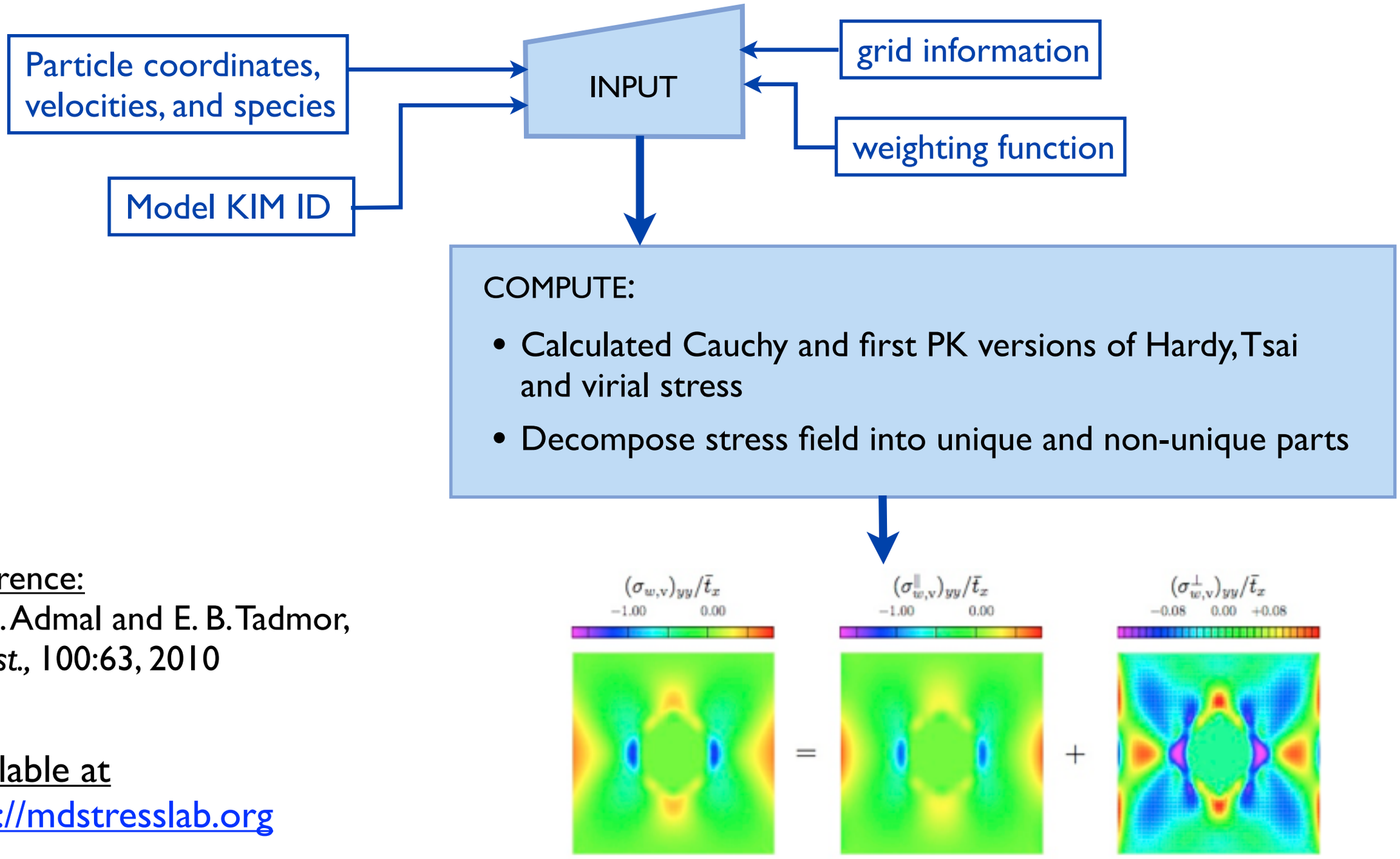
```
pair_style      kim LAMMPSvirial EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_001
pair_coeff      * * Al
mass            1 26.98
```

- Run as usual

For more info, see http://lammps.sandia.gov/doc/pair_kim.html

MDStressLab (http://mdstresslab.org)

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



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

Available at
http://mdstresslab.org

Model Verification Checks

- 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;
- ...

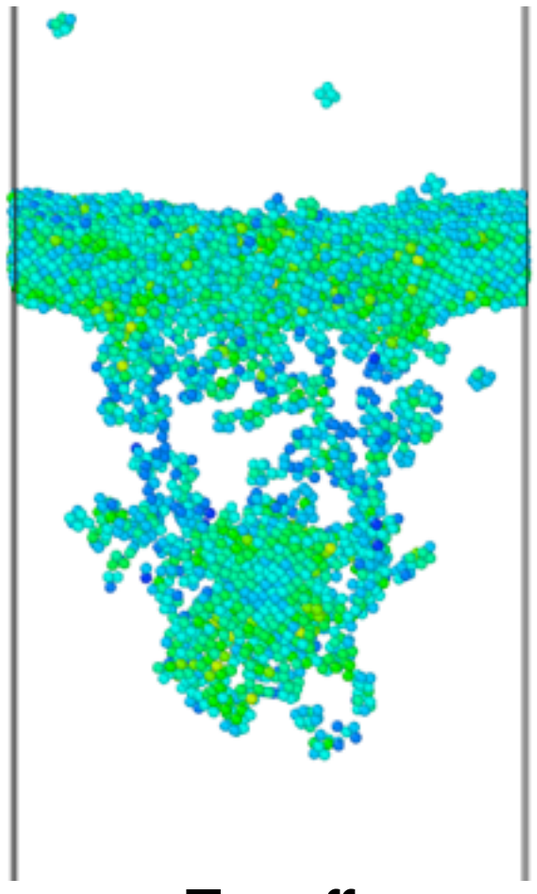
Informational

- Smooth energy, forces, etc. at cutoff;
- Inversion symmetry;
- Coding issues: Dependence on optimiztion, memory leaks, etc.
- ...

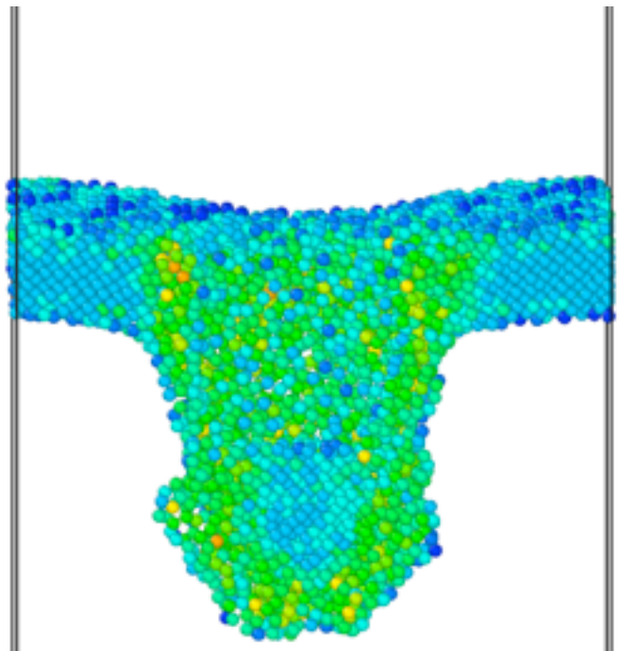
A Simulation is only as good as the Potential

- 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.

Bulk
- lattice constants
- cohesive energy
- elastic constants
- phonon spectrum
- ..

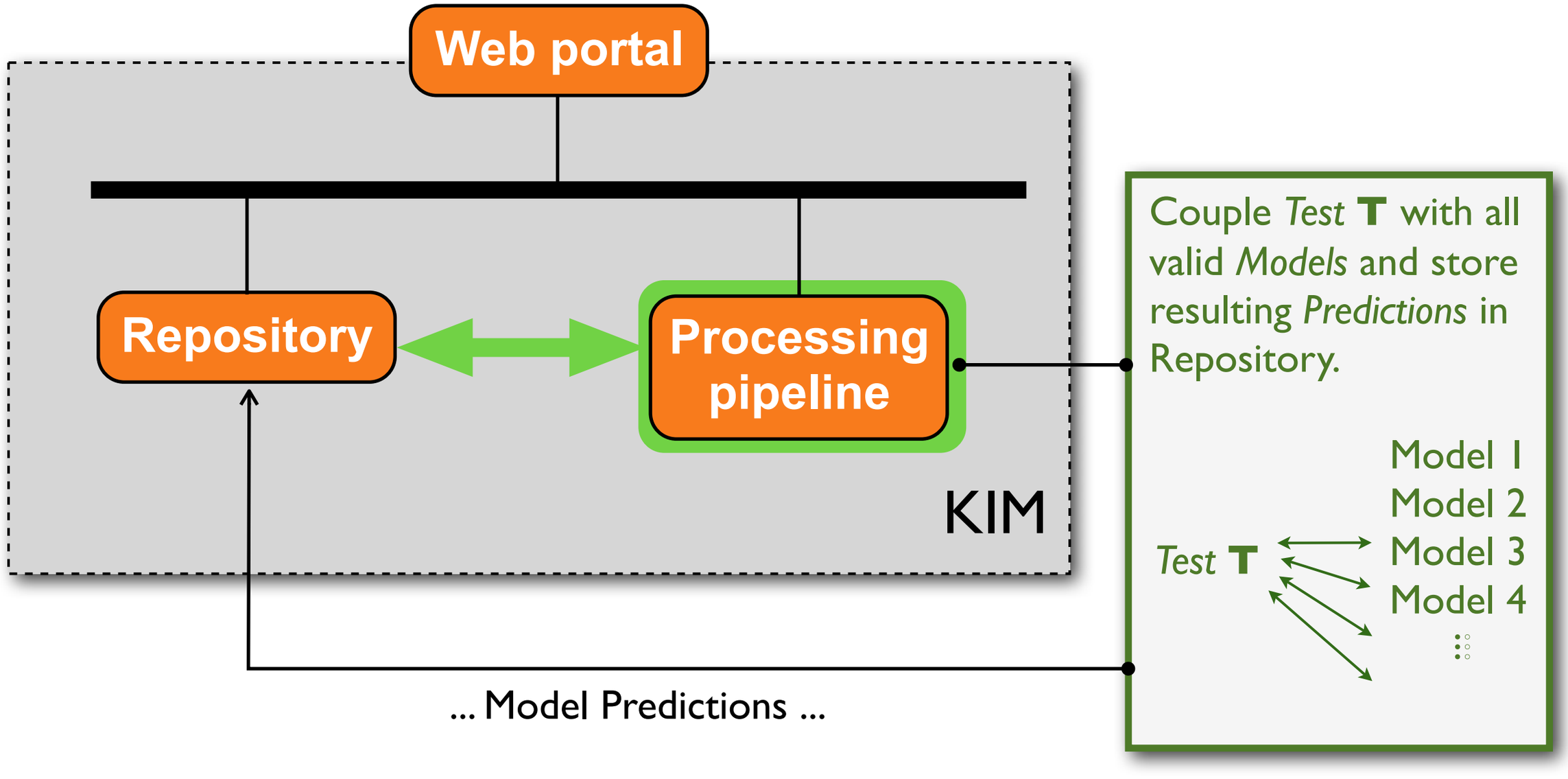
Wall
- surface energy
- surface structure
- gamma surface
- grain boundary structure
- ...

Line
- dislocation core structure
- dislocation core energy
- Peierls barrier
- ...

Point
- vacancy formation energy
- vacancy migration barrier
- ...

Interacting with KIM

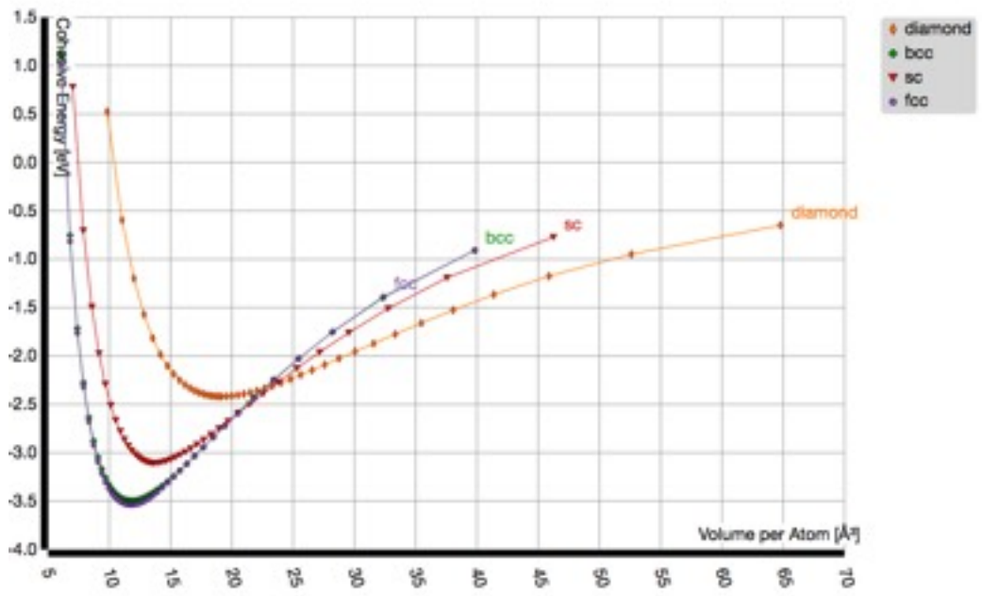
Uploading new KIM Test to the OpenKIM Repository



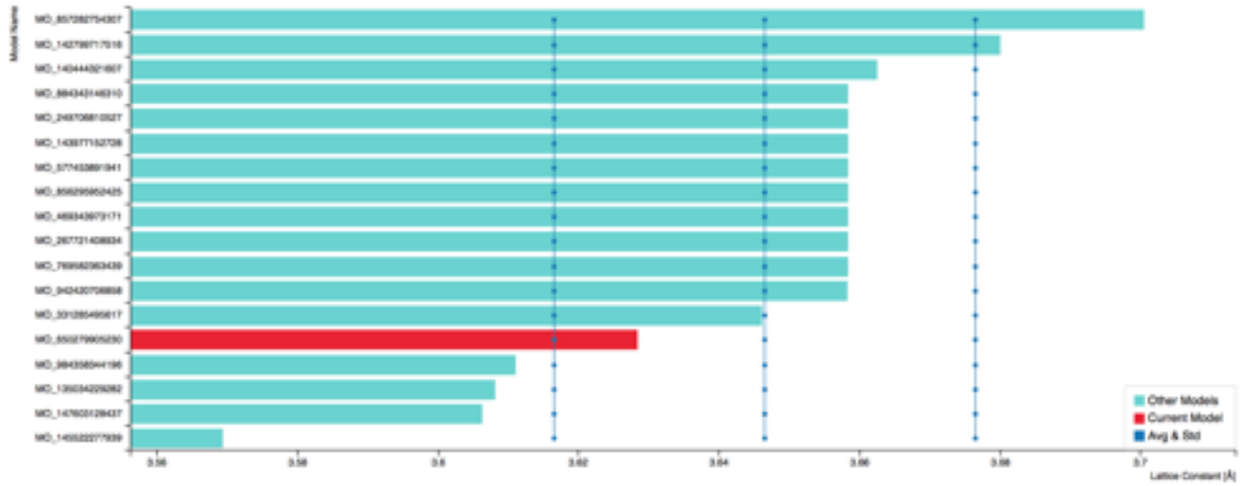
KIM Visualization

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

Cohesive energy curve



FCC Lattice Constant



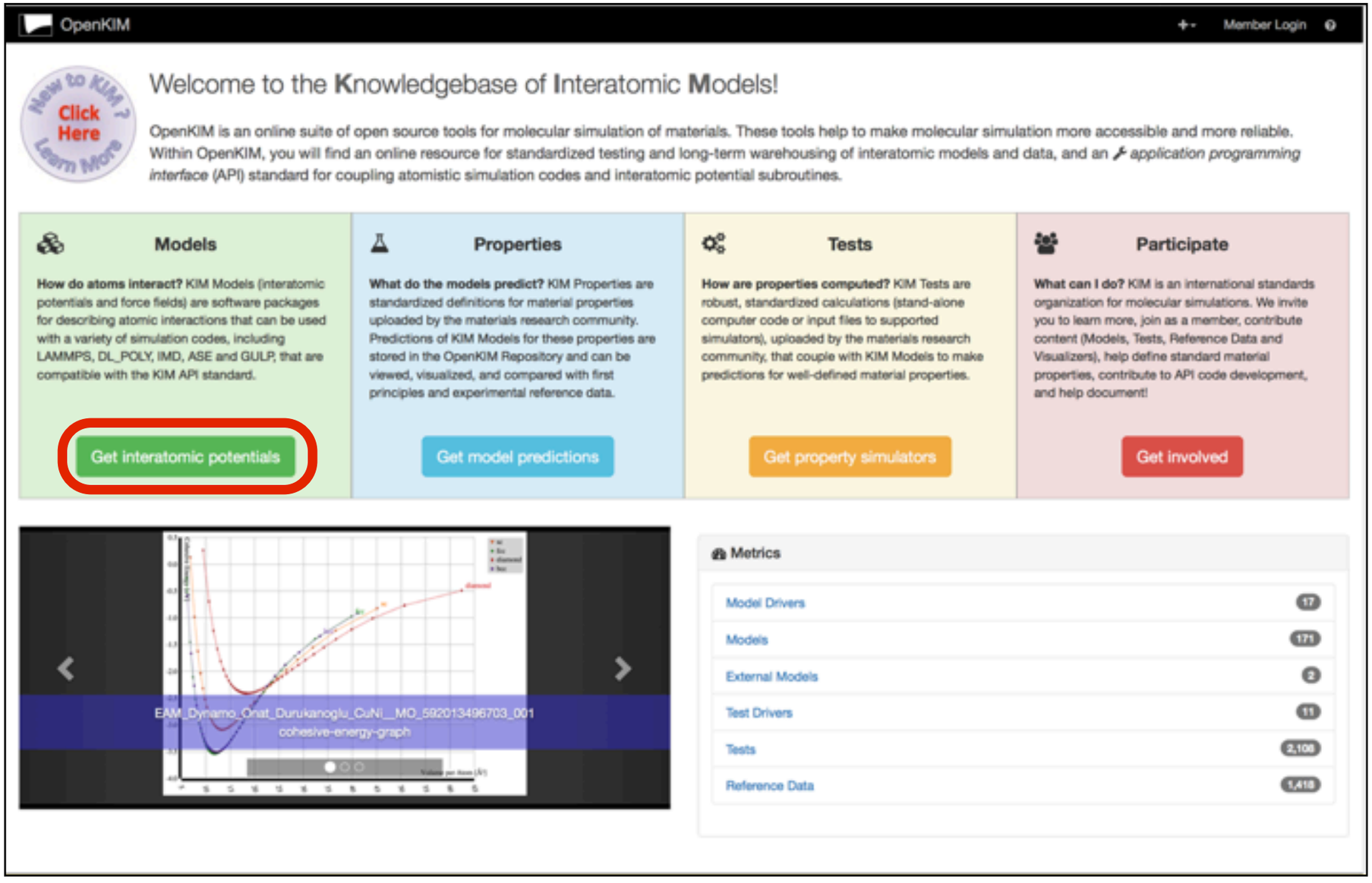
KIM Visualizers work by

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

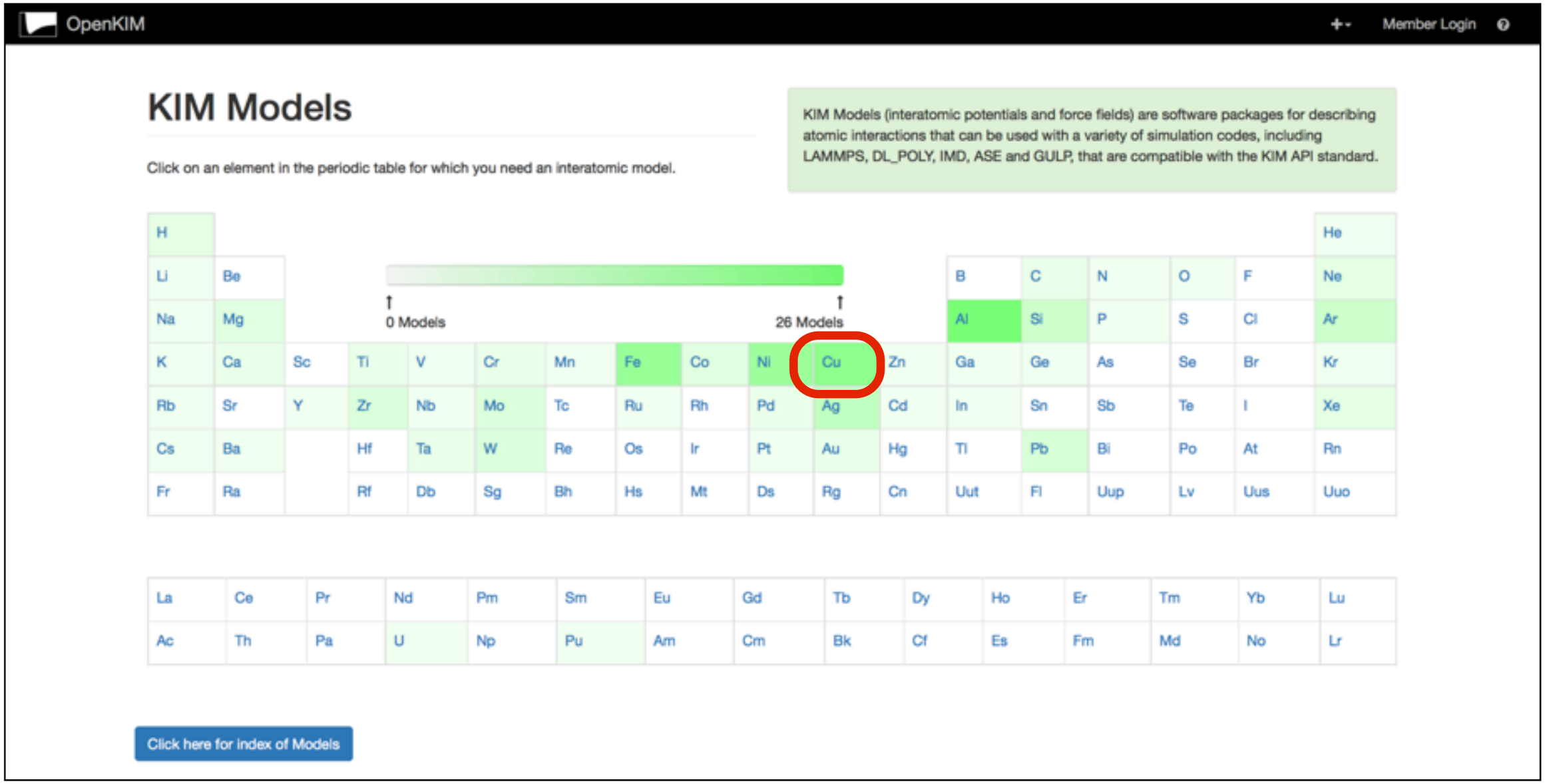
Follow the tutorials to adapt a visualizer to your own needs

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)

Cu

Extended KIM ID	Title
EAM_Dynamo_Ackland_Tichy_Cu__MO_179025990738_001	Finnis Sinclair potential for Cu
EAM_Dynamo_Bonny_Pasianot_FeCuNi__MO_469343973171_001	FeCuNi potential to model reactor pressure vessel steels
EAM_Dynamo_Cai_Ye_AlCu__MO_942551040047_001	EAM potential for Al-Cu binary system
EAM_Dynamo_Foiles_Baskes_Universal3_Cu__MO_666348409573_000	Third universal Cu potential of Foiles, Baskes, and Daw; obtained from LAMMPS
EAM_Dynamo_Hoyt_Garvin_PbCu__MO_119135752160_001	Embedded Atom Method parametrization of the Pb-Cu system
EAM_Dynamo_Mendelev_King_Cu__MO_748636486270_001	FS potential for Cu
EAM_Dynamo_Mendelev_Kramer_Cu__MO_945691923444_001	FS/EAM potential for Cu
EAM_Dynamo_Mendelev_Kramer_CuZr__MO_600021860456_001	FS potential for Cu-Zr
EAM_Dynamo_Mendelev_Sordelet_CuZr__MO_120596890176_001	FS potential for Cu-Zr
EAM_Dynamo_Mishin_Mehl_Cu__MO_346334655118_001	EAM Cu Potential
EAM_Dynamo_Onat_Durukanoglu_CuNi__MO_592013496703_001	An optimized EAM potential for Cu–Ni alloys
EAM_Dynamo_Williams_Mishin_CuAg__MO_128703483589_001	EAM alloy potential for the Cu-Ag system.
EAM_Dynamo_Wu_Trinkle_CuAg__MO_270337113239_001	EAM potential for Cu/Ag(111) Surface Diffusion.
EAM_Dynamo_Zhou_Johnson_Cu__MO_127245782811_001	EAM alloy potential set table, compatible with LAMMPS
EAM_Johnson_NearestNeighbor_Cu__MO_887933271505_001	This is an analytical NN EAM model for Cu by Johnson.
EMT_Asap_MetalGlass_CuMgZr__MO_655725647552_002	Effective Medium Theory potential for CuMg and CuZr alloys, in particular metallic glasses.
EMT_Asap_Standard_Jacobsen_Stoltze_Norskov_AlAgAuCuNiPdPt__MO_118428466217_002	Standard Effective Medium Theory potential for face-centered cubic metals as implemented in ASE/Asap.
MEAM_2NN_Fe_to_Ga__MO_145522277939_001	Model parameterization of 2NN MEAM model
Pair_Morse_Modified_MacDonaldMacDonald_Cu__MO_034823476734_000	Modified Morse pair potential for copper due to MacDonald and MacDonald
Pair_Morse_Shifted_GirifalcoWeizer_HighCutoff_Cu__MO_151002396060_001	This is a Cu Morse Model Parameterization by Girifalco and Weizer using a high accuracy cutoff distance.
Pair_Morse_Shifted_GirifalcoWeizer_LowCutoff_Cu__MO_673777079812_001	This is a Cu Morse Model Parameterization by Girifalco and Weizer using a low accuracy cutoff distance.
Pair_Morse_Shifted_GirifalcoWeizer_MedCutoff_Cu__MO_173787283511_001	This is a Cu Morse Model Parameterization by Girifalco and Weizer using a medium accuracy cutoff distance.

KIM Models (https://openkim.org)

EAM_Dynamo_Mishin_Mehl_Cu__MO_346334655118_002

Title	EAM Cu Potential
Short KIM ID	MO_346334655118_002
Extended KIM ID	EAM_Dynamo_Mishin_Mehl_Cu__MO_346334655118_002
KIM Item Type	Parameterized Model using Model Driver EAM_Dynamo__MD_120291908751_002
Contributor	ymishin
Maintainer	ymishin
Author	Yuri Mishin
Publication Year	2016
Species	Cu
Description	EAM Cu potential fit to experimental and first-principles data
Disclaimer	
Source Citations	Y. Mishin, M.J. Mehl, D.A. Papaconstantopoulos, A.F. Voter, and J.D. Kress, "Structural stability and lattice defects in copper: Ab initio, tight-binding, and embedded-atom calculations," Phys. Rev. B, 63, 224106 (2001).
Programming Language(s)	N/A
Link to NIST	http://www.ctcms.nist.gov/potentials/Cu.html
	EAM Dynamo Mishin Mehl Cu MO_346334655118_002
Item Citation	Click here to download a citation in BibTeX format.
Previous Version	EAM_Dynamo_Mishin_Mehl_Cu__MO_346334655118_001

Click to contribute a fork of this item

Unique archival KIM ID for citation in papers

Scientific reference for the potential.

KIM Models (https://openkim.org)

Further down the model page for
EAM_Dynamo_Mishin_Mehl_Cu__MO_346334655118_002

Tests

ElasticConstantsCubic__TD_011862047401_002

Test	Test Results	Link to Test Results page	Bechmark time
ElasticConstantsCubic_fcc_Cu__TE_188557531340_002	expand	view	1674
ElasticConstantsCubic_sc_Cu__TE_319353354686_002	expand	view	1635

Full results page.

Expand a property synopsis.

Usertime mulip … hark. This number can be used (approximately) to compare the performance of different models independently of the architecture on which the test was run.

KIM Models (https://openkim.org)

Further down the model page for
EAM_Dynamo_Mishin_Mehl_Cu__MO_346334655118_002

Tests

ElasticConstantsCubic__TD_011862047401_002

ElasticConstantsCubic_fcc_Cu__TE_188557531340_002	expand	view	1674
ElasticConstantsCubic_sc_Cu__TE_319353354686_002	collapse	view	1635

instance-id: 1
Isothermal elastic constants for a cubic crystal at constant temperature and stress
(For more information, see the property definition elastic-constants-isothermal-cubic-crystal-npt)

Crystal type = ["sc"]

a = 2.3928461 angstrom
Species = ["Cu"]
Basis atom coordinates = [[0.0 0.0 0.0]]

Temperature = 0 K
Cauchy stress = [0 0 0 0 0 0] GPa

c11 = 321.391497278 GPa
c12 = 24.9933292762 GPa
c44 = -19.950592869 GPa

Elastic constants (note that c44 is negative indicating the sc structure is unstable).

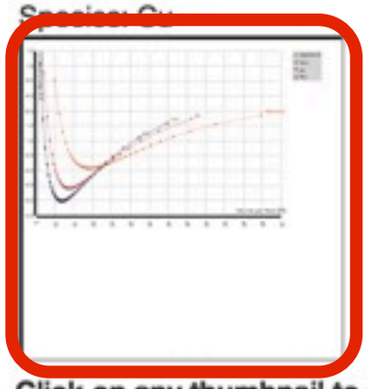
KIM Models (https://openkim.org)

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.

Species: Cu

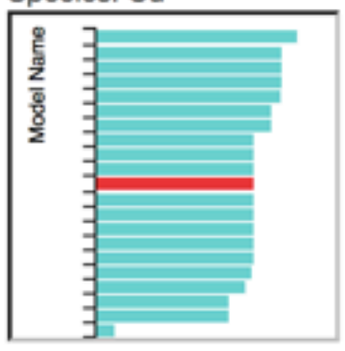


Click on any thumbnail to get a full size image.

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.

Species: Cu



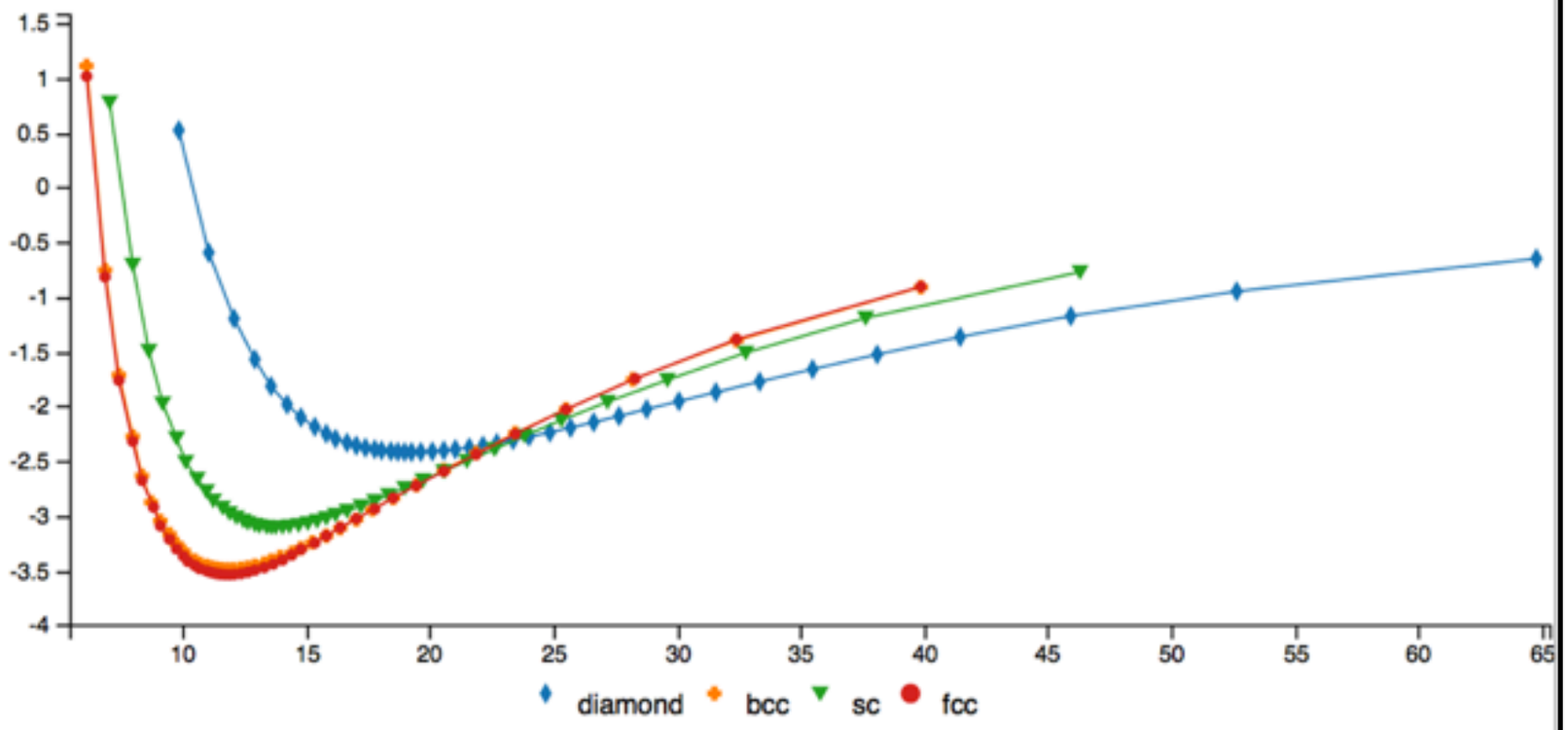
Click on any thumbnail to get a full size image.

KIM Models (https://openkim.org)

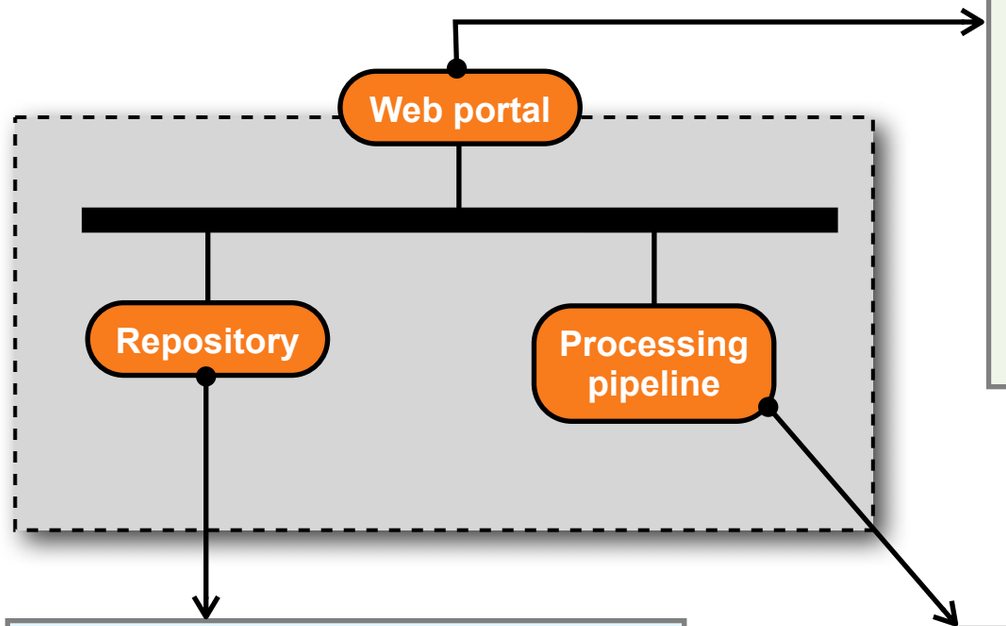
OpenKIM

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)



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

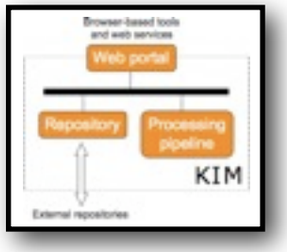
- 189 Models
- 2612 Tests
- 53 property definitions
- 9 visualizers

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

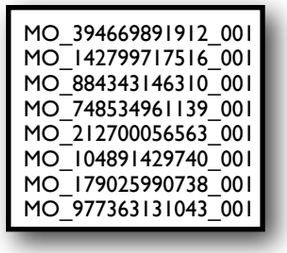
Software supporting KIM API:

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

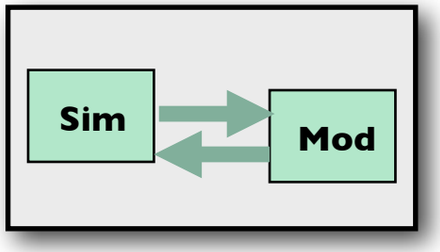
Summary



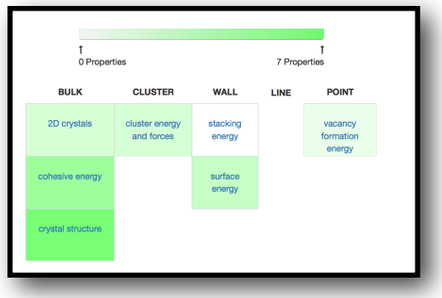
KIM provides archival permanent storage of interatomic models, tests, and reference data with known provenance.



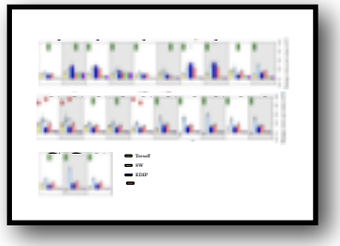
All KIM content is citable with unique permanent identifiers. This makes it possible to reproduce simulation results in the future.



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.

https://openkim.org