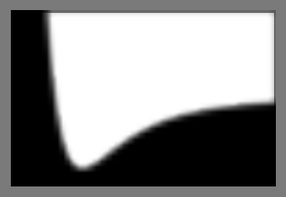

OpenKIM

An Online suite of open source tools for molecular simulation of materials

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NSF CDI and CDS&E programs

LAMMPS Users' Workshop, Albuquerque, NM, August 5–7, 2015

Knowledgebase of Interatomic Models (KIM)

The Open Knowledgebase of Interatomic Models (OpenKIM) is funded through the NSF CDS&E program (https://OpenKIM.org).

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)

KIM Community

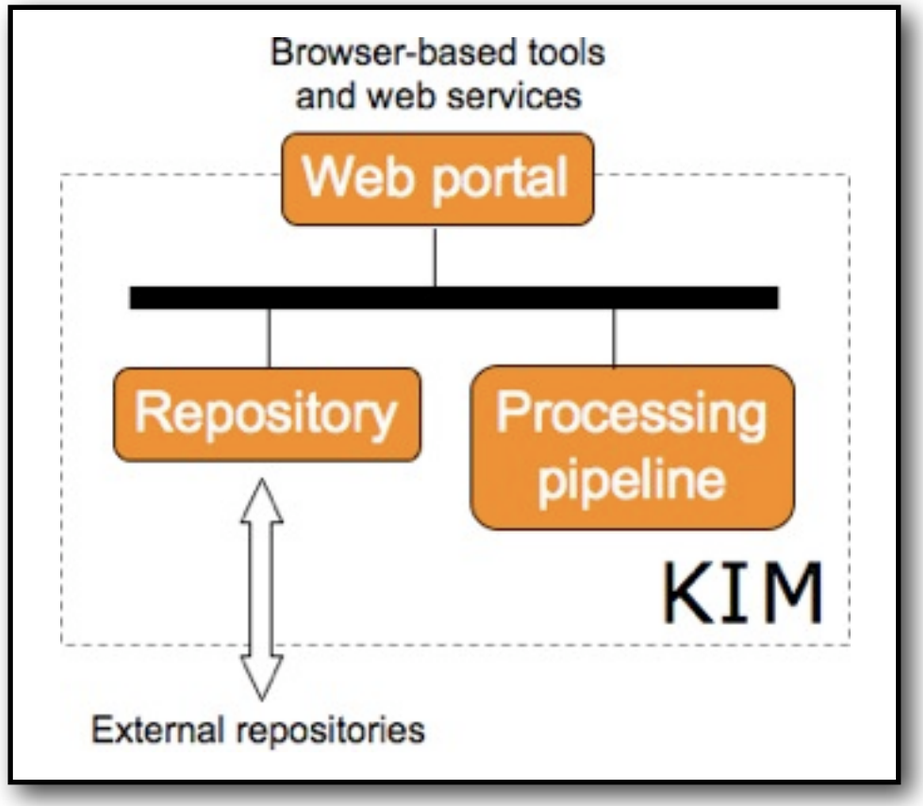
- KIM Inaugural Meeting held in San Diego, Feb 26-27, 2011

  - 63 participants from 7 countries
    - Canada, Germany, Japan, South Korea, Sweden, UK, USA
  - Many key model developers present
  - Major MD code developers present
    - LAMMPS, IMD, GROMACS, SPaSM, DL_POLY
  - KIM Requirements Document defined and has been posted online: http://openkim.org/requirements
  - KIM organizational structure voted on.
  - 355 registered KIM Members (August 2015)

KIM Inaugural Meeting, San Diego, February 2011

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

What is 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

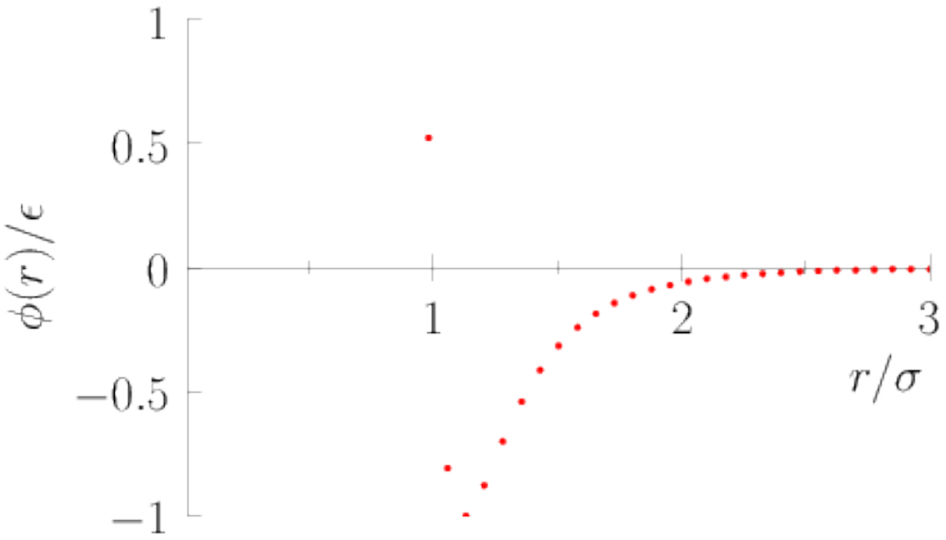
This is common in EAM potentials where the parameter file is considered to be *the* potential.

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:

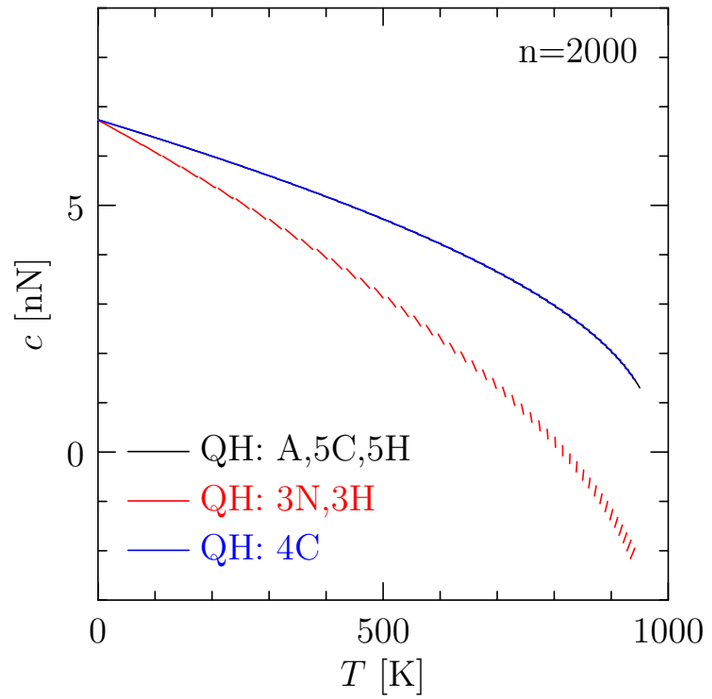


r_1	$\phi(r_1)$
r_2	$\phi(r_2)$
r_3	$\phi(r_3)$
...	...

- 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:

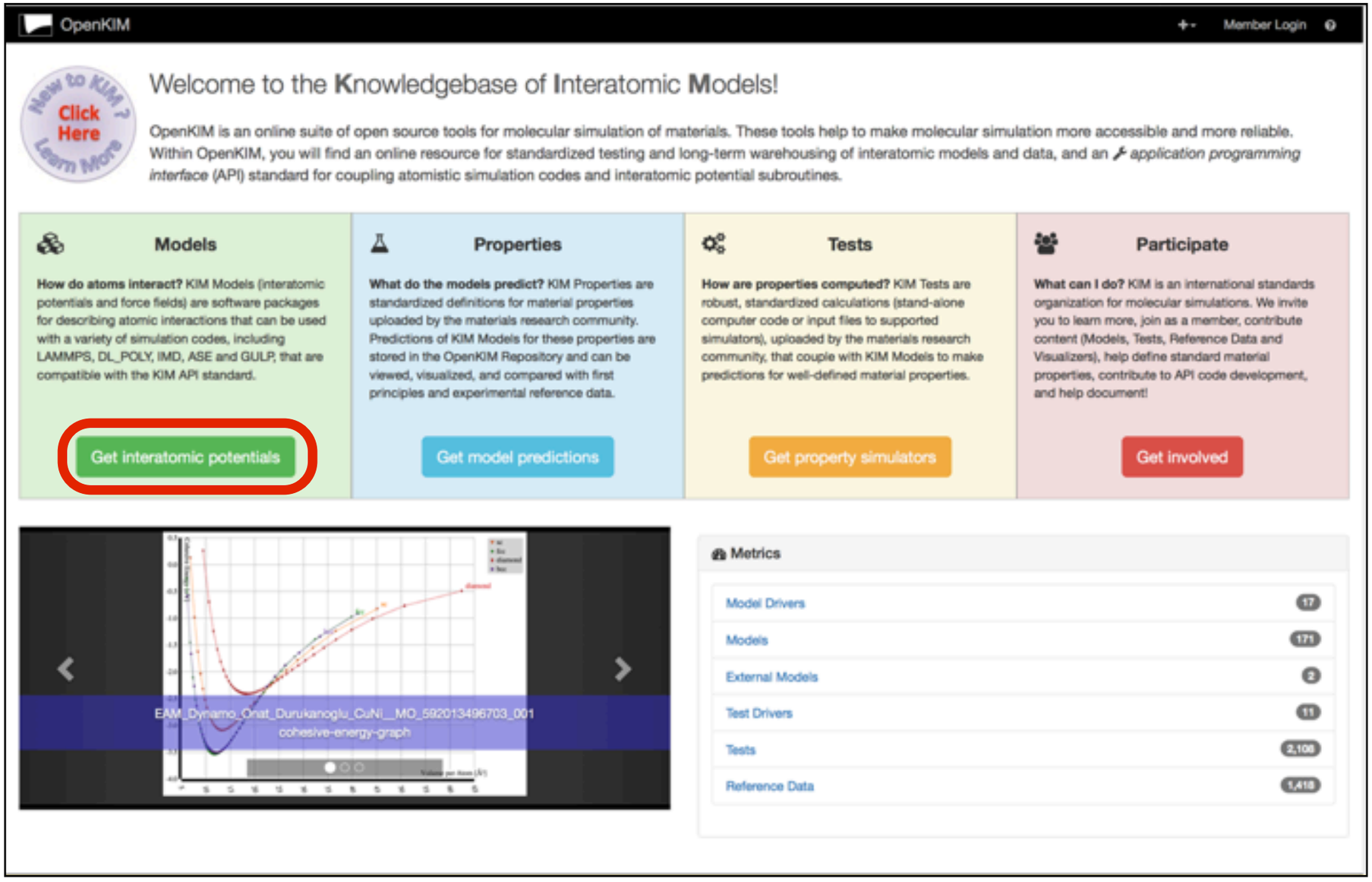
$$c = a\left[\phi''(a) + \frac{k_B T}{2}\frac{\phi^{(4)}(a)\phi''(a) - (\phi''(a))^2}{(\phi''(a))^2}\right]$$



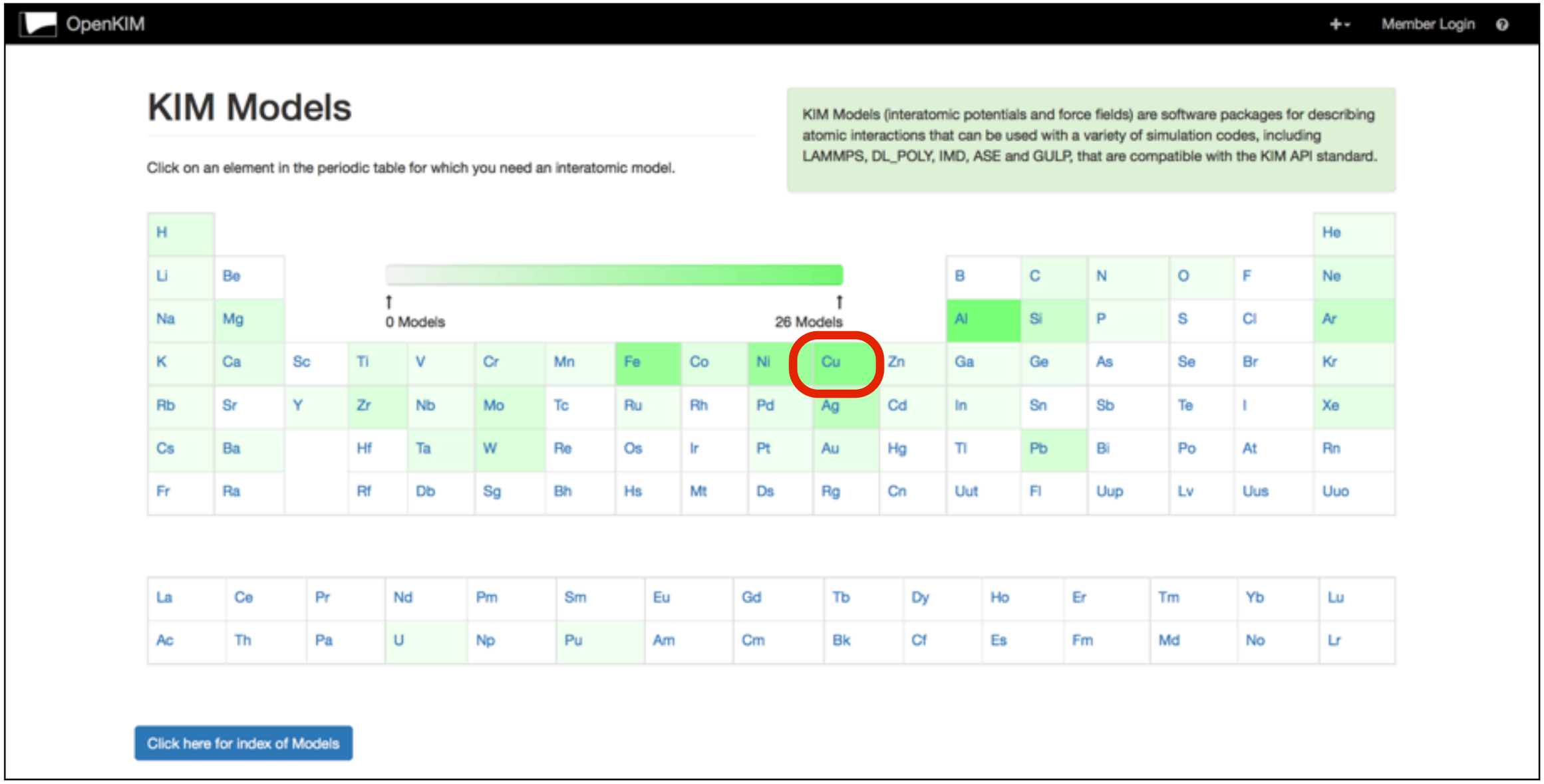
Wen et al., *MSMSE*, in press (2015)

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_001

Title	EAM Cu Potential
Short KIM ID	MO_346334655118_001
Extended KIM ID	EAM_Dynamo_Mishin_Mehl_Cu__MO_346334655118_001
KIM Item Type	Parameterized Model using Model Driver EAM_Dynamo__MD_120291908751_001
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

Unique archival KIM ID for citation in papers

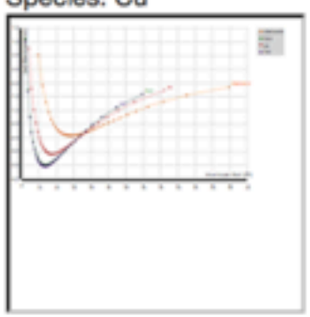
Scientific reference for the potential.

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.

Visualization of various properties computed within KIM system to help select the appropriate potential for the application.

Citing KIM Models

- Example of citing a KIM Model:

In this case, the large compressive stress resulted in an Yttria-stabilized zirconia phase with cubic symmetry. Due to the large system size needed to accurately model the process of oxygen migration, the dipole-based empirical potential of Umeno *et. al* [1] archived in OpenKIM [2-4] was employed.

References

1. Y. Umeno, A. M. Iskandarov, A. Kubo and J. M. Albina, "Atomistic Modeling and Ab Initio Calculations of Yttria-Stabilized Zirconia", ECS Transactions 57-1 (2013) pp.2799-2809.

2. Y. Umeno, "Dipole model potential optimized for YSZ (Yttria-stabilized zirconia)." https://openkim.org/cite/MO_394669891912_000

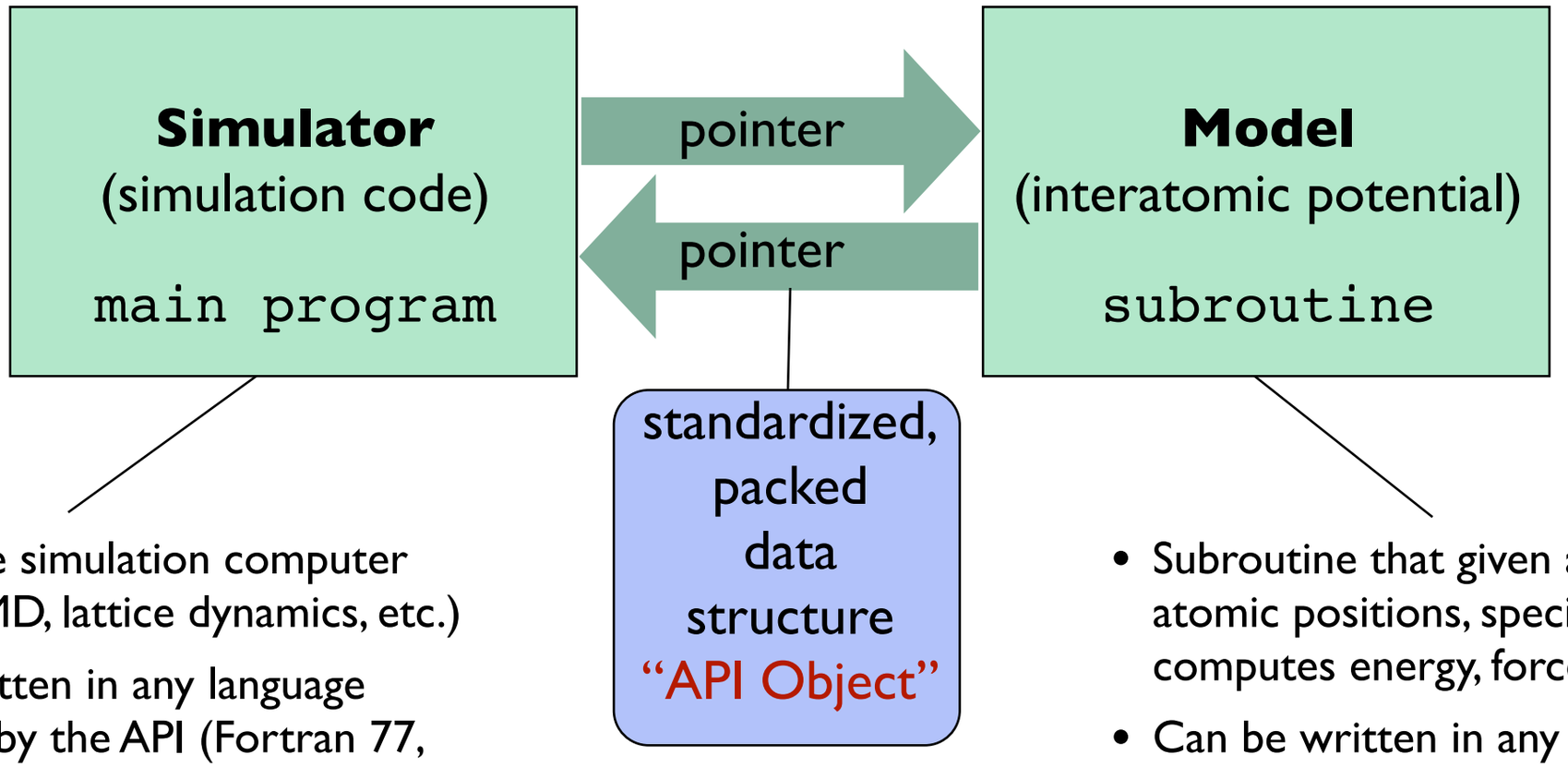
3. E. B. Tadmor, R. S. Elliott, J. P. Sethna, R. E. Miller and C. A. Becker, "The Potential of Atomistic Simulations and the Knowledgebase of Interatomic Models" *JOM*, **63**, 17 (2011).

4. Future publication about the KIM API will be featured here.

The ability to cite a KIM ID and have access to the archived Model makes it possible to reproduce atomistic simulations.

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, C, C++, ...)

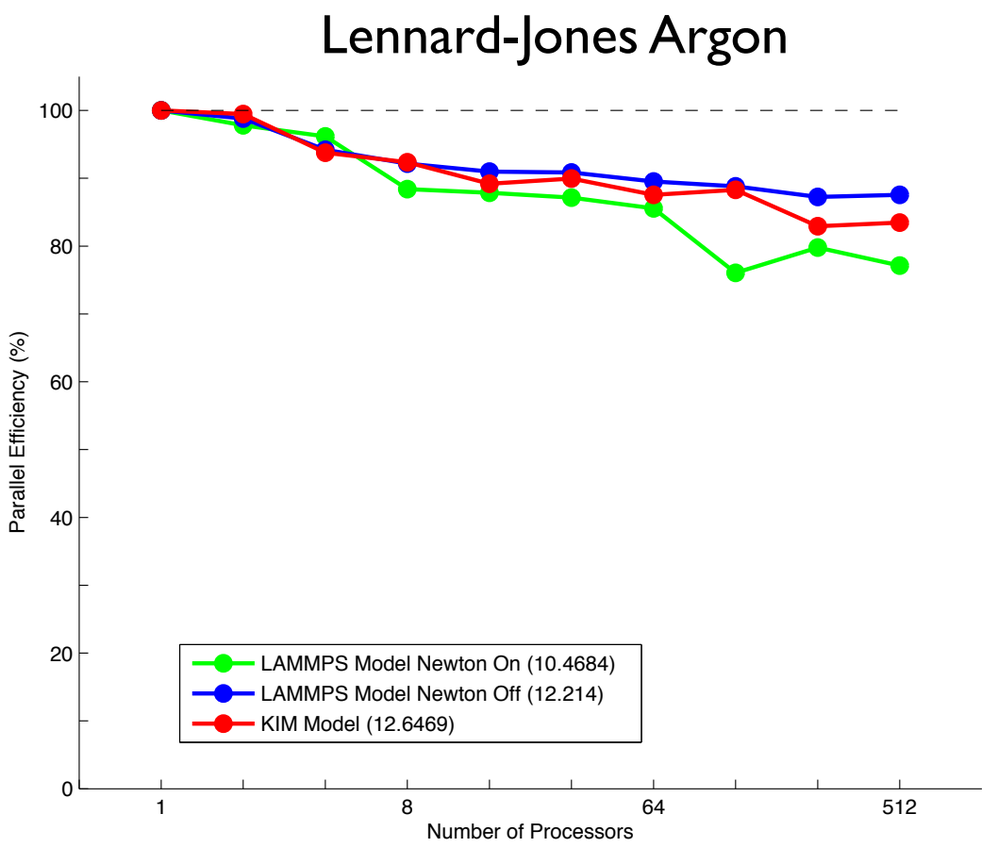
- Subroutine that given a set of atomic positions, species, ... computes energy, forces, ...
- Can be written in any language (Fortran 77, Fortran 90, C, C++, ...)

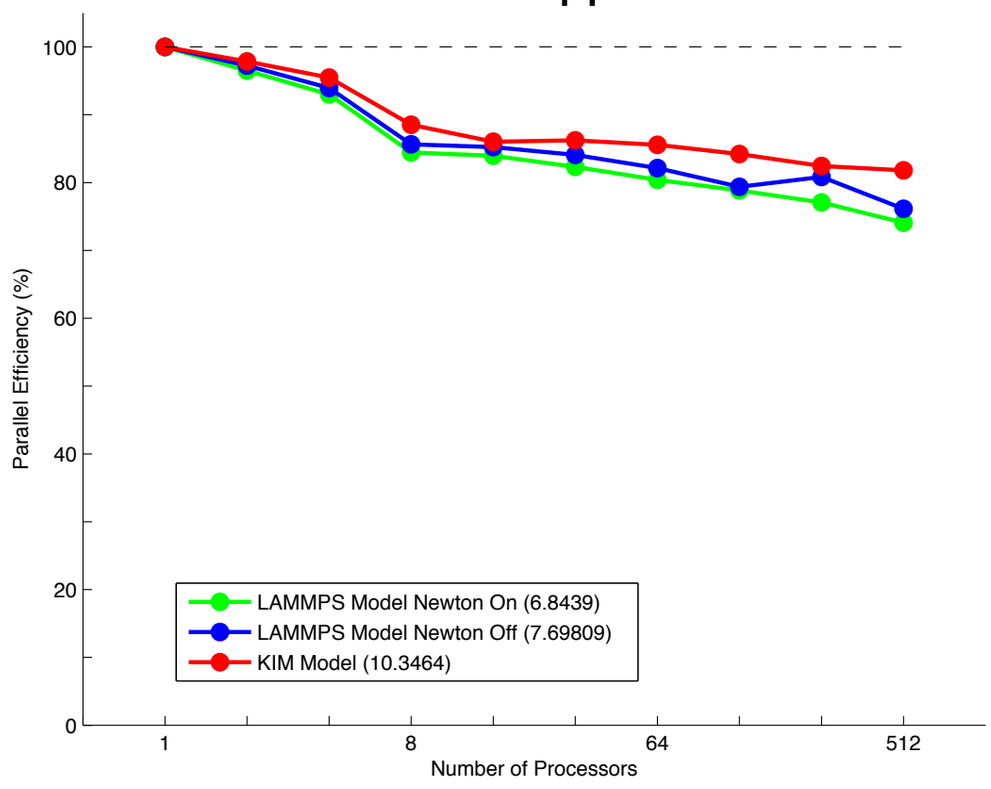
- Currently working on support for electrostatics and charge equilibration.

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

QuasiContinuum Method
the original source for information, publications, and downloads

LAMMPS

MDStressLab

LAMMPS

- Using KIM Models with **LAMMPS** is straightforward:
  - Install the KIM API (packages available for Ubuntu, others in development)
  - Precede LAMMPS installation with "`make yes-kim`"
  - Add the KIM Models that you want to use. (Ubuntu package has 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
```

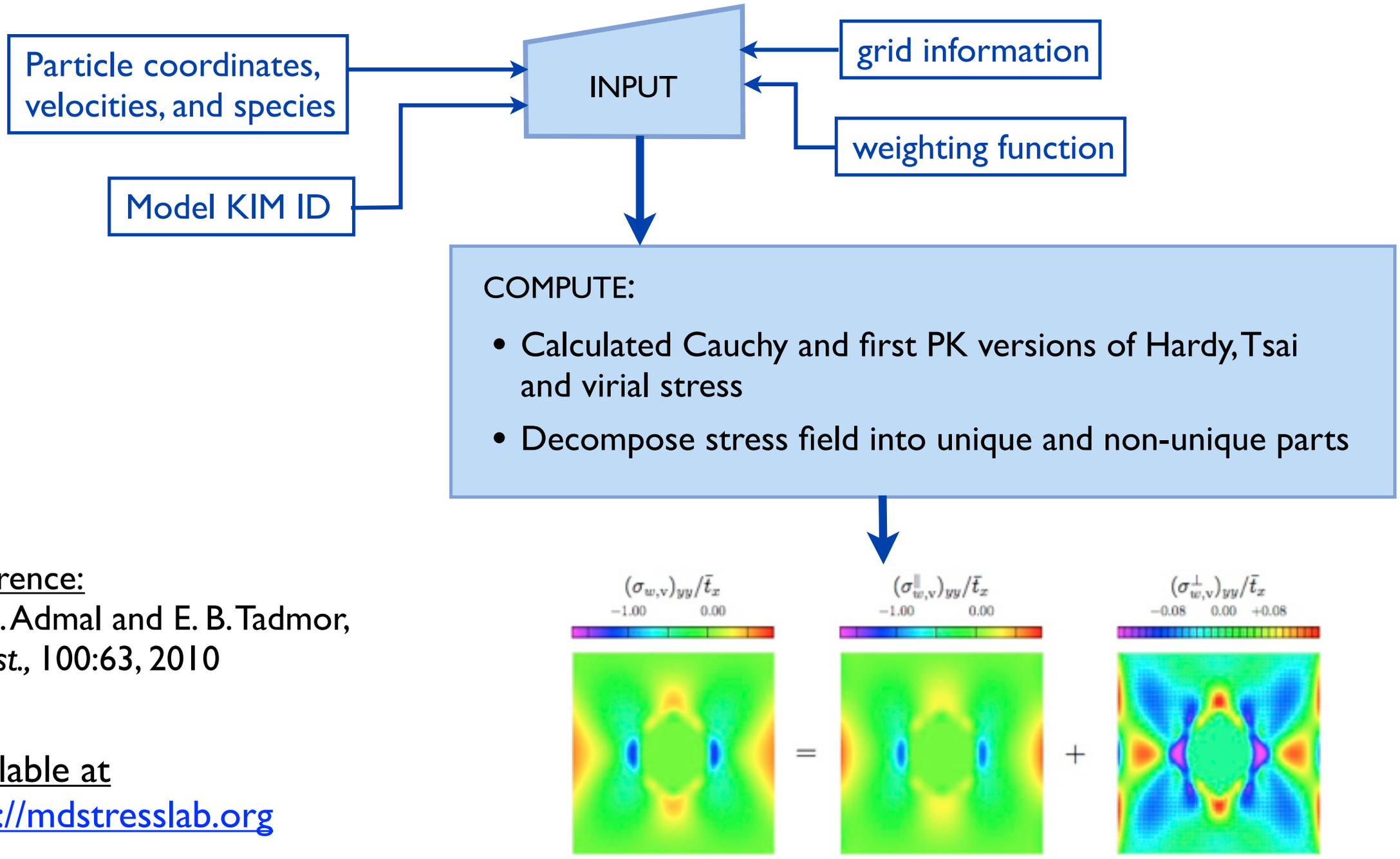
```
pair_style      kim LAMMPSvirial EAM_Dynamo_Ercolessi_Adams_Al__MO_123629422045_001
pair_coeff      * * Al
mass            1 26.98
```

- 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

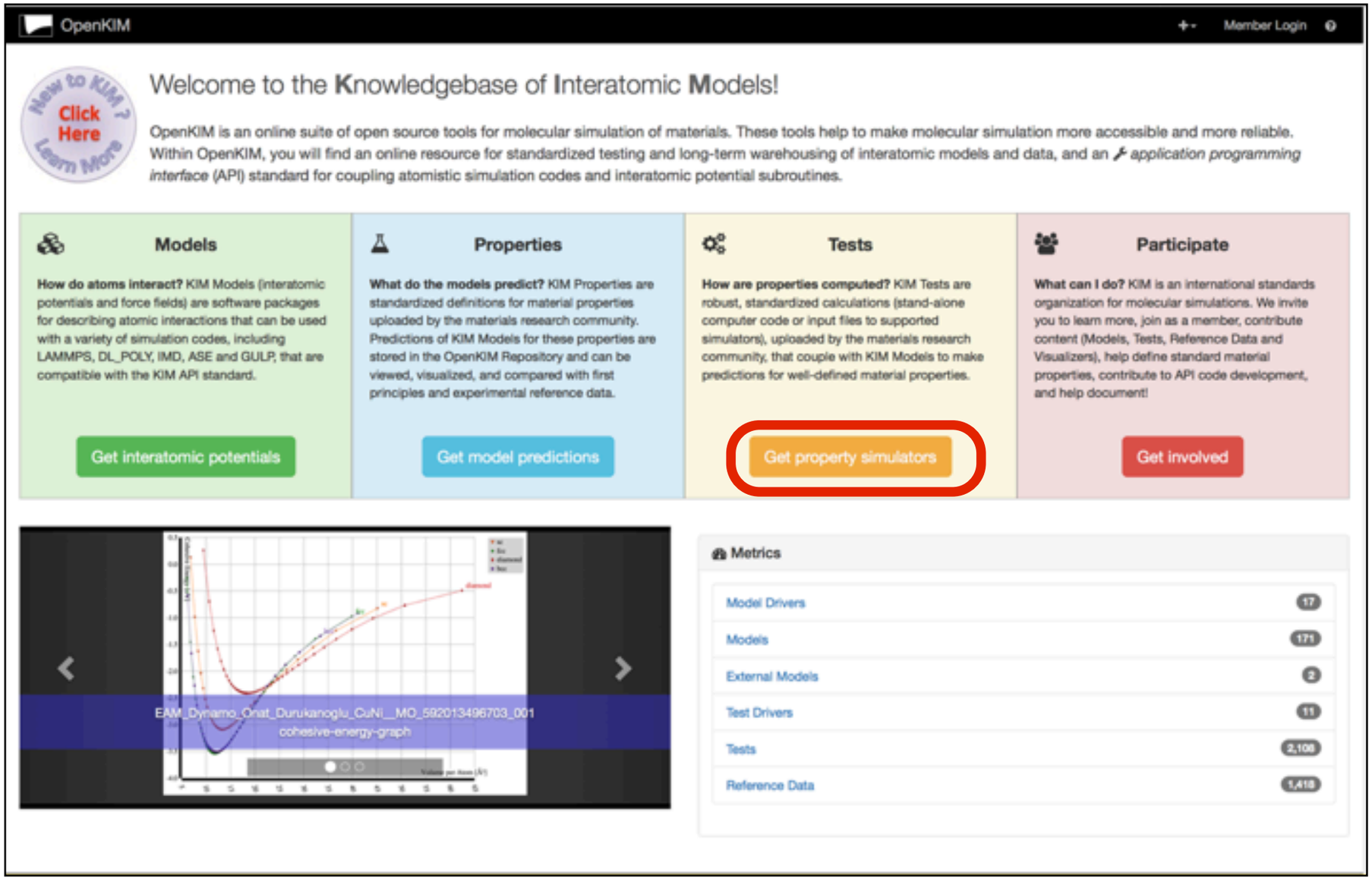


Reference:
N. C. Admal and E. B. Tadmor,
J. Elast., 100:63, 2010

Available at
http://mdstresslab.org

Testing Model Predictions (https://openkim.org)

- User uploadable KIM Tests compute the predictions of archived KIM Models for different properties:



Testing Model Predictions (https://openkim.org)

KIM Tests

Click on a category in the properties table for which you need a KIM Test.

KIM Tests are robust, standardized calculations (stand-alone computer code or input files to supported simulators), uploaded by the materials research community, that couple with KIM Models to make predictions for well-defined material properties.

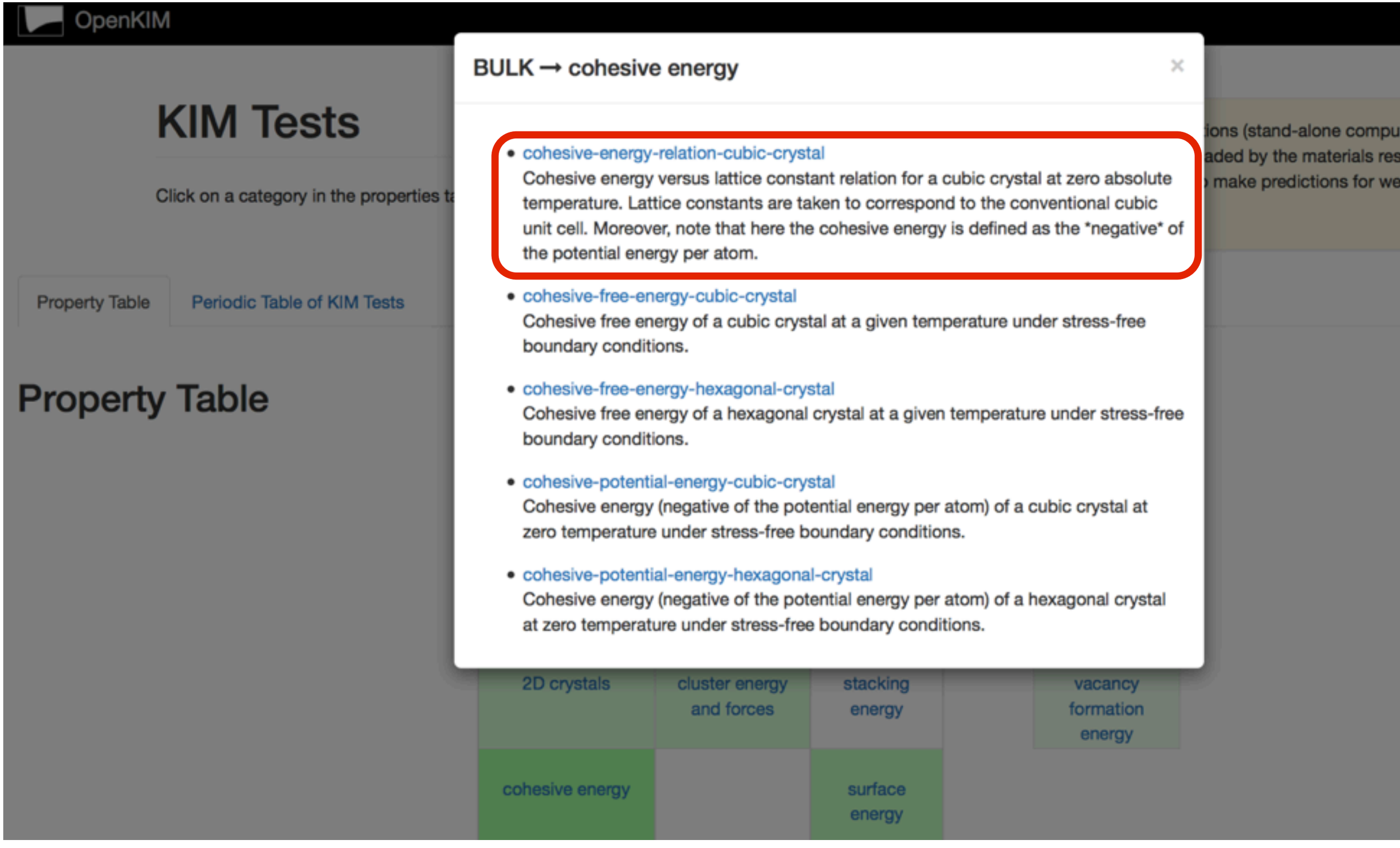
Property Table | Periodic Table of KIM Tests

Property Table

0 Properties — 7 Properties

BULK	CLUSTER	WALL	LINE	POINT
2D crystals	cluster energy and forces	stacking energy		vacancy formation energy
cohesive energy		surface energy		
crystal structure				
elastic constant				
melting temperature				

Testing Model Predictions (https://openkim.org)



Testing Model Predictions (https://openkim.org)

Tests for cohesive-energy-relation-cubic-crystal

By Species | By Test Driver | Alphabetical

Link to Property Definition: cohesive-energy-relation-cubic-crystal

Ag

Test ID	Test Title
CohesiveEnergyVsLatticeConstant_bcc_Ag__TE_776768886429_001	Cohesive energy versus lattice constant curve for bcc Silver
CohesiveEnergyVsLatticeConstant_diamond_Ag__TE_267703329770_001	Cohesive energy versus lattice constant curve for diamond Silver
CohesiveEnergyVsLatticeConstant_fcc_Ag__TE_295388173914_001	Cohesive energy versus lattice constant curve for fcc Silver
CohesiveEnergyVsLatticeConstant_sc_Ag__TE_229146981356_001	Cohesive energy versus lattice constant curve for sc Silver

Al

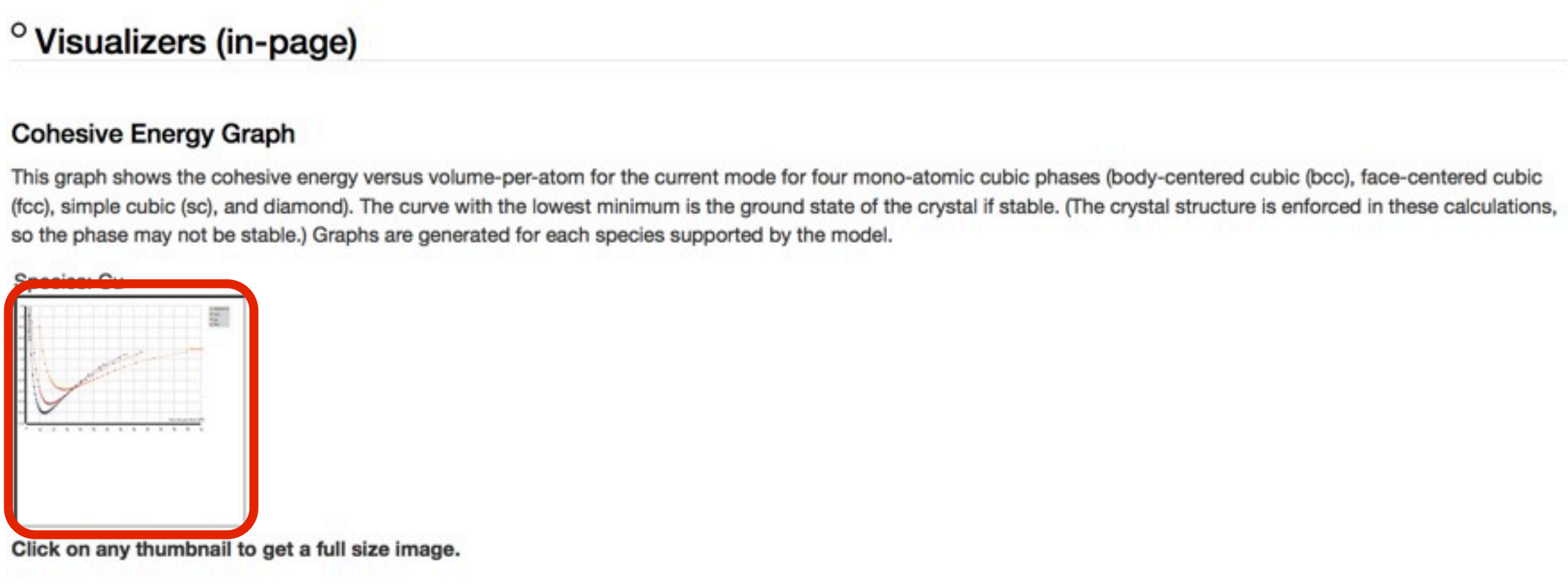
Test ID	Test Title
CohesiveEnergyVsLatticeConstant_bcc_Al__TE_320860761056_001	Cohesive energy versus lattice constant curve for bcc Aluminum
CohesiveEnergyVsLatticeConstant_diamond_Al__TE_024193005713_001	Cohesive energy versus lattice constant curve for diamond Aluminum
CohesiveEnergyVsLatticeConstant_fcc_Al__TE_380539271142_001	Cohesive energy versus lattice constant curve for fcc Aluminum
CohesiveEnergyVsLatticeConstant_sc_Al__TE_549565909158_001	Cohesive energy versus lattice constant curve for sc Aluminum

Visualizers

- You can also see Test results through user uploadable visualizers on the Model Pages:

  Model page for EAM_Dynamo_Mishin_Mehl_Cu__MO_346334655118_001

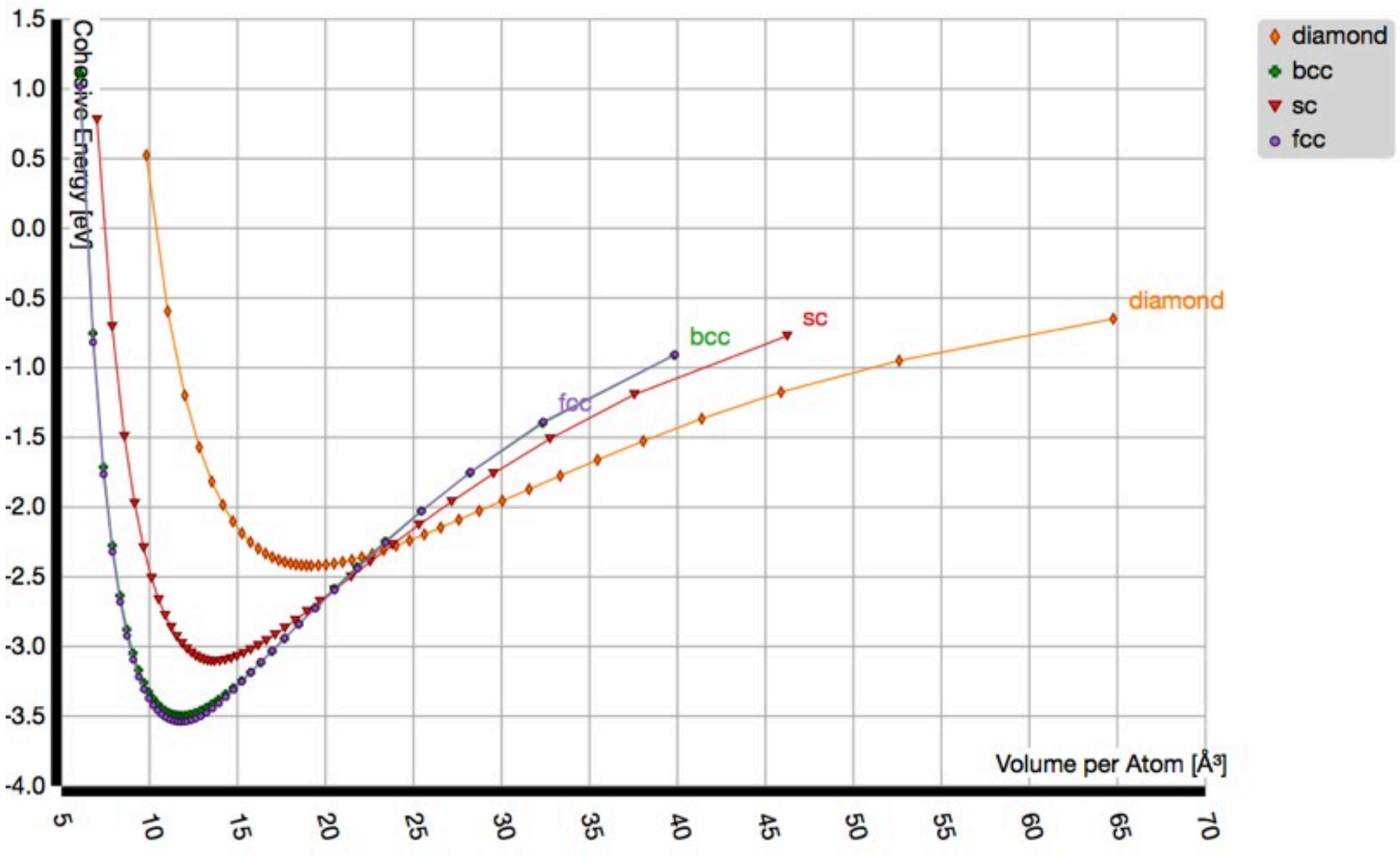
  ⋮



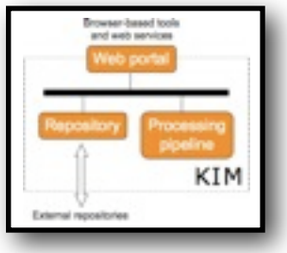
Visualizers

Model: EAM_Dynamo_Mishin_Mehl_Cu__MO_346334655118_001

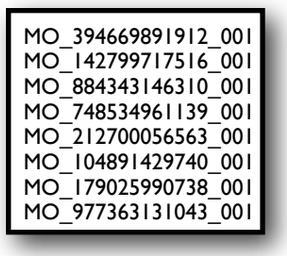
Species: Cu



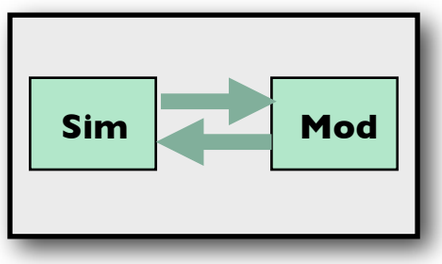
Summary



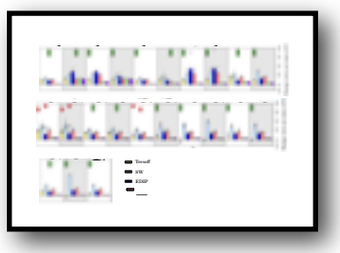
KIM provides archival permanent storage of interatomic models, tests, and reference data with known provenance.



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.



Transferability is quantified through exhaustive testing using KIM Tests uploaded by users for properties of interest.

Come to breakout session:

- Learn more about Testing framework and how to contribute Tests
- How to select the appropriate model for a given application (RATE)
- Discuss future of KIM and your wish list for the project