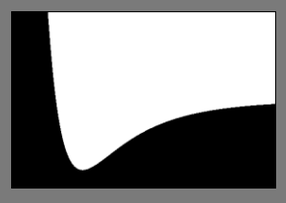

OpenKIM: Tested, portable interatomic models for molecular and multiscale simulations

Daniel S. Karls, Ryan S. Elliott, and Ellad B. Tadmor

Department of Aerospace Engineering and Mechanics, University of Minnesota

NSF CDS&E programs

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-)

OpenKIM Survey on the Future of Molecular Simulation

- Recent survey (Jan 2018) on the needs of researchers engaged in molecular and multiscale simulations with interatomic models. (449 respondents, 25% response rate)

  The respondents identified the following as the most pressing needs:

  - Access to archived interatomic potentials that can be cited in publications (like a DOI), so that simulations can be reproduced
  - Portable implementations of interatomic potentials that can be used in "plug-and-play" fashion with different molecular simulation codes
  - Tools that assist researchers in selecting the most accurate interatomic potential for a specific application
  - Tools that estimate the uncertainty (error bars) associated with the predictions of a given potential (for example, through sensitivity analysis)

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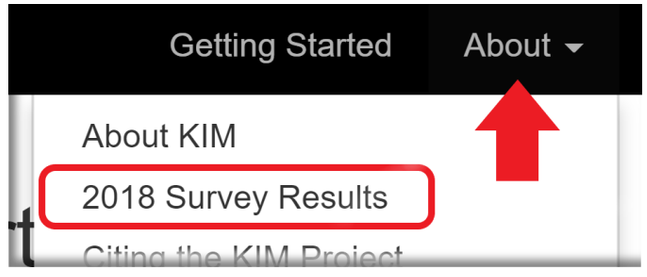
Full survey results available at:

https://openkim.org/survey/2018-future/ or



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:

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

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II. The LJ parameter set for a specific material:

Argon

ε = 0.0104 eV

σ = 3.40 Å

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

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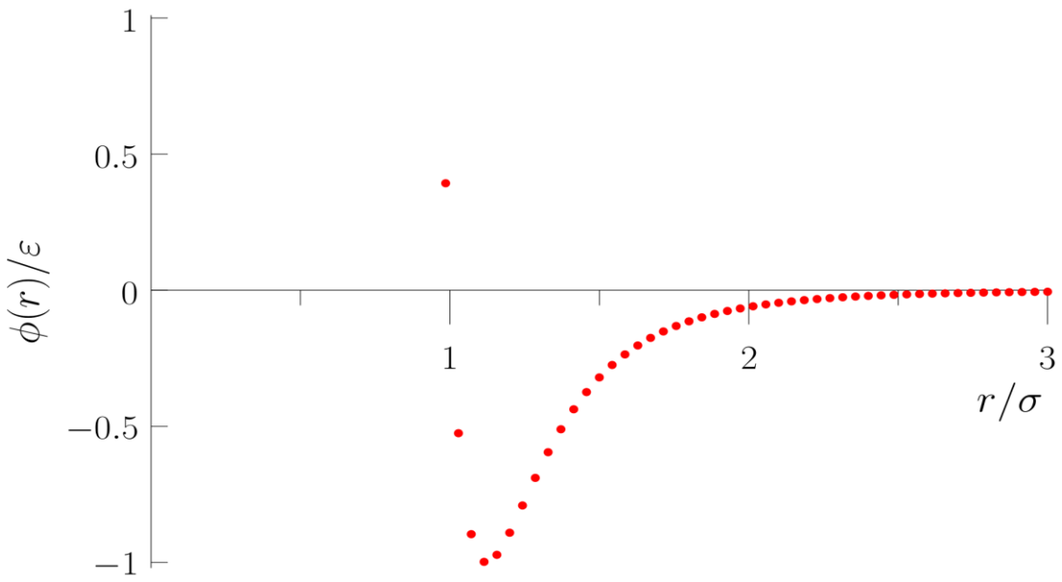
III. A computer implementation of the LJ potential:

```
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
```

Is a parameter set enough?

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



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

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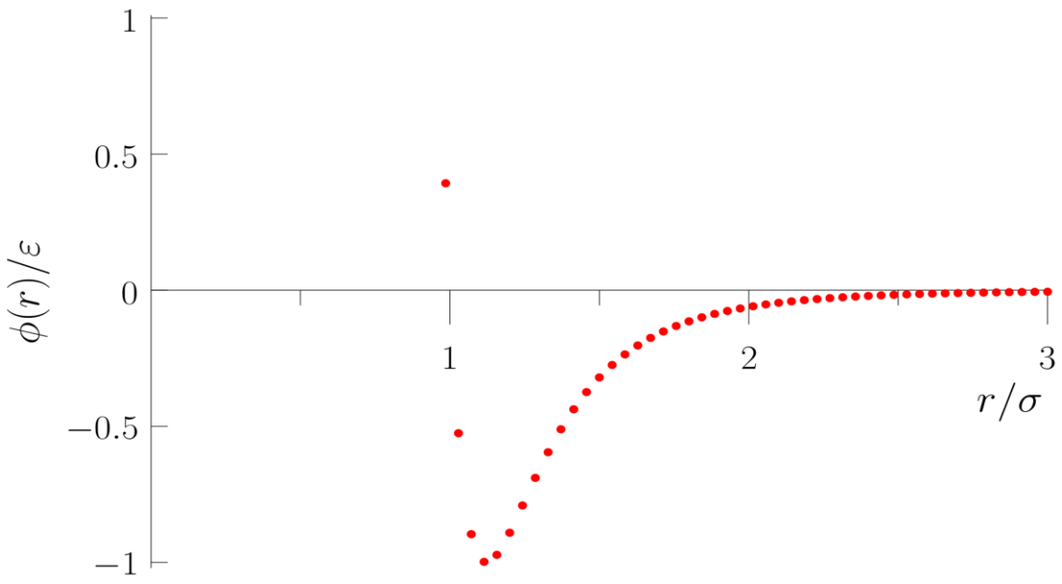

r_1	$\phi(r_1)$
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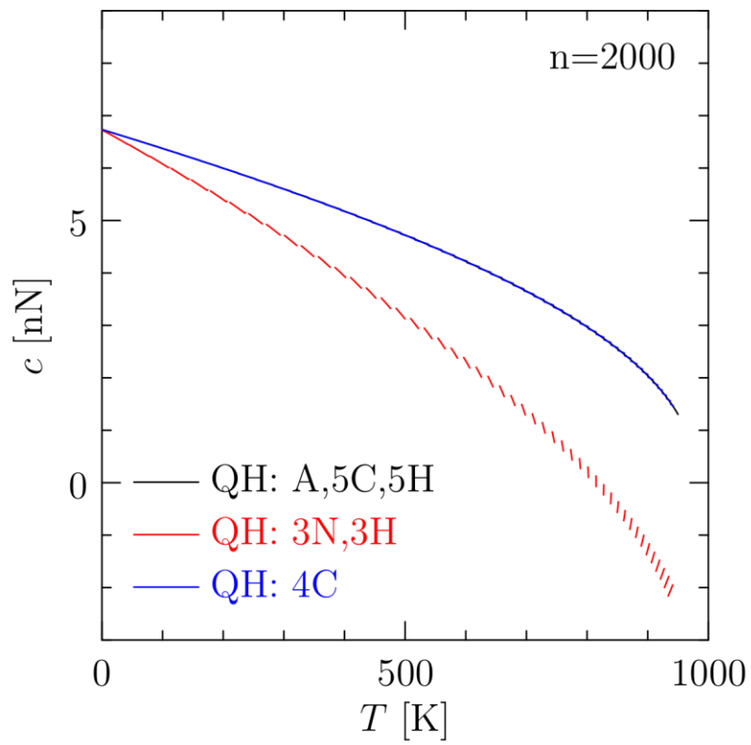
- The interpolation choice (e.g. spline order) affects some results,

  e.g. Quasi-harmonic estimate of the elastic constant for a 1D chain of atoms interacting via a nearest-neighbor Morse pair potential:

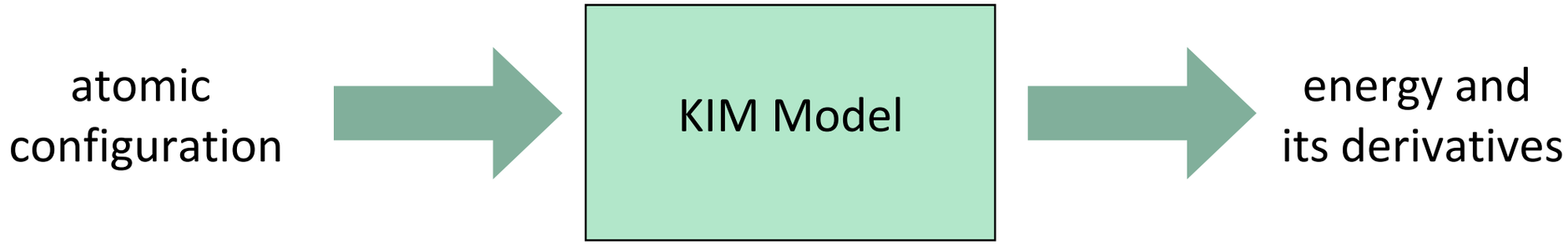
$$c = a\left[\phi''(a) + \frac{k_B T}{2}\frac{\phi^{(4)}(a)\phi''(a) - \left(\phi''(a)\right)^2}{\left(\phi''(a)\right)^2}\right]$$



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

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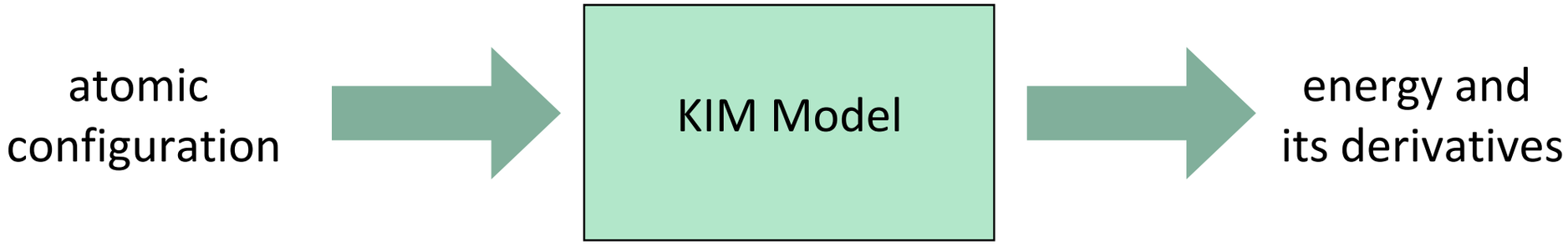

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    1. Stand-alone Model – functional form implementation and parameters for <u>one</u> material

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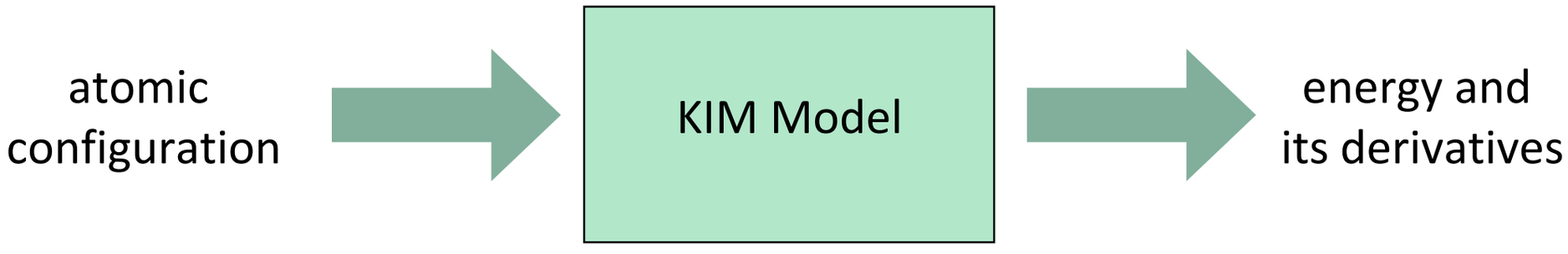


  - KIM Models can have two forms

1. Stand-alone Model – functional form implementation and parameters for <u>one</u> material

2. Parameterized Model – parameter set that is read in by a Model Driver, e.g.:

Lennard-Jones Model Driver:

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

(Computer implementation including any interpolations or other data processing)

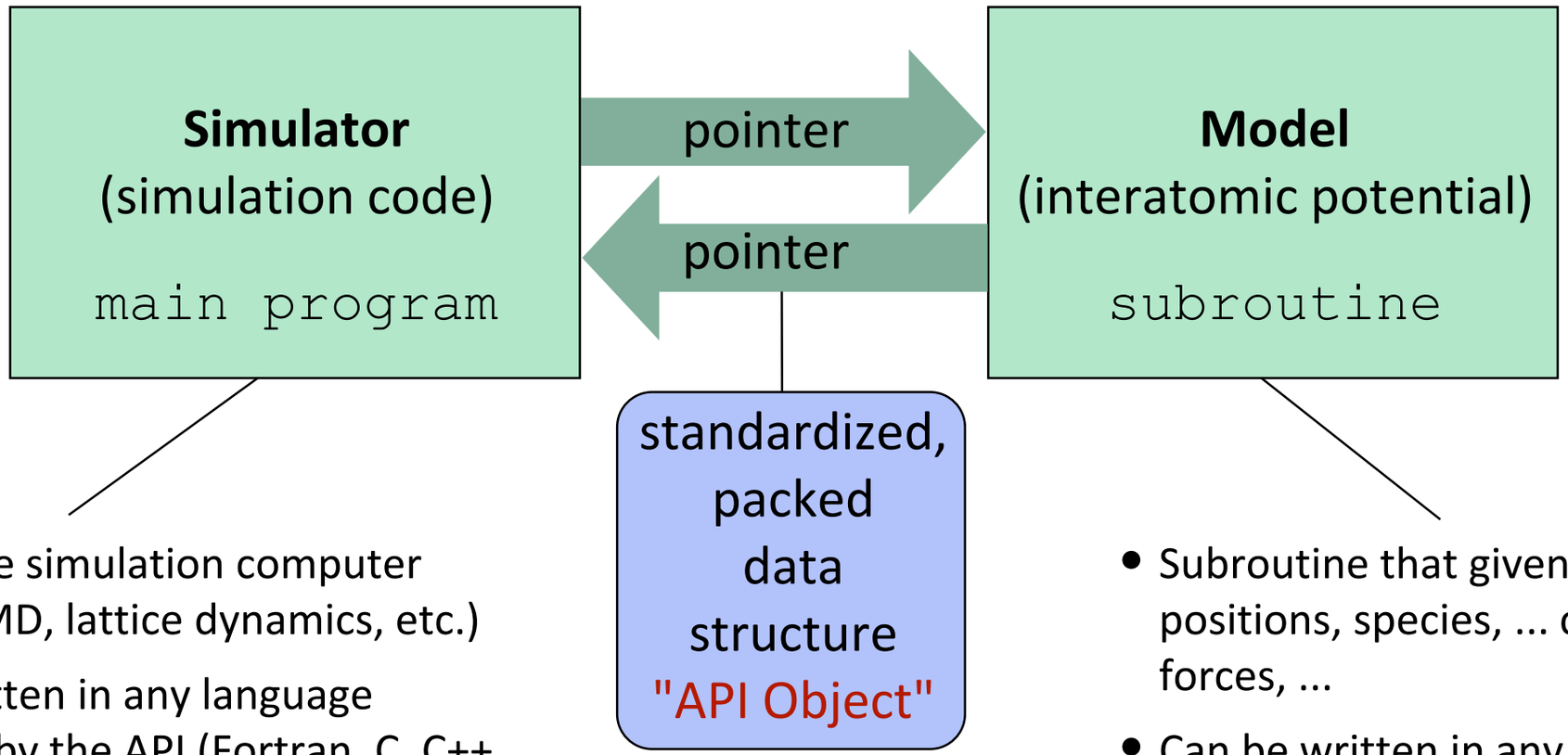
Material-specific LJ Models:

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) standard 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, C, C++, Python)

- Subroutine that given a set of atomic positions, species, ... computes energy, forces, ...
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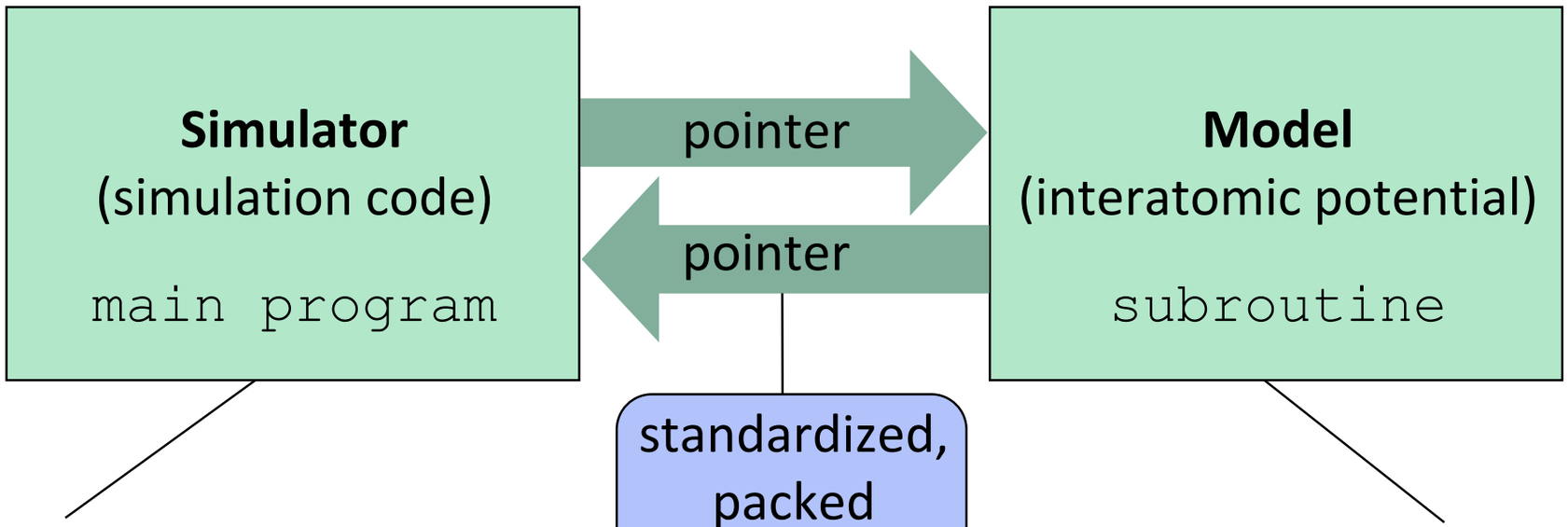

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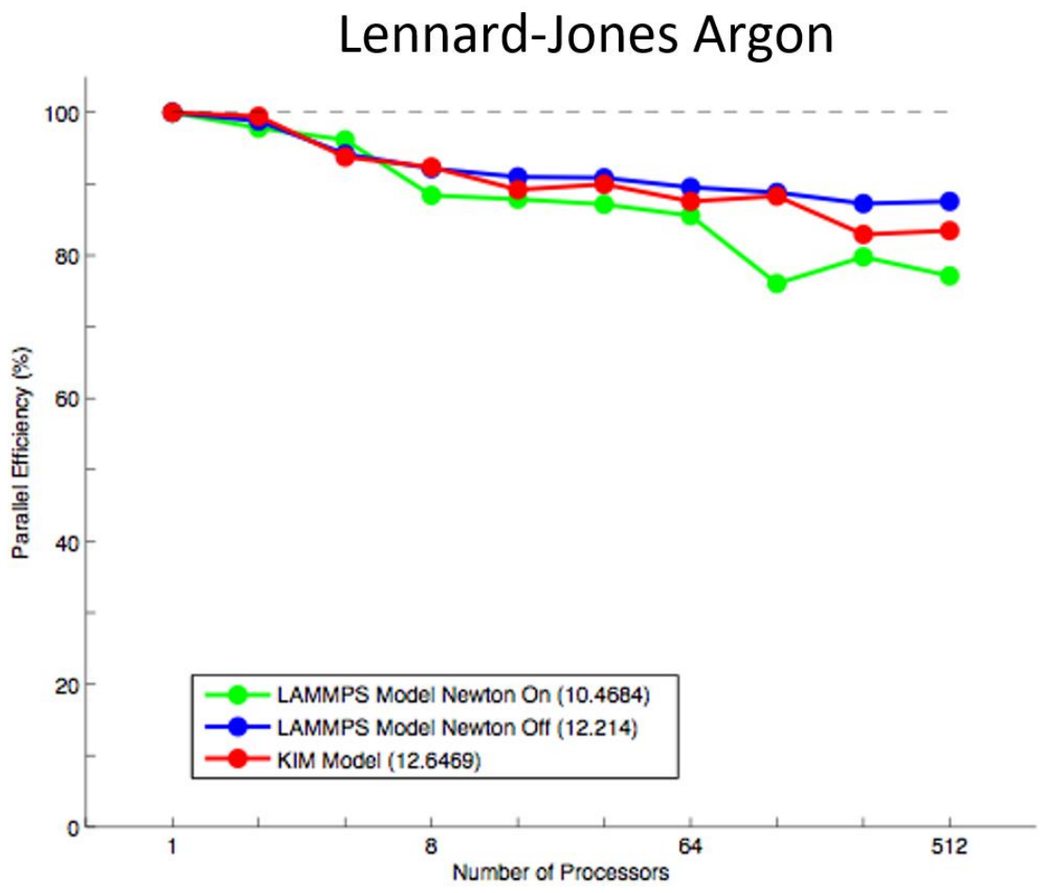
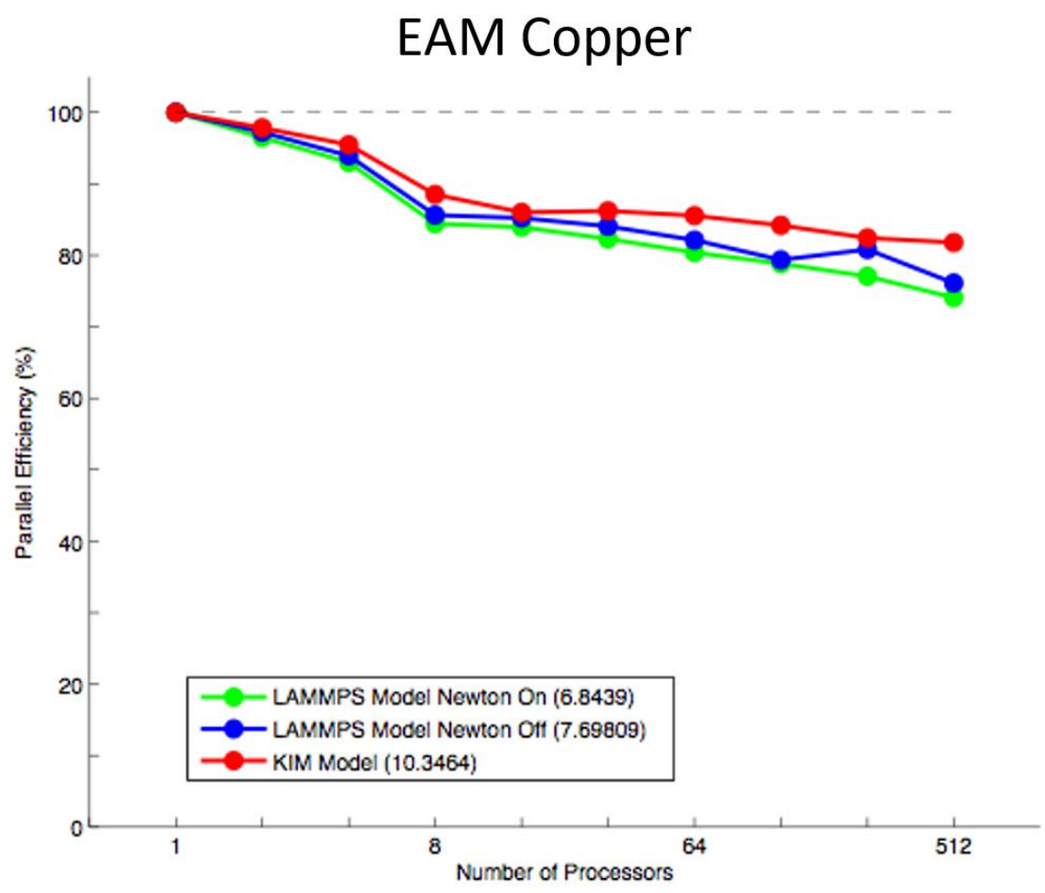
- Currently working on support for electrostatics and charge equilibration

Efficiency of the KIM API

- The KIM API is a lightweight, efficient interface

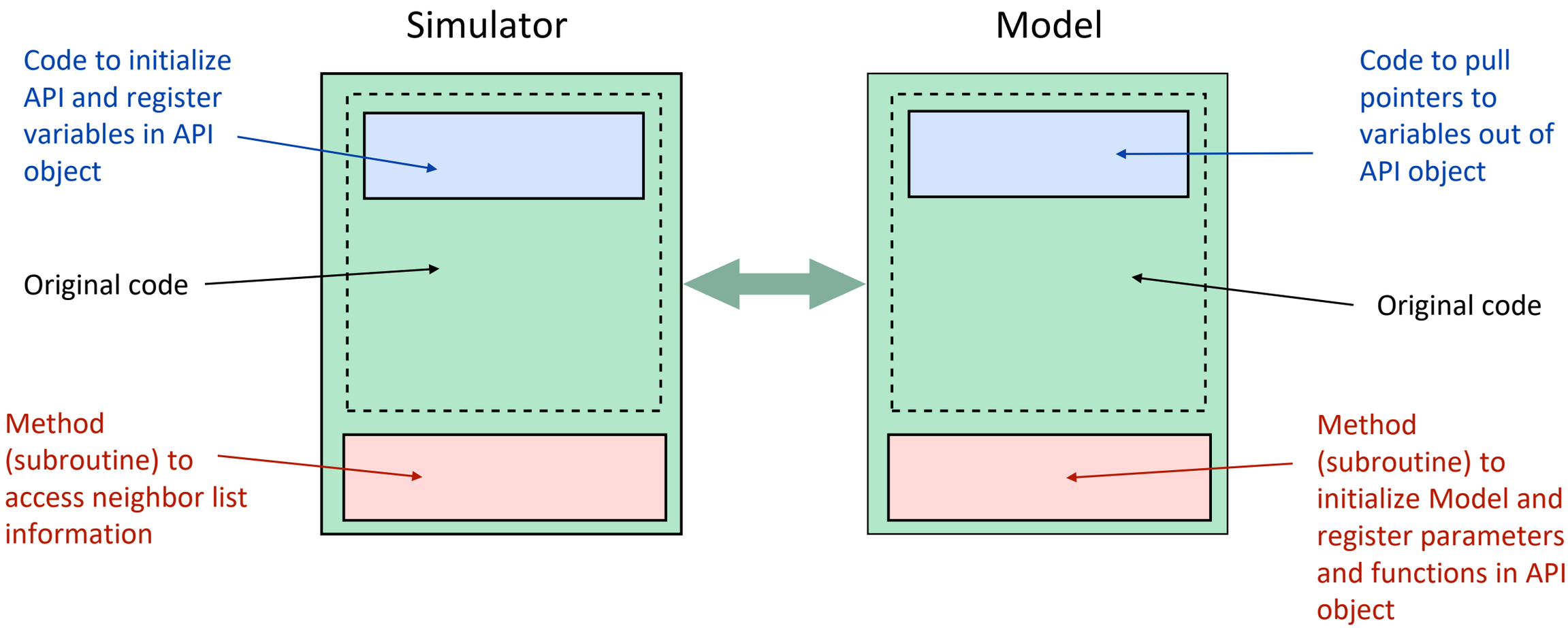
LAMMPS benchmark results (scaled size with 32,000 atoms per core)





Using the KIM API

- Changes to existing codes to make them KIM-compliant are relatively minor:



- By supporting the KIM API:
  - A developer can make their Model available to all KIM-compliant simulation codes
  - A simulator has instant access to all Models in the KIM Repository

KIM-Compliant Codes

Asap

ASE

DL_POLY

GULP

LAMMPS

libAtoms + QUIP

potfit

nanoHUB

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

MDStressLab

Example: Using KIM Models with LAMMPS

- Every KIM Model is uniquely identified by a KIM ID:

EAM_Dynamo_ErcolessiAdams_Al__MO_123629422045_004

human-readable prefix — ID for citation (12 digit + 3 digit version)

- Using KIM Models with LAMMPS is straightforward:
  - Install the KIM API, build LAMMPS with `make yes-kim`
  - Install the KIM Models that you want to use with the collections management utility (included with the API) or download source from openkim.org
  - Use 'pair_style kim' and the KIM ID

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

```
pair_style      kim KIMvirial EAM_Dynamo_ErcolessiAdams_Al__MO_123629422045_004
pair_coeff      * * Al
mass            1 26.98
```

Citing KIM Models

- Example of citing a KIM Model:

...the potential employed was Johnson's nearest neighbor EAM potential [1] archived in OpenKIM [2–3].

References

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

Model Verification Checks

- All KIM Models are subjected to Verification Checks when uploaded to openkim.org

  Mandatory (Pass/Fail)

  - Species supported as stated
  - Unit conversion handled correctly
  - Domain decomposition handled correctly
  - …

  Consistency (A,B,C,D,F)

  - Numerical derivative check of forces, virial, hessian, ...
  - Translational and rotational invariance
  - …

  Informational (Pass/Fail or A,B,C,D,F)

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

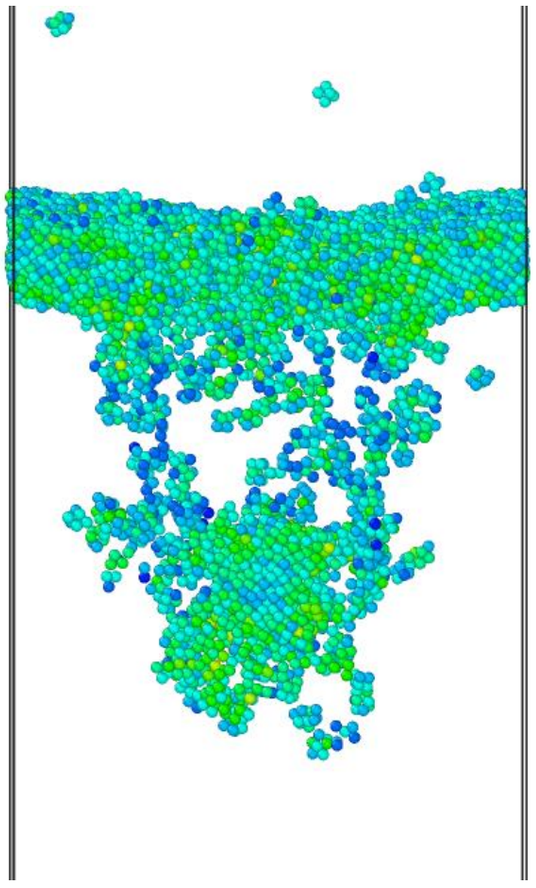
A simulation is only as good as the potential

- The predictive capability of an atomistic simulation is dependent on the fidelity of the interatomic model

Example: Projectile impacting silicon plate

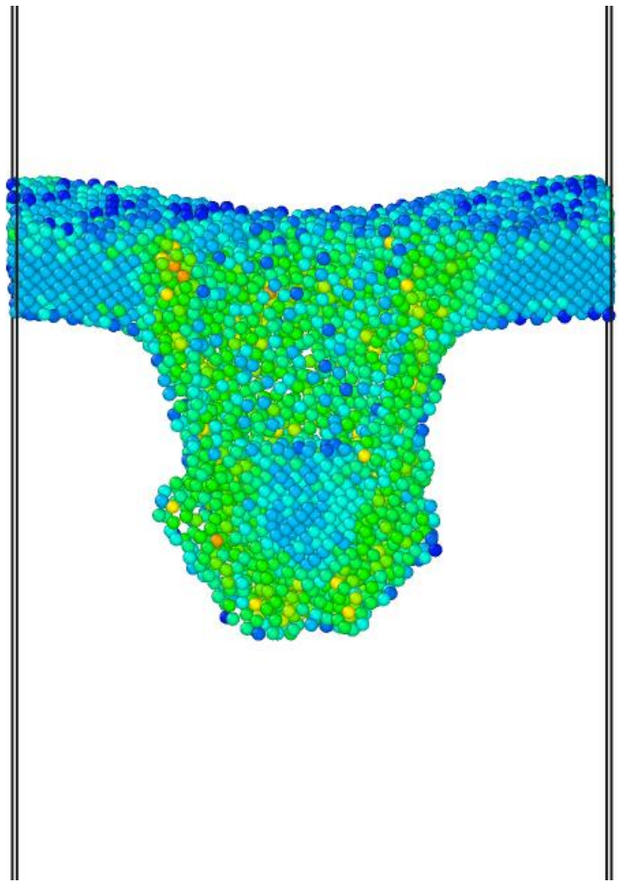
Tersoff Potential

exhibits brittle behavior



Stillinger-Weber Potential

exhibits ductile behavior



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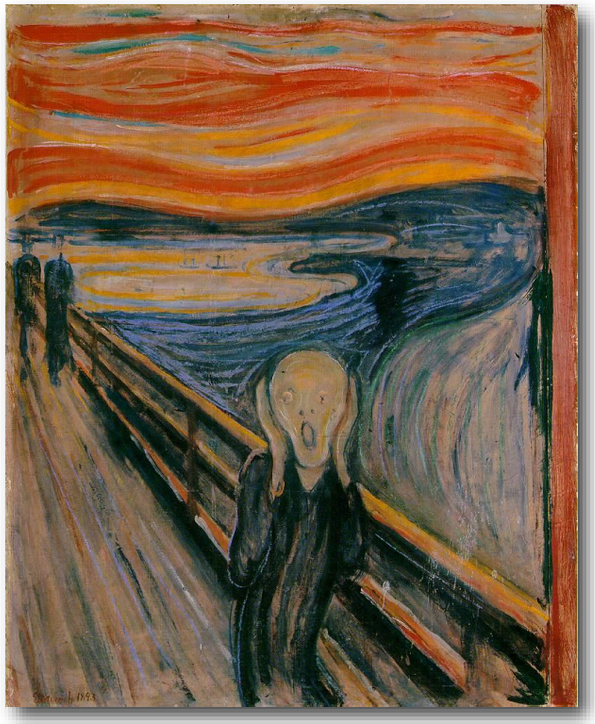

The Scream, Edvard Munch

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

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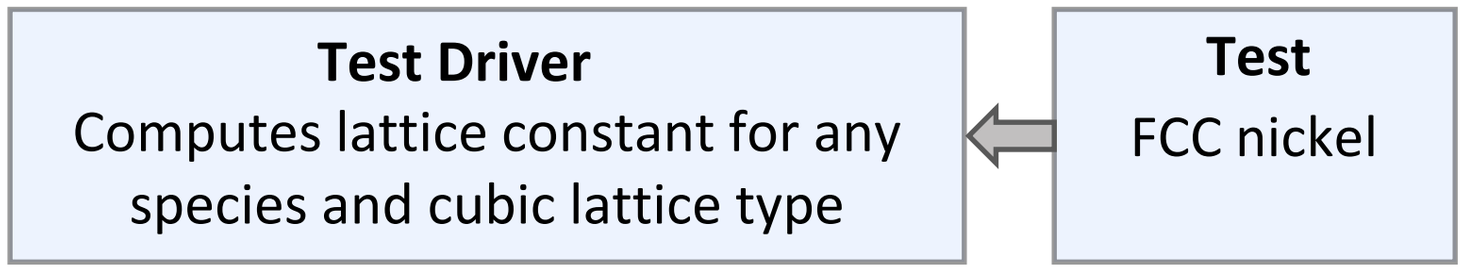
- Usually a parameter set that is read in by a *Test Driver*, e.g.:



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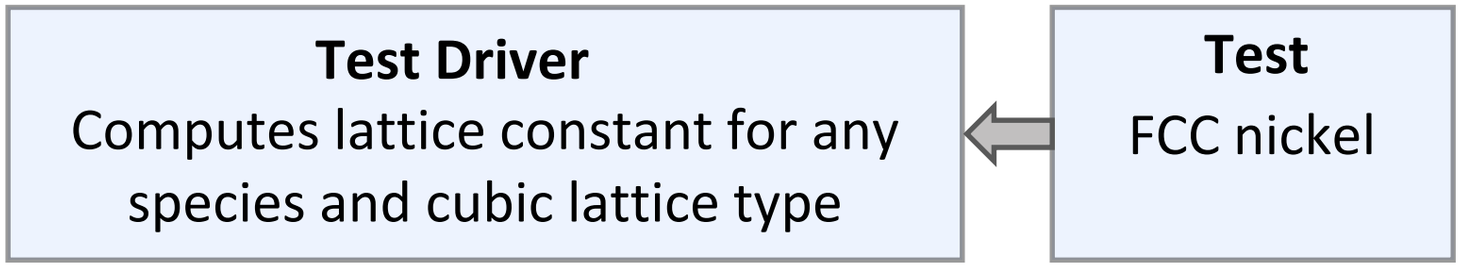

- Can be a program or an input file to a supported Simulator (e.g. ASE, LAMMPS, ...)

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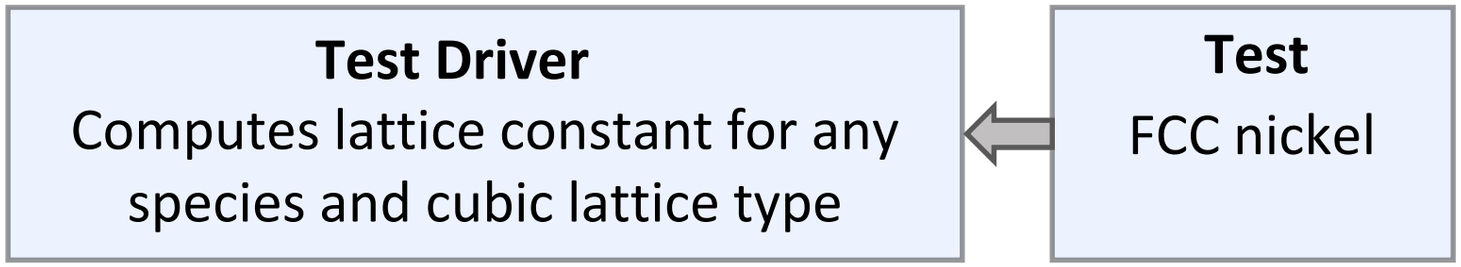
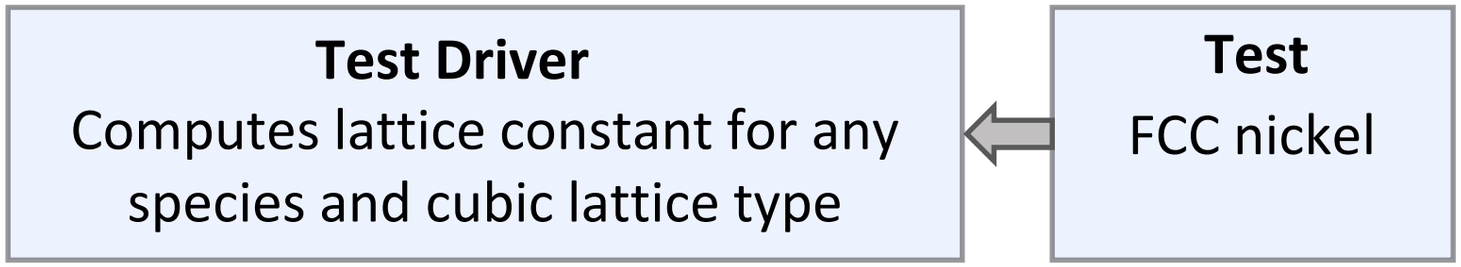


- Can be a program or an input file to a supported Simulator (e.g. ASE, LAMMPS, ...)
- What constitutes a KIM Property?

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

- Usually a parameter set that is read in by a *Test Driver*, e.g.:



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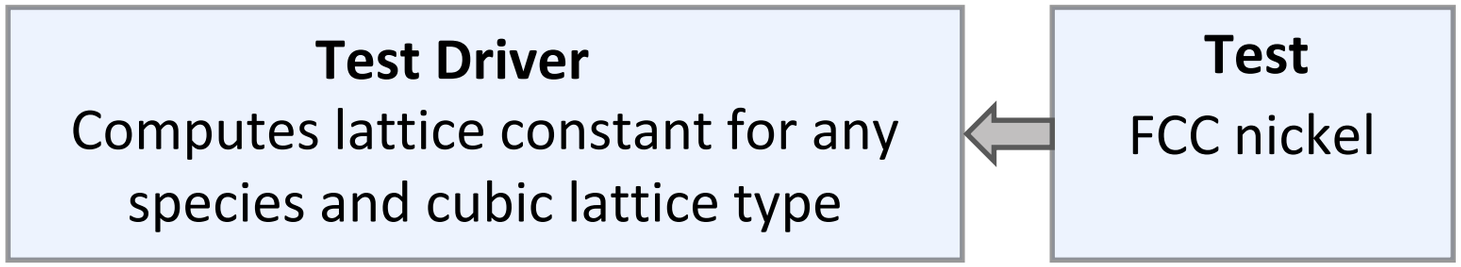

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  - A "canonical property," i.e. a basic atomistic property to which Models are often fitted and from which larger-scale behavior might be inferred

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

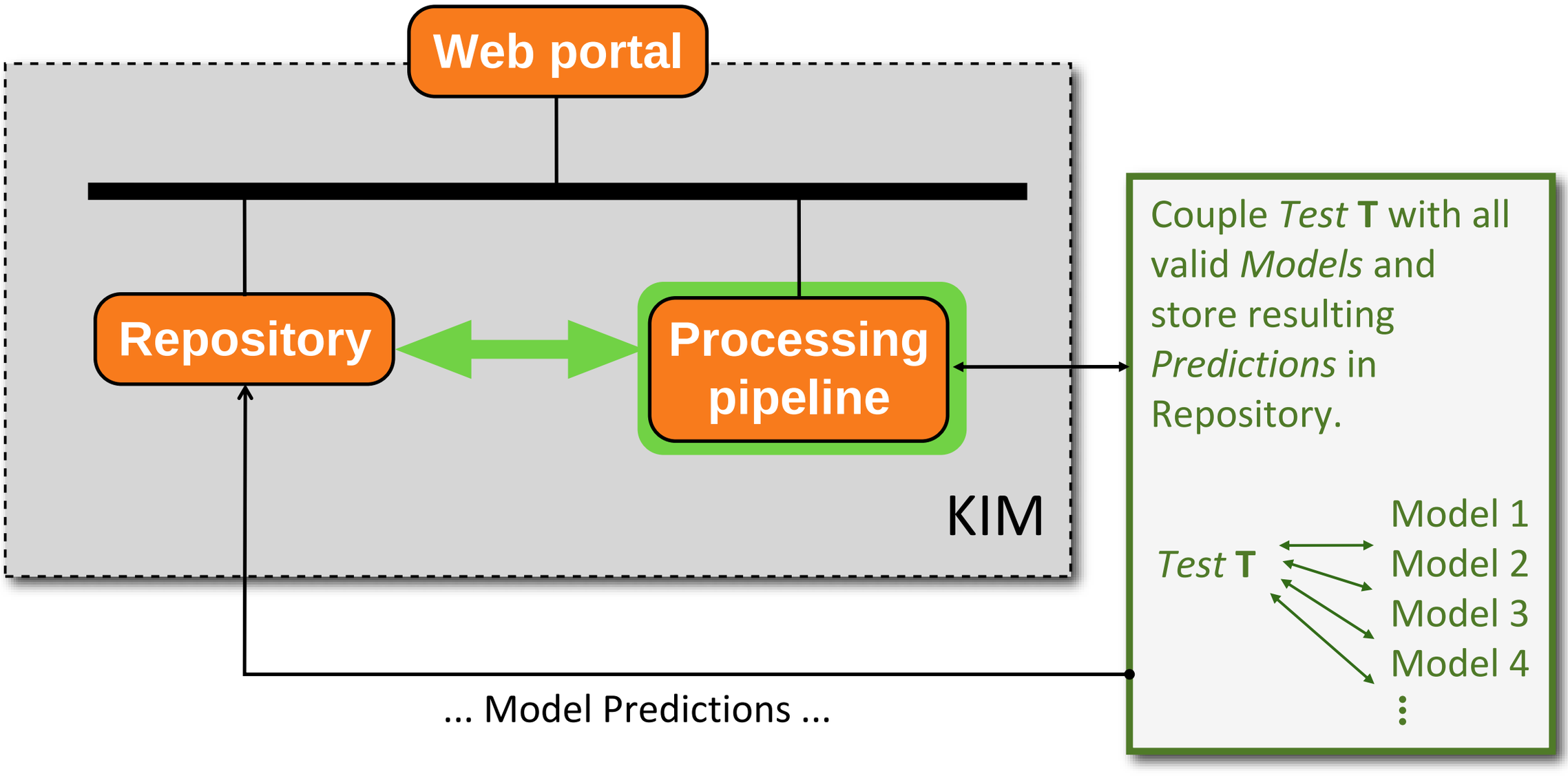
Wall
- surface energy
- surface structure
- gamma surface
- grain boundary structure
- ...

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

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

Interacting with KIM

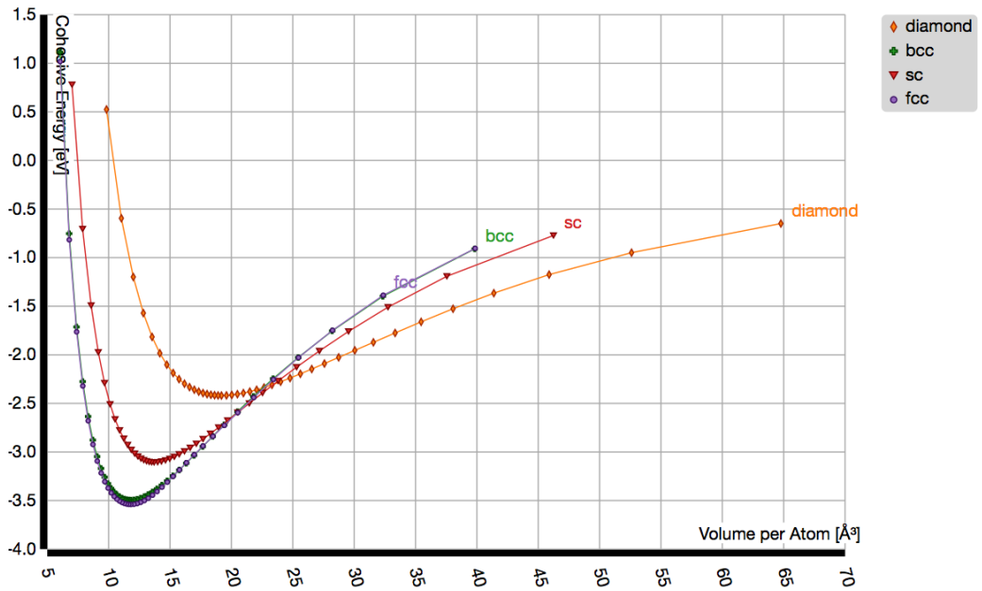
Uploading new KIM Test to the OpenKIM Repository



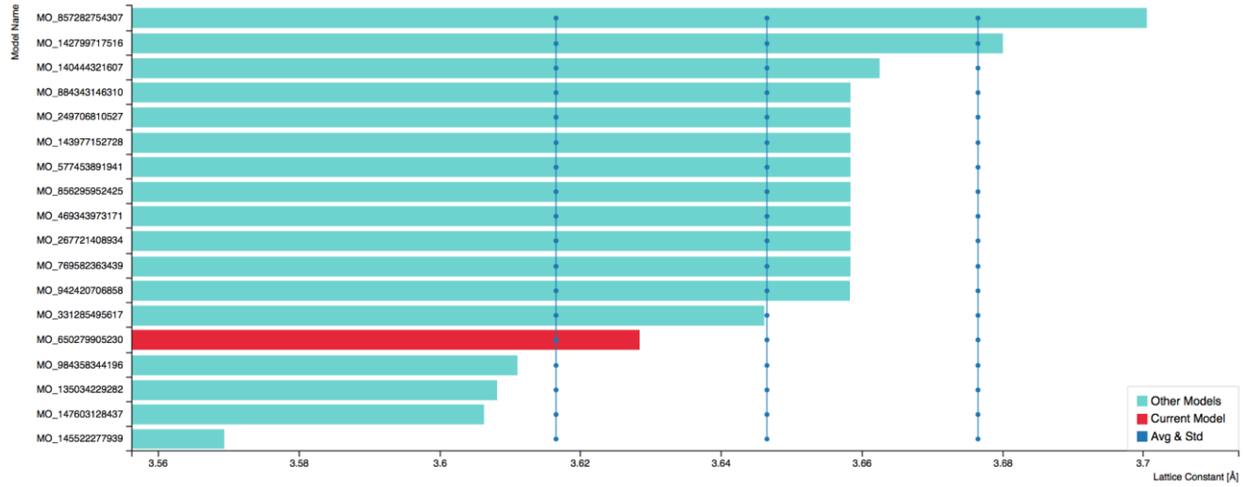
KIM Visualization

- KIM Visualizers are designed to display/analyze Test results 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 (C3, D3) and templates developed in KIM

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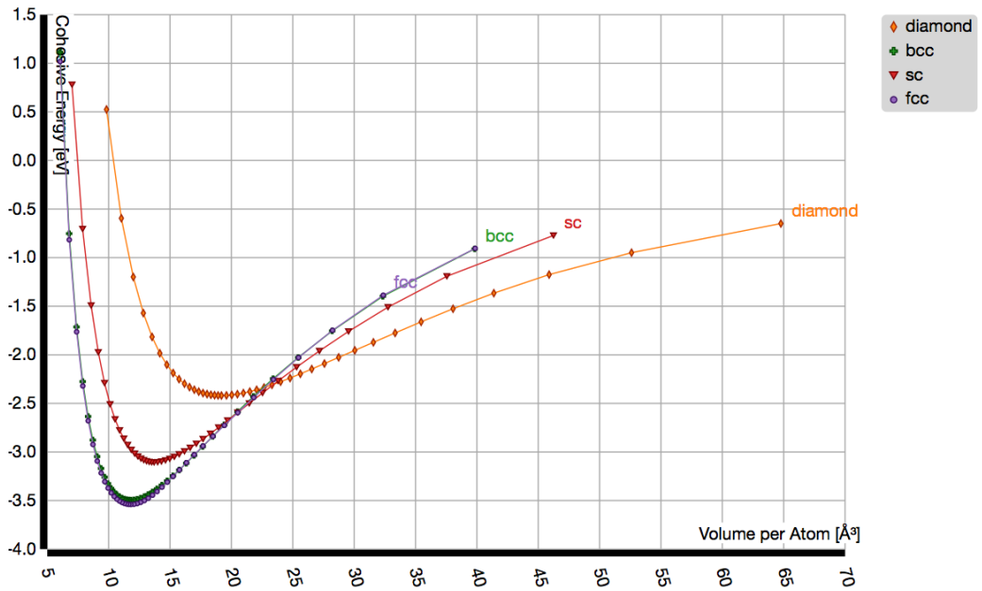

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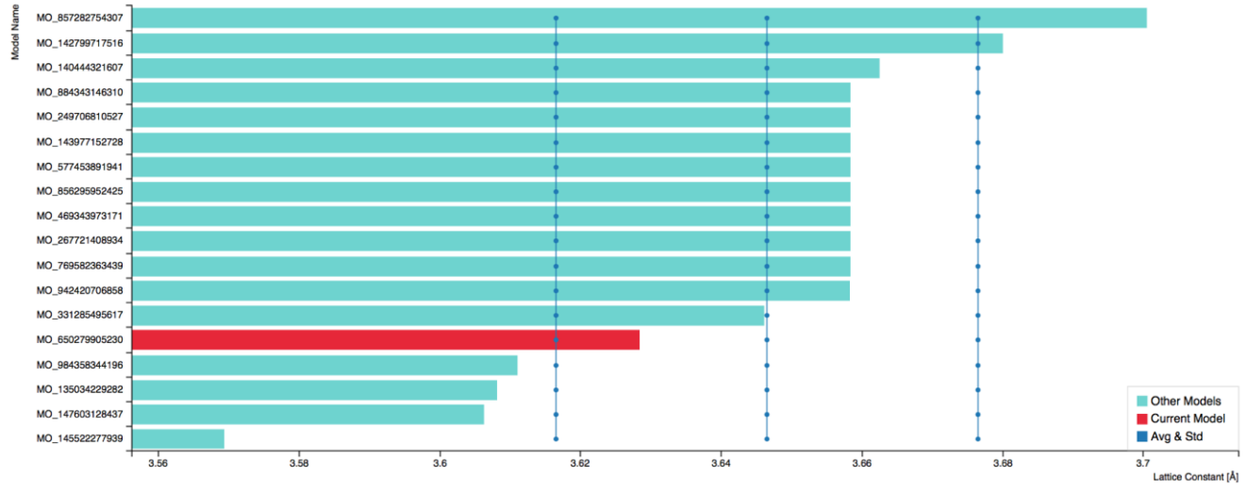

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➡ Submit your own (tutorials available)

KIM Models (https://openkim.org)

OpenKIM | Getting Started | About | Developers | Repository | Support | Member Login

"All models are wrong but some are useful."
— George E. P. Box

Welcome to the **K**nowledgebase of **I**nteratomic **M**odels!

OpenKIM is an online framework for making molecular simulations reliable, reproducible, and portable. Computer implementations of interatomic models are archived in OpenKIM, verified for coding integrity, and tested by computing their predictions for a variety of material properties. Models conforming to the KIM *application programming interface* (API) work seamlessly with major simulation codes that have adopted the KIM API standard.

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07-Jul-2018
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Metrics

Model Drivers 23

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KIM Models

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KIM Models (interatomic potentials and force fields) are software packages for describing atomic interactions that can be used with a variety of simulation codes, including LAMMPS, DL_POLY, IMD, ASE and GULP, that are compatible with the KIM API standard.

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra		Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo

La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

0 Models — 30 Models

Click here for index of Models

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Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra		Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo

0 Models — 30 Models

La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Click here for index of Models

KIM Models (https://openkim.org)

Cu

Extended KIM ID	Title
EAM_Dynamo_Ackland_Tichy_Cu__MO_179025990738_004	Finnis-Sinclair potential for Cu developed by Ackland et al. (1987)
EAM_Dynamo_Bonny_Pasianot_FeCuNi__MO_469343973171_004	FeCuNi potential to model reactor pressure vessel steels
EAM_Dynamo_Cai_Ye_AlCu__MO_942551040047_004	EAM potential for Al-Cu binary system
EAM_Dynamo_Foiles_Baskes_Universal3_Cu__MO_666348409573_003	Third universal Cu potential of Foiles, Baskes, and Daw; obtained from LAMMPS
EAM_Dynamo_Hoyt_Garvin_PbCu__MO_119135752160_004	Embedded Atom Method parametrization of the Pb-Cu system
EAM_Dynamo_Mendelev_King_Cu__MO_748636486270_004	FS potential for Cu
EAM_Dynamo_Mendelev_Kramer_Cu__MO_945691923444_004	FS/EAM potential for Cu
EAM_Dynamo_Mendelev_Kramer_CuZr__MO_600021860456_004	FS potential for Cu-Zr
EAM_Dynamo_Mendelev_Sordelet_CuZr__MO_120596890176_004	FS potential for Cu-Zr
EAM_Dynamo_Mishin_Mehl_Cu__MO_346334655118_004	EAM Cu Potential
EAM_Dynamo_Onat_Durukanoglu_CuNi__MO_592013496703_004	An optimized EAM potential for Cu-Ni alloys
EAM_Dynamo_Williams_Mishin_CuAg__MO_128703483589_004	EAM alloy potential for the Cu-Ag system.
EAM_Dynamo_Wu_Trinkle_CuAg__MO_270337113239_004	EAM potential for Cu/Ag(111) Surface Diffusion.
EAM_Dynamo_Zhou_Johnson_Cu__MO_127245782811_004	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.
LennardJones612_UniversalShifted__MO_959249795837_002	Efficient "universal" shifted Lennard-Jones model for all KIM API supported species
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KIM Models (https://openkim.org)

KIM Items / Models / EAM_Johnson_NearestNeighbor_Cu__MO_887933271505_001

Jump to: Tests | Visualizers | Files | Wiki

EAM_Johnson_NearestNeighbor_Cu__MO_887933271505_001

Title	This is an analytical NN EAM model for Cu by Johnson.
Description	This is an analytical NN EAM model for Cu by Johnson.
Species	Cu
Disclaimer	None
Contributor	Ryan
Maintainer	Ryan
Author	Ryan S. Elliott
Publication Year	2014
Source Citations	Johnson RA (1988) Analytic nearest-neighbor model for fcc metals. *Physical Review B* 37(8):3924–3931. doi:10.1103/PhysRevB.37.3924
Item Citation	Click here to download a citation in BibTeX format.
Short KIM ID	MO_887933271505_001
Extended KIM ID	EAM_Johnson_NearestNeighbor_Cu__MO_887933271505_001
Citable Link	https://openkim.org/cite/MO_887933271505_001
KIM Item Type	Stand-alone Model
Programming Language(s)	100.00% C

KIM Models (https://openkim.org)

- Further down the model page for
  EAM_Johnson_NearestNeighbor_Cu_MO_887933271505_001

Verification Check Dashboard

(Click here to learn more about Verification Checks)

Grade	Name	Category	Brief Description	Full Results	Aux File(s)
P	**vc-species-supported-as-stated**	mandatory	The model supports all species it claims to support; see full description.	Results	Files
P	**vc-periodicity-support**	mandatory	Periodic boundary conditions are handled correctly; see full description.	Results	Files
P	**vc-permutation-symmetry**	mandatory	Total energy and forces are unchanged when swapping atoms of the same species; see full description.	Results	Files
A	**vc-forces-numerical-derivative**	consistency	Forces computed by the model agree with numerical derivatives of the energy; see full description.	Results	Files
F	**vc-dimer-continuity-c1**	informational	The energy versus separation relation of a pair of atoms is C1 continuous (i.e. the function and its first derivative are continuous); see full description.	Results	Files
P	**vc-objectivity**	informational	Total energy is unchanged and forces transform correctly under rigid-body translation and rotation; see full description.	Results	Files
P	**vc-inversion-symmetry**	informational	Total energy is unchanged and forces change sign when inverting a configuration through the origin; see full description.	Results	Files
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P	**vc-thread-safe**	mandatory	The model returns the same energy and forces when computed in serial and when using parallel threads for a set of configurations. Note that this is not a guarantee of thread safety; see full description.	Results	Files

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Numerical differentiation check of forces using Richardson extrapolation

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Memory leak check using the valgrind memory debugging tool

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Python-based verification releasing the Global Interpreter Lock (GIL) to test thread parallelism.

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Cutoff smoothness and discontinuity detection using 5th order local difference formula

KIM Models (https://openkim.org)

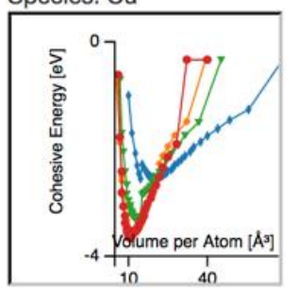
Further down the model page for
EAM_Johnson_NearestNeighbor_Cu_MO_887933271505_001

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.

Diamond Lattice Constant

This bar chart plot shows the mono-atomic face-centered diamond lattice constant predicted by the current model (shown in the unique color) 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.

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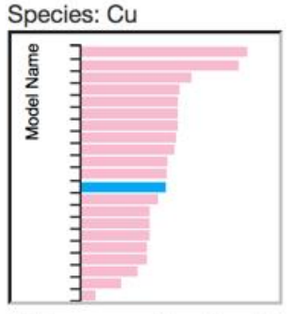

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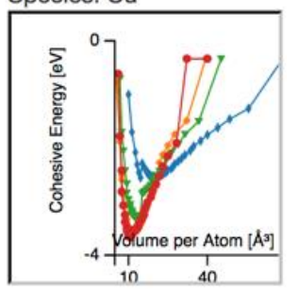
Species: Cu

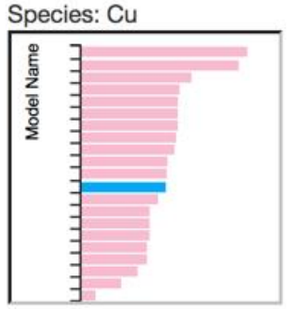


Click on any thumbnail to get a full size image.

Diamond Lattice Constant

This bar chart plot shows the mono-atomic face-centered diamond lattice constant predicted by the current model (shown in the unique color) 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



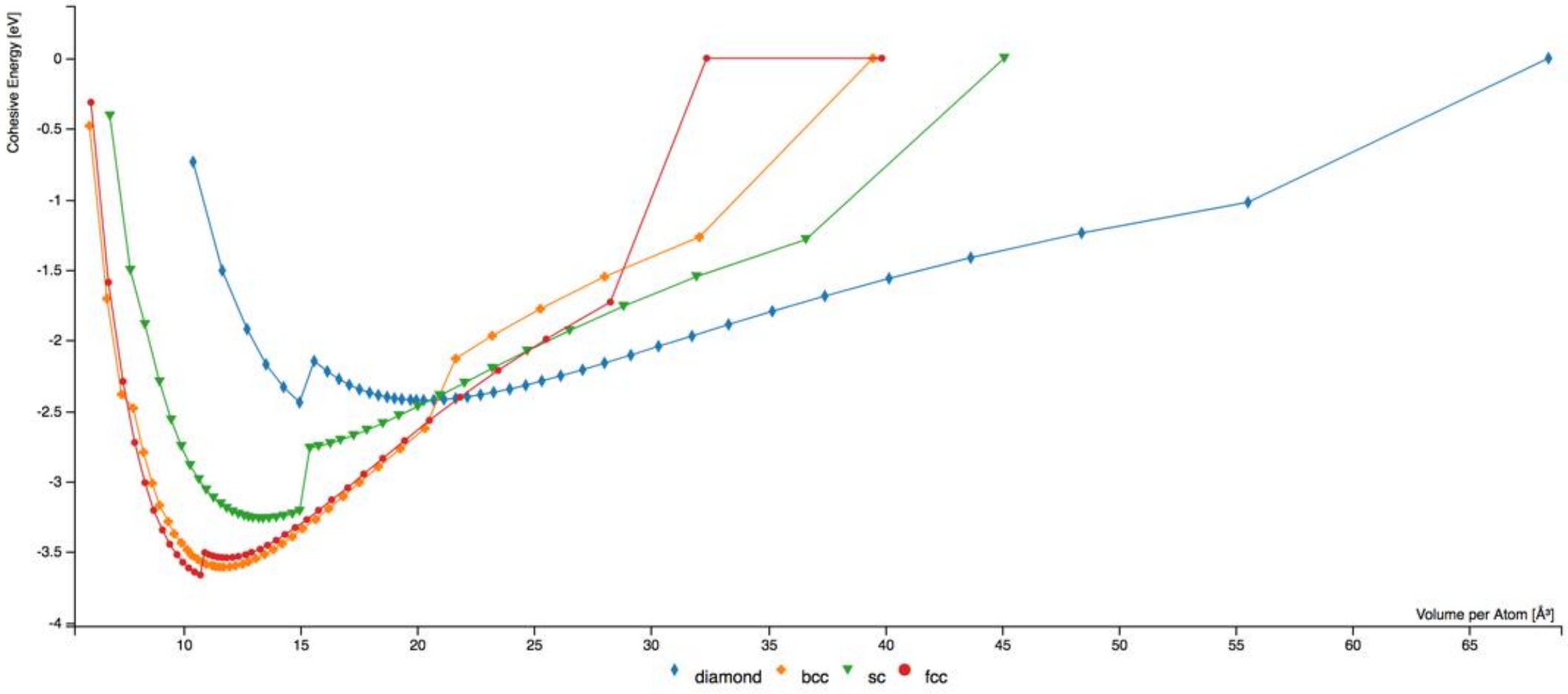
Click on any thumbnail to get a full size image.

KIM Models (https://openkim.org)

OpenKIM

Model: EAM_Johnson_NearestNeighbor_Cu__MO_887933271505_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.



KIM Models (https://openkim.org)

Further down the model page for
EAM_Johnson_NearestNeighbor_Cu_MO_887933271505_001

Cubic Crystal Basic Properties Table

Species: Cu

	Model	Lattice Constant [Å]	Cohesive Energy [eV]	c11 [GPa]	c12 [GPa]	c44 [GPa]
bcc Expand	EAM_Johnson_NearestNeighbor_Cu__MO_887933271505_001	2.85939610004	3.6063831577047547	146.260877653000002	137.952175647000002	91.9367752334
diamond Expand	EAM_Johnson_NearestNeighbor_Cu__MO_887933271505_001	5.450421601530001	2.4241832490740016	N/A	N/A	N/A
fcc Expand	EAM_Johnson_NearestNeighbor_Cu__MO_887933271505_001	3.61472985148	3.540000123312368	184.172808464	115.324864339	68.8519693906
sc Expand	EAM_Johnson_NearestNeighbor_Cu__MO_887933271505_001	2.372449815270004	3.263473577969841	270.847253148	24.4996165814	-17.5854303931

KIM Models (https://openkim.org)

- Further down the model page for
  EAM_Johnson_NearestNeighbor_Cu_MO_887933271505_001

Cubic Crystal Basic Properties Table

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diamond Expand	EAM_Johnson_NearestNeighbor_Cu__MO_887933271505_001	5.450421601530001	2.4241832490740016	N/A	N/A	N/A
fcc Expand	EAM_Johnson_NearestNeighbor_Cu__MO_887933271505_001	3.61472985148	3.540000123312368	184.172808464	115.324864339	68.8519693906
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KIM Models (https://openkim.org)

- Further down the model page for EAM_Johnson_NearestNeighbor_Cu_MO_887933271505_001

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diamond Expand	EAM_Johnson_NearestNeighbor_Cu__MO_887933271505_001	5.450421601530001	2.4241832490740016	N/A	N/A	N/A
fcc Collapse	EAM_Johnson_NearestNeighbor_Cu__MO_887933271505_001	3.61472985148	3.540000123312368	184.172808464	115.324864339	68.8519693906
	EAM_Dynamo_Ackland_Tichy_Cu__MO_179025990738_004	3.61500008404	3.519353152563151	169.863009714000001	122.098874641000001	76.6212942879

KIM Models (https://openkim.org)

- Further down the model page for
  EAM_Johnson_NearestNeighbor_Cu_MO_887933271505_001

Tests

ElasticConstantsCubic__TD_011862047401_003

Measures the cubic elastic constants for some common crystal types (fcc, bcc, sc) by calculating the hessian of the energy density with respect to strain. Error estimate is reported due to the numerical differentiation.

This version fixes the number of repeats in the species key.

Test	Test Results	Link to Test Results page	Benchmark time
ElasticConstantsCubic_bcc_Cu__TE_091603841600_003	expand	view	2375
ElasticConstantsCubic_fcc_Cu__TE_188557531340_003	expand	view	48734
ElasticConstantsCubic_sc_Cu__TE_319353354686_003	expand	view	47151

KIM Models (https://openkim.org)

Further down the model page for
EAM_Johnson_NearestNeighbor_Cu_MO_887933271505_001

Tests

ElasticConstantsCubic__TD_011862047401_003

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ElasticConstantsCubic_fcc_Cu__TE_188557531340_003	expand	view	48734
ElasticConstantsCubic_sc_Cu__TE_319353354686_003	expand	view	47151

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.

KIM Models (https://openkim.org)

- Further down the model page for EAM_Johnson_NearestNeighbor_Cu_MO_887933271505_001

Tests

ElasticConstantsCubic__TD_011862047401_003

Measures the cubic elastic constants for some common crystal types (fcc, bcc, sc) by calculating the hessian of the strain. Error estimate is reported due to the numerical differentiation.

This version fixes the number of repeats in the species key.

Full results page.

Test	Test Results	Link to Test Results page	Benchmark time
ElasticConstantsCubic_bcc_Cu__TE_091603841600_003	expand	view	2375
ElasticConstantsCubic_fcc_Cu__TE_188557531340_003	expand	view	48734
ElasticConstantsCubic_sc_Cu__TE_319353354686_003	expand	view	47151

KIM Models (https://openkim.org)

- Further down the model page for
  EAM_Johnson_NearestNeighbor_Cu_MO_887933271505_001

- **Tests**

ElasticConstantsCubic__TD_011862047401_003

Measures the cubic elastic constants for some common crystal types (fcc, bcc, sc) by calculating the hessian of the energy density with respect to strain. Error estimate is reported due to the numerical differentiation.

This version fixes the number of repeats in the species key.

Test	Test Results	Link to Test Results page	Benchmark time
ElasticConstantsCubic_bcc_Cu__TE_091603841600_003	expand	view	2375
ElasticConstantsCubic_fcc_Cu__TE_188557531340_003	expand	view	48734
ElasticConstantsCubic_sc_Cu__TE_319353354686_003	expand	view	47151

Expand a property synopsis.

KIM Models (https://openkim.org)

- Further down the model page for EAM_Johnson_NearestNeighbor_Cu_MO_887933271505_001

Tests

ElasticConstantsCubic__TD_011862047401_003

Measures the cubic elastic constants for some common crystal types (fcc, bcc, sc) by calculating the hessian of the energy density with respect to strain. Error estimate is reported due to the numerical differentiation.

This version fixes the number of repeats in the species key.

Test	Test Results	Link to Test Results page	Benchmark time
ElasticConstantsCubic_bcc_Cu__TE_091603841600_003	expand	view	2375
ElasticConstantsCubic_fcc_Cu__TE_188557531340_003	expand	view	48734
ElasticConstantsCubic_sc_Cu__TE_319353354686_003	collapse	view	47151

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 = 2.37244981527 angstrom
Species = ["Cu"]
Basis atom coordinates = [[0.0 0.0 0.0]]

c11 = 270.847253148 GPa
c12 = 24.4996165814 GPa
c44 = -17.5854303931 GPa

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

KIM Models (https://openkim.org)

- Further down the model page for EAM_Johnson_NearestNeighbor_Cu_MO_887933271505_001

  - **Wiki**

Description

This **Model** implements the potential developed by R.A. Johnson for fcc metals as described in the reference above (see Source Citations). In particular, this model is applied to copper (Cu).

Parameters

Symbols (matching the reference):

$$r_e, \phi_e, \gamma, f_e, \beta, E_c, \alpha, \rho_e.$$

Corresponding variables in code:
JEAM_R0, JEAM_PHI0, JEAM_GAM, JEAM_G0, JEAM_BET, JEAM_EC, JEAM_ALF, JEAM_RHO0, where the prefix JEAM emphasizes the fact that each variable corresponds to the "Johnson Embedded Atom Potential".

Warning: The model uses other parameters DIM, SPECCODE and MODEL_CUTOFF denoting the dimensionality of the space (3 by default), the number of species (1, by default) and the cut-off radius (3.5 Angstrom by default), respectively. Default values have been hardcoded and, in principle, they should not be modified.

Details

The total potential energy of a system of N atoms is assumed to take the form $E = \sum_{i=1}^{N} E_i$, such that

$$E_i = \sum_{i=1}^{N} \left[F(\rho_i) + \frac{1}{2} \sum_{j=1}^{m} \phi(r_{ij}) \right],$$

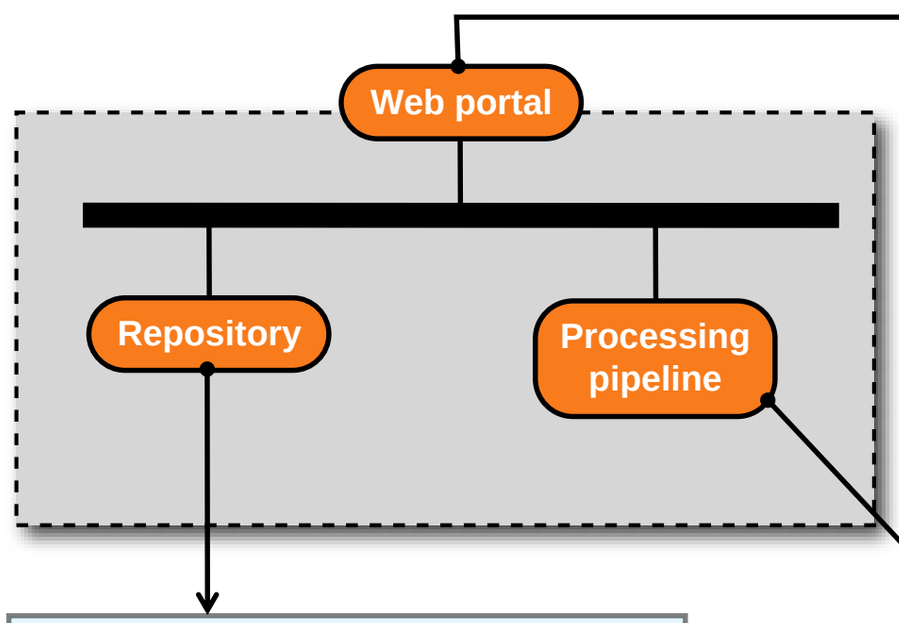
and

$$\rho_i = \sum_{j=1}^{m} f(r_{ij}),$$

where E_i denotes the energy per atom i, $F(\rho_i)$ is the embedding function contribution, $\frac{1}{2} \sum_{j=1}^{m} \phi(r_{ij})$ is the two-body contribution to the energy, ρ_i stands for the electron density at atom i, and $f(r_{ij})$ is the atomic electron density of atom j as a function of the distance from its center r_{ij}, while j is one of the m neighbors of the atom i.

...

Current Status (Aug. 2, 2018)



- Interface to explore content
- Content upload by members
- Forums and Wikis for member input

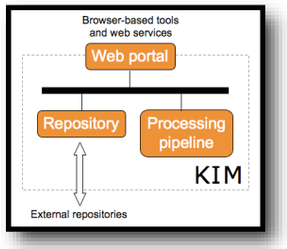
- 190 Models
- 2481 Tests
- 53 property definitions
- 9 Verification Checks

- Cloud-deployable
- Handling of dependencies
- User VM

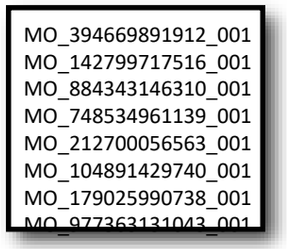
Software supporting KIM API:

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

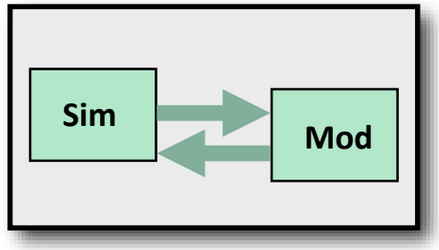
Summary



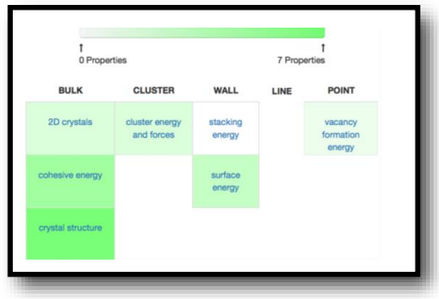
KIM provides archival permanent storage of interatomic models, tests, and reference data with known provenance.



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.

KIM API v2.0 coming soon!

KIM Models (https://openkim.org)

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"All models are wrong but some are useful."
— George E. P. Box

Welcome to the **K**nowledgebase of **I**nteratomic **M**odels!

OpenKIM is an online framework for making molecular simulations reliable, reproducible, and po
interatomic models are archived in OpenKIM, verified for coding integrity, and tested by computi
material properties. Models conforming to the KIM *application programming interface* (API) work
that have adopted the KIM API standard.

Become a member to get updates and vote on KIM policy

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Start here if you are new to KIM

News

07-Jul-2018
kim-api-v2.0.0-beta.1 and kim-api-v1.9.7 released

Metrics

Model Drivers 23