The OpenKIM project: Reproducibility, Portability and Metadata Standards in Molecular Simulation

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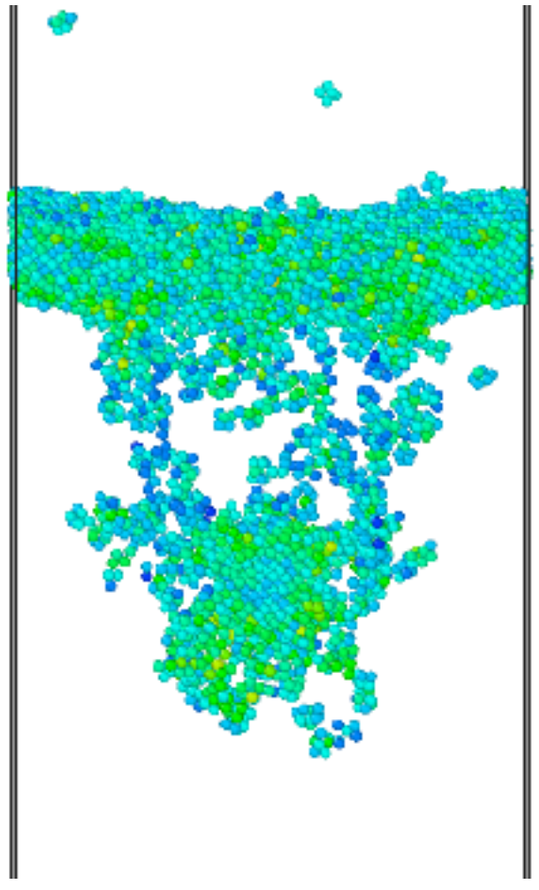
NSF CDI (2009-2014); NSF CDS&E (2014-2018); NSF CMMT (2019-)

A Simulation is Only as Good as the Potential

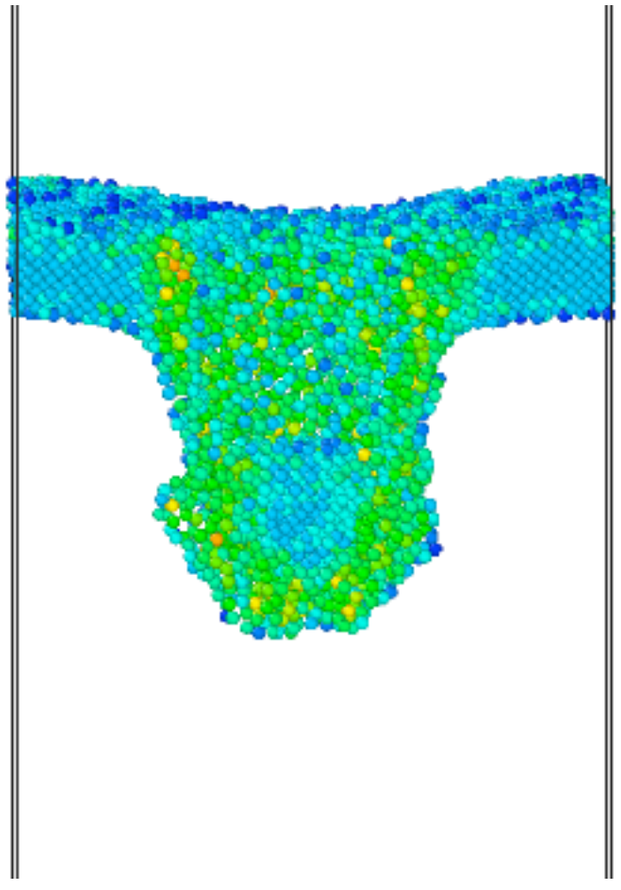
- The predictive capability of an atomistic simulation is dependent on the fidelity of the interatomic model (IM).

Example: Projectile impacting silicon plate

Tersoff Potential
exhibits brittle behavior



Stillinger-Weber Potential
exhibits ductile behavior



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

Interatomic Potentials for Silicon

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The Scream, Edvard Munch

The Problems with Molecular Modeling

- The KIM effort addresses key problems faced by molecular modelers:

Problem 1: **Reproducibility**. It is currently very difficult or even impossible for a researcher to reproduce published results obtained using molecular simulations with a given IM or to use the same IM in a different study.

Archival Storage DOIs

Problem 2: **Portability**. It is very difficult to port IMs between simulation codes that have different program architectures and may be written in different computer languages. (Interoperable)

KIM API

Problem 3: **Re-inventing the wheel.** A great deal of researcher time is spent redeveloping methods for computing complex material properties (e.g. melting temperature, thermal conductivity, phonon spectra, etc.). (Accessible, Recyclable)

KIM Tests

The Problems with Molecular Modeling

- The KIM effort addresses key problems faced by molecular modelers:

Problem 4: **Coding Errors.** Programming errors in IM implementations can lead to systematic errors that can go unnoticed, or result in strange behavior that can be extremely difficult and time-consuming to debug.

KIM Verification Checks

Problem 5: **Diffuse Knowledge.** Researchers do not have a central location to exchange information about specific IMs and share analysis and visualization tools that they have developed related to molecular simulation. (Findable, Accessible)

KIM Model Pages Central Discussion Forum

Problem 6: **Too many options.** Researchers do not have a systematic way of choosing an IM for a given application. (Recyclable)

RATE Multitask Learning of Transferability

The Problems with Molecular Modeling

- The KIM effort addresses key problems faced by molecular modelers:

Problem 7: **Uncertainty.** Researchers rarely estimate the predictive uncertainty of IMs, i.e. systematic errors due to the mathematical representation of the IM (functional forms and parameters).

Model Ensembles UQ

Problem 8: **Access.** Researchers do not have easy and reliable access to predictions of an IM for certain properties needed for problem setup or analysis, e.g. an equilibrium lattice constant is required to build a crystal or a bulk cohesive energy is required in a surface energy calculation. (Findable, Accessible)

KIM Queries

Knowledgebase of Interatomic Models

The Open Knowledgebase of Interatomic Models (KIM) is a cyberinfrastructure funded by the U.S. National Science Foundation (NSF) with the following features:

- Curated repository interatomic models (IMs) (potentials and force fields) with comprehensive provenance and version control.
- Application Programming Interface (API) standards connecting molecular simulation codes ("simulators") with IMs.
- Standardized testing framework for archived IMs including their predictions for material properties and checks on their coding integrity.
- Source and binary distribution framework for easy installation and use of the KIM API and KIM IMs with conforming simulators.
- Rigorous transferability and uncertainty estimation for KIM IMs based on machine learning approaches to select IMs for target application and providing error bounds on their predictions. (under development)

KIM Community

- KIM is a collaborative effort.

  It began with the KIM Inaugural meeting 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 Inaugural Meeting, San Diego, February 2011

- KIM currently has 460 registered members in 43 countries (June 28, 2019)
- The project actively collaborates with many researchers:
  - Nikhil Admal (UIUC)
  - Noam Bernstein (NRL)
  - Richard Berger (Temple)
  - Tobias Brink (TU Darmstadt)
  - David Cereceda (Villanova)
  - Lauren Dupuy (CEA)
  - Julian Gale (Curtin)
  - Anton Gladky (Debian)
  - Ben Haley (nanoHUB)
  - Christoph Junghans (LANL)
  - Axel Kohlmeyer (Temple)
  - Jim Madge (STFC)
  - Jens Mortensen (DTU)
  - Brandon Runnels (U. Colorado)
  - Enrique Martinez Saez (LANL)
  - Jakob Schiøtz (DTU)
  - Daniel Schopf (Cinemo GmbH)
  - Amit Singh (IIT Bombay)

KIM Governance

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Mark Transtrum
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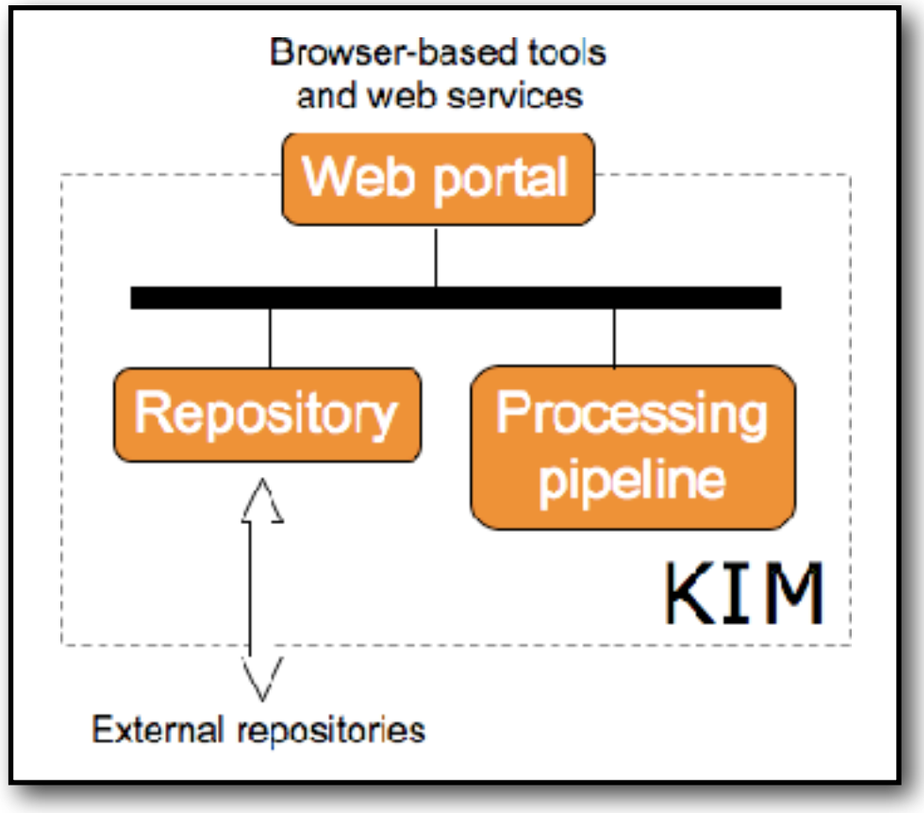
(U, Minnesota)

KIM Research Assoc

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)
- *Verification Checks* (coding integrity scripts)

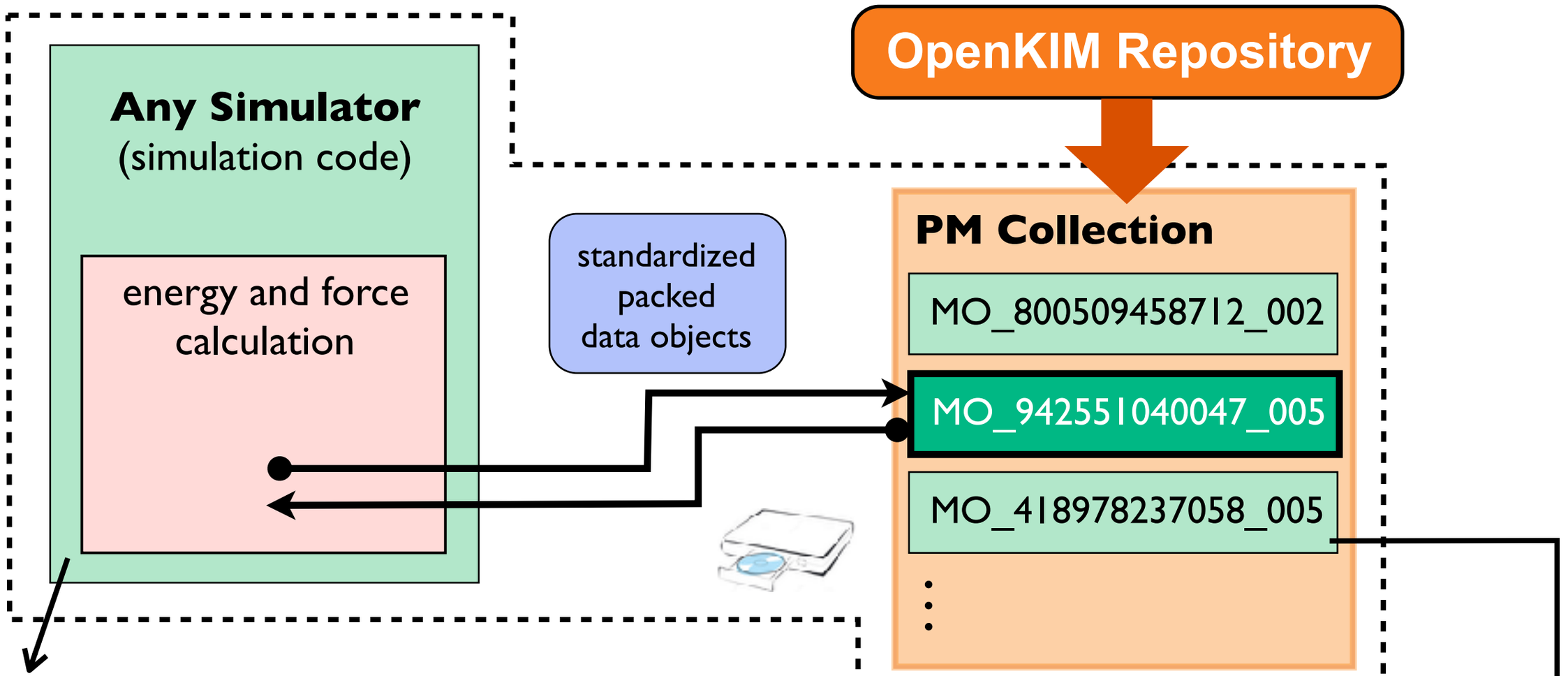


Web portal: A web interface that facilitates:
- user upload and download of Tests, Models, and Reference Data
- searching and querying the repository
- comparing and visualizing Predictions and Reference Data
- recording user feedback

Processing pipeline: An automatic system for generating results by mating *Tests* and *Verification Checks* with *Models* in the KIM Repository.
- puts the "knowledge" in "knowledgebase"
- employs OS virtualization and cloud-based computing

KIM API — Portable Models

- KIM Models employ the KIM Application Programming Interface (API).
  - Portable Models (PMs) conform to the KIM API Portable Model Interface (PMI)

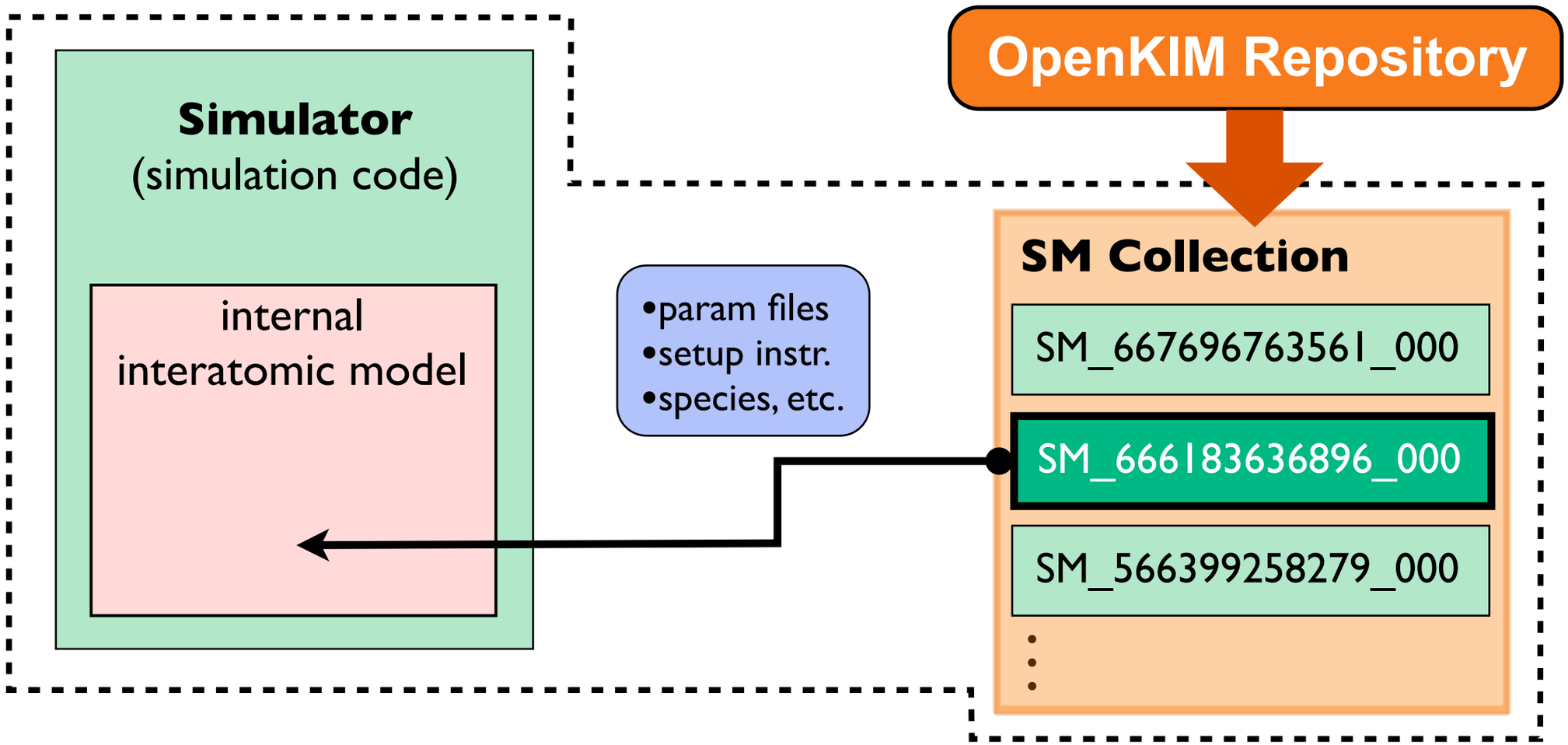


- Stand-alone simulation computer program (MD, lattice dynamics, etc.)
- Can be written in any language supported by the API (Fortran, C, C++, Python)

- Autonomous code that given a set of atomic positions, species, ... computes energy, forces, ...
- Can be written in any language supported by the API (Fortran, C, C++)

KIM API — Simulator Models

- KIM Models employ the KIM Application Programming Interface (API).
  - Simulator Models (SMs) conform to the KIM API Simulator Model Interface (SMI)



- The KIM API v2 is designed with simplicity in mind and adheres to API best practices:

• Implementation hiding (pimpl idiom)	• Ease of use (discoverable, consistent, orthogonal)	• Use of namespaces
• Loose coupling	• Static factory methods	• Const-correctness
• Minimal-completeness		• Avoid abbreviations

KIM-Compliant Simulators

Asap

ase

nanoHUB

DL_POLY

potfit

GULP

LAMMPS

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

libAtoms + QUIP

MDStressLab

Example: Using KIM PMs or SMs with LAMMPS

- Every KIM PM and SM is uniquely identified by a KIM ID:

EAM_Dynamo_ErcolessiAdams_1994_Al__MO_123629422045_005

human-readable prefix | Unique identifier (12 digit + 3 digit version)

- Using KIM PMs or SMs with LAMMPS is straightforward:
  - Install the KIM API from source or binary (packages available for Ubuntu, CentOS, Fedora, OpenSUSE, Homebrew).
  - Add the KIM Models that you want to use. (Binary packages have option to add all models.)
  - Replace native potential with kim commands to select a model based on its KIM ID:*

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

```
kim_init          kim EAM_Dynamo_ErcolessiAdams_1994_Al__MO_123629422045_005 metal
kim_interactions Al
```

Citing KIM Models (PMs and SMs)

- KIM is a member of DataCite and issues DOIs to content on openkim.org, which can be cited in publications:

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

References

1. R. A. Johnson, "Analytic nearest-neighbor model for fcc metals", *Phys. Rev. B*, **37**, 3924–3931, 1988.

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The ability to cite a DOI and have access to the archived KIM PMs and SMs makes it possible to reproduce atomistic simulations.

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. ASE, 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
- ...

KIM Property Definition Format

- A Property Definition is stored in a subset of EDN format and contains an unordered set of three required key-value pairs followed by an arbitrary number of key-map pairs:

required

```
{
  "property-id" "<unique ID in Tag URI scheme>"
  "property-title" "<one-line title of property>"
  "property-description" "<brief description of property>"
```

one or more keys

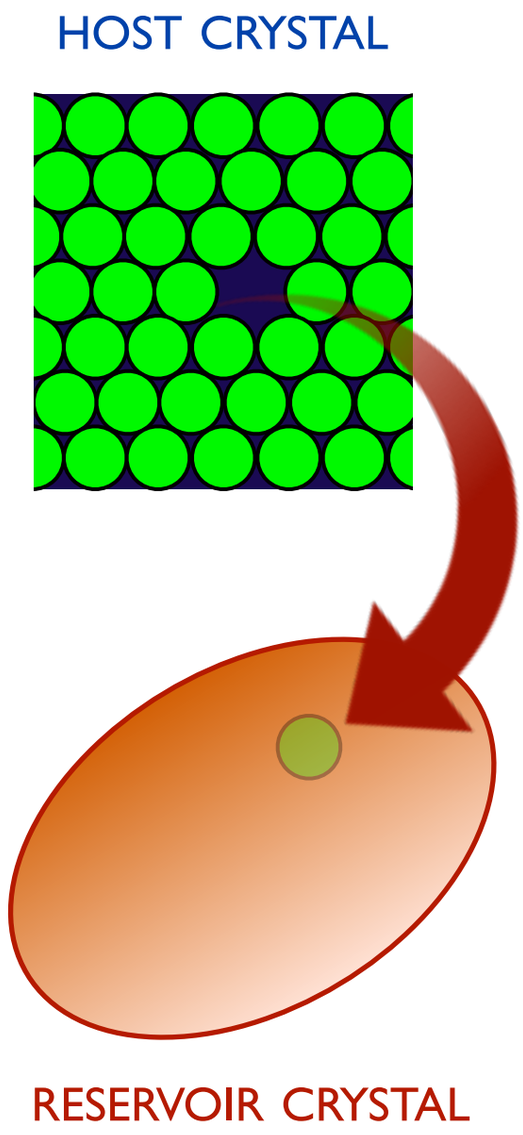
```
  "<key name>" {
     "type"  "string | float | int | bool"
     "has-unit"  "true | false"
     "extent"  "<bounds specification>"
     "required"  "true | false"
     "description"  "<brief description of the key>"
  }
  .
  .
  .
}
```

Property Definition Example

monovacancy-formation-free-energy-crystal-npt

host-short-name	reservoir-short-name
host-a	reservoir-a
host-b	reservoir-b
host-c	reservoir-c
host-alpha	reservoir-alpha
host-beta	reservoir-beta
host-gamma	reservoir-gamma
host-space-group	reservoir-space-group
host-wyckoff-multiplicity	reservoir-wyckoff-multiplicity
host-wyckoff-coordinates	reservoir-wyckoff-coordinates
host-wyckoff-species	reservoir-wyckoff-species
host-temperature	reservoir-temperature
host-cauchy-stress	reservoir-cauchy-stress
host-removed-atom	reservoir-cohesive-free-energy

formation-free-energy



Example of a Property Definition

monovacancy-formation-free-energy-crystal-npt

```
{
  "property-id" "tag:staff@noreply.openkim.org,2014-08-21:property/monovacancy-formation-..."

  "property-title" "Formation free energy of a monovacancy in a crystal at finite temperature and ..."

  "property-description" "Gibbs free energy of formation a monovacancy in a ..."

  "host-short-name" {
    "type"         "string"
    "has-unit"     false
    "extent"       [":"]
    "required"     false
    "description"  "Short name describing the host crystal type (e.g. fcc, bcc, diamond)."
  }
  "host-a" {
    "type"         "float"
    "has-unit"     true
    "extent"       []
    "required"     true
    "description"  "The average length of the host crystal unit cell vector <a>. The associated ..."
  }
...
```

Property Instance

- A Property Instance is either a Prediction or Reference Data conforming to the specification in the associated Property Definition:

required

```
{
  "property-id" "<unique ID in Tag URI scheme>"

  "instance-id" <ID for multiple instances>
```

one or more keys

```
  "<key name>" {
     "source-value"  <value of the variable>
     "source-unit"  "<physical units>"
     "source-unit-uncert-value" <value of uncertainty>
     .
     .
     .
     "digits"  <number of reported digits>
  }
  .
  .
  .
}
```

Uncertainty measures conforming to the ISO standard.

Example of a Property Instance

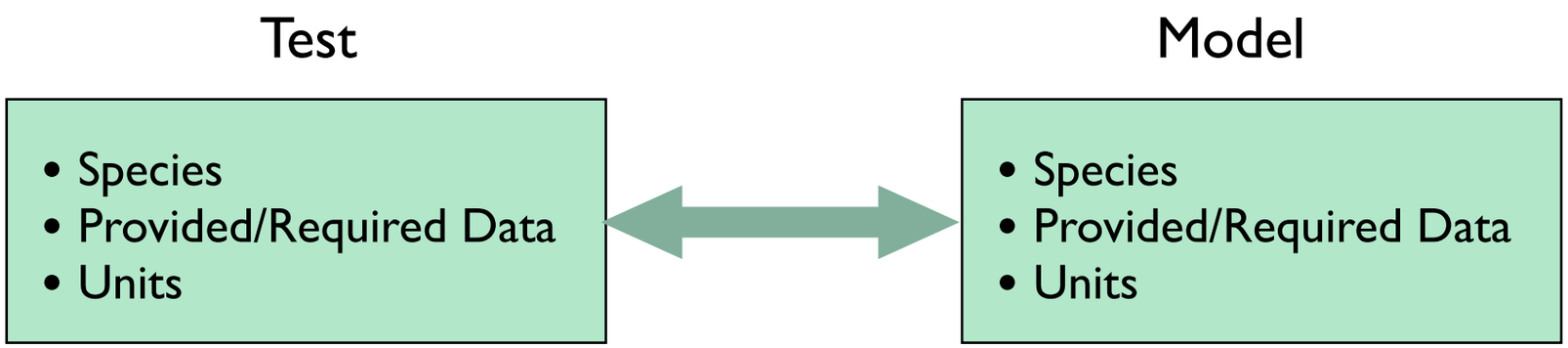
monovacancy-formation-free-energy-crystal-npt

```
{
  "property-id" "tag:staff@noreply.openkim.org,2014-08-21:property/monovacancy-formation-..."

  "instance-id" 1

  "host-short-name" {
     "source-value" [ "fcc" ]
  }
  "host-a" {
     "source-value" 4.032
     "source-unit" “angstrom”
     "digits" 5
   }
   "host-b" {
     "source-value" 4.032
     "source-unit" “angstrom”
     "digits" 5
   }
   "host-c" {
     "source-value" 4.032
      ...
}
```

KIM Processing Pipeline: Test/VC–PM/SM Coupling

Processing pipeline: An automatic cloud-based system for generating results due to new *Test/VC* or *Portable/Simulator Model* upload or changes in the OpenKIM Repository:

- Detect viable Test–PM/SM couplings (VCs run with all PMs and SMs)

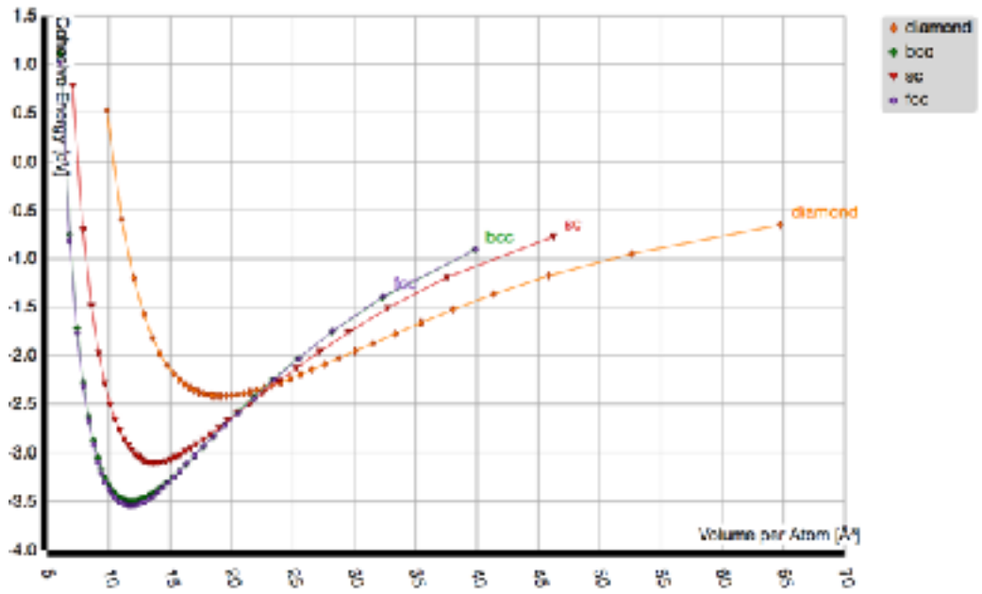


- Uses Celery (an asynchronous queuing system based on message passing) to assign tasks to virtual machine workers.
- Handles dependencies between Tests
- Coordinates with WebApp to Store Test and VC Results in the OpenKIM Repository
- Written in Python

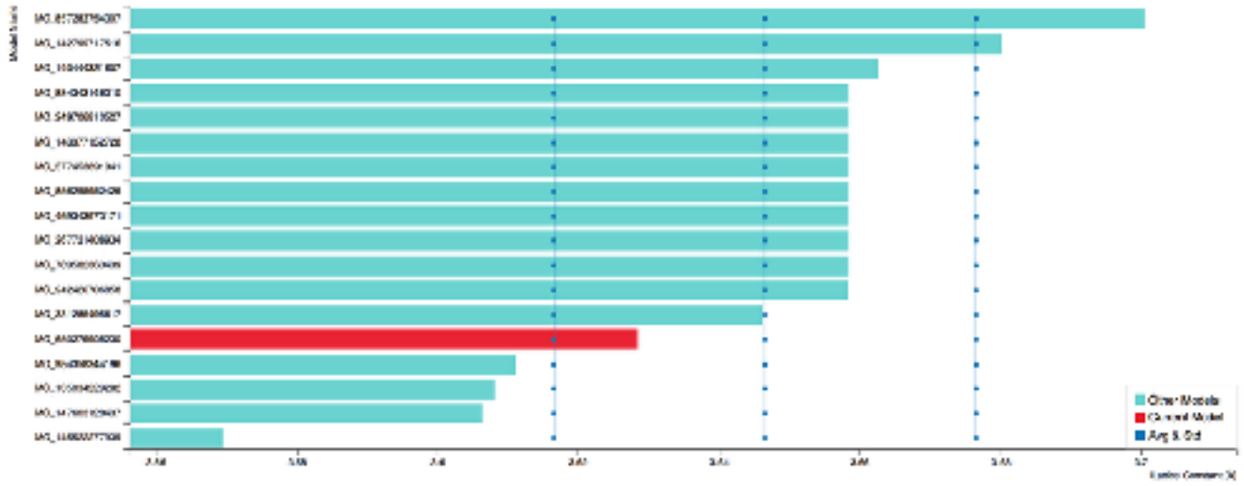
KIM Visualization

- 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

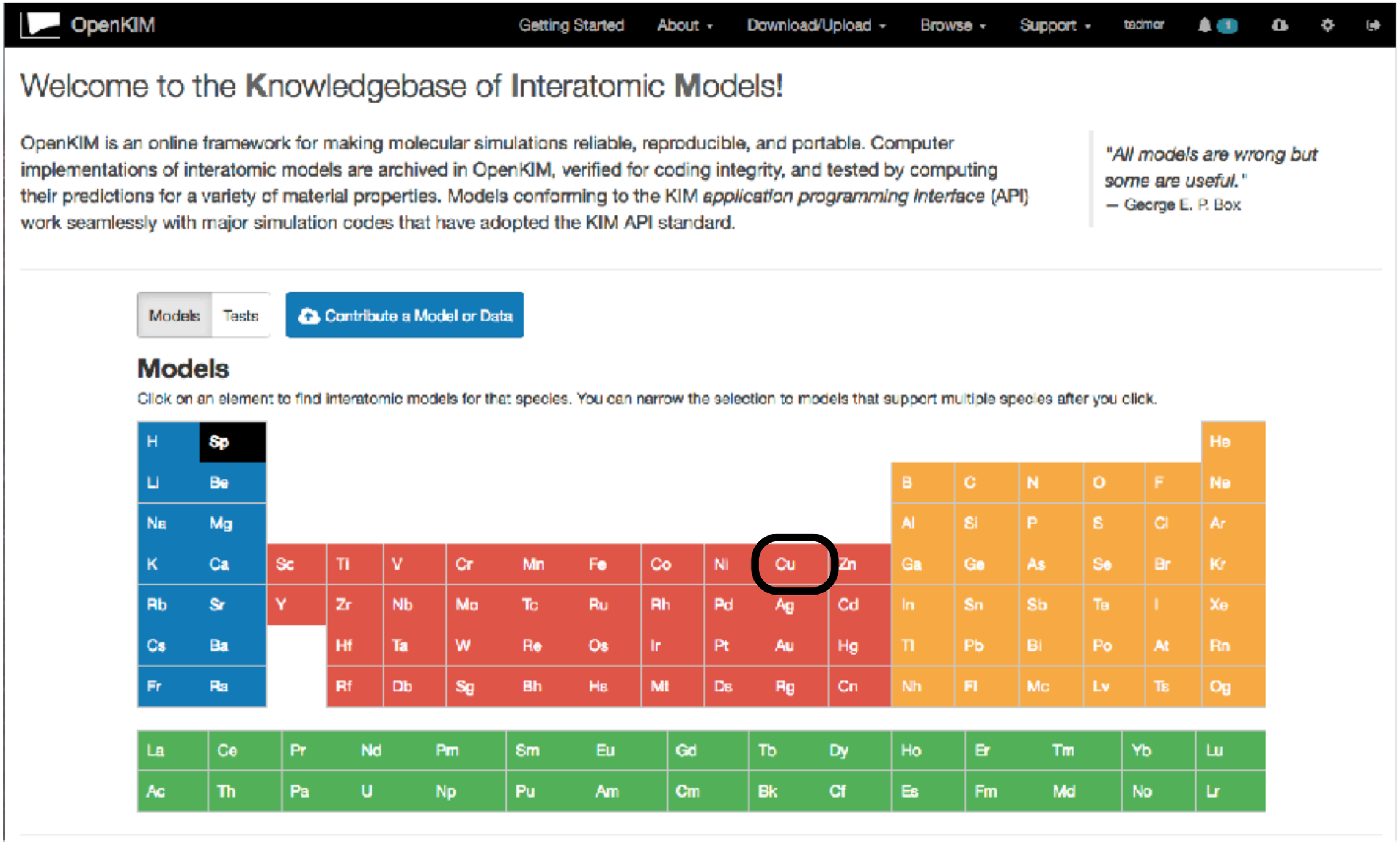


KIM Visualizers work by

- 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

Models on openkim.org



Models on openkim.org

Cu

Extended KIM ID	Title
EAM_Dynamo_AcklandTichyVitek_1987_Cu__MO_179025990738_005	Finnis-Sinclair potential (LAMMPS cubic hermite tabulation) for Cu developed by Ackland et al. (1987) v005
EAM_Dynamo_AcklandTichyVitek_1987v2_Cu__MO_762736677654_000	Finnis-Sinclair potential (LAMMPS cubic hermite tabulation) for Cu developed by Ackland et al. (1987), version 2 refitted for radiation studies v000
EAM_Dynamo_AcklandVitek_1990_Cu__MO_542748370524_000	Finnis-Sinclair potential (LAMMPS cubic hermite tabulation) for Cu developed by Ackland and Vitek (1990) v000
EAM_Dynamo_AdamsFoiles_1989Universal6_Cu__MO_145873821697_000	EAM potential (LAMMPS cubic hermite tabulation) for Cu [Universal6] developed by Adams and Foiles (1989) v000

-
-
-

EAM_Dynamo_ZhouWadleyJohnson_2001_CuTa__MO_547741193826_000	EAM potential (LAMMPS cubic hermite tabulation) for the Cu-Ta system developed by Zhou, Wadley and Johnson (2001) v000
[illegible]	EAM potential (LAMMPS cubic hermite tabulation) for Cu developed by Zhou, Wadley and Johnson (2001) v000
EAM_NN_Johnson_1968_Cu__MO_887933271503_002	EAM Potential (analytical nearest-neighbor) for Cu developed by Johnson (1968) v002
EMT_Asap_MetalGlass_BaileySchiotzJacobsen_2004_CuMg__MO_226059236215_001	EMT potential for Cu-Mg metallic glasses developed by Bailey, Schiotz, and Jacobsen (2004) v000
EMT_Asap_MetalGlass_CuMgZr__MO_655725647552_002	Effective Medium Theory potential for CuMg and CuZr alloys, in particular metallic glasses.
EMT_Asap_MetalGlass_PaduraruKenoufiBailey_2007_CuZr__MO_967541074959_001	EMT potential for Cu-Zr metallic glasses developed by Paduraru et al. (2007) v000
EMT_Asap_Standard_JacobsenStoltzeNorskov_1996_AlAgAuCuNiPdPt__MO_115316750986_001	EMT potential for Al, Ni, Cu, Pd, Ag, Pt and Au developed by Jacobsen, Stoltze, and Norskov (1996) v000
EMT_Asap_Standard_JacobsenStoltzeNorskov_1996_Cu__MO_396616545191_001	EMT potential for Cu developed by Jacobsen, Stoltze, and Norskov (1996) v000
EMT_Asap_Standard_Jacobsen_Stoltze_Norskov_AlAgAuCuNiPdPt__MO_118425166217_002	Standard Effective Medium Theory potential for face-centered cubic metals as implemented in ASE/Asap.
LJ_ElliottAkerson_2015_Universal__MO_959249795837_003	Efficient 'universal' shifted Lennard-Jones model for all KIM API supported species developed by Elliott and Akerson (2015) v003
MEAM_2NN_Fe_to_Ga__MO_145522277939_001	Model parameterization of 2NN MEAM model
Morse_Shifted_GirifalcoWeizer_1959HighCutoff_Cu__MO_151002396060_002	Morse potential (shifted) for Cu by Girifalco and Weizer (1959) using a high-accuracy cutoff distance v002
Morse_Shifted_GirifalcoWeizer_1959LowCutoff_Cu__MO_673777079812_002	Morse potential (shifted) for Cu by Girifalco and Weizer (1959) using a low-accuracy cutoff distance v002
Morse_Shifted_GirifalcoWeizer_1959MedCutoff_Cu__MO_173767283511_002	Morse potential (shifted) for Cu by Girifalco and Weizer (1959) using a medium-accuracy cutoff distance v002
Pair_Morse_Modified_MacDonaldMacDonald_Cu__MO_034823476734_000	Modified Morse pair potential for copper due to MacDonald and MacDonald

Models on openkim.org

KIM Items / Models / EAM_NN_Johnson_1988_Cu__MO_887933271505_002

Jump to: Tests | Visualizers | Files | Wiki

EAM_NN_Johnson_1988_Cu__MO_887933271505_002

Title	EAM Potential (analytical nearest-neighbor) for Cu developed by Johnson (1988) v002
Description	Analytical nearest-neighbor EAM model for Cu by Johnson
Species	Cu
Contributor	Ryan
Maintainer	Ryan
Author	Ryan S. Elliott
Publication Year	2018
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_002
Extended KIM ID	EAM_NN_Johnson_1988_Cu__MO_887933271505_002
DOI	10.25950/3ccd9f3b https://doi.org/10.25950/3ccd9f3b https://search.datacite.org/works/10.25950/3ccd9f3b
Citable Link	https://openkim.org/cite/MO_887933271505_002
KIM Item Type	Stand-alone Model
KIM API Version	2.0
Programming Language(s)	100.00% C

Models on openkim.org

Further down the model page for
EAM_NN_Johnson_1988_Cu__MO_887933271505_002

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				
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	consisten			
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	informatio			
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
P	vc-memory-leak	informational	The model code does not have memory leaks (i.e. it releases all allocated memory	Results	Files
P	vc-thread-safe	mandatory			

Numerical differentiation check of forces using Richardson extrapolation

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

Memory leak check using the valgrind memory debugging tool

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

Models on openkim.org

- Further down the model page for EAM_NN_Johnson_1988_Cu__MO_887933271505_002

Cubic Crystal Basic Properties Table

Species: Cu

	Model	Lattice Constant [Å]	Cohesive Energy [eV]	c11 [GPa]	c12 [GPa]	c44 [GPa]
bcc Expand	EAM_NN_Johnson_1988_Cu__MO_887933271505_002	2.85939610749000 03	3.60638315770475 47	146.260887382000 02	137.952181442	91.9367817649000 2
diamond Expand	EAM_NN_Johnson_1988_Cu__MO_887933271505_002	5.45042160153000 1	2.42418324907400 16	N/A	N/A	N/A
fcc Expand	EAM_NN_Johnson_1988_Cu__MO_887933271505_002	3.61472985148	3.54000012331236 8	184.172808464	115.324884335	68.8519693905
sc Collapse	EAM_NN_Johnson_1988_Cu__MO_887933271505_002	2.37244981527000 04	3.26347357796984 1	270.847253148	24.4996165814	-17.5854303931
	EAM_Dynamo_AcklandTichyVitek_1987_Cu__MO_179025990738_005	2.41274794936	2.93498774633736 6	296.901843605	90.8334172056000 1	54.1961445689
	EAM_Dynamo_Ackl	2.39571615309	2.94757703382590	186.096823759000	61.7775700379000	24.2576222484000

Models on openkim.org

- Further down the model page for EAM_NN_Johnson_1988_Cu__MO_887933271505_002

Tests

ElasticConstantsCubic__TD_011862047401_004

Computes the cubic elastic constants for some common crystal types (fcc, bcc, sc) by calculating the hessian of the energy density with respect to strain. An estimate of the error associated with the numerical differentiation performed is reported.

Test	Test Results	Link to Test Results page	Benchmark time
ElasticConstantsCubic_bcc_Cu__TE_091603841600_004	expand	view	2602
ElasticConstantsCubic_fcc_Cu__TE_188557531340_004	expand	view	3665
ElasticConstantsCubic_sc_Cu__TE_319353354686_004	expand	view	3079

Full results page.

Expand a property synopsis.

Usertime muliplied 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.

Models on openkim.org

- Further down the model page for EAM_NN_Johnson_1988_Cu__MO_887933271505_002

Tests

ElasticConstantsCubic__TD_011862047401_004

Computes the cubic elastic constants for some common crystal types (fcc, bcc, sc) by calculating the hessian of the energy density with respect to strain. An estimate of the error associated with the numerical differentiation performed is reported.

Test	Test Results	Link to Test Results page	Benchmark time
ElasticConstantsCubic_bcc_Cu__TE_091603841600_004	expand	view	2602
ElasticConstantsCubic_fcc_Cu__TE_168557531340_004	expand	view	3665
ElasticConstantsCubic_sc_Cu__TE_319363364686_004	collapse	view	3079

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 = 2.372443881627 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 = 270.8472531475441 GPa
c12 = 247.4996155813950 9 GPa
c44 = -17.585430393063543 GPa

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

Models on openkim.org

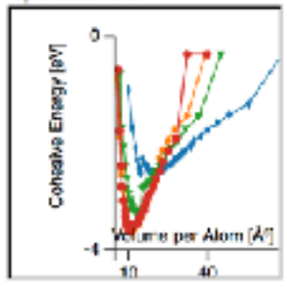
Further down the model page for
EAM_NN_Johnson_1988_Cu__MO_887933271505_002

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

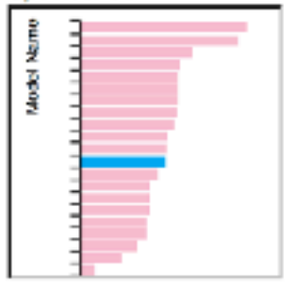


Click on any thumbnail to get a full size image.

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.

Species: Cu



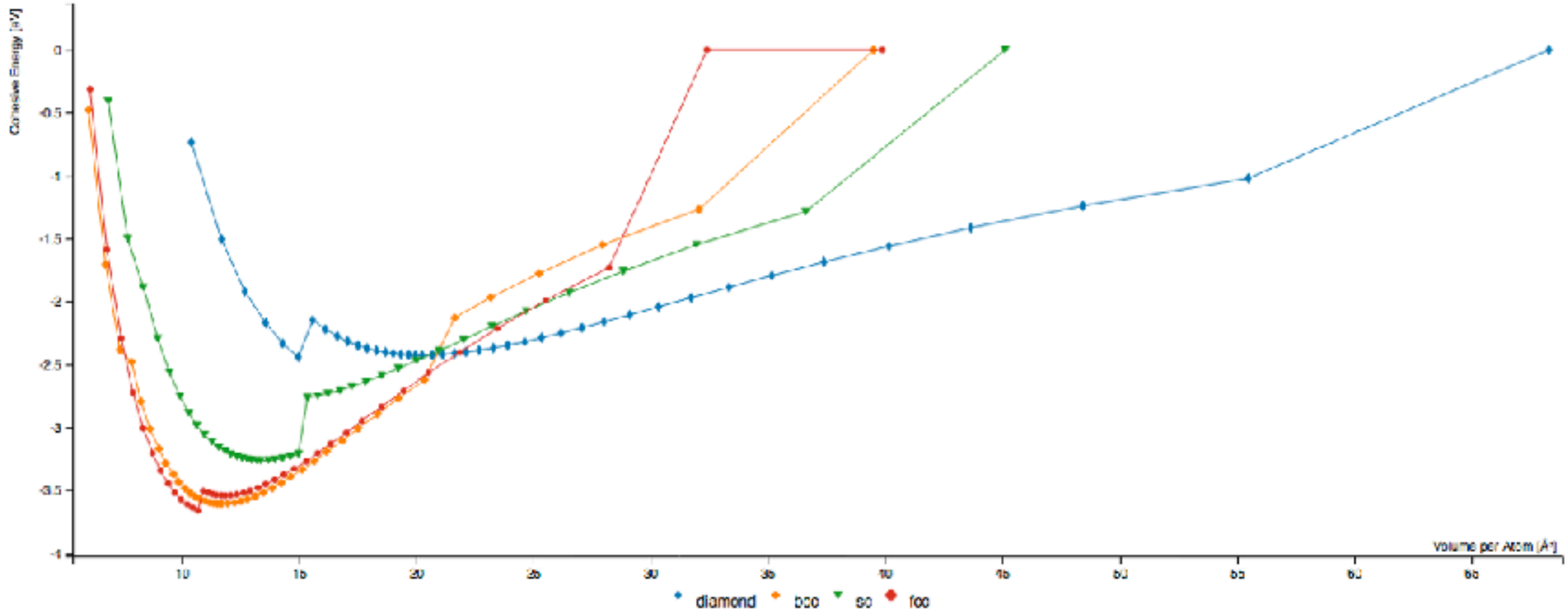
Click on any thumbnail to get a full size image.

Models on openkim.org

OpenKIM

Model: EAM_NN_Johnson_1988_Cu__MO_887933271505_002
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.



Models on openkim.org

Further down the model page for
EAM_NN_Johnson_1988_Cu__MO_887933271505_002

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

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

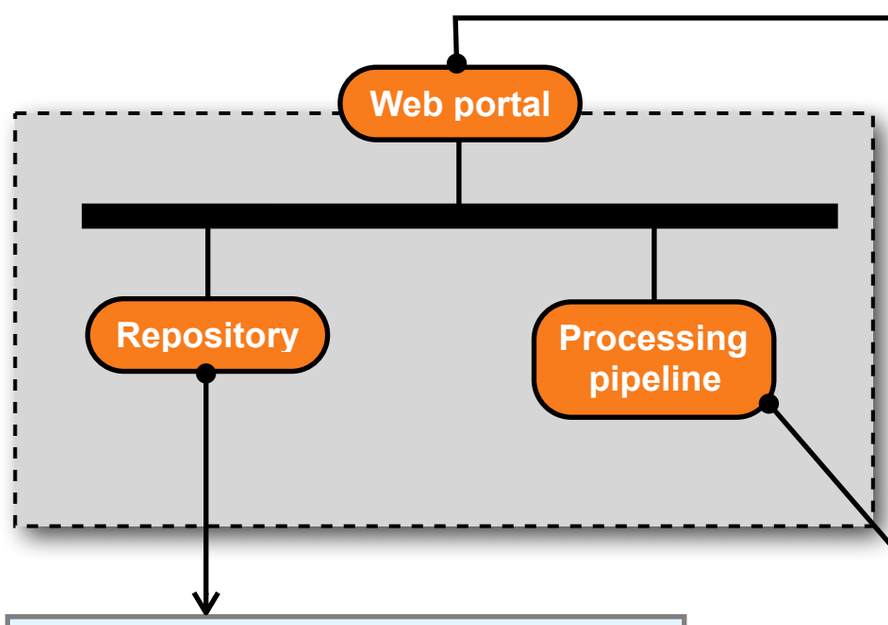
and

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

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 (June 28, 2019)



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

- 388 Models
- 2588 Tests
- 53 property definitions
- 10 Verification Checks
- 9 visualizers

- Automatic cloud-based computations
- Downloadable User Docker container
- Handling of dependencies

Software supporting KIM API:

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

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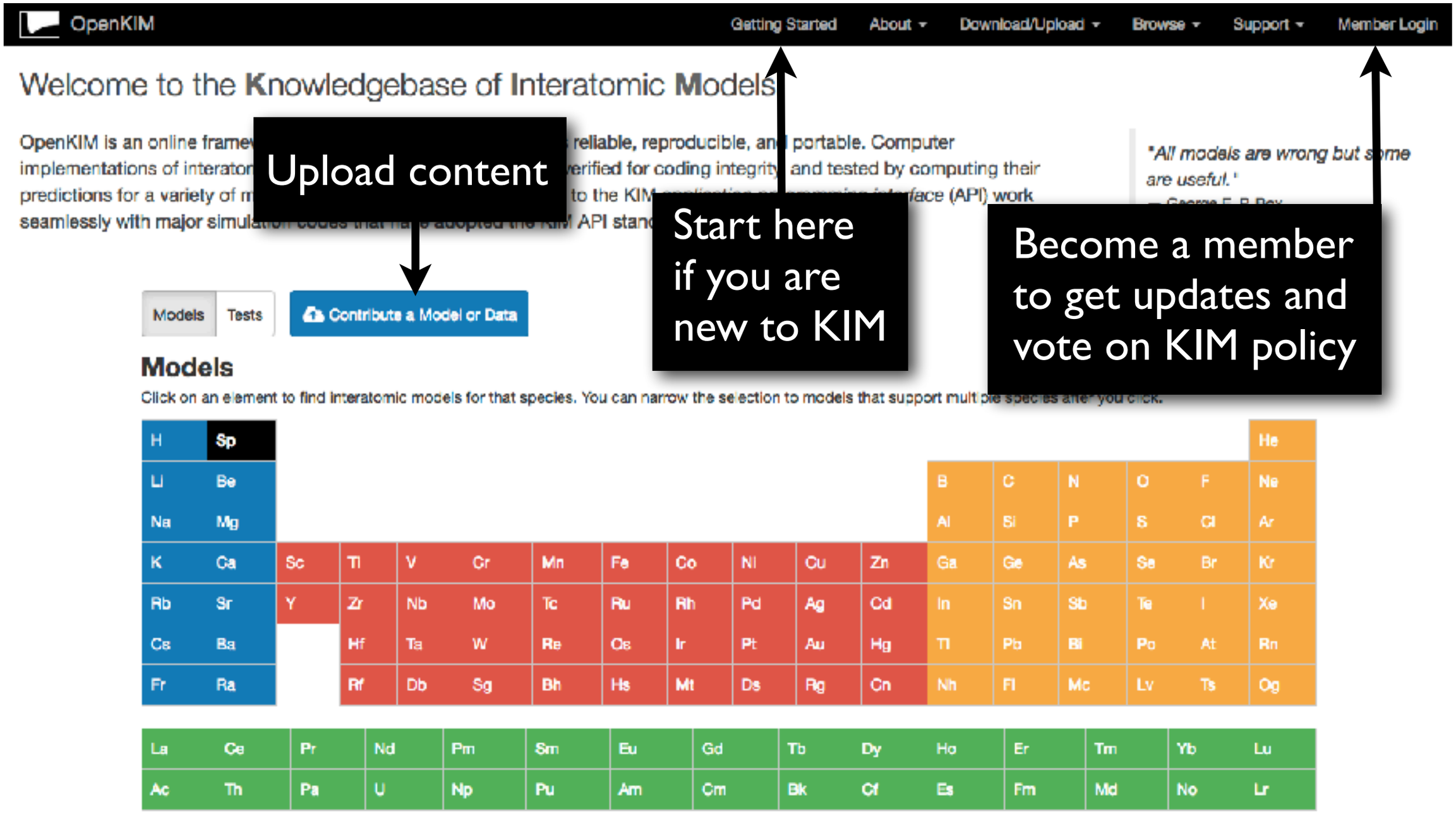
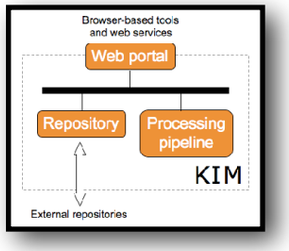
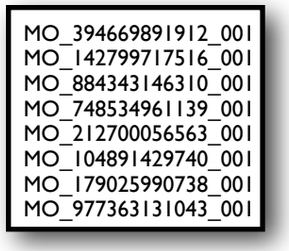


https://openkim.org

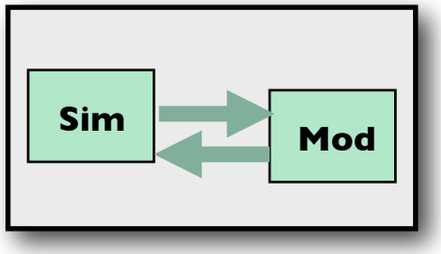
Summary



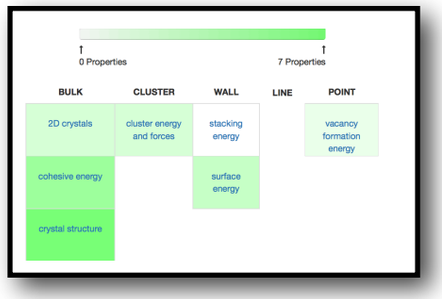
KIM provides archival permanent storage of interatomic models, tests, and reference data with known provenance.



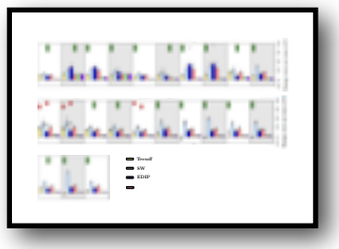
All KIM content is citable using issued DOIs. This makes it possible to reproduce simulation results in the future.



KIM Portable Models stored in the OpenKIM Repository 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 and verified for coding integrity using an automated processing pipeline.



Machine learning based tools for assessing interatomic model transferability and topology based uncertainty quantification tools are in development.