OpenKIM: Streamlining the use of Interatomic Models with LAMMPS

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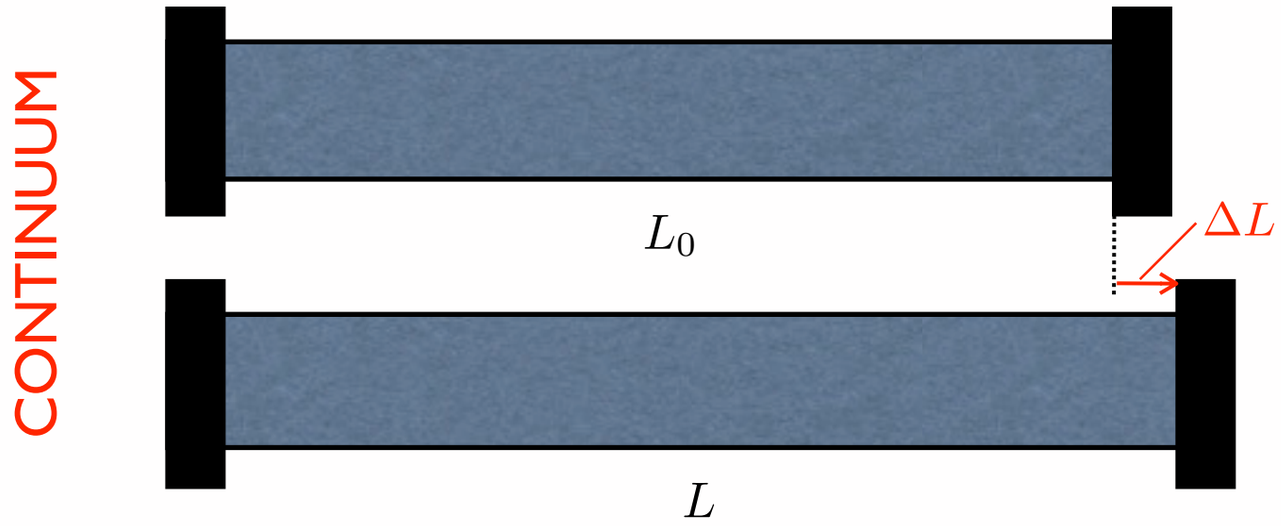
The Promise of Atomistic and Multiscale Simulations

- Consider the simple problem of a bar in tension:

  As long as the bar is not stretched too much, linear elasticity is an excellent model:



$$\epsilon = \Delta L / L_0$$

$$\sigma = E\epsilon = E\frac{\Delta L}{L_0}$$

One adjustable parameter fit to experiment (E = Young's modulus)

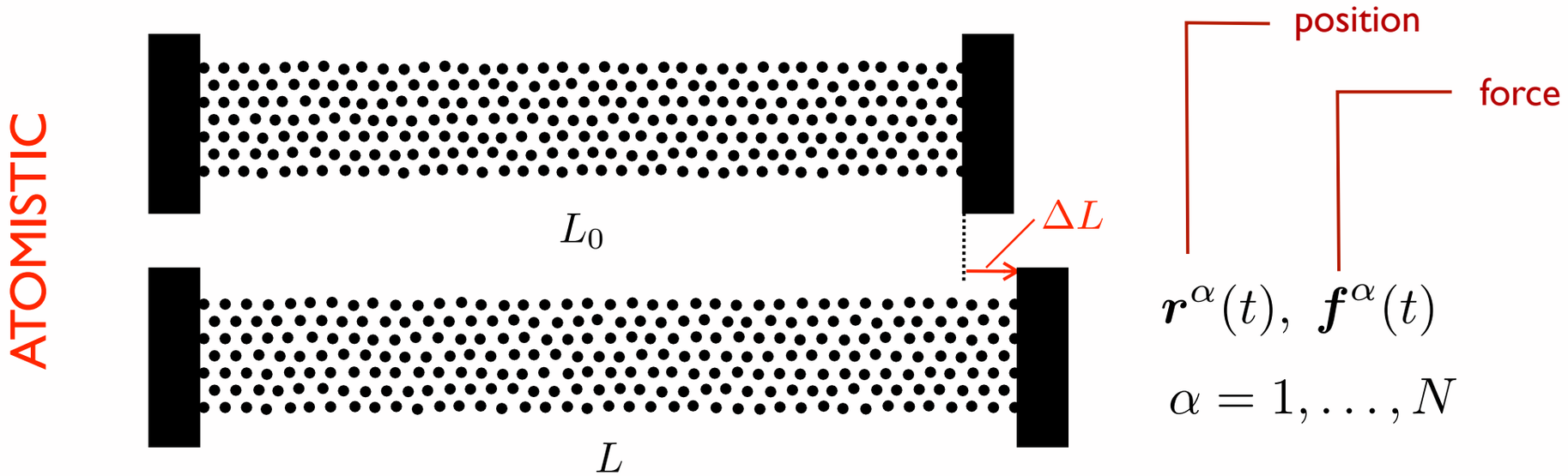
If we stretch the bar more, we could use a nonlinear elasticity theory, or a plasticity theory, or some other suitable phenomenological theory.

But what if the unexpected occurs?

- fracture (due to defect distribution)
- phase transformations
- deformation twinning
- chemical reactions (e.g. oxidation)
- fatigue (thermal, mechanical, ...)
- strain rate effects
- boundary effects
- etc. etc. etc.

The Promise of Atomistic and Multiscale Simulations

- Atomistic and multiscale methods promise predictive modeling based on a more fundamental model of the material:



The interactions between the atoms are described using an interatomic model (IM):

$$\mathcal{V} = \mathcal{V}(\boldsymbol{r}^1, \ldots, \boldsymbol{r}^N); \qquad \boldsymbol{f}^\alpha = -\nabla_{\boldsymbol{r}^\alpha}\mathcal{V}$$

But what if the unexpected occurs?

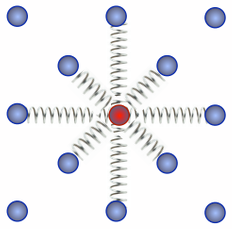
- fracture (due to defect distribution)
- phase transformations
- deformation twinning
- chemical reactions (e.g. oxidation)
- fatigue (thermal, mechanical, ...)
- strain rate effects
- boundary effects
- etc. etc. etc.

Can the IM capture the new effect?

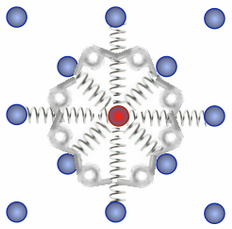
Menagerie of Interatomic Models

- Many different kinds of IMs have been developed over the years:

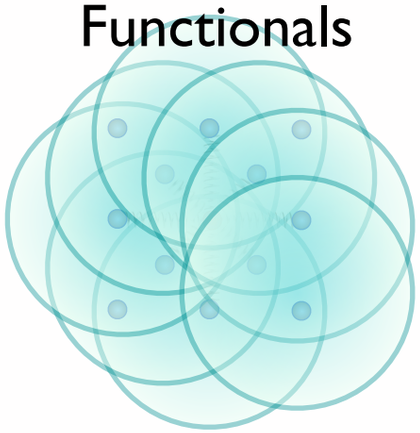
Pair Potentials



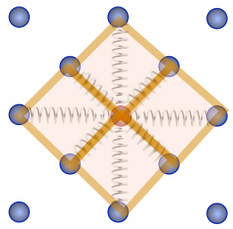
Cluster Potentials



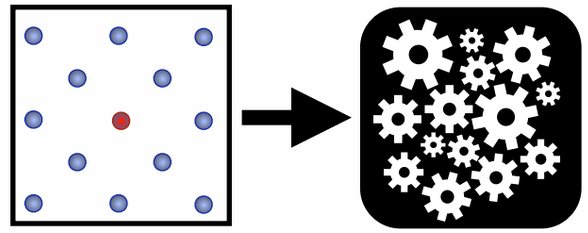
Pair/Cluster Functionals



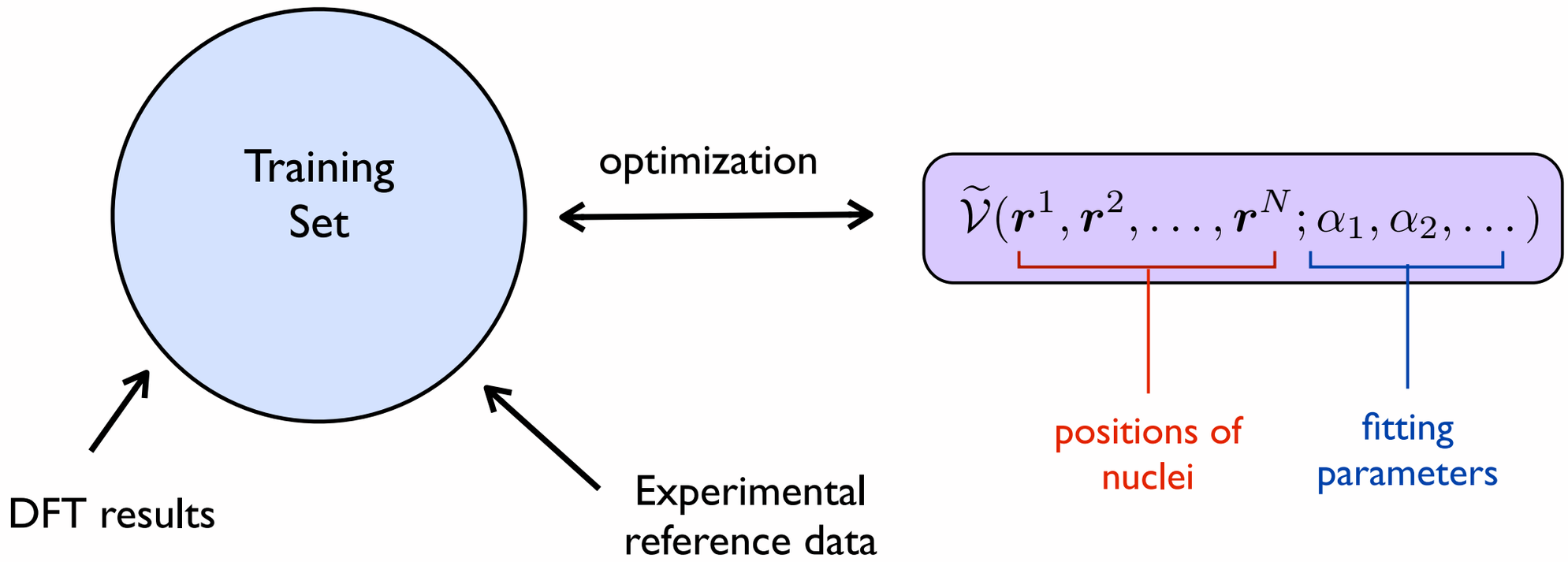
Bond-order Potentials



Machine learning Potentials



- They have a functional form (physics-based or machine learning) and are fit to a training set:



Which one should you use?

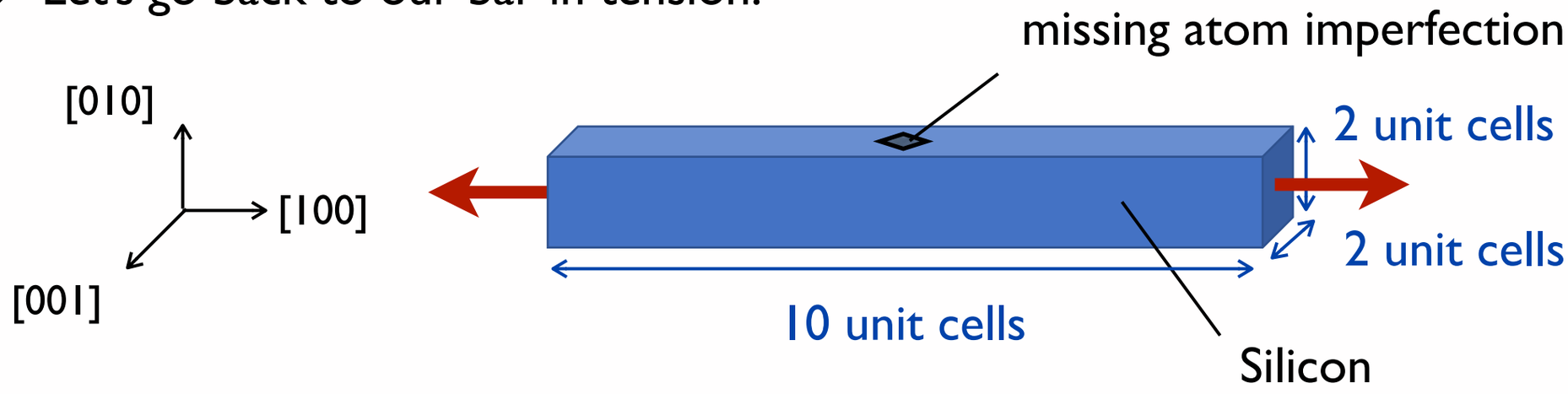
Silicon IMs since the 1980s:

1. Keating (Valence), *Phys. Rev.*, **145**, 637 (1966).
2. Altmann,...,Tomassini (Valence), *J. Phys. C,* **15**, 5581 (1982).
3. Pearson, Takai, Halicioglu, Tiller (PTHT), *J. Cryst. Growth*, **70**, 33 (1984).
4. Stillinger-Weber (SW), *PRB*, **31**, 5262 (1985).
5. Tersoff (T1), *PRL*, **56**, 632 (1986).
6. Brenner, Garrison, *PRB*, **34**, 1304 (1986).
7. Dodson (DOD), *PRB*, **35**, 2795 (1987).
8. Biswas, Hamann (BH), *PRB*, **36**, 6434 (1987).
9. Baskes (EAM-Si), *PRL*, 2666 (1987).
10. Tersoff (T2), *PRB*, **37**, 6991 (1988).
11. Tersoff (T3), *PRB*, **38**, 9902 (1988).
12. Khor, Das Sarma, *PRB*, **38**, 3318 (1988).
13. Kaxiras, Pandey, *PRB*, **38**, 12736 (1988).
14. Baskes, Nelson, Wright (MEAM-Si), *PRB*, **40**, 6085 (1989).
15. Ackland, *PRB*, **40**, 10351 (1989).
16. Chelokowsky, Phillips, Kamal, Strauss, *PRL*, **62**, 292 (1989).
17. Mistriotis, Flytzanis, Farantos (4-body), *PRB,* **39**, 1212 (1989).
18. Erkoç, *Phys. Stat. Sol. (b)*, **152**, 447 (1989).
19. Bolding, Anderson, *PRB*, **41**, 10568 (1990).
20. Carlsson, Fedders, Myles, *PRB*, **41**, 1247 (1990).
21. Murrell, Mottram, *Mol. Phys.*, **69**, 571 (1990).
22. Wang, Rockett, *PRB*, **43**, 12571 (1991).
23. Chelikowsky, Glassford, Phillips, *PRB*, **44**, 1538 (1991).
24. Li, Johnson, Murrell, *Chem. Soc. Faraday Trans.*, **88**, 1229 (1992).
25. Gong, *PRB*, **47**, 2329 (1993).
26. Liu, *Thermocem. J. Molec. Struct.*, **341**, 253 (1995).
27. Omote, Waseda (Pair Potential), *Jap. J. Appl. Phys. 1*, **35**, 151 (1996).
28. Stephenson, Radny, Smith (modifed SW), *Surf. Sci.*, **366**, 177 (1996).
29. Bazant, Kaxiras, Justo (EDIP), *PRB*, **56**, 8542 (1997).
30. Cai, *Phys. Stat. Sol. B*, **212**, 9 (1999).
31. Lenosky,...,Kress (MEAM), *Mod. Sim. Mater. Sci. Eng., **8**, 825 (2000).*
32. van Duin,...,Goddard (ReaxFF), *J. Phys. Chem. A* **107**, 3803 (2003).
33. Erhart, Albe (Bond Order), *PRB*, **71**, 035211 (2005).
34. Kumagai, Izumi, Hara, Sakai, *Comp. Mat. Sci*, **39**, 457 (2007).
35. Lee, *Calphad-Comp. Coupling Phase Diag. Thermochem.,* **31**, 95 (2007).
36. Yu, Sinnott, Phillpot, *PRB,* **75**, 085311 (2007).
37. Timonova, Lee, Thijsse (MEAM), *Nuc. Inst. Meth. Phys. Res. B,* **255**, 195 (2007).
38. Gillespie,...,Pettifor (Bond Order), *PRB*, **75**, 155207 (2007).
39. Behler and Parrinello (NN), *Phys. Rev. Lett.* **98**, 146401 (2007).
40. Vashishta et al. (3-body), *J. Appl. Phys.* **101**, 103515 (2007).
41. Sanville (NN), *J. Phys. Cond. Matt.* **20**, 285219 (2008).
42. Schelling (Bond order), *Comp. Mat. Sci.* **44**, 274-279 (2008)
43. Malshe et al. (NN), *J. Chem. Phys.* **129**, 044111 (2008).
44. Ohta et al. (SW), *Jap. J. Appl. Phys.* **48**, 020225 (2009).
45. Hossain et al. (DFT-ArSi), *Nucl. Inst. & Meth. Phys. Res. B* **267**, 1061 (2009).
46. Lucas et al. (EDIP), *J. Phys. Cond. Matt.* **22**, 035802 (2010).
47. Ryu and Cai (MEAM), *J. Phys. Cond. Matt.* **22**, 055401 (2010).
48. Timonova and Thijsse (MEAM), *Comp. Mat.. Sci.* **48**, 609-620 (2010).
49. Grochia et al. (MEAM), *Chem. Phys. Lett.* **493**, 57-60 (2010).
50. Du et al. (MEAM), *Phys. Stat. Solidi B* **248**, 2050-2055 (2011).
51. Tewary (Phenomenological), *Phys. Lett. A* **375**, 3811-3816 (2011).
52. Lee and Hwang (FM-SW), *Phys. Rev. B* **85**, 125204 (2012).
53. Dongare et al. (A-EAM), *MSMSE* **20**, 035007 (2012).
54. Cui et al. (MEAM), *J. Power Sources* **207**, 150-159 (2012).
55. da Cruz et al. (MEAM), *J. Heat Trans.* **134**, 062402 (2012).
56. Briquet et al., (reactive) *J. Phys.: Condens. Matter.* **24**, 395004 (2012).
57. Pastewka et al. (Bond Order). *PRB* **87**, 205410 (2013).
58. Saidi et al. (MEAM). *MSMSE* **22**, 055010 (2014).
59. Jaramillo-Botero et al. (ReaxFF). *J. Chem. Theory Compt.* **10**, 1426 (2014).
60. Takamoto et al. (Tersoff). *J. Appl. Phys.* **120**, 165109 (2016).
61. Pun and Mishin (Tersoff). *PRB* **95**, 224103 (2017).
62. Bartok et al. (machine learning), *PRX* **8**, 041048 (2018).

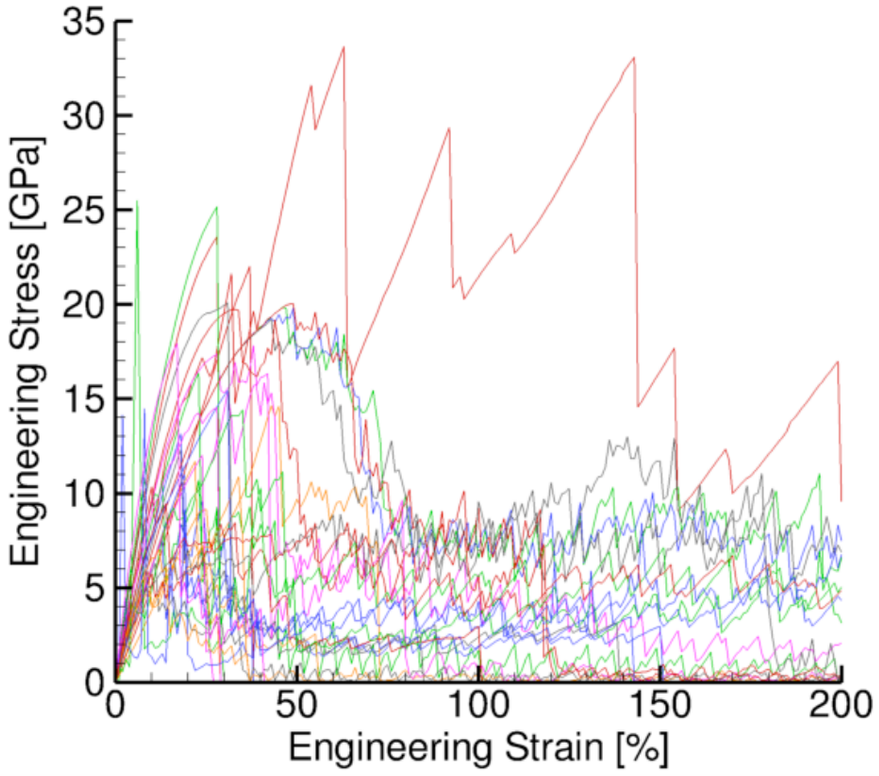
The Scream, Edvard Munch

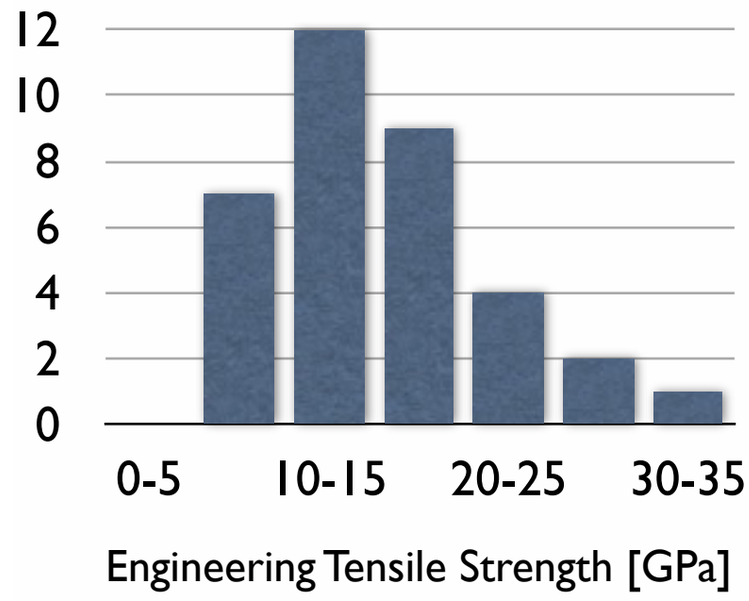
The IM makes a difference...

- Let's go back to our bar in tension.



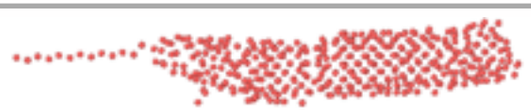
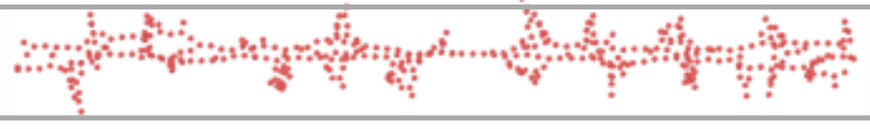
- Stress-strain prediction of 40 silicon models:





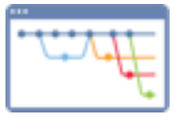
DFT reference: $\sigma_{\mathrm{id}}^{100,\mathrm{bulk}} = 27.8\ \mathrm{GPa}$ (Dubois *et al*, 2006)

The IM makes a difference...

Model	σ_{UTS}	Profile at 200% strain	Model	σ_{UTS}	Profile at 200% strain
GAP	6.2		m-Tersoff-K	14.4	
BH	6.3		MEAM-JGH	14.5	
ADP	7.0		WR	14.6	
MEAM-DLH	8.4		m-Tersoff-P	15.4	
EDIP	9.4		PPM	16.3	
Gong	9.5		Tersoff-EA-II	17.8	
KP	10.7		MFF	17.9	
Tersoff-T2	10.9		Tersoff-T3	19.2	
SW-ZXH-1	11.0		Tersoff-ZBL	20.0	
SW-LH-GGA	12.0		SRS	22.0	
SW	12.3		SW-BHS	25.2	
EDIP-JMS	13.0		GWZBL	25.5	
SW-BHT	13.1		KDS	33.7	

OpenKIM

The Open Knowledgebase of Interatomic Models (OpenKIM) addresses IM challenges:



IM version tracking and citation

- Curated repository of interatomic models (IMs) (potentials and force fields) with comprehensive provenance and version control.
- Digitial Object Identifiers (DOIs) issued to all archived IMs by OpenKIM via DataCite.

Reliable IMs that integrate with researcher codes and workflows.

- IMs archived in https://openkim.org conform to an Application Programming Interface (API) that allows them to work in plug-and-play fashion with major simulators.

Asap ASE DL_POLY GULP LAMMPS nanoHUB MDStressLab potfit QuasiContinuum Method

- Source and binary distribution framework for easy installation and use of the KIM API and KIM IMs with conforming simulators.

Testing IM predictions and bug detection to help with IM selection.

- Standardized testing framework for archived IMs including their predictions for material properties and checks on their coding integrity.
- Web-based query system to obtain IM predictions for any computed properties.

KIM Testing Framework

- All KIM IMs are subjected to Verification Checks (VCs) for coding integrity

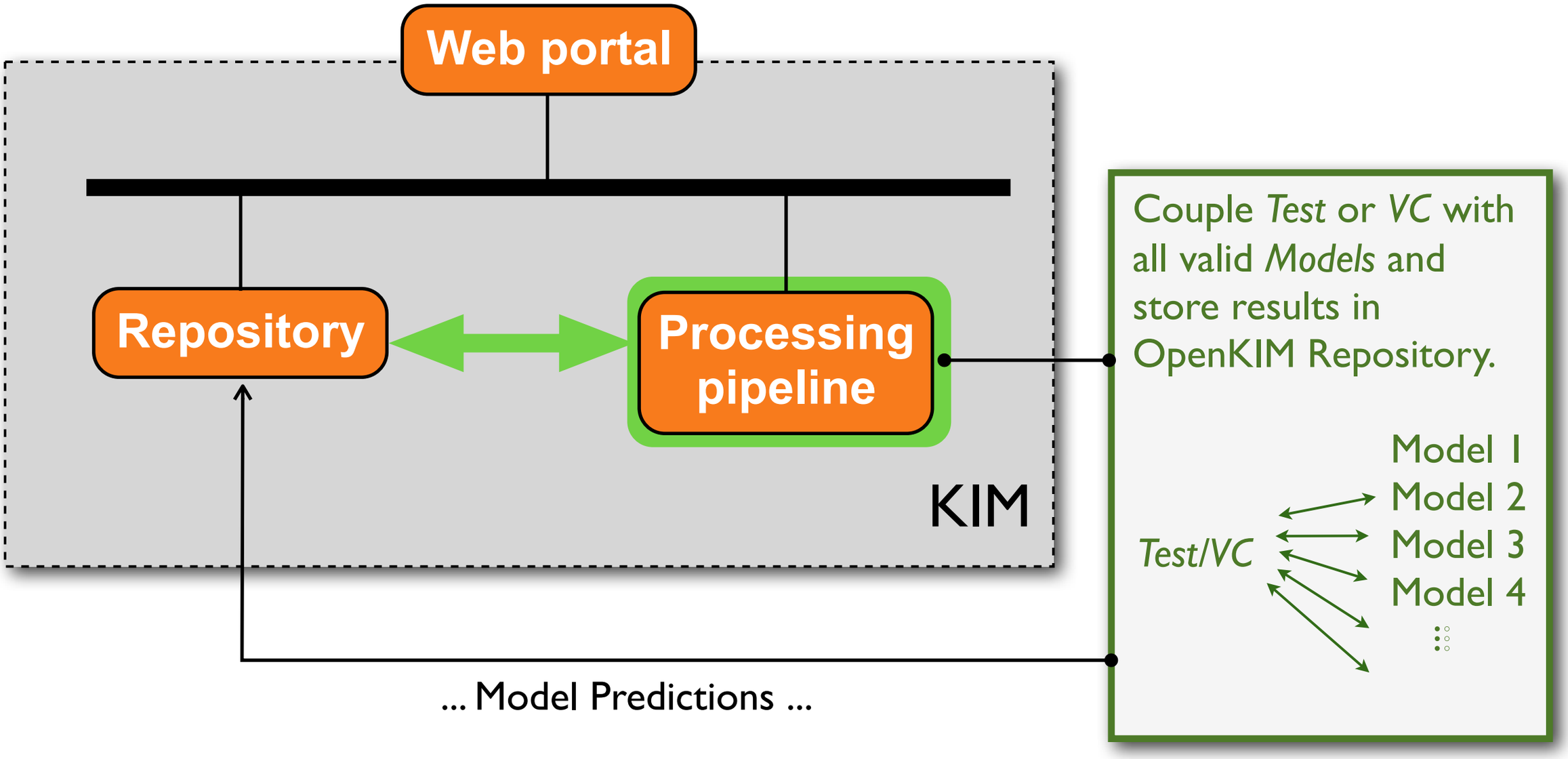
Mandatory	Consistency	Informational
▪ Species supported as stated; ▪ Unit conversion handled correctly; ▪ Domain decomposition handled correctly; ▪ ...	▪ Numerical derivative check of forces, virial, hessian, ...; • Translational and rotational invariance; ▪ ...	▪ Continuity, smooth cutoff; • Inversion symmetry; ▪ Coding issues: memory leaks, optimization dependence, ... ▪ ...

- All KIM IMs are run against all compatible KIM Tests to compute material properties:

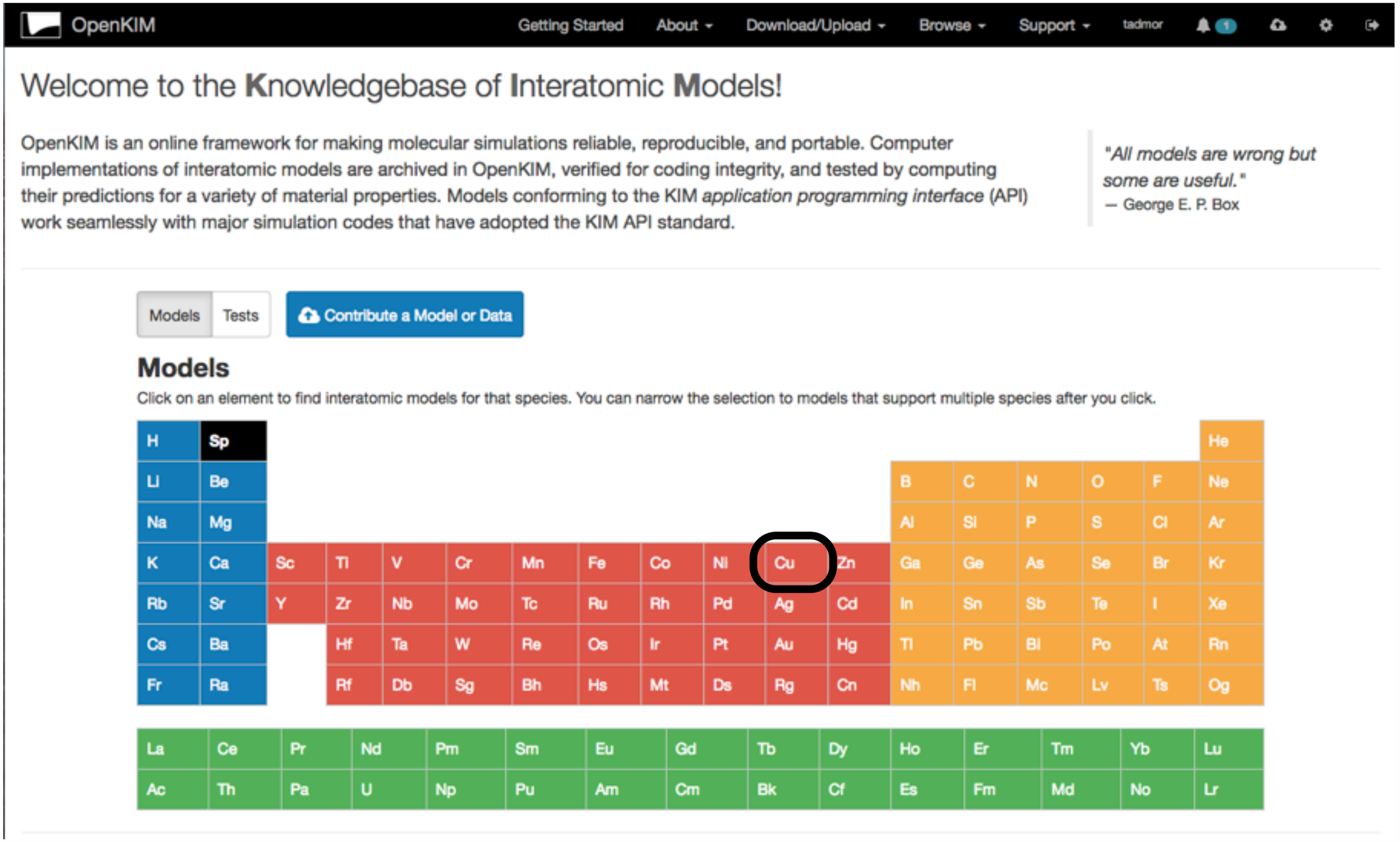
Bulk	Wall	Line
- cohesive energy	- antiphase boundary	- dislocation core structure
- elastic constants	- gamma surface	- dislocation core energy
- lattice constants	- grain boundary structure	- Peierls barrier
- phonon spectrum	- stacking fault energy	- ...
- thermal conductivity	- surface energy	Point
- thermal expansion	- surface structure	- vacancy formation energy
- ..	- ...	- vacancy migration barrier

Interacting with KIM

Uploading new KIM Test/VC to the OpenKIM Repository



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_762798677854_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_642748370624_000	Finnis-Sinclair potential (LAMMPS cubic hermite tabulation) for Cu developed by Ackland and Vitek (1990) v000
EAM_Dynamo_AdamsFoiles_1989Universal6_Cu__MO_145873824897_000	EAM potential (LAMMPS cubic hermite tabulation) for Cu (Universal6) developed by Adams and Foiles (1989) v000

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-
-
-

EAM_Dynamo_ZhouWadleyJohnson_2001_CuTa__MO_547744193826_000	EAM potential (LAMMPS cubic hermite tabulation) for the Cu-Ta system developed by Zhou, Wadley and Johnson (2001) v000
EAM_NN_Johnson_1988_Cu__MO_887933271505_002	EAM Potential (analytical nearest-neighbor) for Cu developed by Johnson (1988) v002
EMT_Asap_MetalGlass_BaileySchiotzJacobsen_2004_CuMg__MO_228059236215_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_987541074959_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_118428466217_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_173787283511_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

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
Item Citation	This Model originally published in [1] is archived in OpenKIM [2-4]. [1] Johnson RA. Analytic nearest-neighbor model for fcc metals. Physical Review B. 1988Mar;37(8):3924–31. doi:10.1103/PhysRevB.37.3924 [2] Elliott RS. EAM Potential (analytical nearest-neighbor) for Cu developed by Johnson (1988) v002. OpenKIM; 2018. doi:10.25950/3ccd9f3b [3] Tadmor EB, Elliott RS, Sethna JP, Miller RE, Becker CA. The potential of atomistic simulations and the Knowledgebase of Interatomic Models. JOM. 2011;63(7):17. doi:10.1007/s11837-011-0102-6 [4] Elliott RS, Tadmor EB. Knowledgebase of Interatomic Models (KIM) Application Programming Interface (API). OpenKIM; 2011. doi:10.25950/ff8f563a Click here to download the above 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
KIM Item Type	Portable Model
KIM API Version	2.0
Programming Language(s)	100.00% C
Previous Version	EAM_NN_Johnson_1988_Cu__MO_887933271505_001

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**	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
P	**vc-memory-leak**	informational	The model code does not have memory leaks (i.e. it releases all allocated memory at the end); see full description.	Results	Files
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

Models on openkim.org

- Further down the model page for
  EAM_NN_Johnson_1988_Cu__MO_887933271505_002

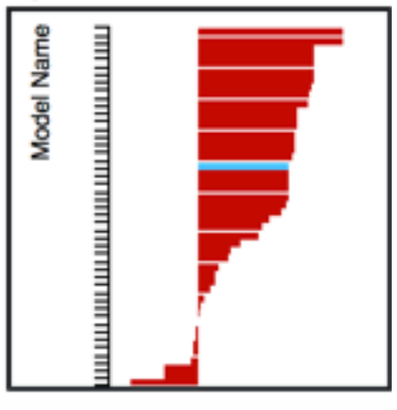
Tests

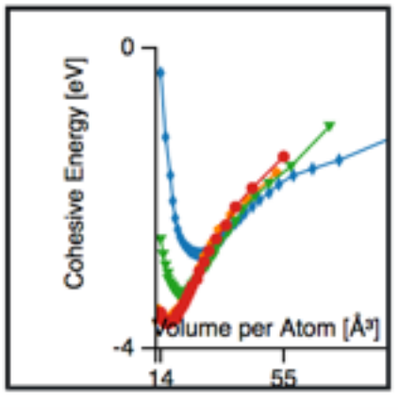
ElasticConstantsCubic__TD_011862047401_004

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

	Model	Lattice Constant [Å]	Cohesive Energy [eV]	c11 [GPa]	c12 [GPa]	c44 [GPa]
bcc Expand	EAM_NN_Johnson_1988_Cu__MO_887933271505_002	2.8593961074900003	3.6063831577047547	146.26088738200002	137.952181442	91.93678176490002
diamond Expand	EAM_NN_Johnson_1988_Cu__MO_887933271505_002	5.450421601530001	2.4241832490740016	N/A	N/A	N/A
fcc Expand	EAM_NN_Johnson_1988_Cu__MO_887933271505_002	3.61472985148	3.540000123312368	184.172808464	115.324864335	68.8519693905
sc Expand	EAM_NN_Johnson_1988_Cu__MO_887933271505_002	2.3724498152700004	3.263473577969841	270.847253148	24.4996165814	-17.5854303931





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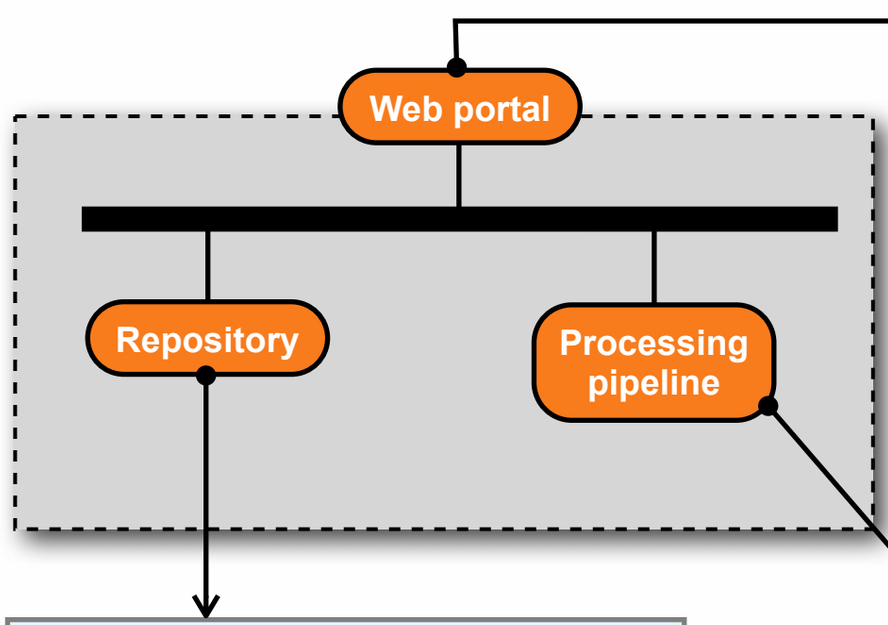
Current Status (August 14, 2019)



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

- 390 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 nanoHUB MDStressLab potfit QuasiContinuum Method

LAMMPS ALL-IN-KIM CAMPAIGN

GOAL: Gather into OpenKIM all interatomic potentials used in publications that cite the LAMMPS project

1995 1996 1997 1998 1999 2000 2001 2002

2003 2004 2005 2006 2007 2008 2009 2010

2011 2012 2013 2014 2015 2016 2017 2018

2019 2020 2021 2022 2023 2024 2025 2026