2020 Atomistic Simulations for Industrial Needs Workshop (online)

August 6, 2020

The Platform for the Interatomic Potentials Validation

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ICAMS
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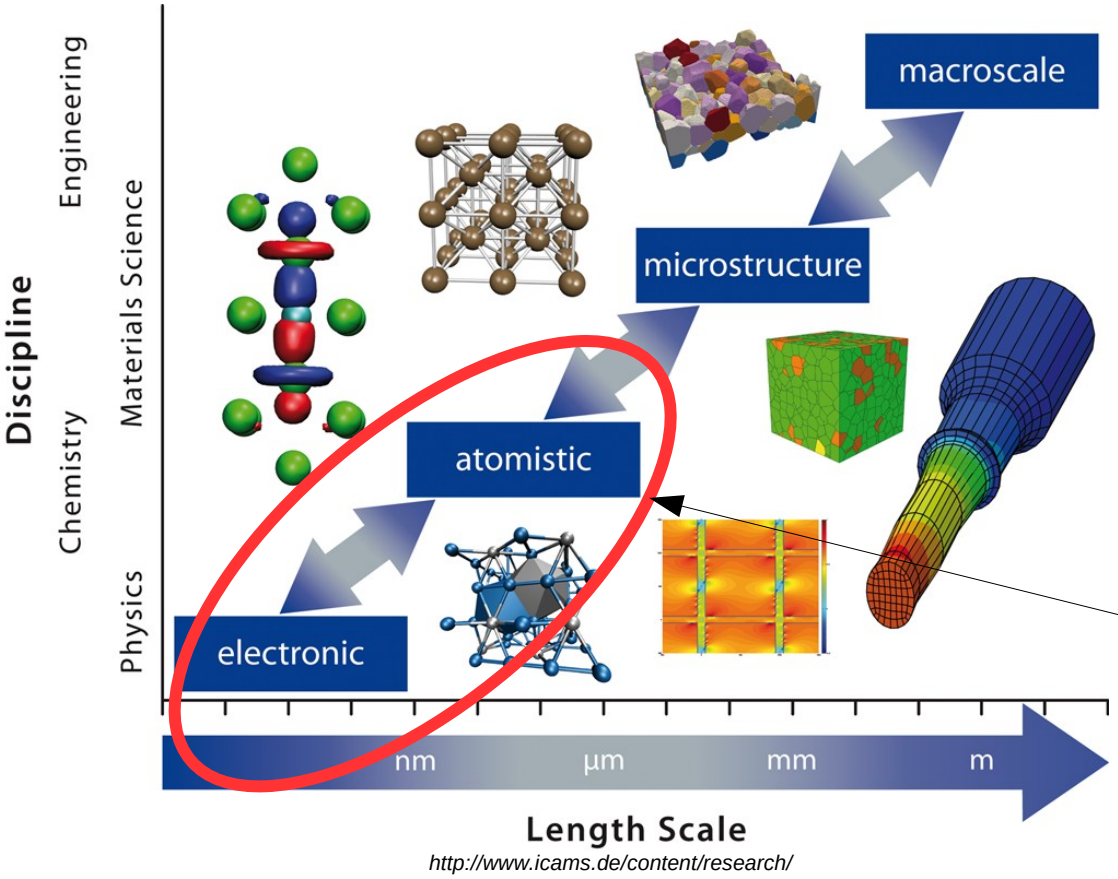
Atomistic simulations



http://www.icams.de/content/research/

ab initio and molecular dynamic simulations

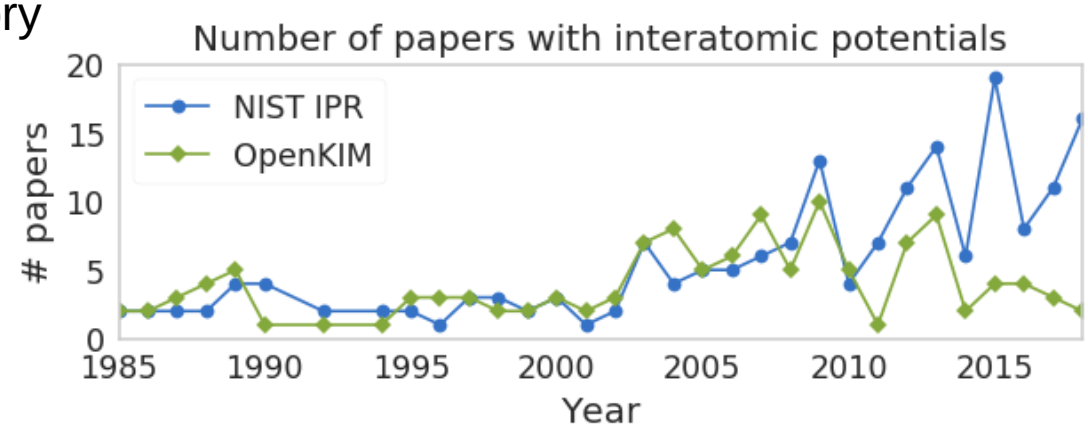
Interatomic potentials (as of 2019)

- NIST interatomic potentials repository

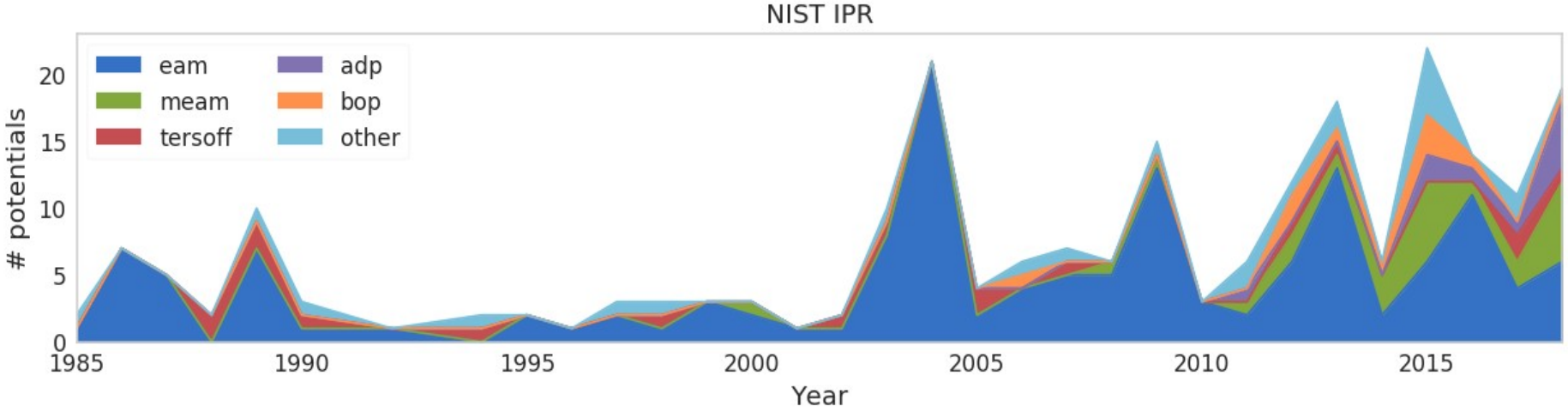
NIST IPR

- OpenKIM

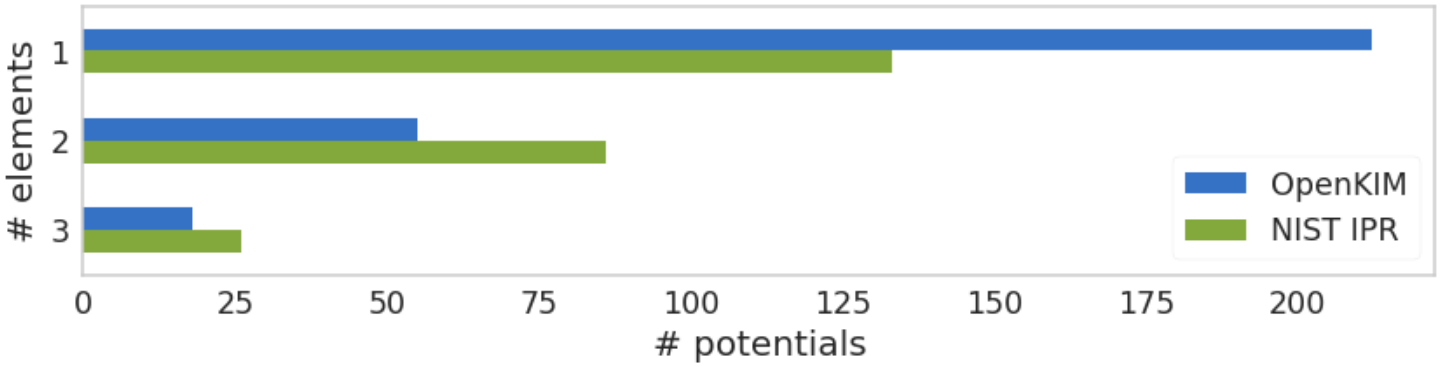
OpenKIM



Interatomic potential types (LAMMPS pair_style)

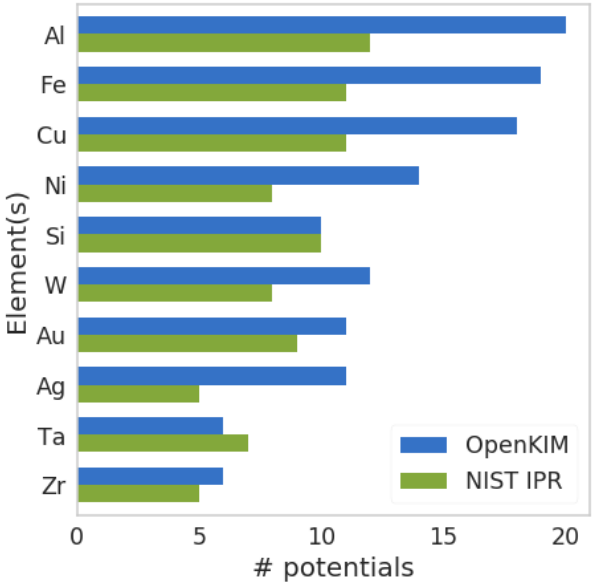


Interatomic potentials statistics (as of 2019)

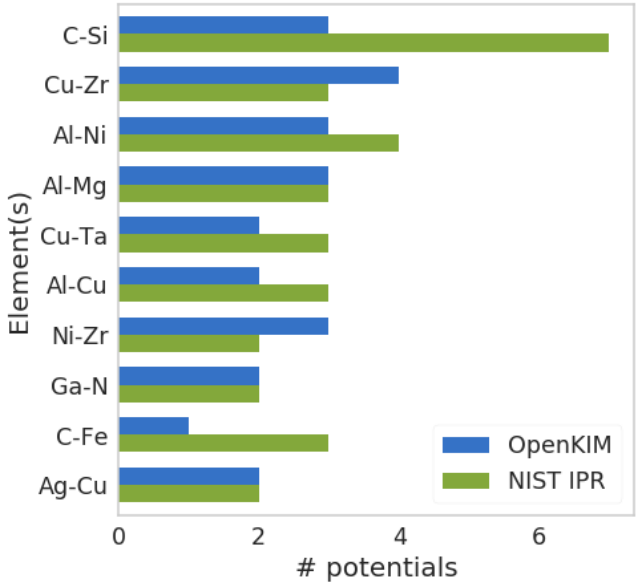


Single-specie interatomic potentials are the most common

Most frequent elements in single-species potentials



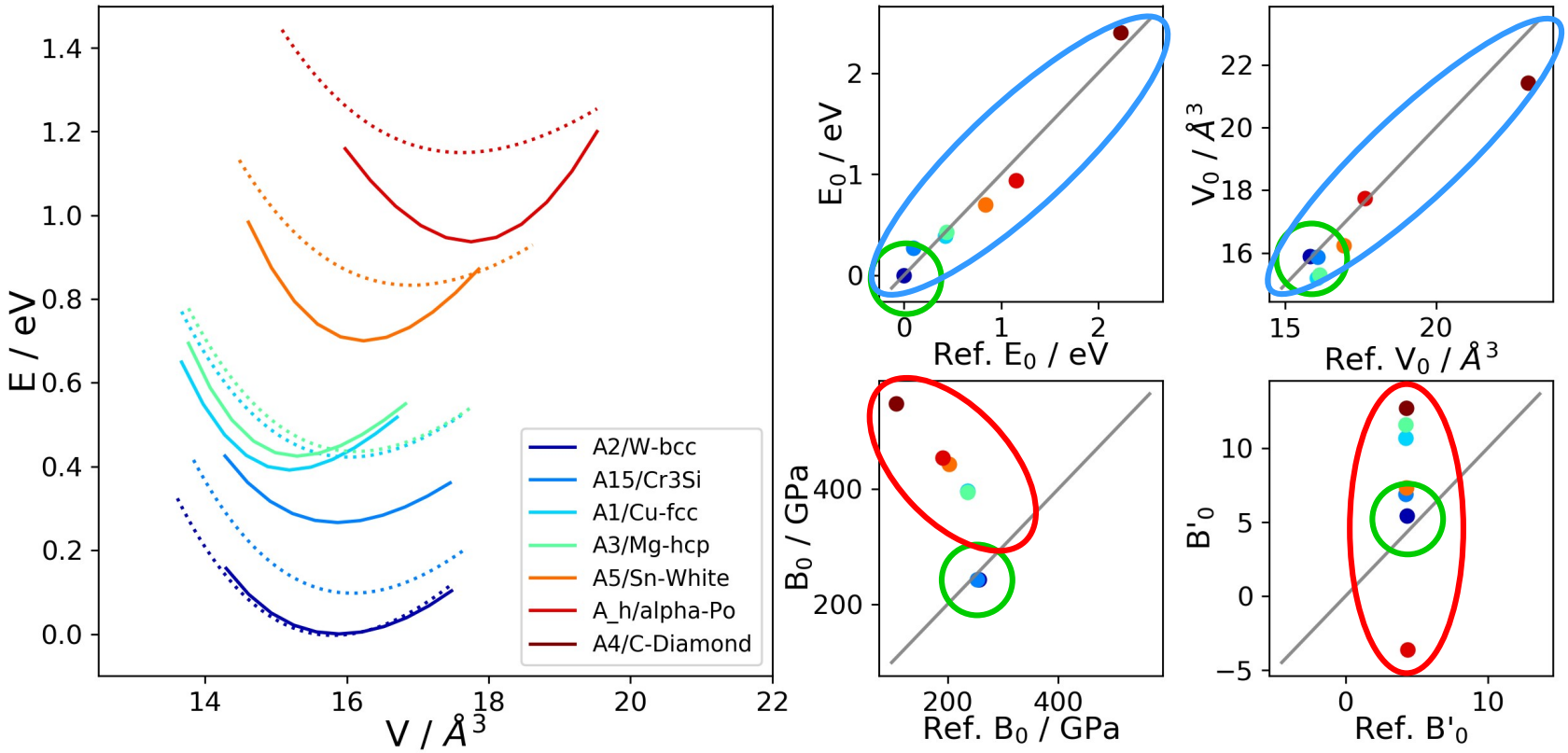
Most frequent binaries in two-species potentials



Transferability

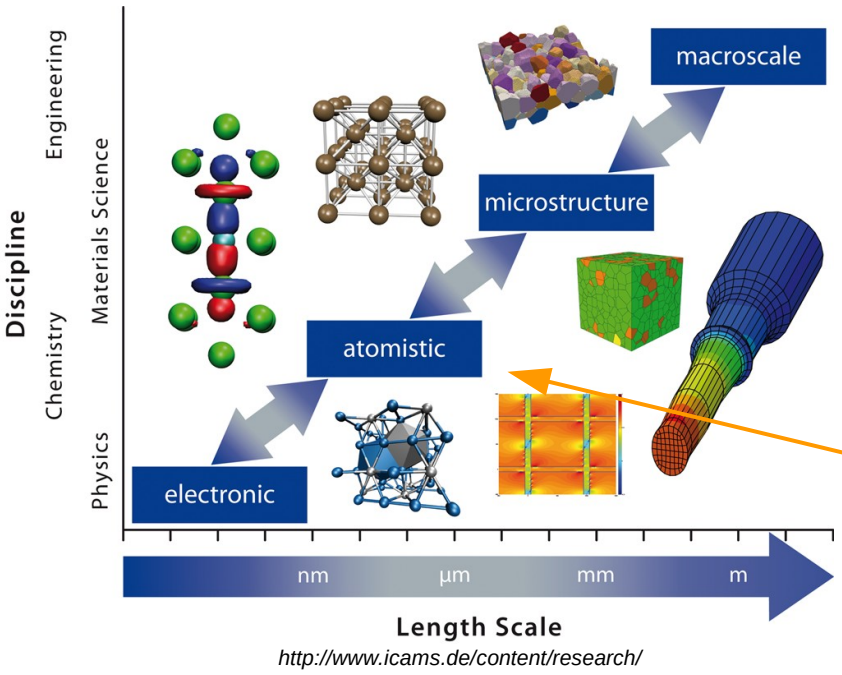
Transferability of interatomic potentials – **reliability** of calculated **properties** for structures which are **not** from potential **training set**

Example:solid line - MEAM Park for Mo [*H.Park et al. Phys. Rev. B 85, 214121]*,
dotted – reference,DFT-PBE



Properties of ground-state (A2/BCC) have small error
Level I properties (energy,volume) – good transferability
Level II properties (B_0, B') – bad transferability

Interatomic potentials



http://www.icams.de/content/research/

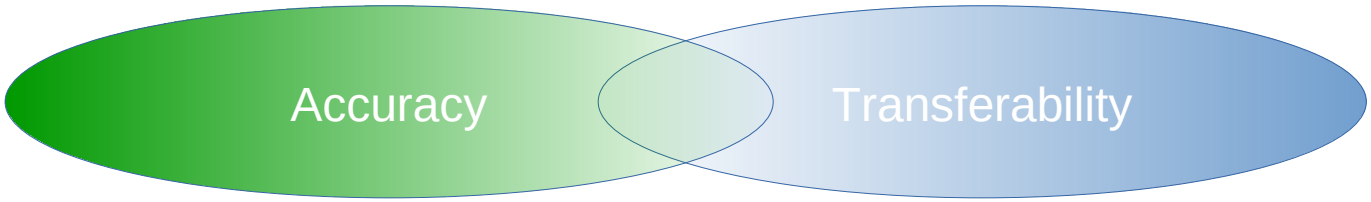
Training set: **DFT**/experimental structures/properties

Potential functional form: MEAM, ADP, BOP, …, ML

Potential fitting (energy-matching, force-matching, property-matching)

Interatomic potential

How reliable are these potentials?



Transferability of interatomic potentials – **reliability** of calculations for structures and/or properties that are **not** from the **training set**

Validate by comparison to reference data

The (basic) needs of atomistic simulation community

Roles

Molecular dynamics simulation user

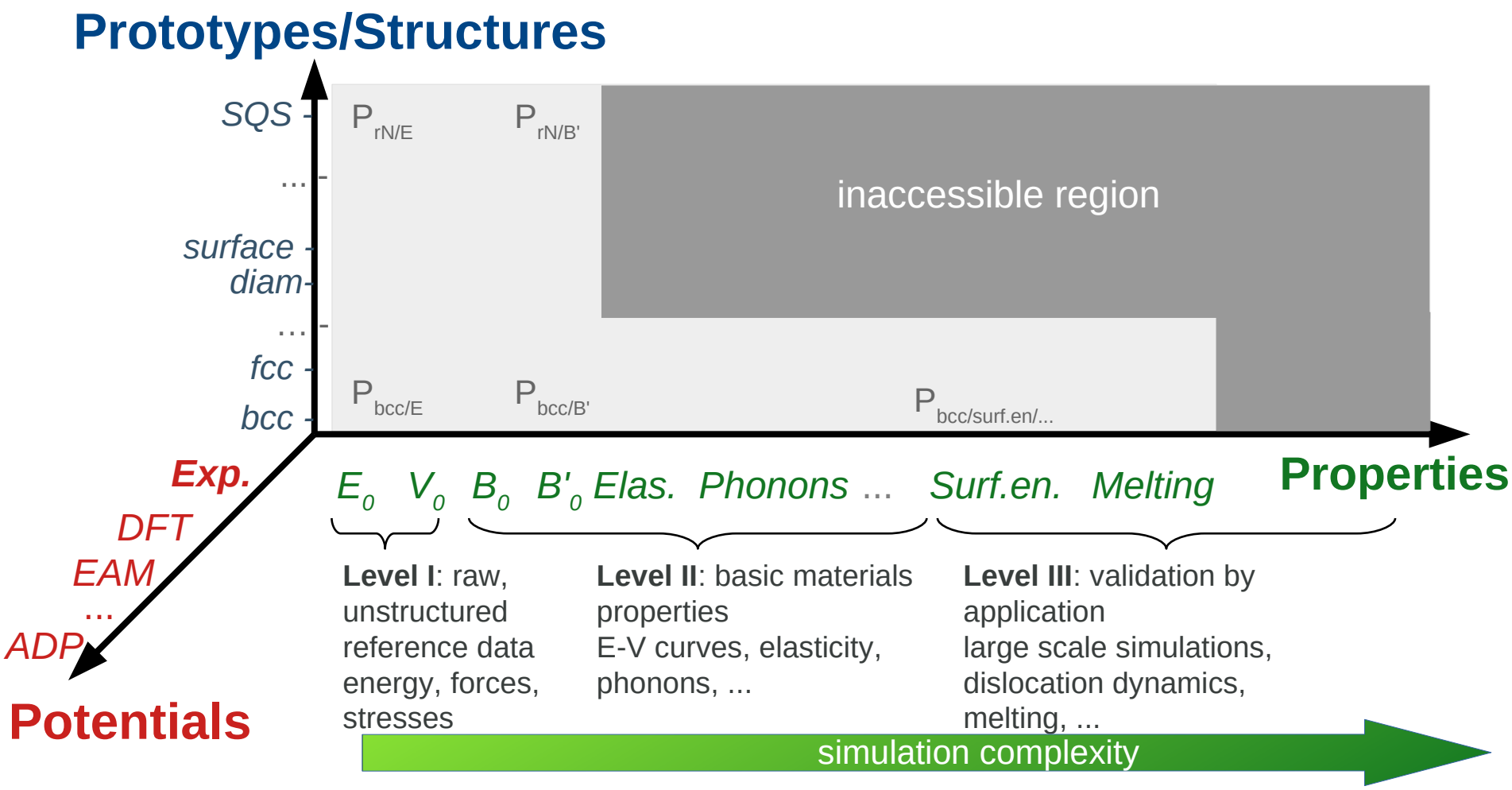
- What is the best/appropriate potentials for my particular purpose ?
- What properties could I simulate (and how)?
- What would be the error of my MD simulations?

Interatomic potentials developer

- How my new potential would perform?
- Are there standard benchmarks which I can use for my new potential?
- Is my potential better than the previous ones?

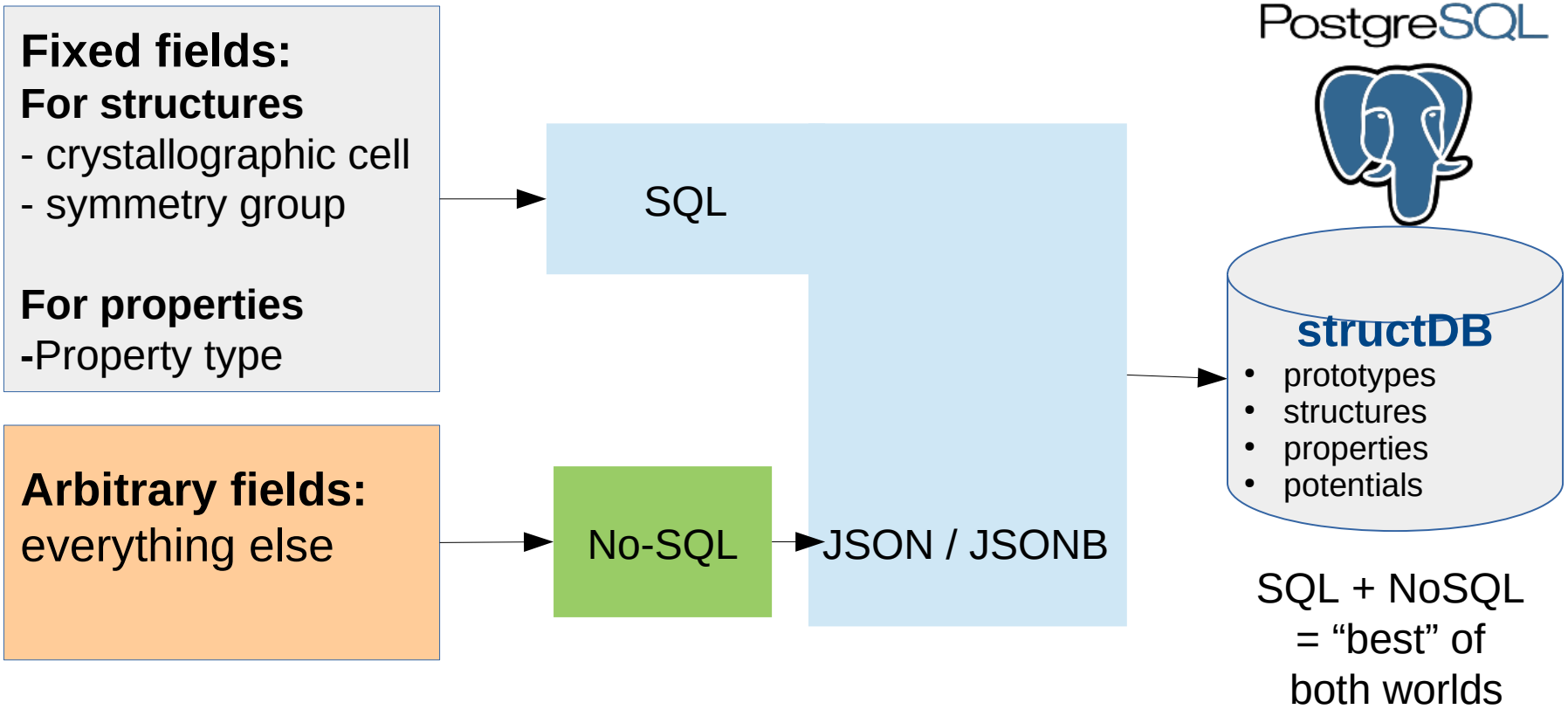
Atomistic simulations PPP-space

Abstract space for the “navigation” in atomistic simulations

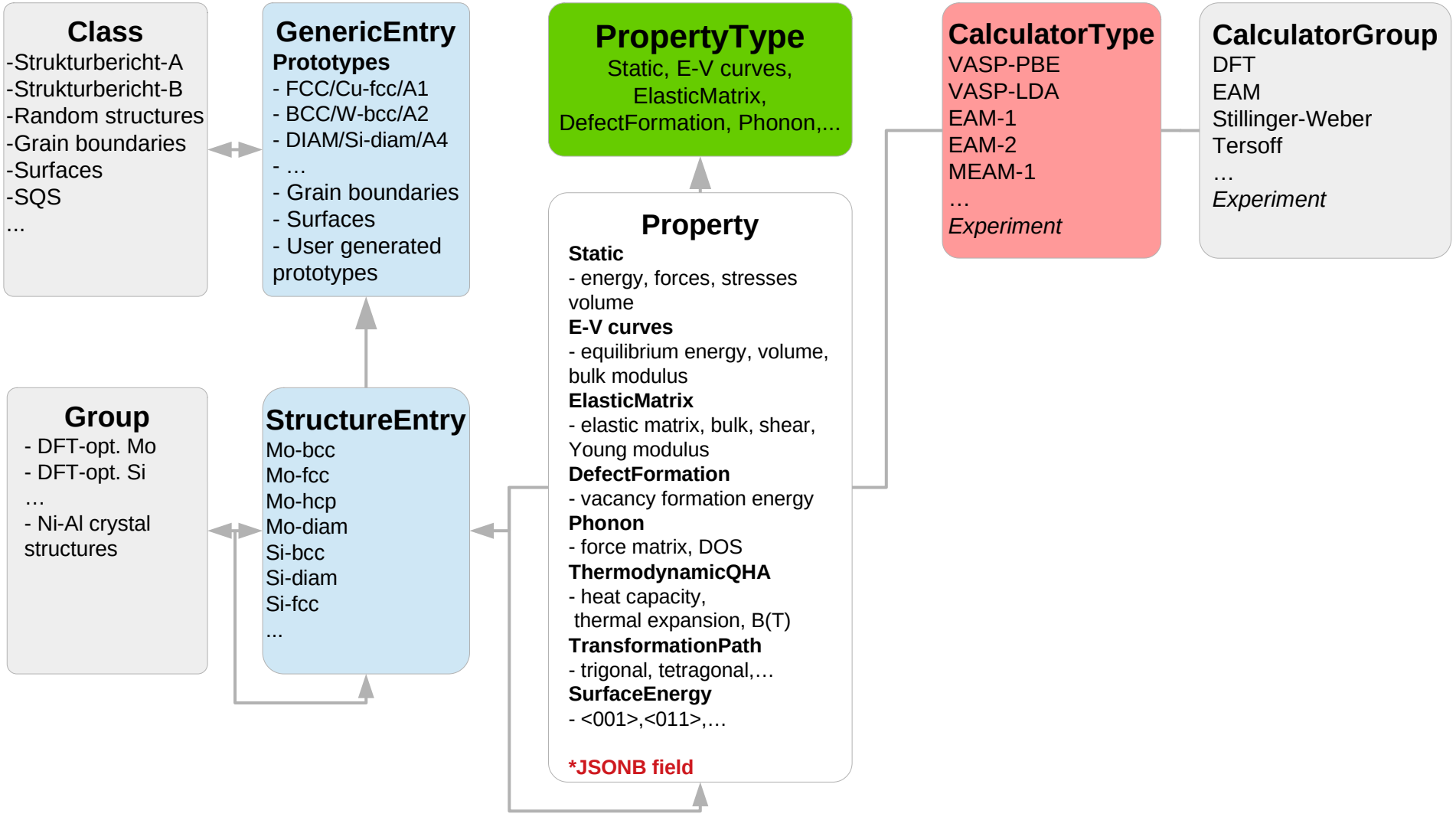


Data types of atomistic simulations

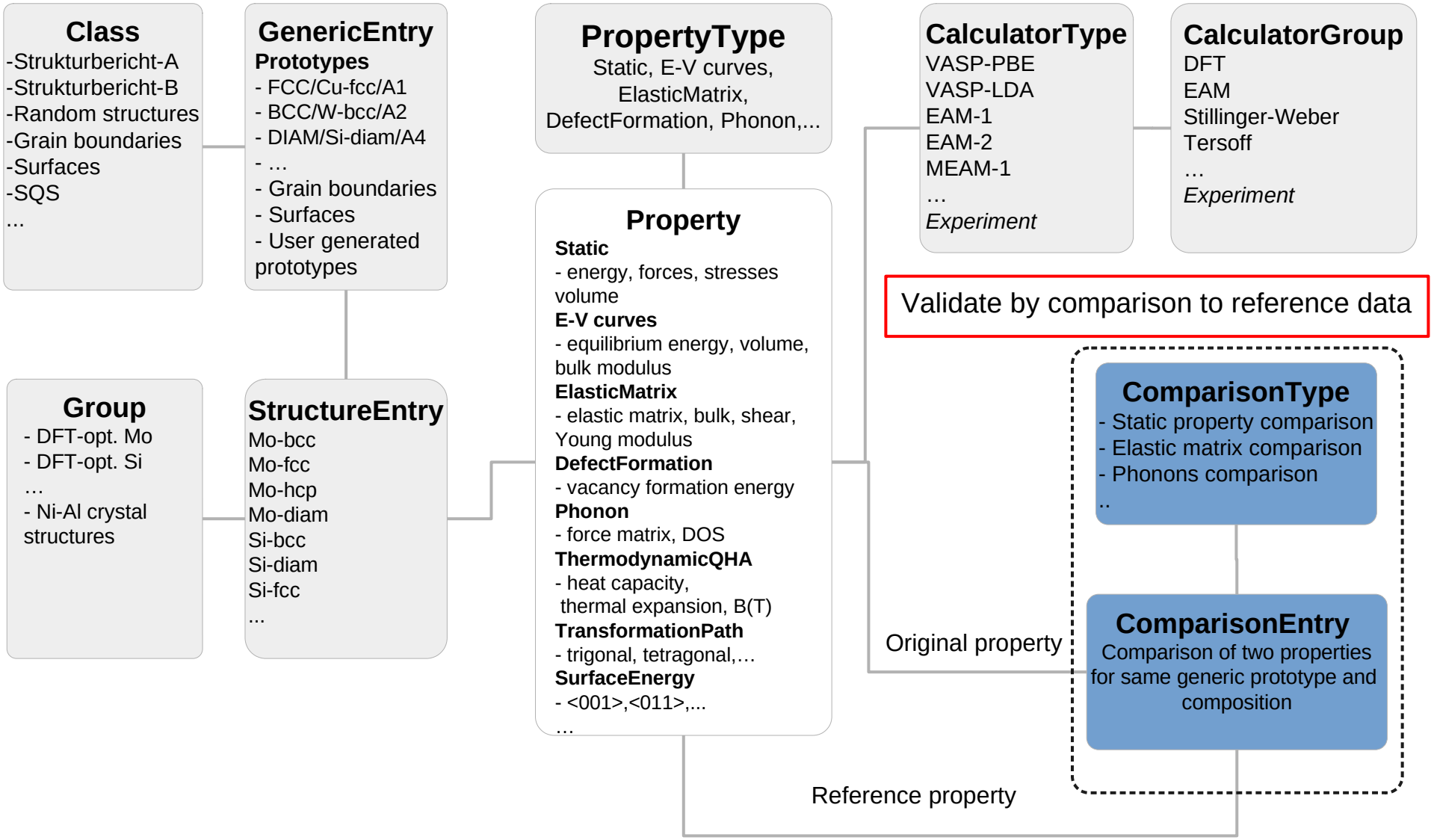
- **Atomic structures:** crystallographic cell, symmetry group, atomic coordinates, composition, etc...
- **Basic data:** energies, forces, volumes, etc...
- **Featured data:** elasticity, defect formation energy, phonon DOS, Cv, Cp, thermal expansion, transformation paths, etc...



Database design

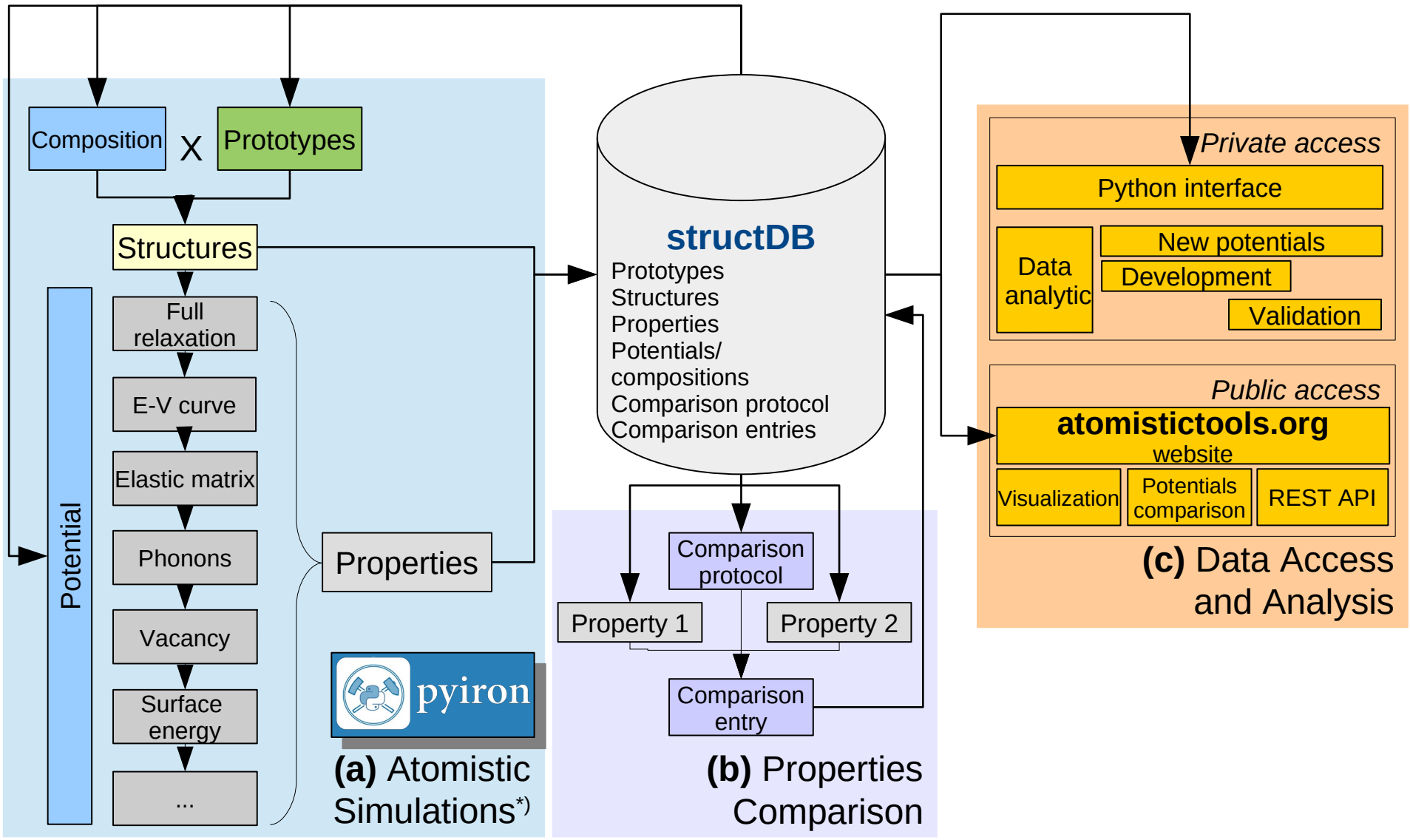


Data management: structDB



Interatomic potentials validation

Data management: structDB

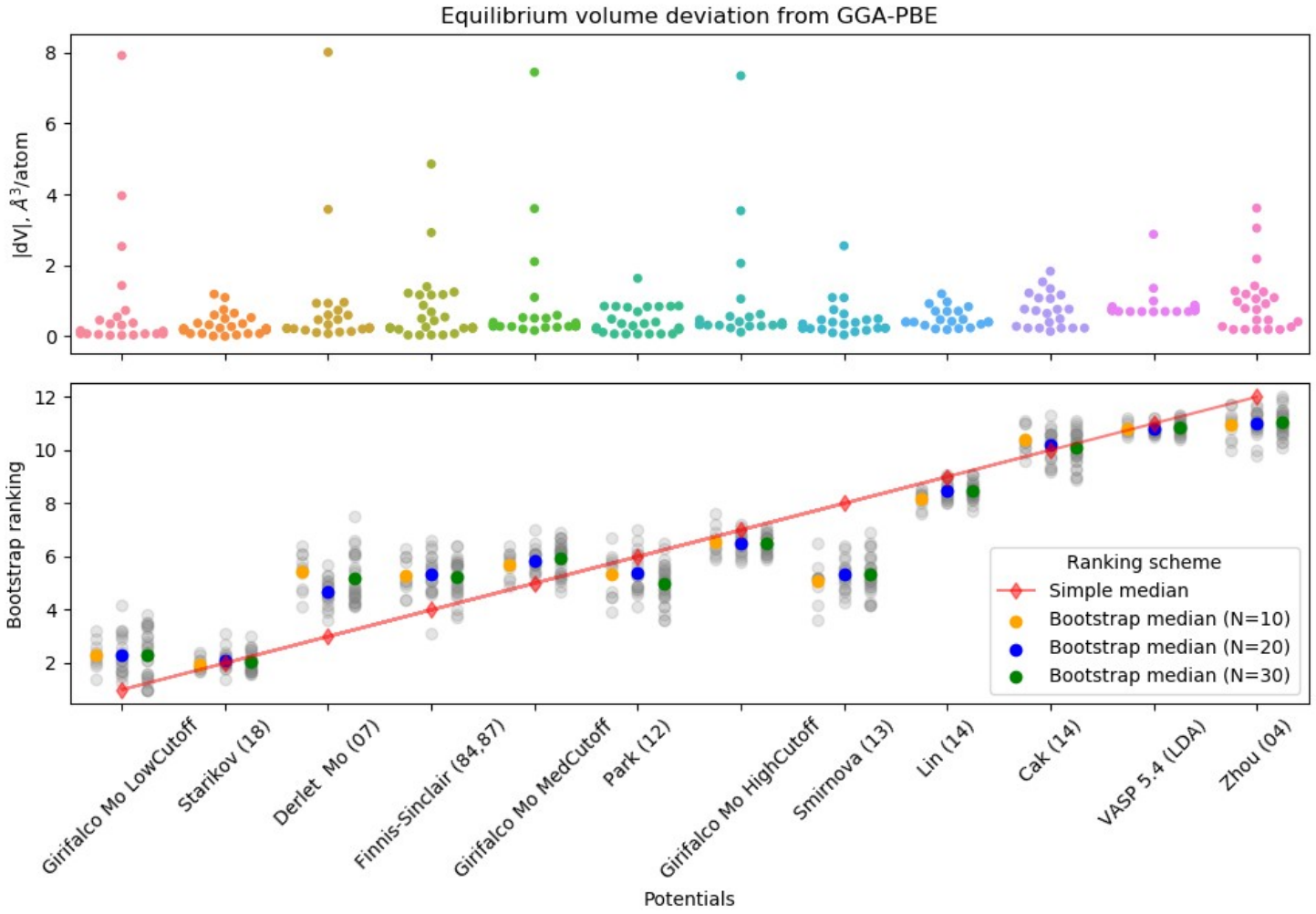


*) calculations are done with *pyiron*

Robust comparison of properties error distributions

Problem: Stability and robustness of potentials comparison wrt. outliers and incomplete sampling

Solution: Bootstrapping of error distributions → averaging → robust continuous ranking



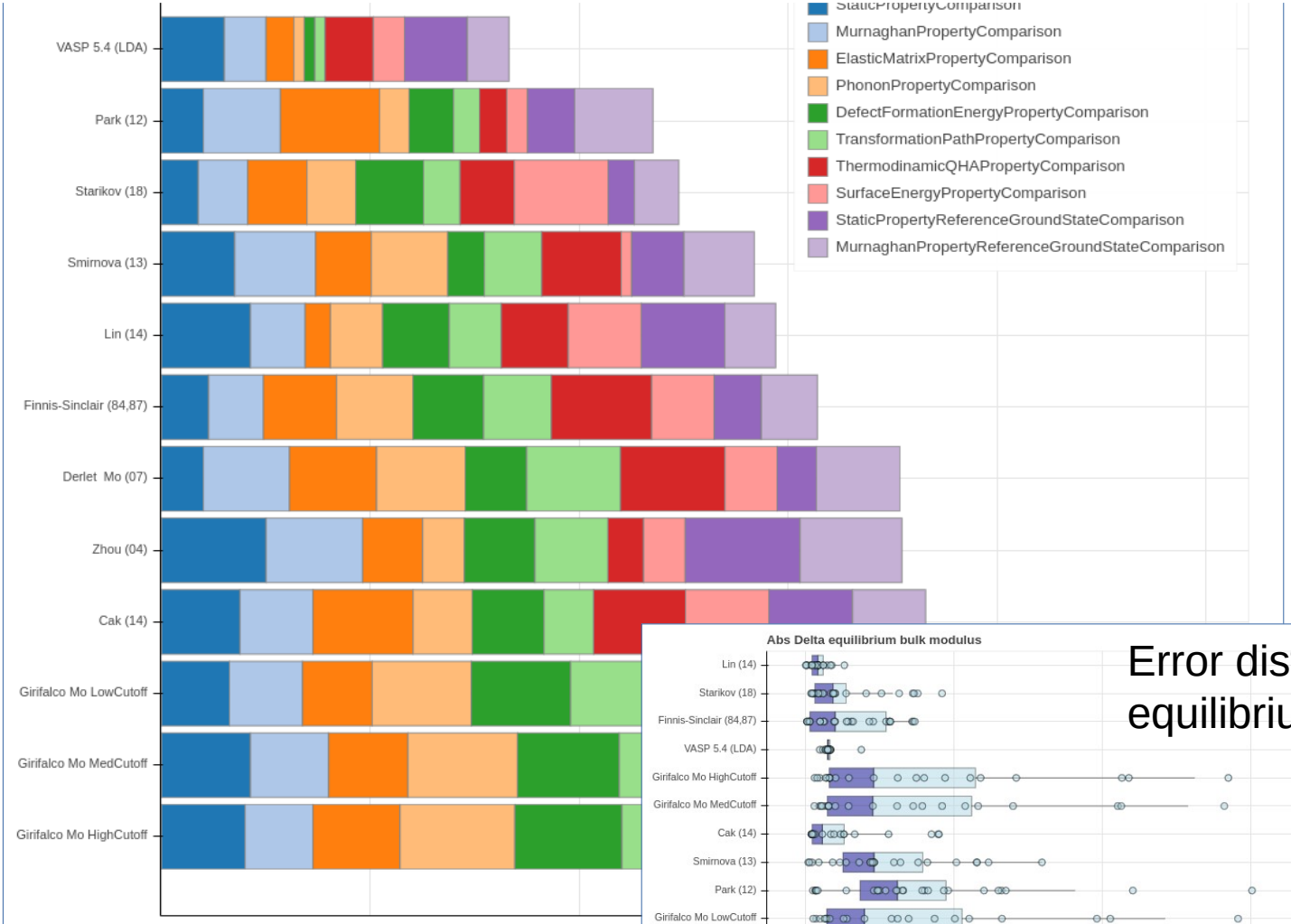
Points - errors for different crystal prototypes
(up to 29 points for the Strukturbericht A group)

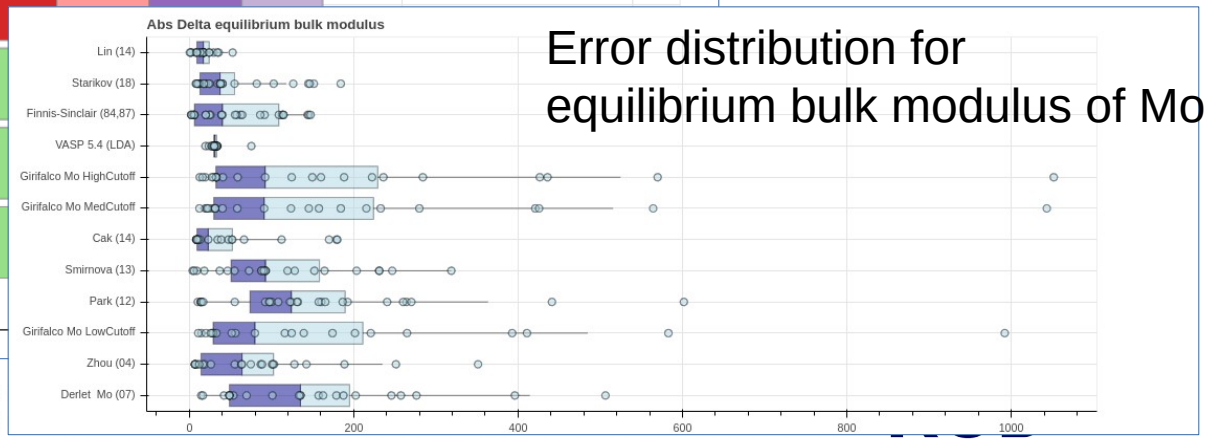
- Bootstrap error distributions 10, 20 and 30 times
- Convergence of the bootstrap ranking
- “Continuous” average rank

Atomistictools.org demo

atomistictools.org

Interatomic potentials performance in comparison wrt. DFT-PBE for Mo





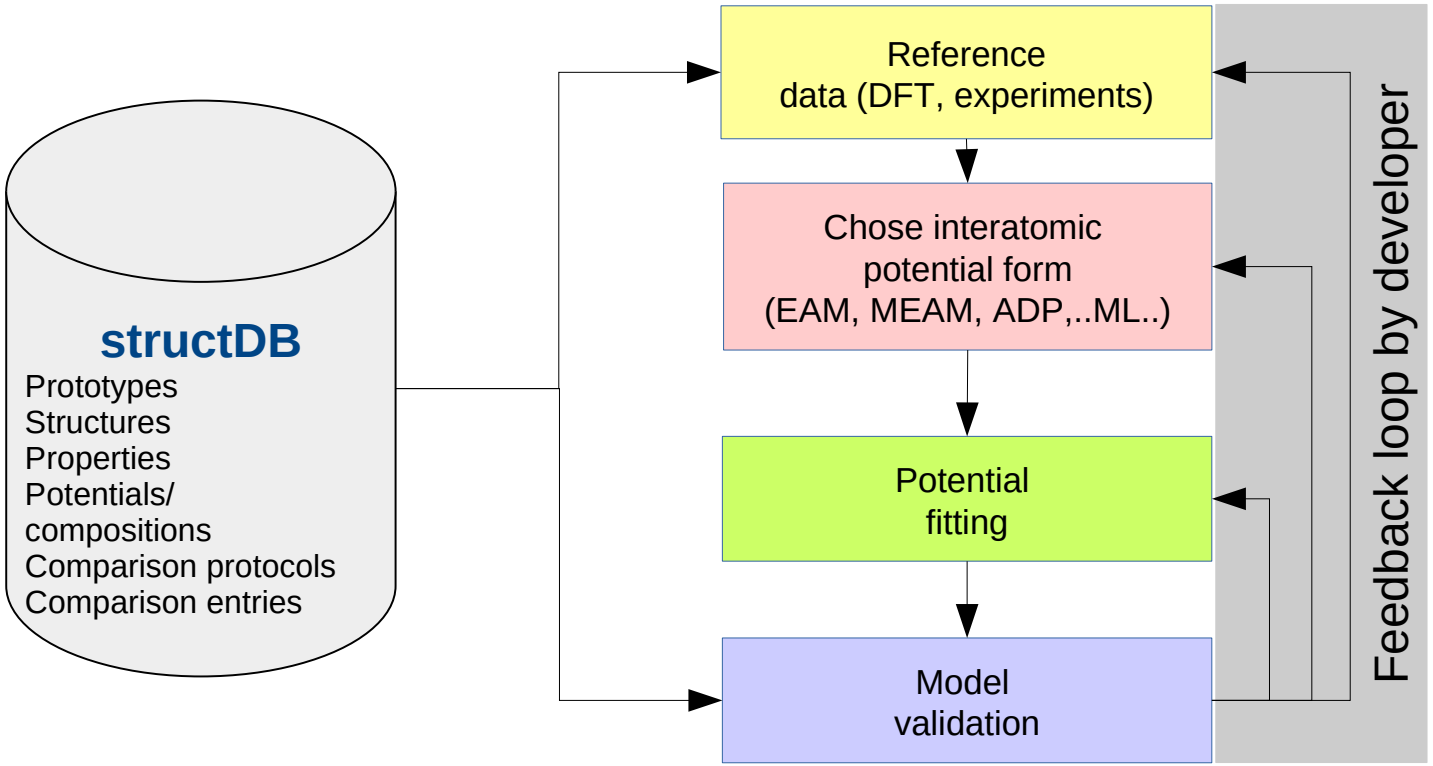
Error distribution for equilibrium bulk modulus of Mo

***YL**, Thomas Hammedschmidt, Ralf Drautz, Validation of the interatomic potentials for the unary compounds, in preparation*

Interatomic potentials development

with Alberto Ferrari and Sergei Starikov

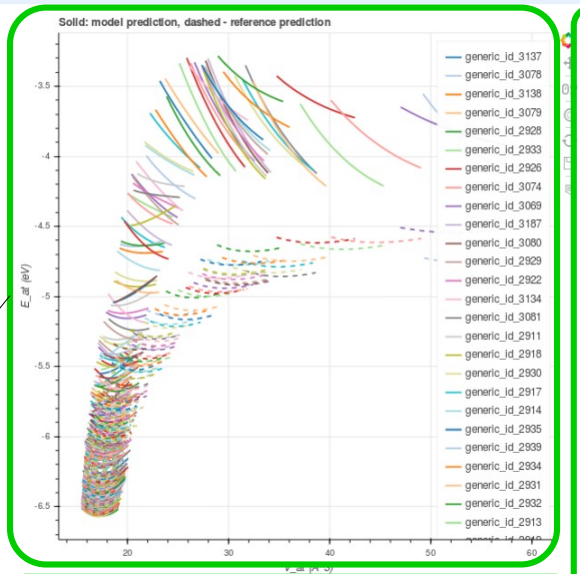
Interatomic potentials development process



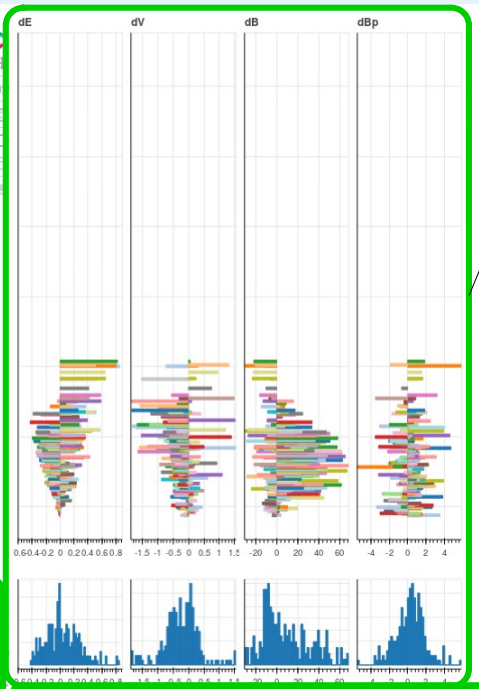
Bond order potential for Ti (by Alberto Ferrari)

Work environment screenshot

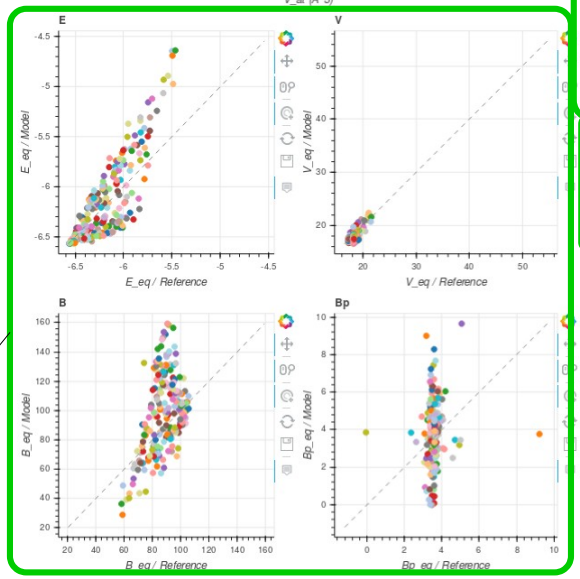
E-V curves for ~200 random structures



Error distributions for diff. properties



#	Stats	Mean	Std.	Min	Max
0	dE	0.191467948456...	0.160001832851...	0.001084865303...	0.8543508699
1	dV	0.455704448278...	0.424010841633...	0.001288255078...	1.8683717418
2	dB	19.06055198150...	16.38544426729...	0.019944958006...	68.707641602
3	dBp	1.253239861371...	1.057479813722...	0.006307481397...	5.8291087496



#	names	E_mod	E_ref	dE	V_mod	V_ref	dV	B_mod	B_ref	dB	Bp_mo	Bp_ref	dBp
0	gen...	-6.5...	-6.5...	-0.0...	17....	17....	-0.1...	101...	105...	-4.2...	4.8...	3.4...	1.4...
1	gen...	-6.5...	-6.5...	-0.0...	16....	17....	-0.2...	109...	105...	4.2...	6.9...	3.4...	3.5...
2	gen...	-6.5...	-6.5...	-0.0...	17....	17....	-0.0...	105...	104...	1.0...	5.0...	3.4...	1.5...
3	gen...	-6.5...	-6.5...	-0.0...	17....	17....	-0.1...	99....	103...	-4.3...	4.0...	3.4...	0.5...
4	gen...	-6.5...	-6.5...	-0.0...	17....	17....	-0.0...	100...	104...	-3.7...	2.8...	3.4...	-0.5...
5	gen...	-6.5...	-6.5...	-0.0...	17....	17....	-0.0...	104...	104...	0.8...	4.7...	3.3...	1.3...
6	gen...	-6.5...	-6.5...	-0.0...	17....	17....	-0.0...	100...	103...	-3.2...	0.4...	3.4...	-2.9...
7	gen...	-6.5...	-6.5...	0.0...	17....	17....	0.2...	98....	100...	-2.4...	3.0...	4.0...	-1.0...
8	gen...	-6.5...	-6.5...	-0.0...	17....	17....	0.1...	101...	98....	2.4...	2.4...	3.1...	-0.7...
9	gen...	-6.5...	-6.5...	-0.0...	17....	17....	-0.0...	95....	103...	-8.3...	2.6...	3.4...	-0.7...
10	gen...	-6.5...	-6.5...	-0.0...	17....	17....	0.0...	105...	103...	1.4...	0.8...	3.3...	-2.5...
11	gen...	-6.5...	-6.5...	-0.0...	17....	17....	0.0...	99....	103...	-3.6...	2.2...	3.4...	-1.2...
12	gen...	-6.5...	-6.5...	-0.0...	17....	17....	0.0...	95....	102...	-6.3...	2.4...	3.4...	-0.9...
13	gen...	-6.5...	-6.5...	0.0...	17....	17....	0.3...	91....	103...	-12....	1.9...	3.4...	-1.4...

Potential quality metrics

Potential-vs-DFT properties pairplots

*A. Ferrari, M. F. Schröder, **YL**, et. al., Phase transitions in titanium with an analytic bond-order potential MSMSE, 27, 085008, (2019)*

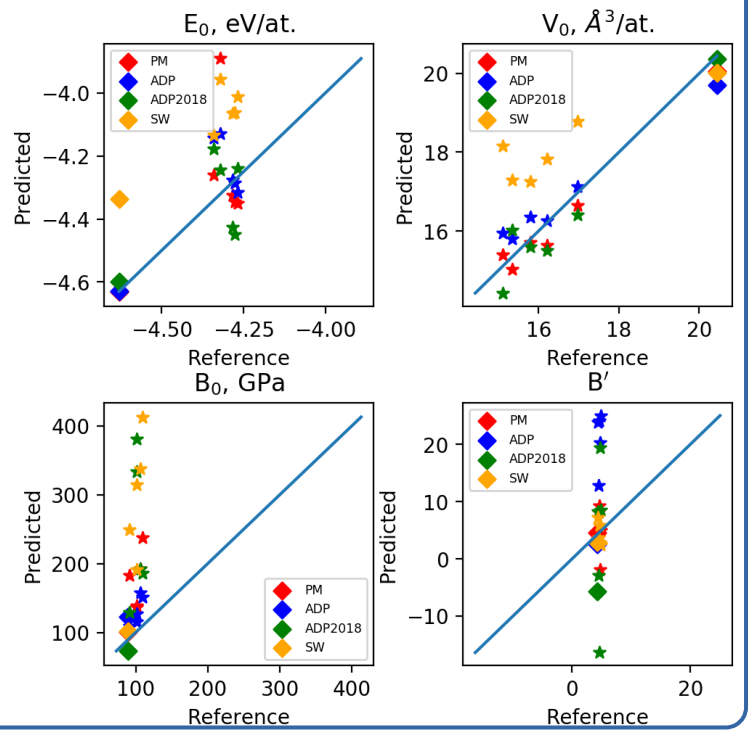
Angular dependent potential potential for Si - validation (by Sergei Starikov)

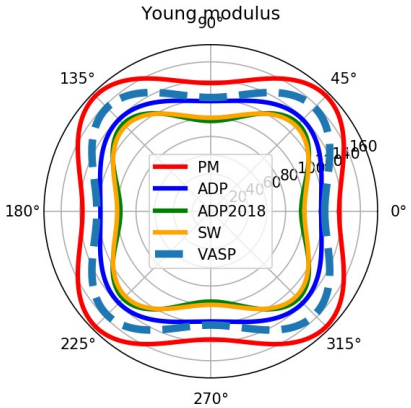
Independent validation of the new potential for Si wrt. reference DFT data (VASP) and comparison with existing potentials

New potential:
ADP2018: ADP Starikov 2018

Existing potentials:
PM: 2017—Purja-Pun-G-P-Mishin-Y--Si
ADP: ADP_Starikov_2017
SW: Three_Body_Stillinger_Weber_Si__MO_405512056662_003

E-V curves for low-energy structures



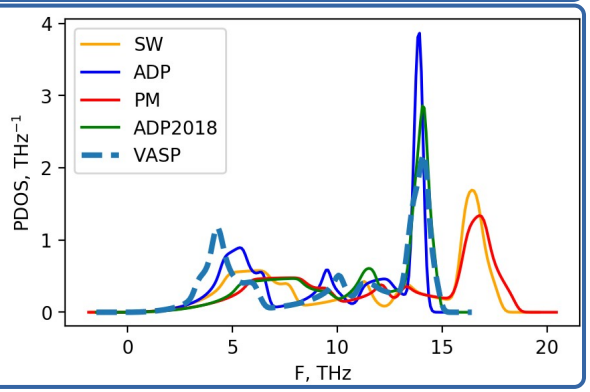


Elastic properties for Si-diam

SHORT_NAME	d_C	d_BH	d_EH	d_abs_Young
PM	41.0267	11.7134	17.1394	17.1507
SW	56.5568	12.5396	26.9793	26.5838
ADP2018	58.3122	16.2173	24.2326	24.7337
ADP	102.143	32.405	16.0617	15.0352

Phonon density-of-states for Si-diam

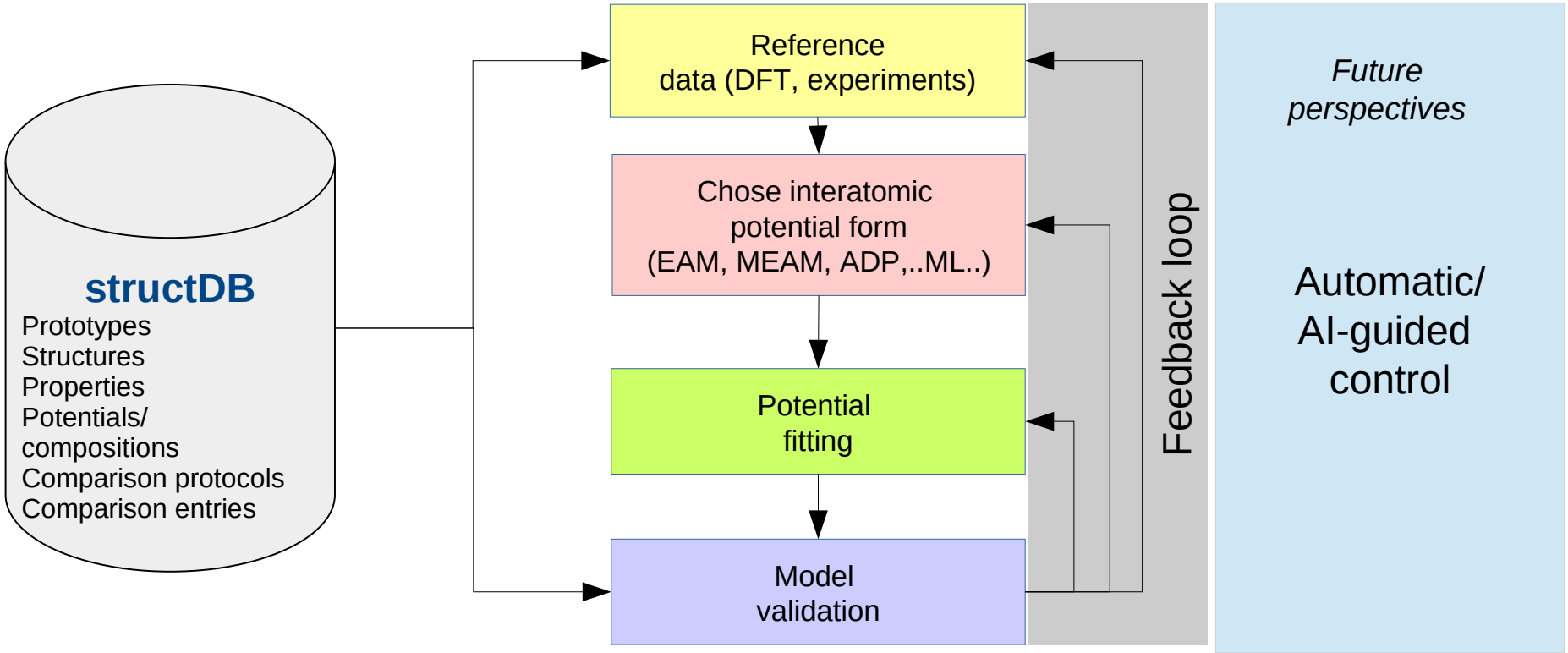
SHORT_NAME	d_DOS_MAE	d_freq_MAE	d_Cv_MAE
ADP	0.0309421	0.377617	0.0341284
ADP2018	0.0283281	1.11505	0.309852
SW	0.0486096	1.68497	0.451345
PM	0.0513959	2.39533	0.647455



*S. Starikov, I. Gordeev, **YL**, L. Kolotova, S. Makarov, Optimized interatomic potential for study of structure and phase transitions in Si-Au and Si-Al systems, Comp.Mat.Sci. 184 (2020): 109891.*

Interatomic potentials development - future perspectives

Automatic/ML/AL/AI-guided fitting procedure based on the potentials quality metric



Use ML/AI to create physical models

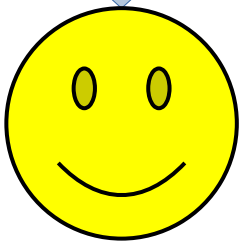
Future perspectives: distributed resources

Future perspectives: use-cases and roles

Atomistic simulations distributed resources
(NIST IPR, OpenKIM, atomistictools.org, ...)

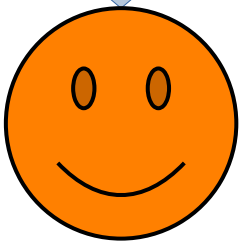
Web interface, REST-API, API

- **Interatomic potentials (IP)**
- **Models validation**
- Protocols validation



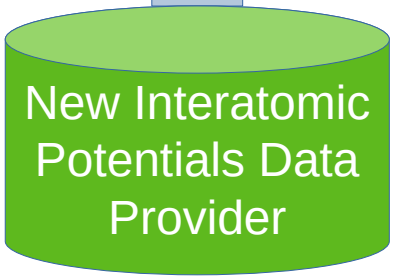
Molecular dynamics simulation user

- **Provide new IP**
- Get test protocols for new IP
- Get reference data for fitting and validation

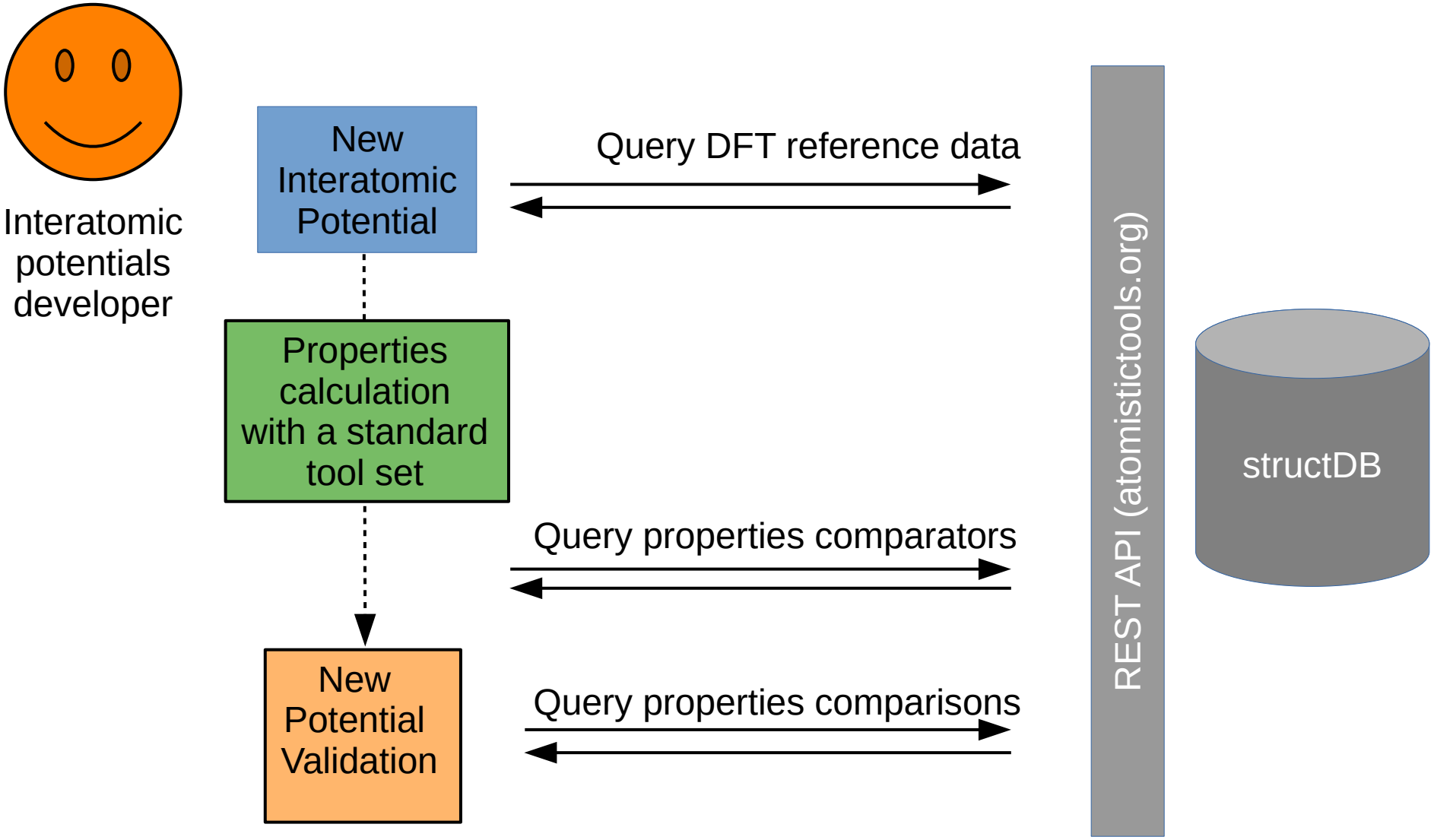


Interatomic potentials developer

Provide new data, validation tests, resources, protocols, etc.



REST API use scenario: new potential validation



REST API interface (proof-of-concept)

Provide functionality for querying the interatomic potentials validation database without direct connection to database (via WEB)

- Crystal prototypes (generic)

```
generics=db_rester.query_generic(prototype_strukturbericht=”A2”)
```

- Structures

```
structures=db_rester.query_structure(prototype_strukturbericht=”A2”,
                                     calculator_name="VASP%PBE%",
                                     structure_composition="Mo%")
```

- Computed properties (i.e. reference DFT data)

```
reference_data=db_rester.query_property(property_type_name="murnaghan",
                                        structure_composition="Si%",
                                        prototype_strukturbericht="%",
                                        calculator_name="VASP%PBE%")
```

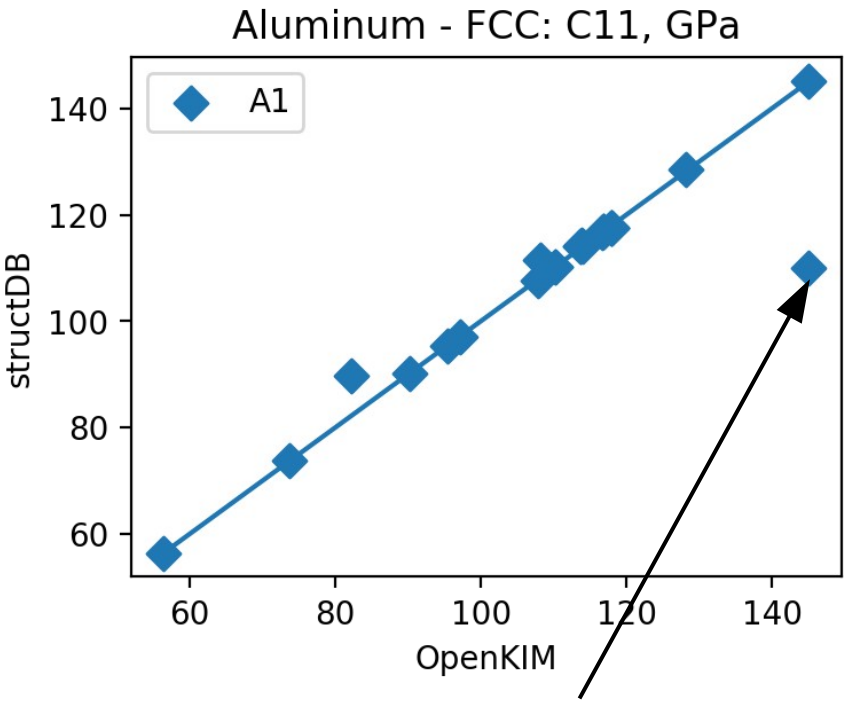
- Properties comparison protocol (comparator)

```
comparator=db_rester.query_comparator(property_type_name="phonons")
```

Data consistency? (open question)

Distributed query to OpenKIM & atomistictools.org*

Query elastic constants of fcc aluminum

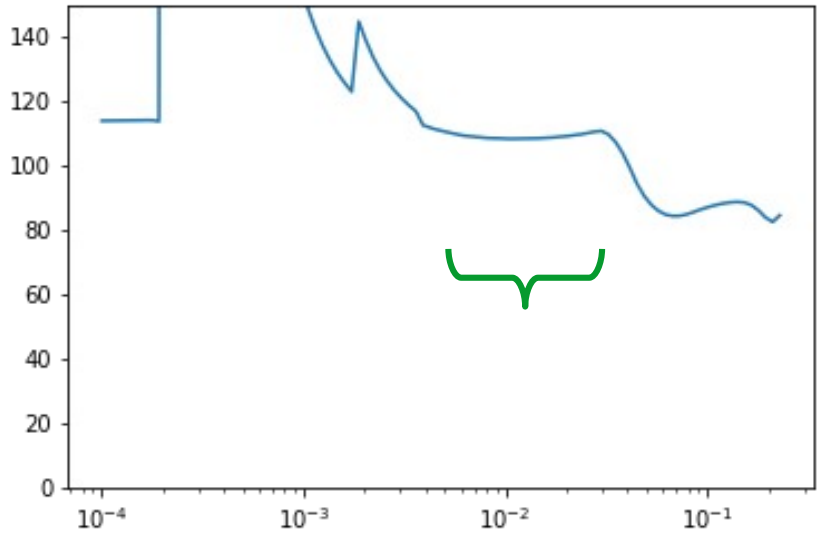


EAM_Dynamo_ZhouJohnsonWadley_2004_Al

- OpenKIM uses small strain range (~1e-8) and numerical derivatives
- Numerical noise of the model implementation
- Instability of properties computational protocol

Each property calculation protocol has it's "hyperparameters", i.e. strain range, number of points, fit order for elastic matrix calculations

EAM_Dynamo_ZhouJohnsonWadley_2004_Al MO_131650261510_005



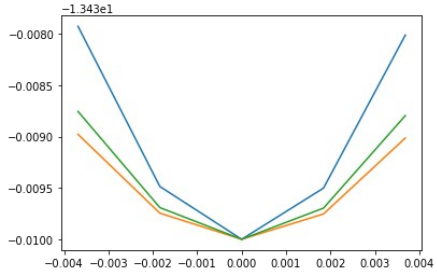
Strain range: 10^{-5} - $2*10^{-1}$

*) *proof-of-concept*

Properties calculation hyper-parameters

Example: elastic matrix property via energy-strain curves

ElasticMatrixCalculator(
num_of_point=5,
eps_range=0.005,
fit_order=2,
optimize_deformed_structure=True,
fmax=0.005)



“hyper-parameters”

- Physically-inspired suggestions (max **num_of_point**, min **eps_range**, min **f_max**) not always correct, due to numerical noise, etc.

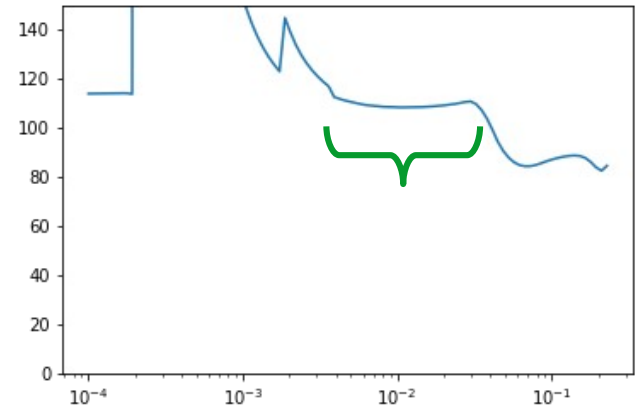
- Sensitivity analysis should be done for each parameter and property type:
  - vary hyperparameters combinatorially
  - compute property
  - find “safety spot” in hyper-parameter space (stable predictions)
- Does this “spot” is transferable to another potentials types and elements?

Properties calculation hyperparameters

Each property calculation protocol has it's "hyperparameters".
Ex.: Elastic matrix calculation: strain range, number of points, fit order, ...

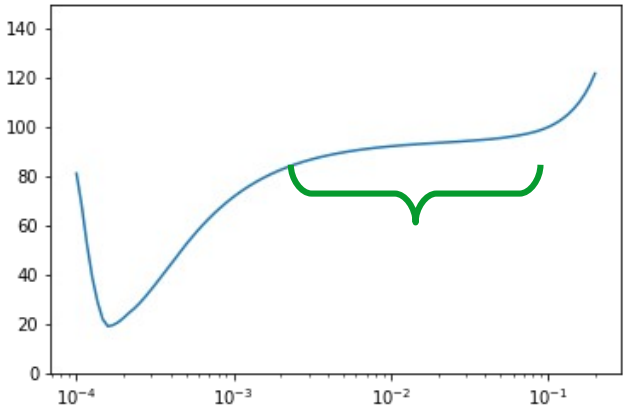
Aluminum-fcc: C11 constant

EAM_Dynamo_
ZhouJohnsonWadley_
2004_Al
MO_131650261510_005



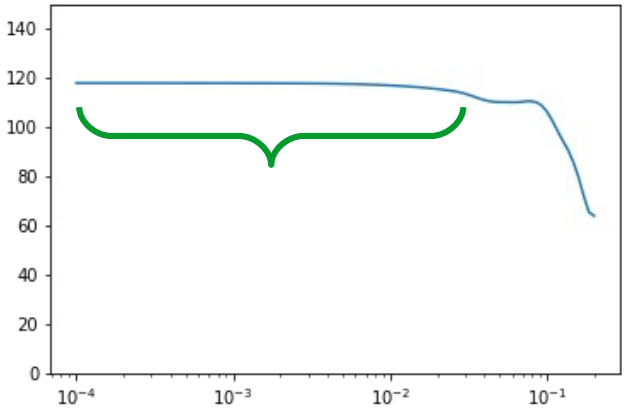
Strain range: 10^{-5} - $2*10^{-1}$

Morse_Shifted
GirifalcoWeizer_
1959HighCutoff_Al
MO_140175748626_003



Strain range: 10^{-5} - $2*10^{-1}$

EAM_
ErcolessiAdams
1994_Al
MO_324507536345_002



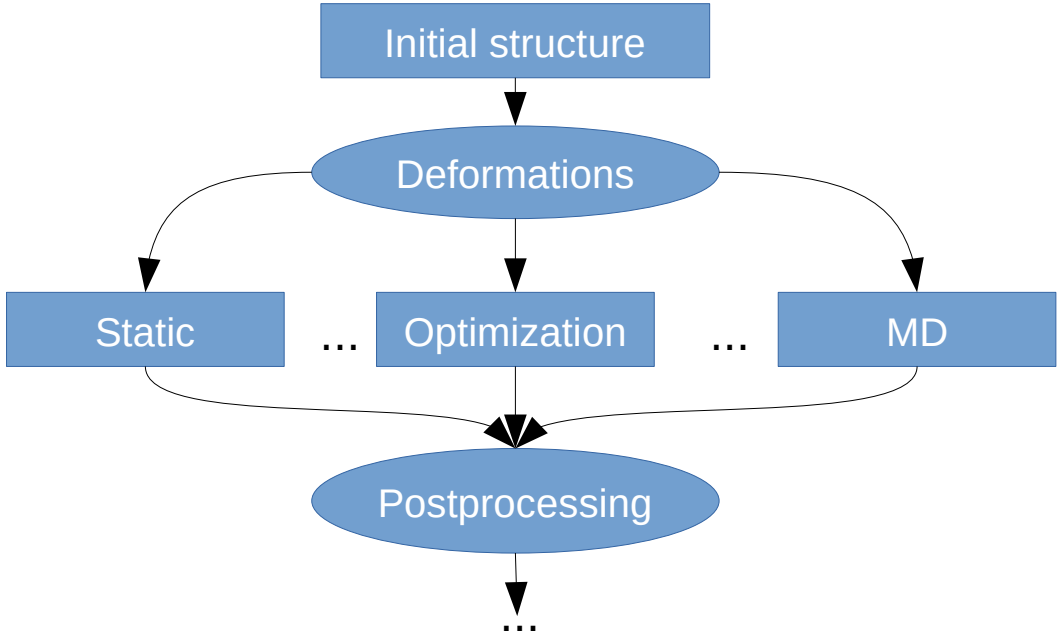
Strain range: 10^{-5} - $2*10^{-1}$

There are an overlapping of "safety-spots" of hyperparameters for properties calculations for different potentials and elements

Generalization of properties calculation protocols

1. Properties calculation protocols are mostly general:

- Initial structure(s)
- Deformations (optional)
- perform
  - Static calculation
  - Optimization
  - Molecular Dynamic
- Post-processing
- … repeat (optional)



2. Different execution "backends/engines":

- ASE, Fireworks/Atomate, AiiDA, AFLOW, pyiron, Atomman, …

Separation between **protocol** and **computation engine(s)** is needed for unification!

- Unified "**language**" to describe the **atomic properties** calculation protocol
- Mapping to different execution "backends"
- Way to achieve interoperability between data producers and data storage
- **Standardize** atomistic simulations

Concluding remarks

Concluding remarks

- Interatomic potentials validation by high-throughput **properties comparison (transferability)**
- Common protocols & tests for interatomic potentials validation and DFT
- Testing of publicly available potentials:
  - **OpenKIM** & **NIST** potentials repositories
- Potential comparison as a service for community:
  - **atomistictools.org** (testing stage, password: "**icams"**)
- Comparison wrt. reference data: usually DFT (VASP 5.4 PBE) or experiment (Pearson Crystallographic Database, Landolt-Boernstein, …)
- REST API with compatible interfaces for unified queries

Further development

- Production stage of **atomistictools.org** (for unaries)
- Increase the amount of properties & comparison metrics
- Sampling strategies for binaries and ternaries compounds
- Data analysis of the potentials transferability, identification of the key metrics
- Testing for ML potentials

Thank you for attention