ASE Workshop 2019

a Summary by Florian Knoop

Intro

ASE:

The **A**tomic **S**imulation **E**nvironment (Intro-Slides by Ask)

Workshop Organizers:

Paul Erhart, Tuomas Rossi, **Ask H. Larsen**, Jens J. Mortensen, Kristian S. Thygesen

Location:

Chalmers University, Gothenburg, Sweden

Scope: Bring the community together (for the first time)

ase-workshop.materialsmodeling.org/

Speakers

- **Jens Jørgen Mortensen (DTU): History of ASE**
- **Adam J. Jackson (STFC UK): Use all the codes!**
- Michael Walter (Uni Freiburg): Non-resonant Raman spectra
- Florian Knoop (FHI): `FHI-vibes`
- **Erik Fransson (Chalmers): `hiphive` and `icet`**
- Jin Hyun Chang (DTU): Cluster expansion with CLEASE
- **Jakob Schiøtz (DTU): KIM framework for force fields**
- Marko M. Melander (Uni Jyväskylä): Grand Canonical Chemistry
- Mikael Kuisma (Uni Jyväskylä): Light-matter interaction with GPAW
- **Peter M. Larsen (DTU): Classification of Bravais lattices w/o tolerance**

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Speakers

- Maxime Van den Bossche (Paris): Global structure optimization w/ DFTB
- **Eric D. Hermes (Sandia Labs): Saddle point search with `sella`**
- Ask Hjorth Larsen (Simune Atomistics): ASE
- **Bjørn Lindi (Norwegian Inst. of Science): Code development**
- **Kirsten T. Winter (SLAC): ASE database applications**
- Morten Gjerding (DTU): Atomic Simulation Recipes (ASR)

+ Tutorials

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Jens Jørgen Mortensen: History of ASE

Contribute to ASE?

```
Think of a contribution like a puppy: you might view it as this cute,
wonderful thing you're giving me while I'm looking at it as over a
decade of feeding, walking, and vet bills.

-- Brett Cannon
```

Not everything is a good fit for ASE

Alternatives:

- Code snippets in a tutorial plus a few helper functions added to ASE.
- Its own thing: PyPI + GitLab + ReadTheDocs + JOSS

Adam J. Jackson

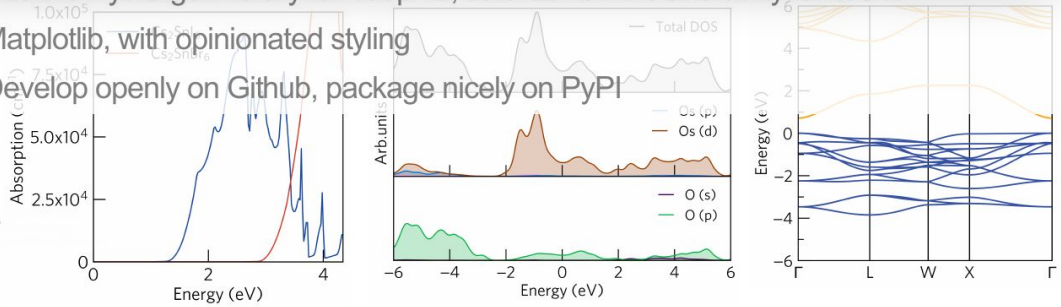
Importance of good tools

Anecdote 2: Sumo

JOSS 10.21105/joss.00717

Interest in plotting nice band structures?
Checkout **sumo** and contact **Adam**!

- Use the Pymatgen library for Vasp IO, data containers and utility functions
- Matplotlib, with opinionated styling
- Develop openly on Github, package nicely on PyPI



Erik Fransson: hiphive

Force constant extraction

hiphive

$$E = E_0 + \sum_i \Phi_i u_i + \frac{1}{2!}\sum_{ij} \Phi_{ij} u_i u_j + \frac{1}{3!}\sum_{ijk} \Phi_{ijk} u_i u_j u_k \ldots$$

"Direct" approach: systematic enumeration

Harmonic approximation → phonopy

Third-order FCs → phono3py, almaBTE

→ Poor scaling with system size and order

$$\Phi_{ij} = \frac{\partial^2 E}{\partial u_i \partial u_j} \approx -\frac{F_i(u_j) - F_i(0)}{u_j}$$

"Regression" approach: fit to snapshots

→ TDEP & ALAMODE

Hellman *et al.* PRB 2011, Tadano *et al.* JPCM 2014

→ Compressive sensing

Zhou, Ozolins *et al.* PRL 2014

$$\Phi_{ij} = \Phi_{ij}(\boldsymbol{x})$$

$$\min(\|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{f}\|_2^2)$$

hiphive

Generalizes regression approach and makes it easily accessible

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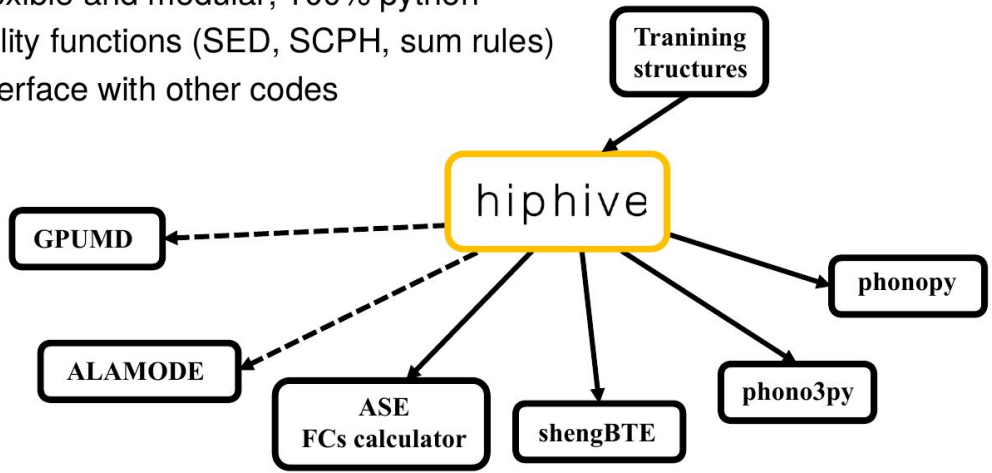
Erik Fransson: hiphive

hiphive

hiphive

Force constants extraction tool

- Flexible and modular, 100% python
- Utility functions (SED, SCPH, sum rules)
- Interface with other codes



python

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Eriksson *et al.*, Adv. Theory Simul. **2019**, 1800184

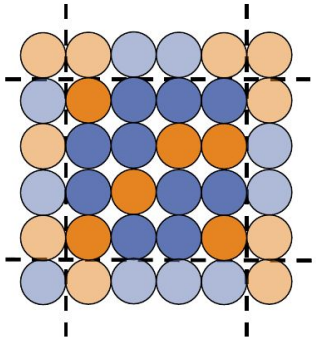
Erik Fransson: icet

Cluster Expansions

icet

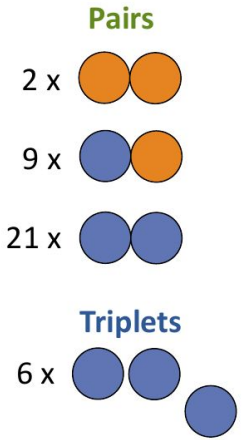
Expansion of the total energy in site occupations

$$E(\boldsymbol{\sigma}) = E_0 + \sum_i J_i \sigma_i + \sum_{ij} J_{ij} \sigma_i \sigma_j + \sum_{ijk} J_{ijk} \sigma_i \sigma_j \sigma_k + \ldots$$



$\boldsymbol{\sigma}$ Occupation vector

Decompose into "clusters"



Need efficient means to extract effective cluster interactions (ECIs) J_α
→ Again a linear problem

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Jakob Schiøtz: KIM force fields

KIM Testing Framework

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

Mandatory

- Species supported as stated;
- Unit conversion handled correctly;
- Domain decomposition handled correctly;
- ...

Consistency

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

Informational

- 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
- cohesive energy
- elastic constants
- lattice constants
- phonon spectrum
- thermal conductivity
- thermal expansion
- ..

Wall
- antiphase boundary
- gamma surface
- grain boundary structure
- stacking fault energy
- surface energy
- surface structure
- ...

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

Point
- vacancy formation energy
- vacancy migration barrier

Ellad B. Tadmor (University of Minnesota) 14

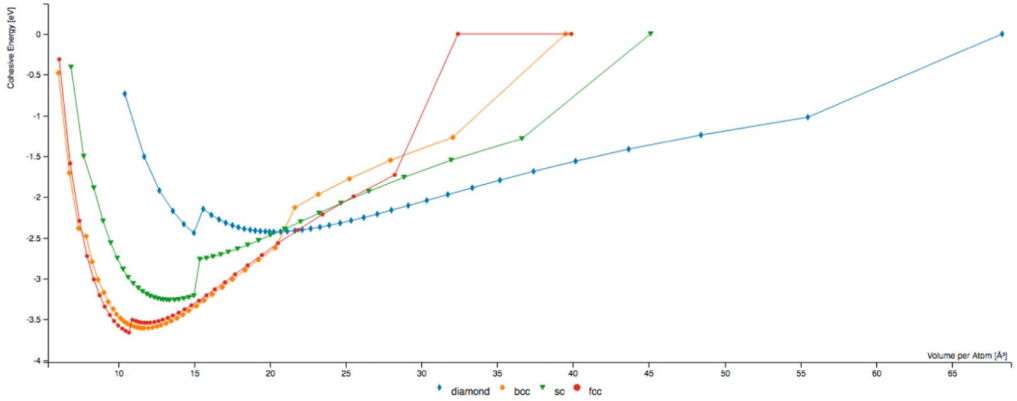
Jakob Schiøtz: KIM force fields

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.



Peter M. Larsen: Symmetry w/ distance functions

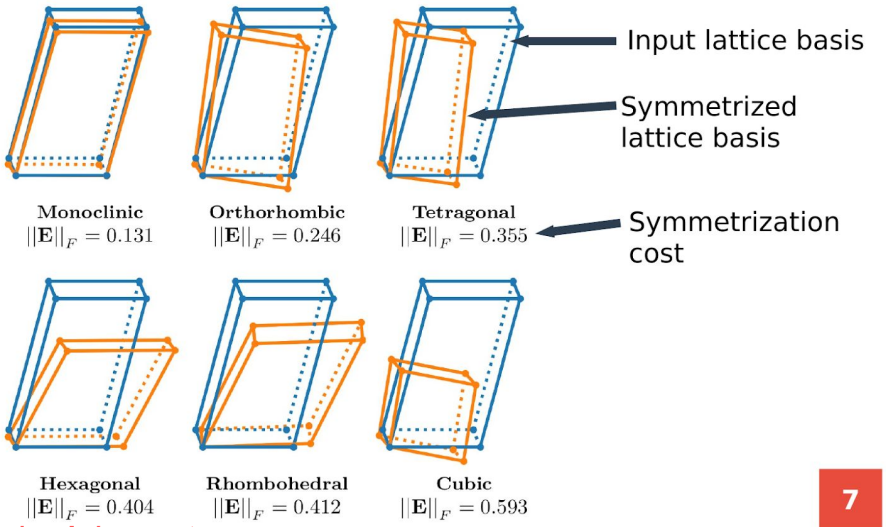
TRATTORIA DEI MATERIALI

Bruschetta	*???*
Risotto con asparagi	*???*
Linguine All'arrabbiata	*???*
Gnocchi ai quattro formaggi	*???*
Melanzane alla parmigiana	*???*

Peter M. Larsen: Symmetry w/ distance functions

A menu for Bravais lattices

Symmetrize by minimizing distance function *d(A, B)*
B is observed lattice basis *(input)*
A is variable lattice which respects symmetry of target Bravais type



https://github.com/pmla/auguste

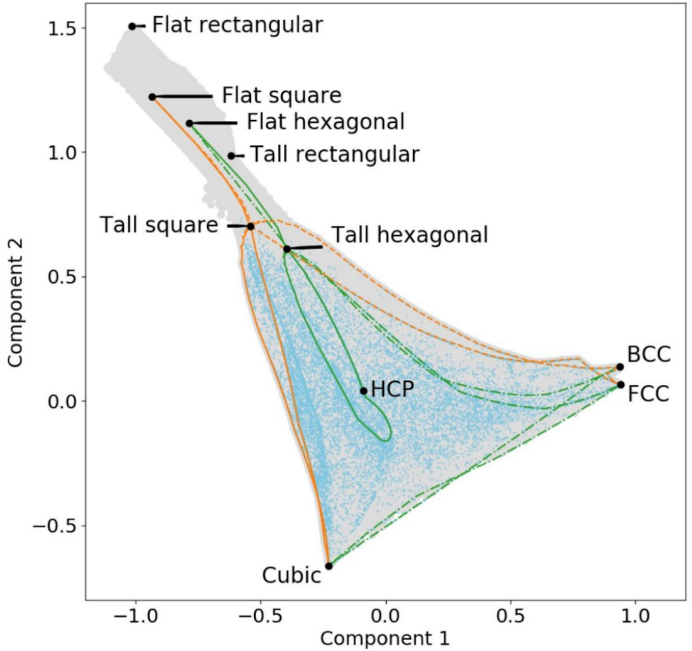
Peter M. Larsen: Symmetry w/ distance functions

Visualizing the Bravais lattice space

-All structures in Crystallography Open Database (blue dots)

-PCA projection of distance vectors

-Distance function aids understanding



https://github.com/pmla/auguste

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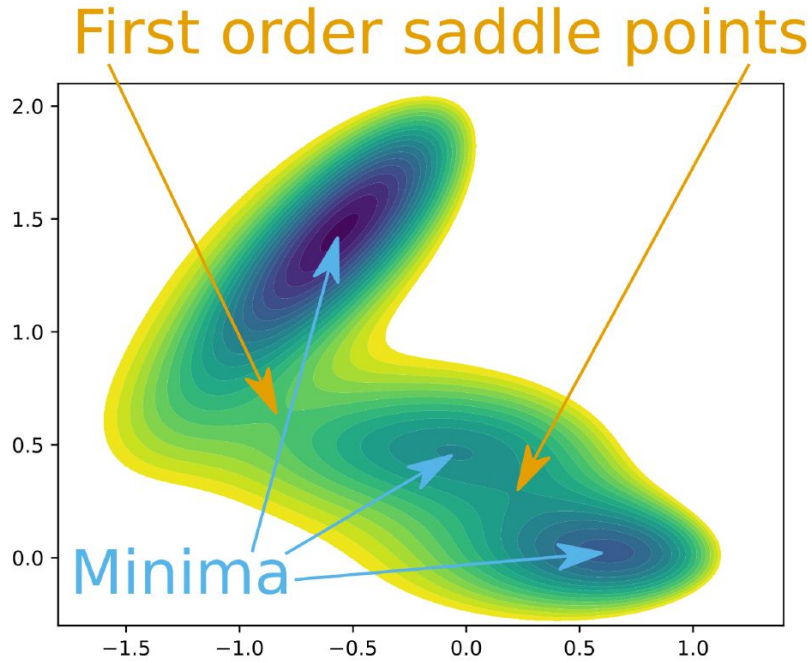
Eric D. Hermes: Saddle points w/ Sella

What is Sella?

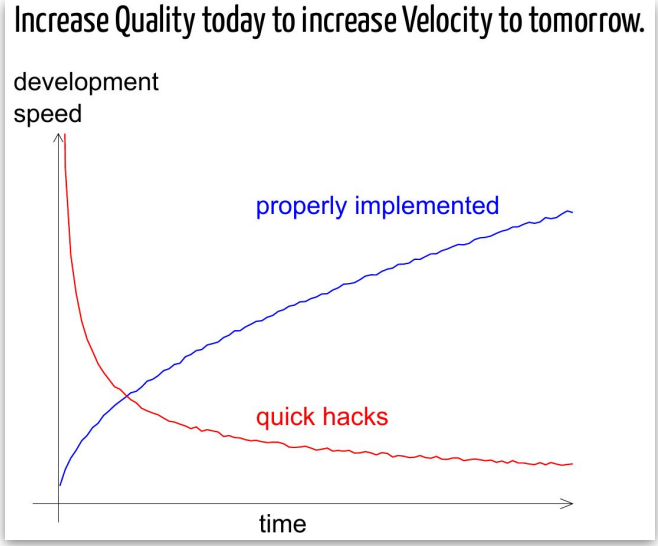
Sella is a tool for finding first order saddle points.



Bjørn Lindi: Write CLEAN code

Fail forward?

Give yourself the freedom to make mistakes, establish short feed back cycles.



Other useful things

"Finnish Stop" for debugging:

- type **`asdf`** (or anything else) to make your code "stop" where you want
- like breakpoint() in python (3.7+) only faster

Python, scipy, etc. have *a lot* of useful stuff built in

- e.g. logging module

The conference was paper free

- organization via up-to-date webpage

Other useful things

You can have beer on tap in the Mensa!

Summary

ASE has a nice and active community centered around DTU Copenhagen

Core developers know what they are doing

ASE is purely FOSS with all the pros and cons

Making decisions is *not* a speciality of ASE's core team

There is a world beyond single-use scripts: Let's write (better) packages!

We (FHI people) should embrace ASE and fully adopt the aims Calculator

Thank you!

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MAX-PLANCK-GESELLSCHAFT

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Florian Knoop