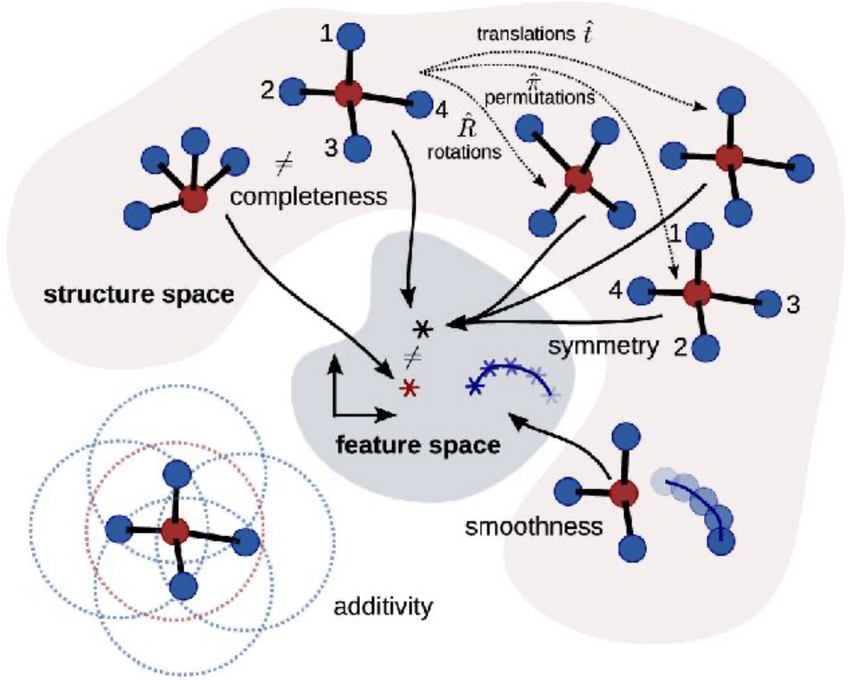
COSMO
COMPUTATIONAL SCIENCE AND MODELING

EPFL



ML-IP 2023

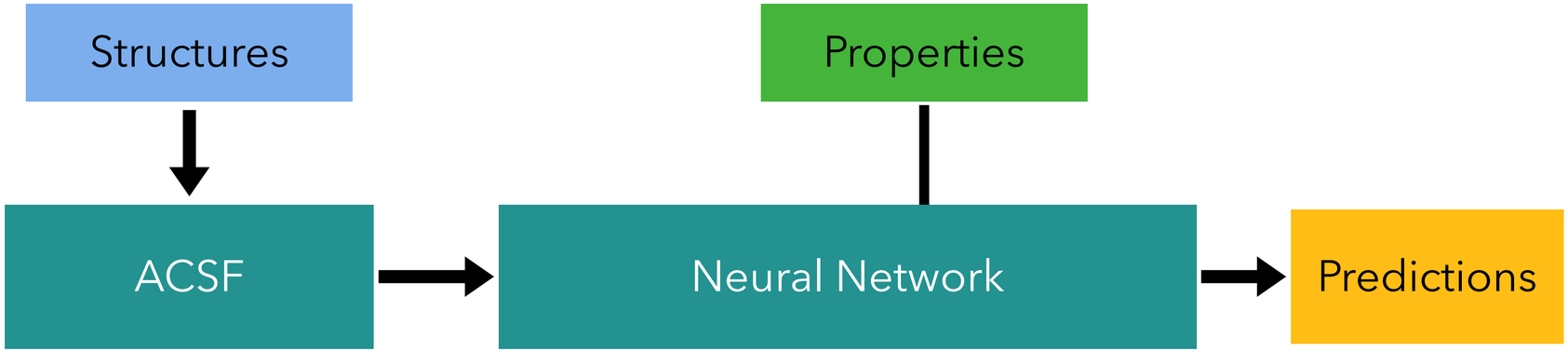
A common language for atomistic machine learning models

Guillaume Fraux

guillaume.fraux@epfl.ch

@Luthaf
@__luthaf__
mas.to/@luthaf

The state of atomistic machine learning



Behler-Parrinello NN

PiNN

SchNET

Snap

n2p2

REANN

DeepMD

ANI

ænet

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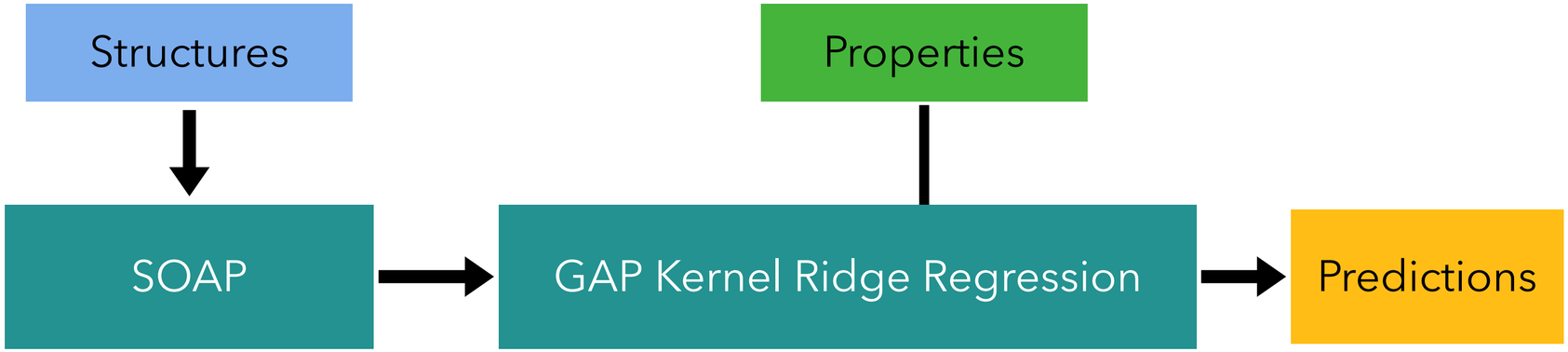

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Kernel models

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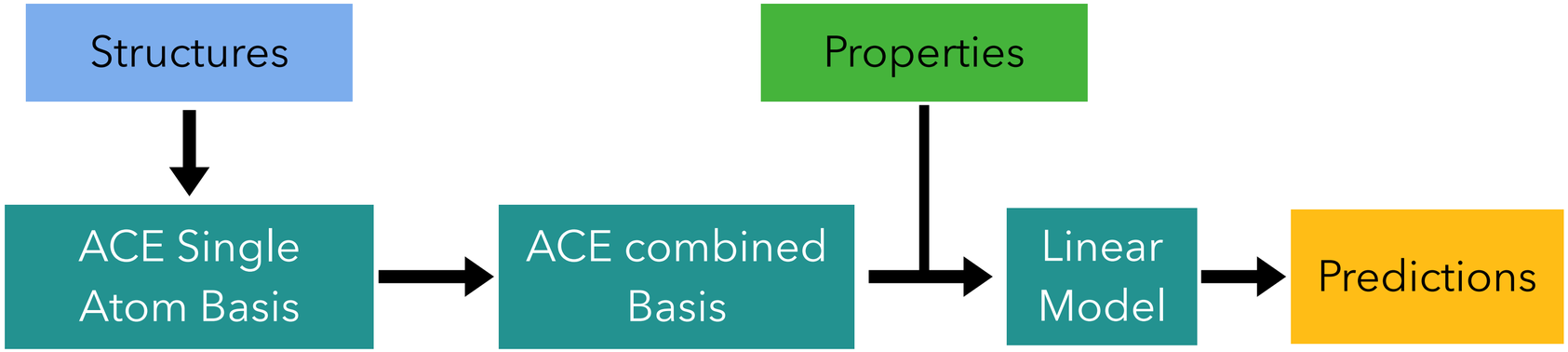

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Body-ordered representations

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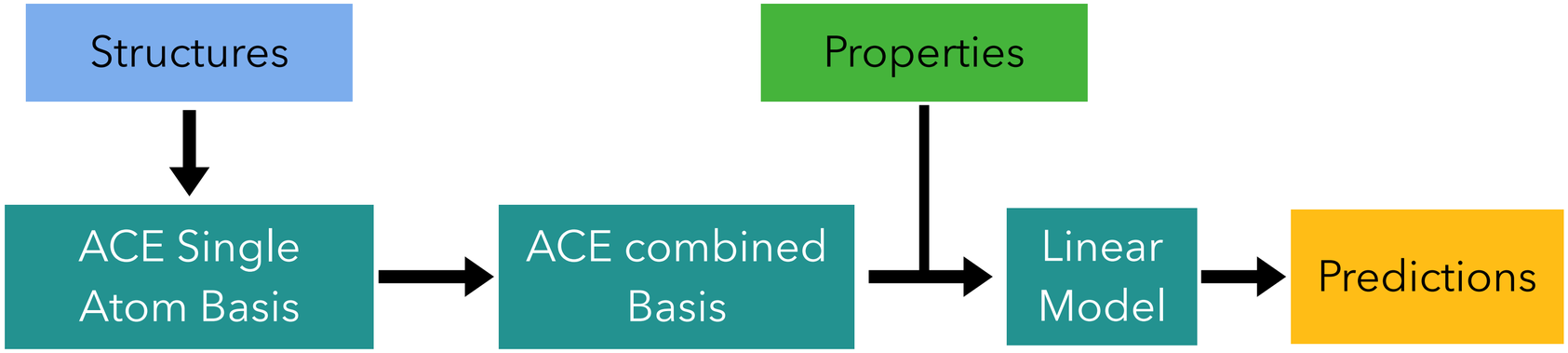

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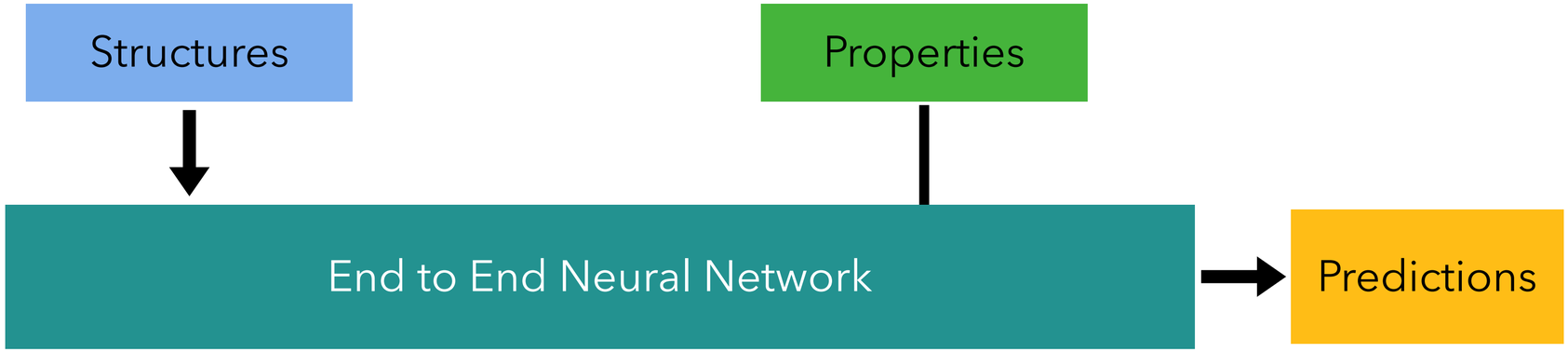

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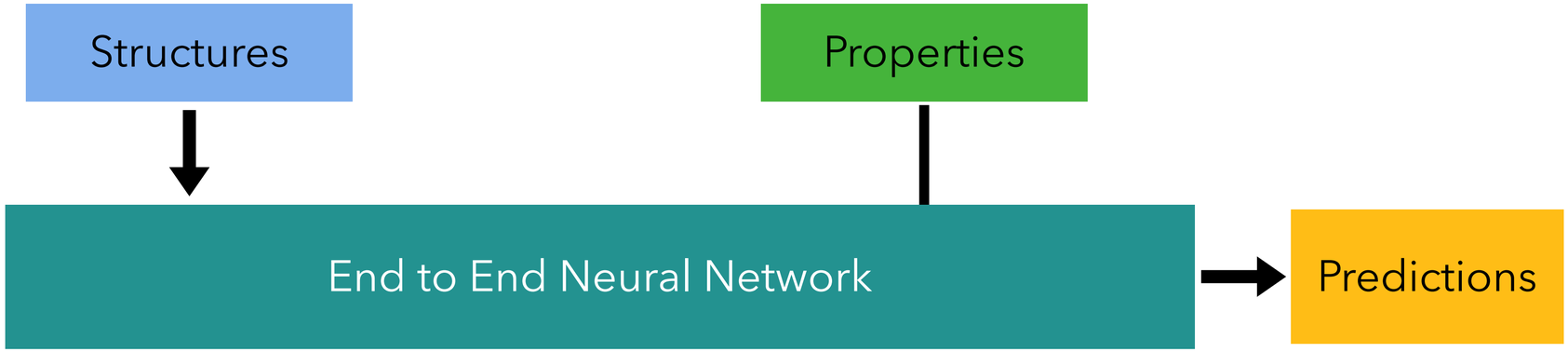

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Software for MLIP is fragmented and siloed

A fragmented ecosystem

Software for MLIP is fragmented and siloed

Harder to **combine** ideas

Harder to **compare** models

Lot of **duplicated** effort
(LAMMPS interface, …)

Harder to **experiment** with new representations/models/architectures

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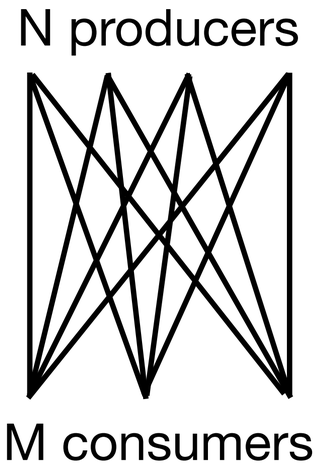

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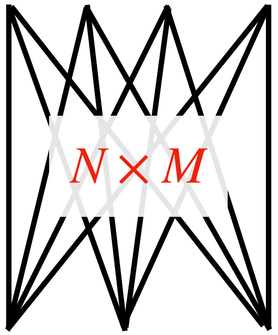

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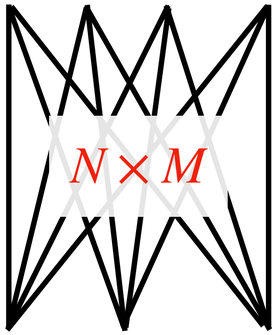

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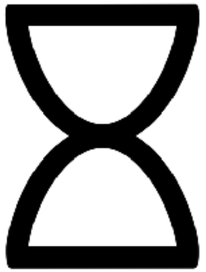

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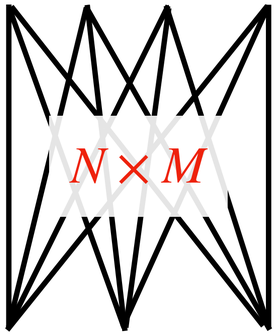

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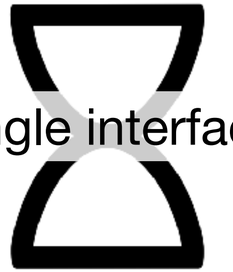

Single interface $N + M$

M consumers

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Sharing data for atomistic machine learning

metatensor

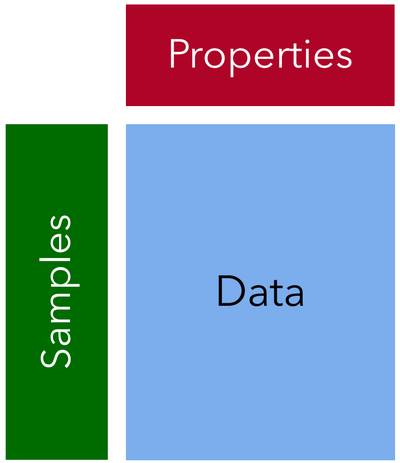
lab-cosmo/metatensor

Sharing data for atomistic machine learning

Store **data** and **metadata**, allow software to share without knowledge of each other

metatensor

lab-cosmo/metatensor



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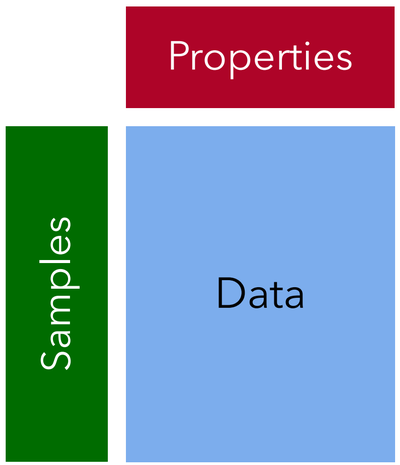


Samples

structure	atom
0	0
0	1
0	…
1	0

Properties

l	m	n
0	0	0
0	0	1
0	0	2
	…	
3	-3	3
3	-2	0
	…	

Sharing data for atomistic machine learning

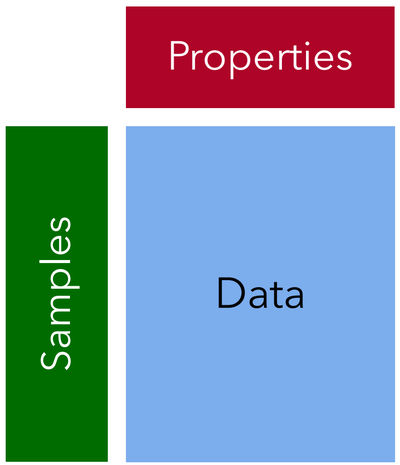
metatensor

Store **data** and **metadata**, allow software to share without knowledge of each other

Store values and **gradients** of these values together

lab-cosmo/metatensor

values



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gradients w.r.t.
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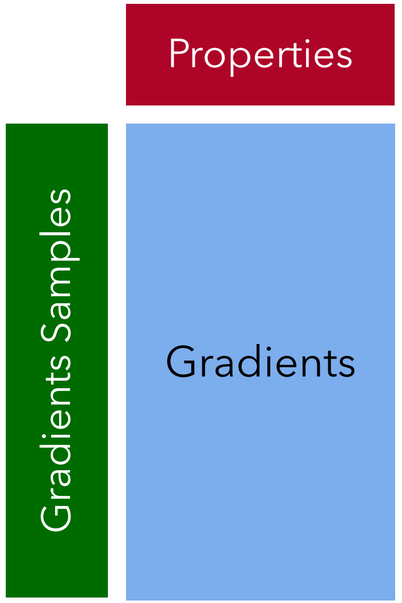

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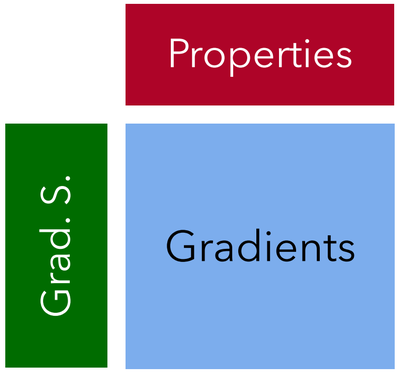

Sharing data for atomistic machine learning

metatensor

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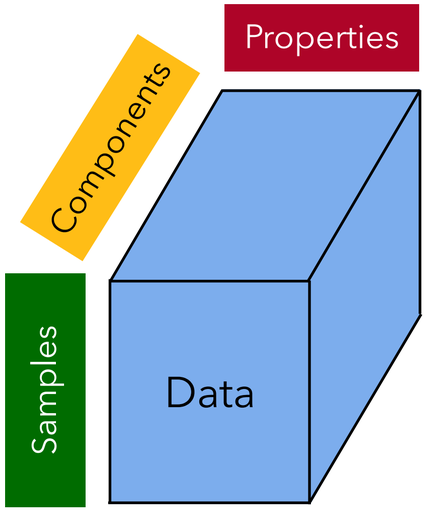
Store **data** and **metadata**, allow software to share without knowledge of each other

Store values and **gradients** of these values together

Handle vectorial components in the data (equivariance, vector quantities)

values



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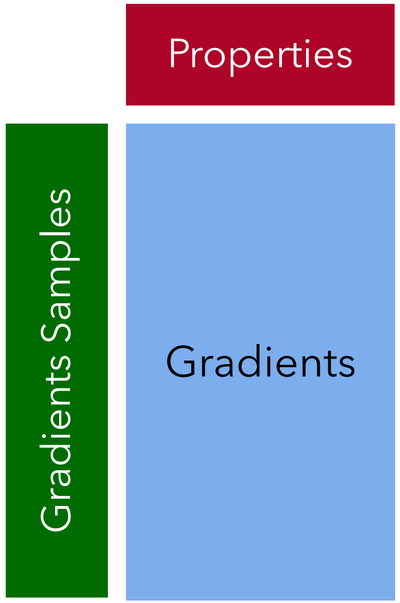

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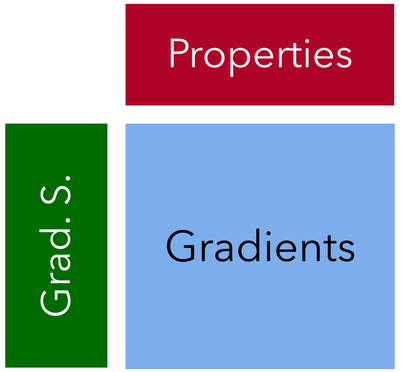

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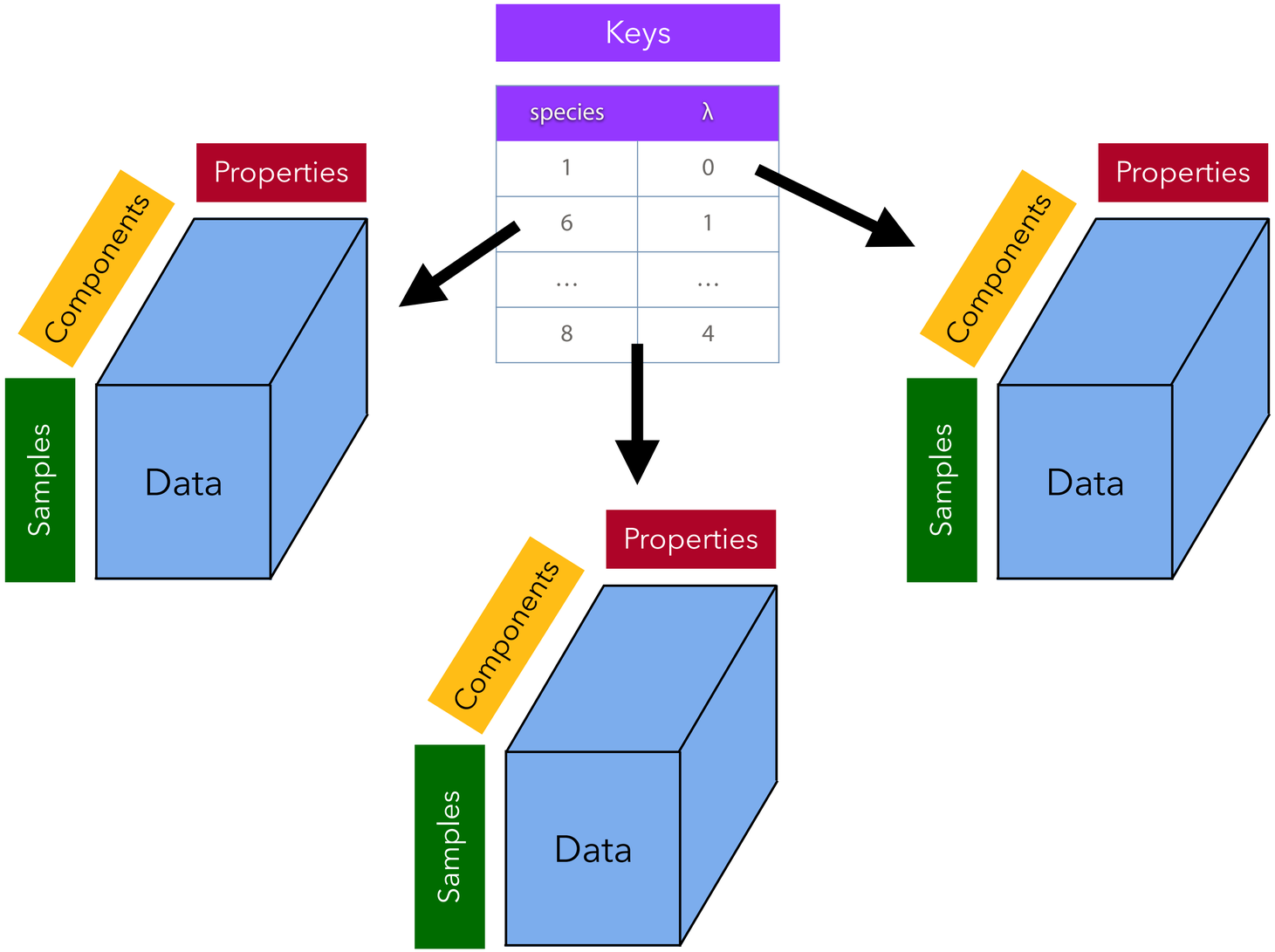
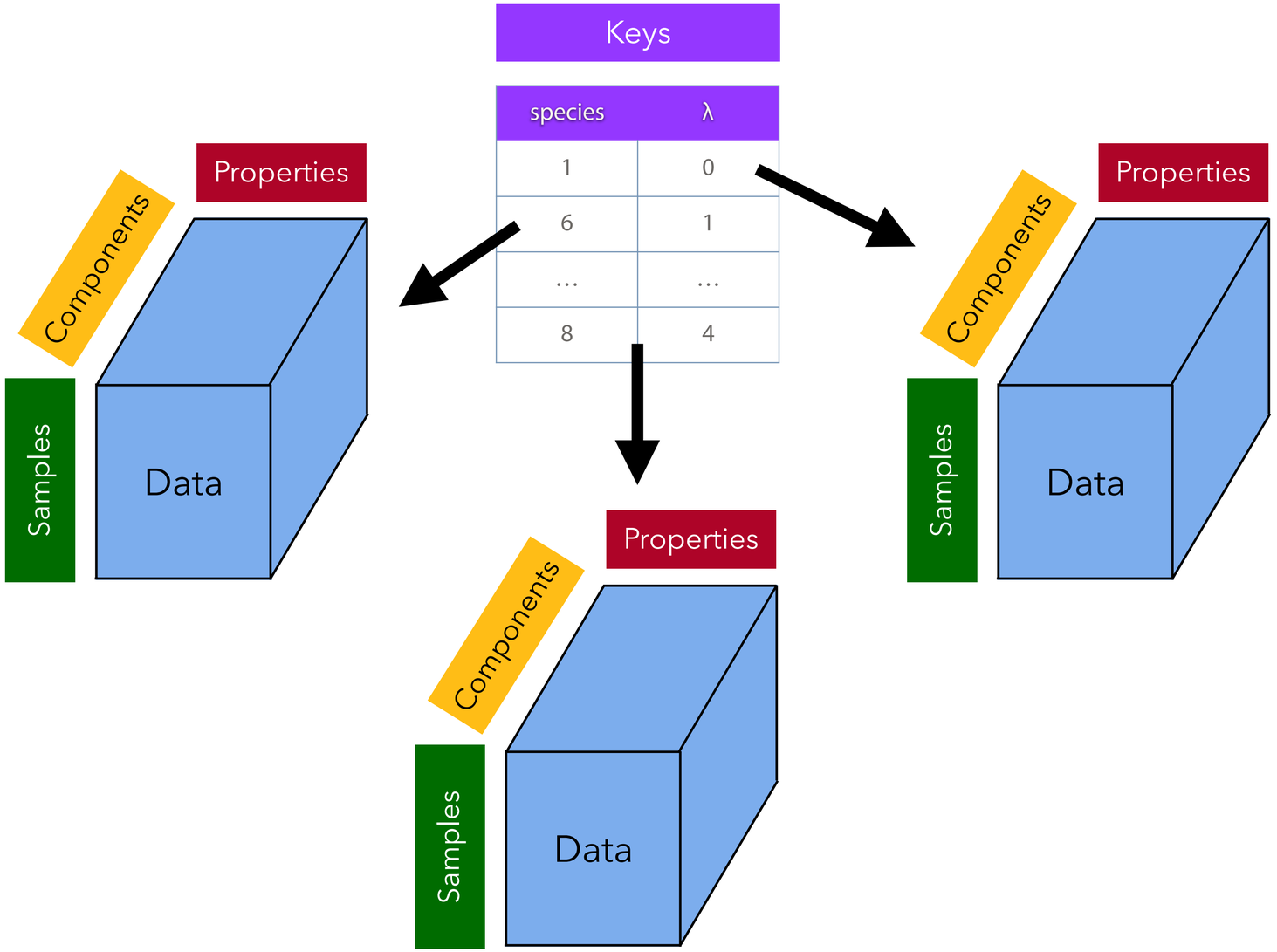


Block sparse data

Sharing data for atomistic machine learning



Block sparse data

Equivariant representations

Handle irreducible representations of the group separately

SO(3): keep λ separated, group the corresponding μ

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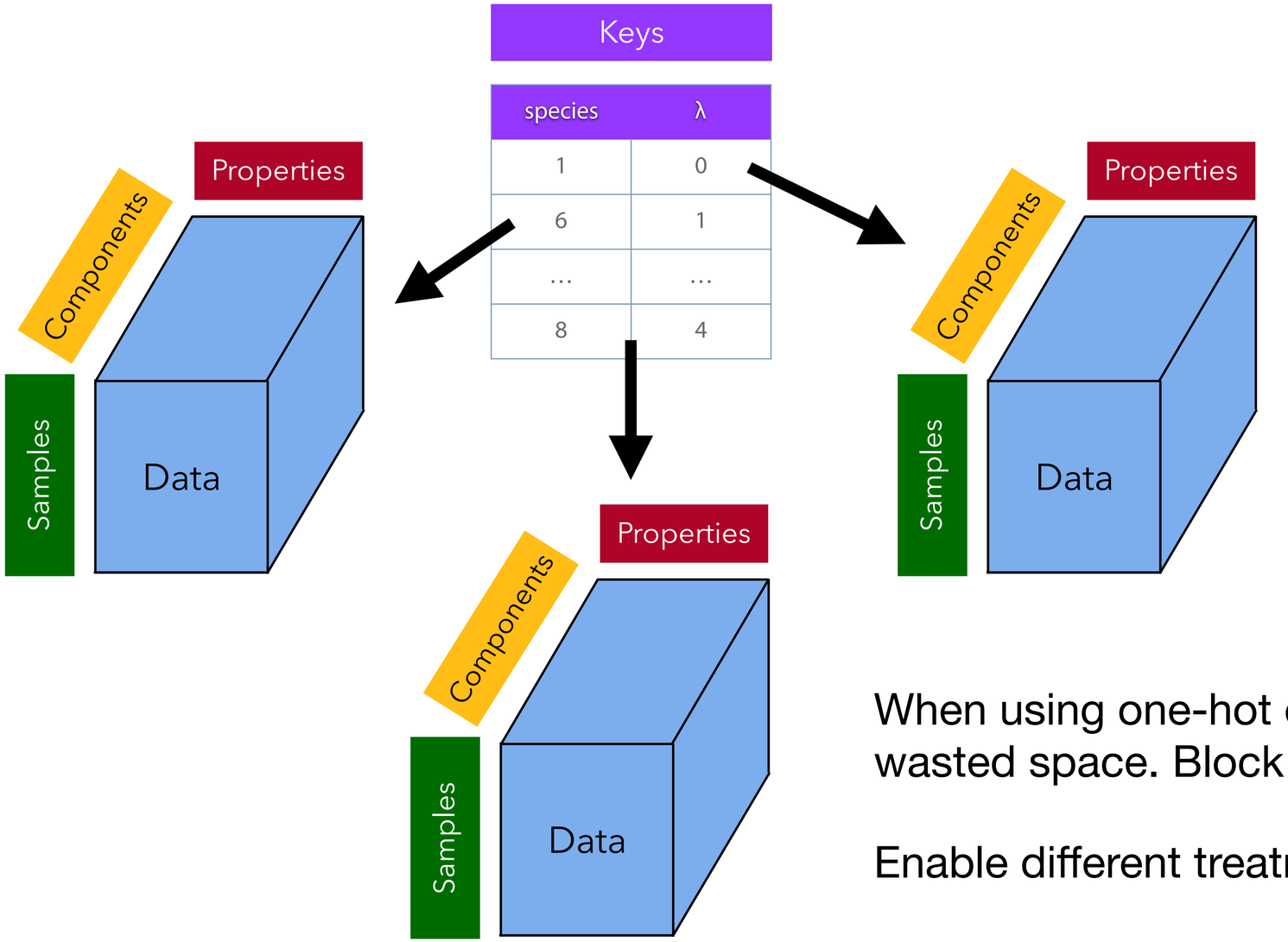

Block sparse data

Equivariant representations

Handle irreducible representations of the group separately

SO(3): keep λ separated, group the corresponding μ

Species handling

When using one-hot encoding of species, potential for a lot of wasted space. Block sparse data only keep the non-zero parts.

Enable different treatment of different species in models

Sharing data across ecosystems

Different researchers use different programming languages, we want to support all of them!

Metatensor is a Rust library, with a **C API**.
This C API can be used from many languages

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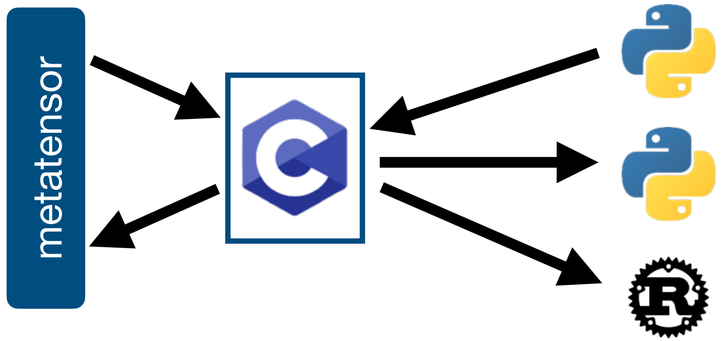

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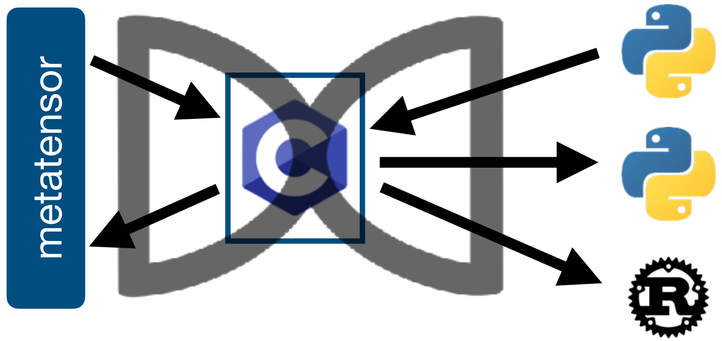

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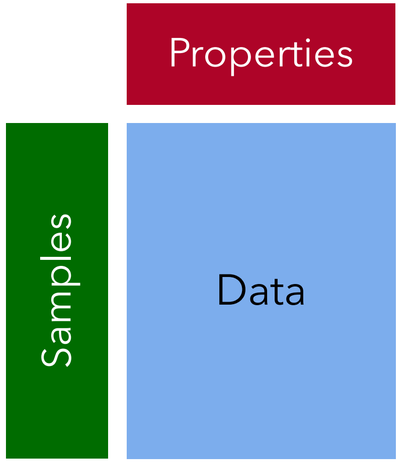

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Even in a single language, multiple ecosystems and data sources

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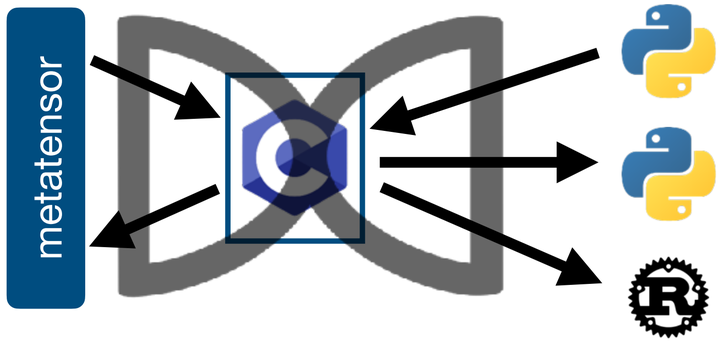

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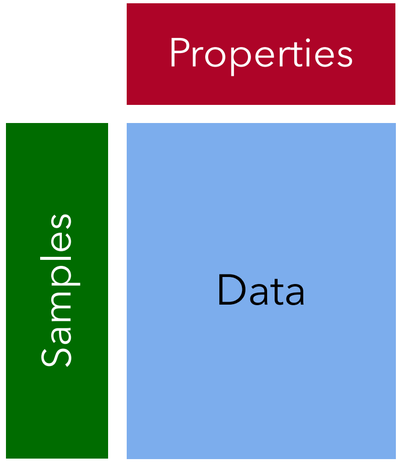

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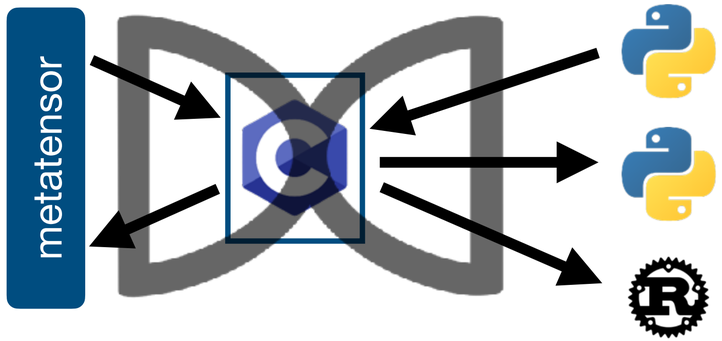

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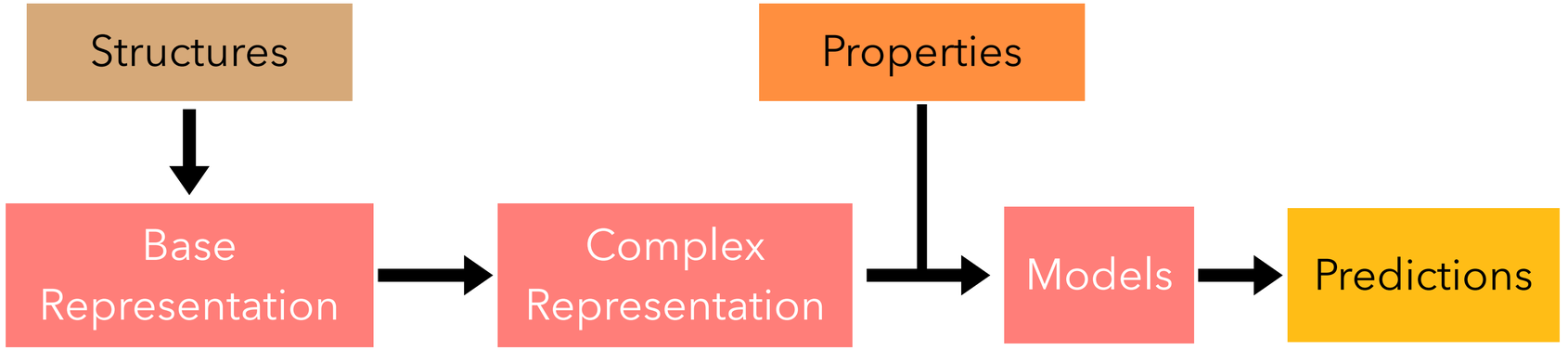
Metatensor need minimal information about the data, can manipulate values on GPU, inside torch Tensor (with full autograd support), …

Data sharing in practice



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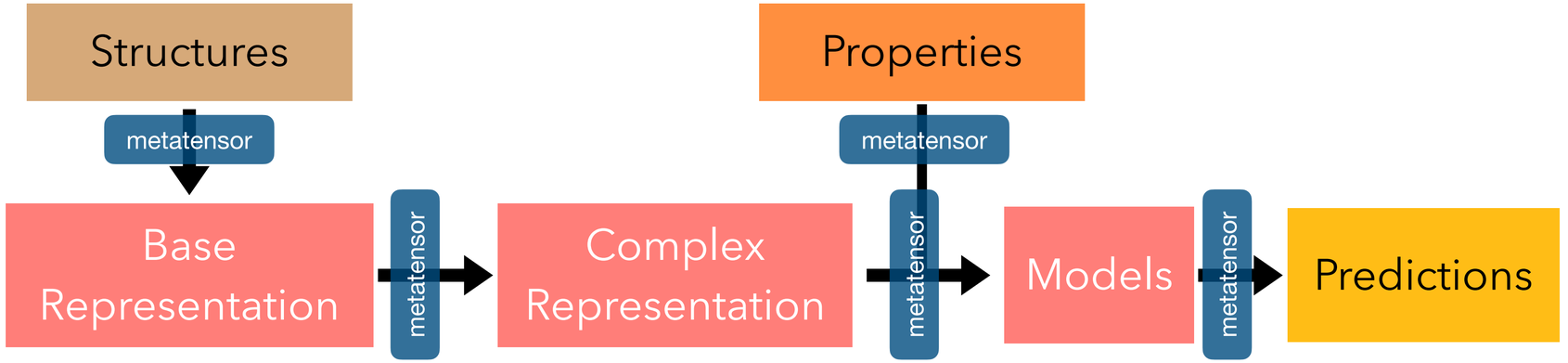

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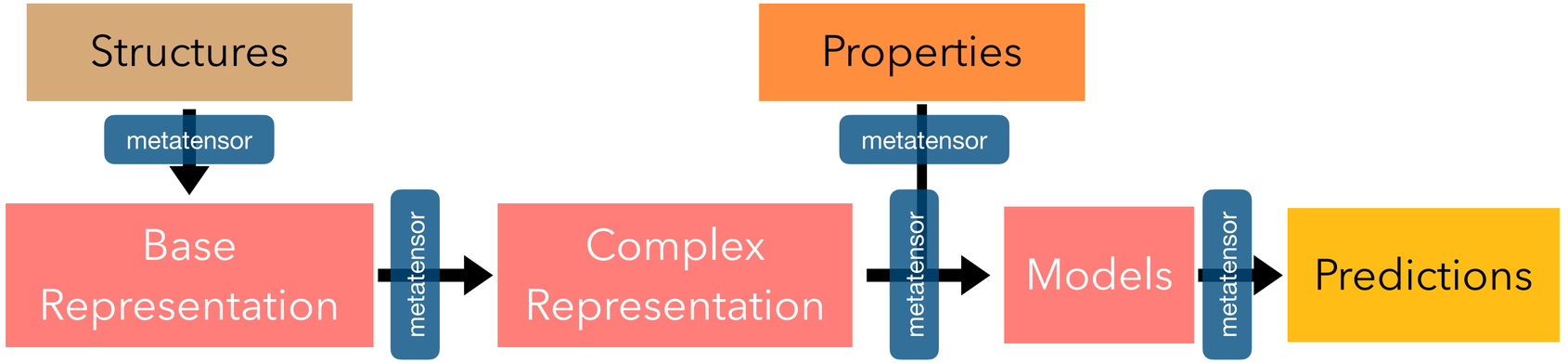

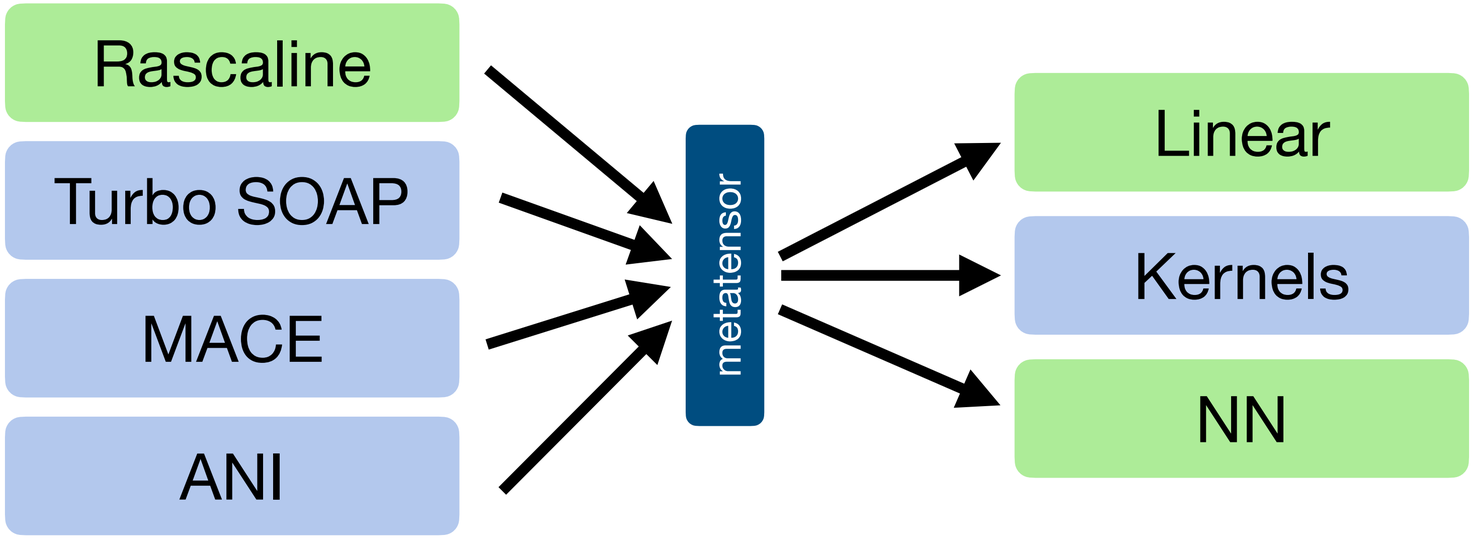

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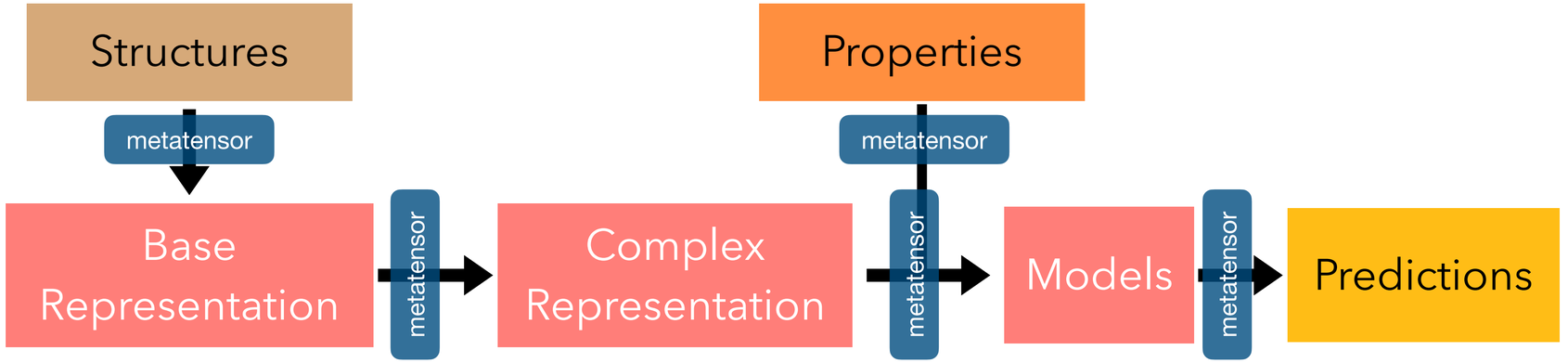

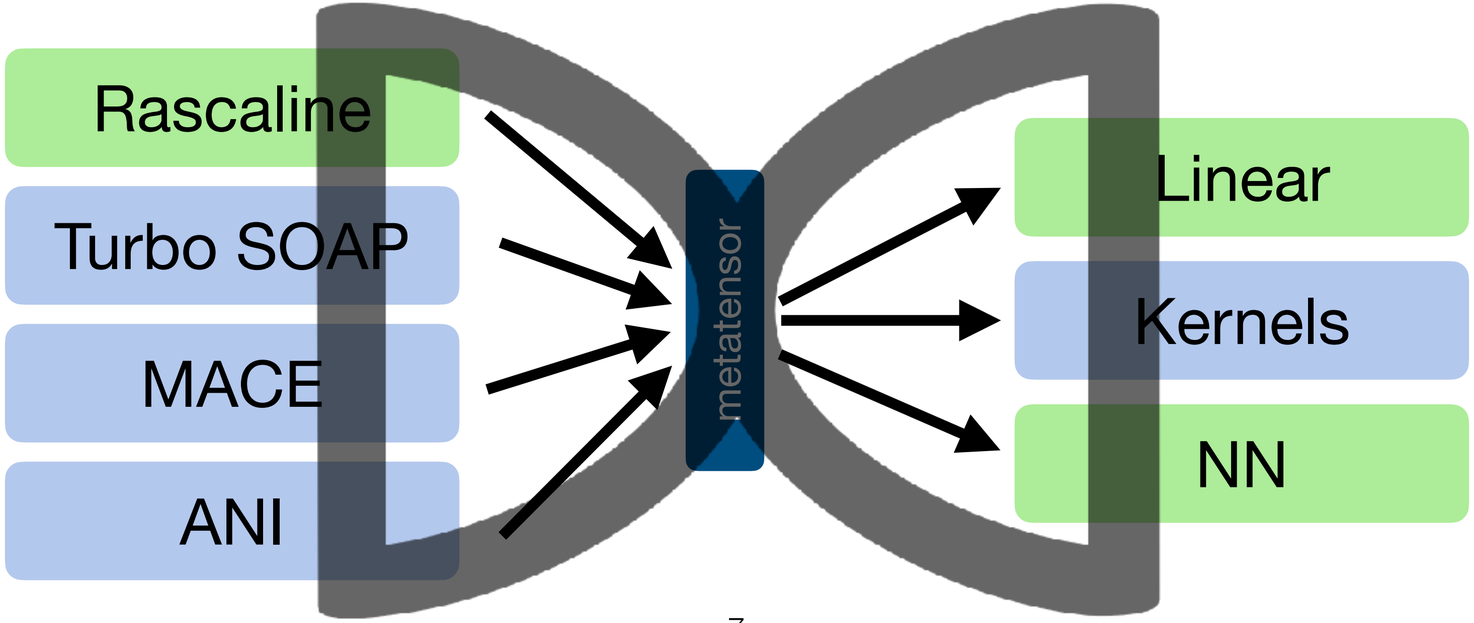

Existing metatensor ecosystem

Operations on metatensor data

lab-cosmo/metatensor

Existing metatensor ecosystem

Operations on metatensor data

lab-cosmo/metatensor

Parallel **representations** calculations (SOAP, LODE, …)

Luthaf/rascaline

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lab-cosmo/metatensor

Models building blocks
Ridge, Kernels, NN

lab-cosmo/equisolve

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Learnable representations

lab-cosmo/torch_spex

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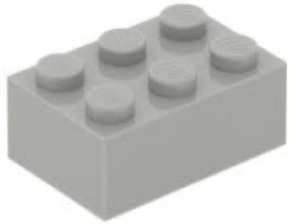

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Electronic structure ML

jwa7/rho_learn

lcmd-epfl/Q-stack
Hamiltonian Learning

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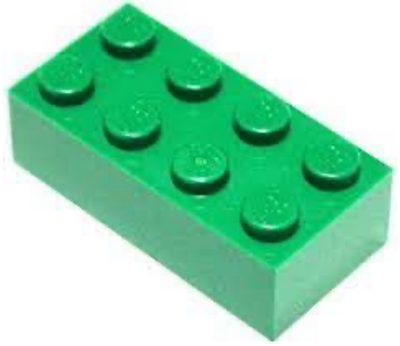

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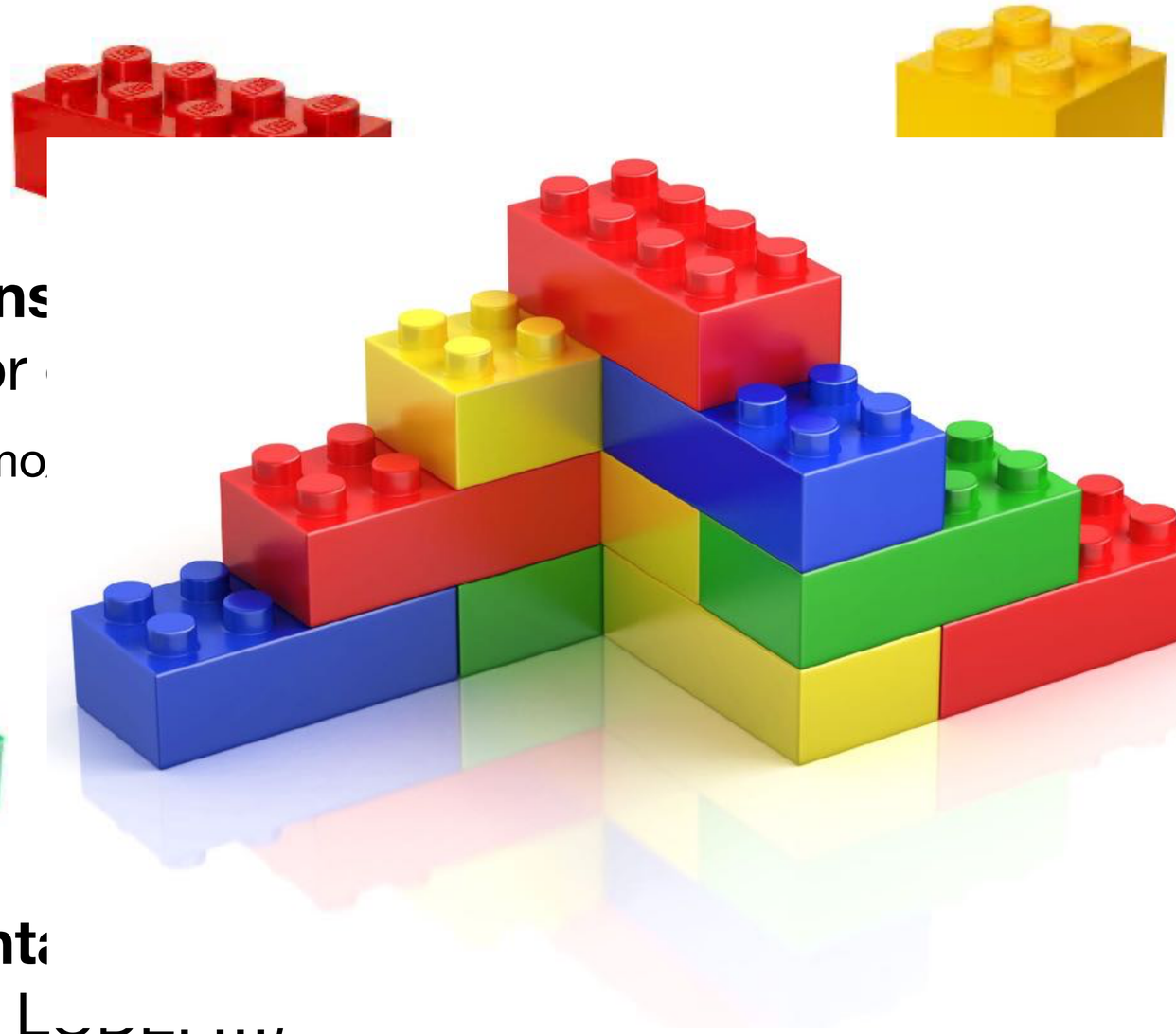
Luthaf/rascaline

Your own software?

Existing metatensor ecosystem



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Rascaline: representation calculations

Library of representations for atomistic machine learning

Output data as metatensor, can also use metatensor for input

rascaline

Luthaf/rascaline

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Luthaf/rascaline

Many different representations

SOAP Pair Spherical Expansion

SOAP Spherical Expansion

SOAP Radial Spectrum

SOAP Power Spectrum

LODE Spherical Expansion

Neighbors Lists

Atomic Composition

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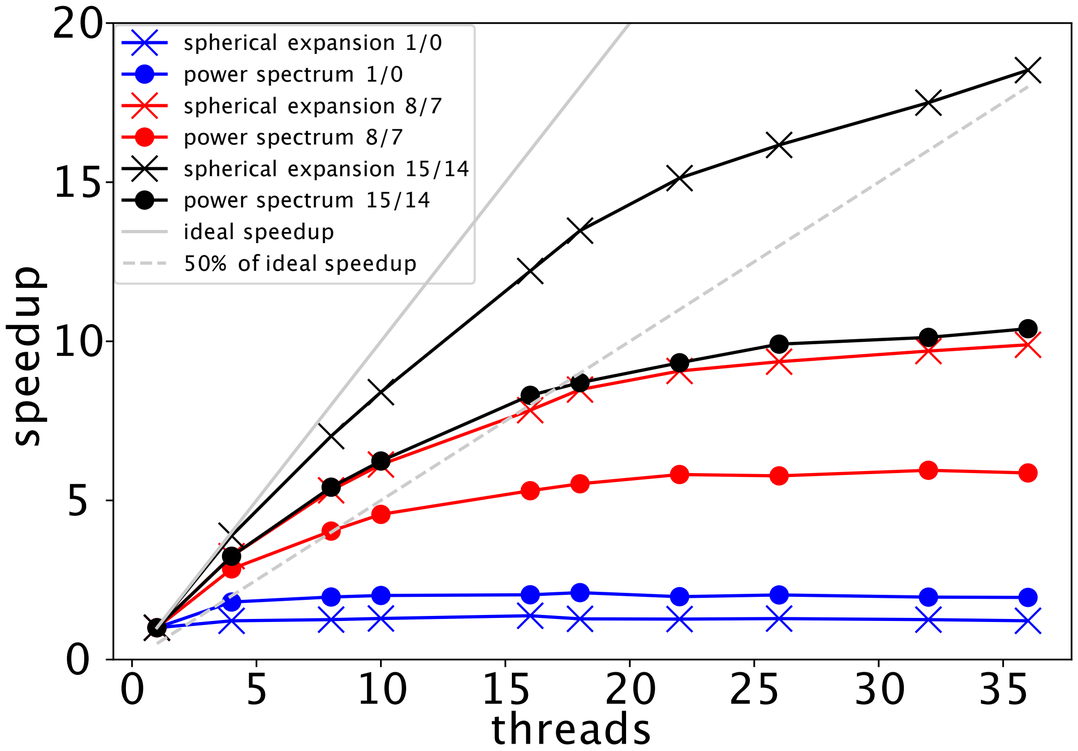
Fast — Parallelism



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Luthaf/rascaline

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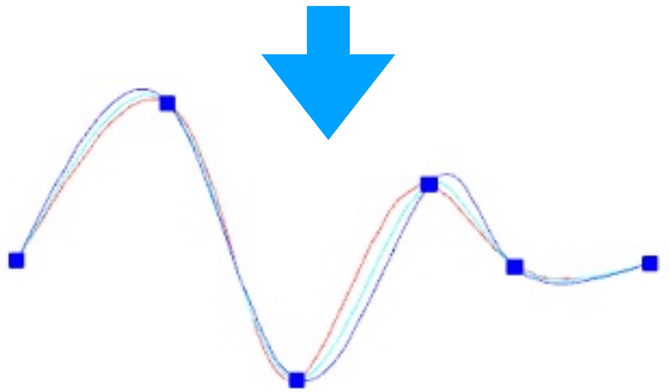
$$I_{nl}(r_{ij}) = \frac{1}{(\pi\sigma^2)^{3/4}} 4\pi e^{-\frac{r_{ij}^2}{2\sigma^2}} \int_0^\infty \mathrm{d}r r^2 R_{nl}(r) e^{-\frac{r^2}{2\sigma^2}} i_l\left(\frac{r r_{ij}}{\sigma^2}\right)$$

Fast — Parallelism

Fast — Radial Basis splining (~3x)

$$I_{nl}(r_{ij}) = \frac{1}{(\pi\sigma^2)^{3/4}} \cdot \pi^{\frac{3}{2}} \frac{\Gamma\left(n_{\text{eff}}\right)}{\Gamma\left(l_{\text{eff}}\right)} \frac{(a r_{ij})^l}{(a+b)^{n_{\text{eff}}}} M\left(n_{\text{eff}}, l_{\text{eff}}, \frac{a^2 r_{ij}^2}{a^2+b^2}\right)$$

Custom Python basis definition



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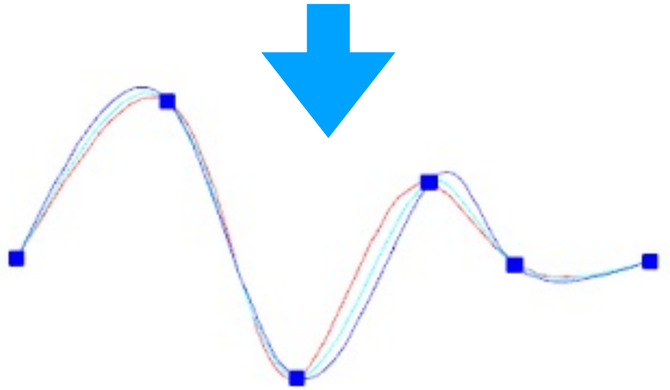

Full integration with PyTorch

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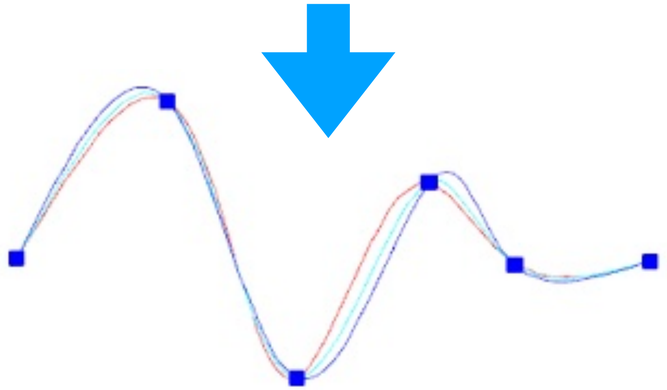

Full integration with PyTorch

Usable from C/C++/Python/Rust/…

Sharing code for atomistic ML

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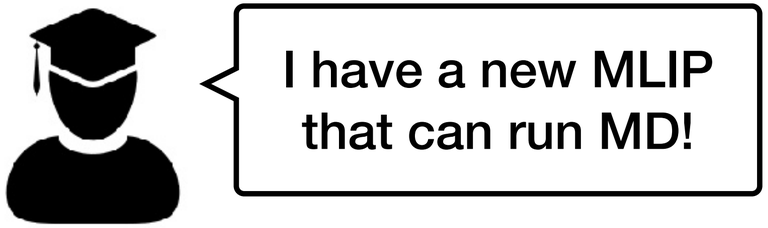

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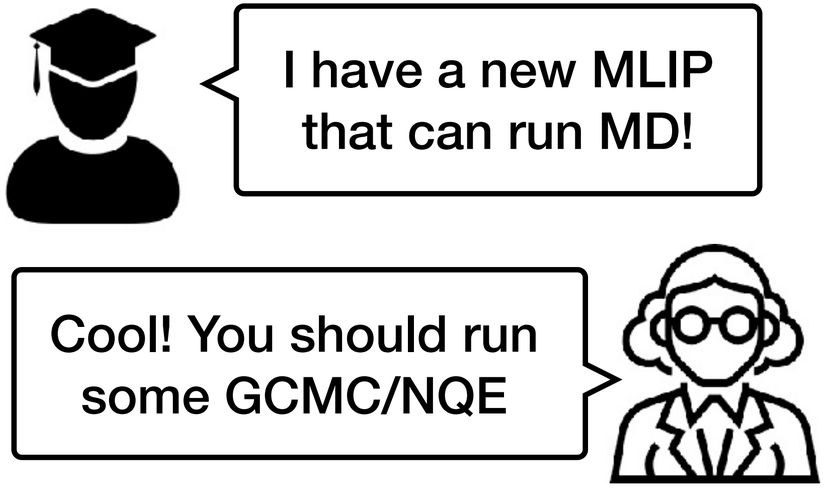

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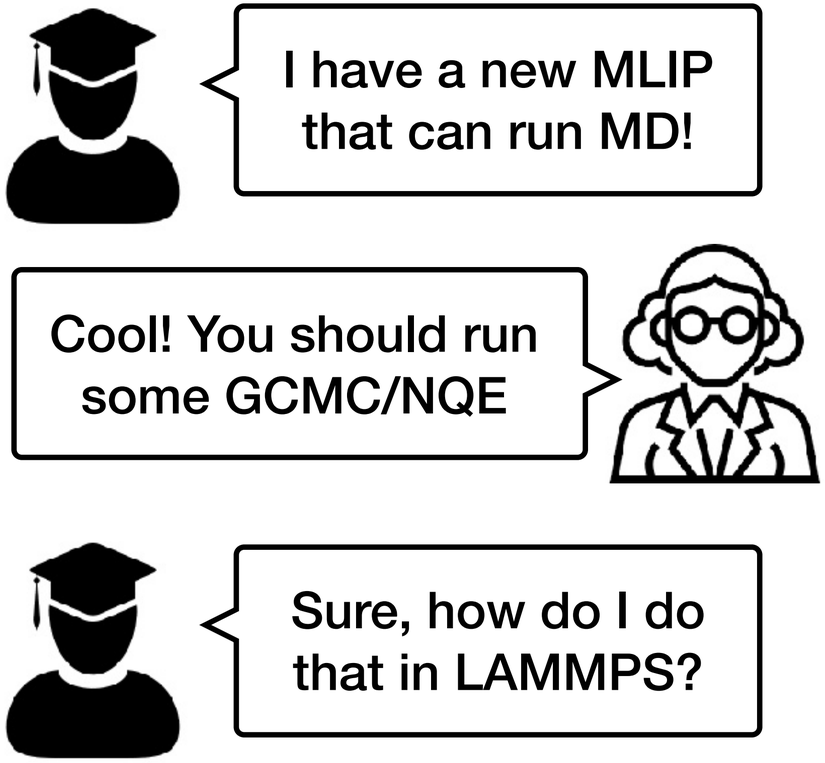

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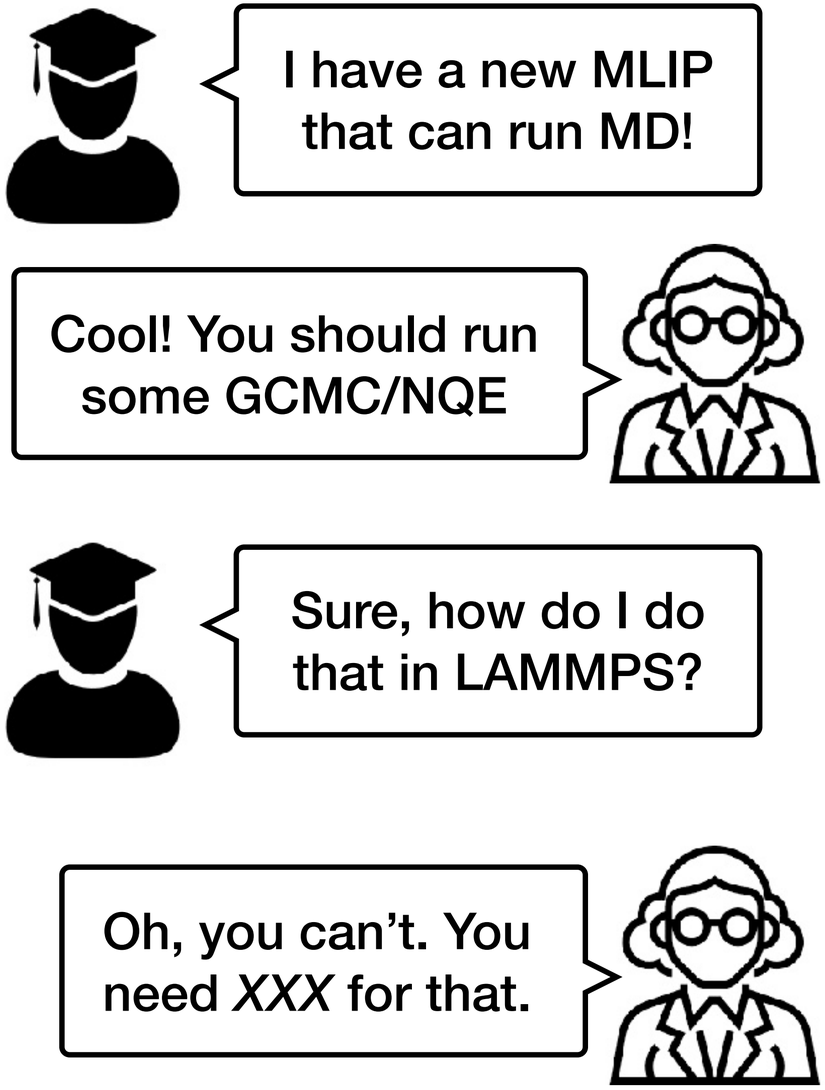

Sharing ~~code~~ for atomistic ML

models

I have a new MLIP that can run MD!

Cool! You should run some GCMC/NQE

Sure, how do I do that in LAMMPS?

Oh, you can't. You need *XXX* for that.

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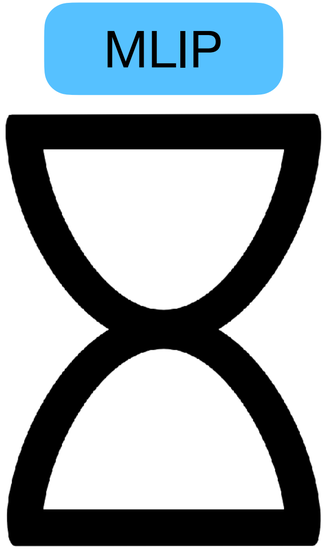

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Train and export the model **once**

Use it in **many** simulations!

Share with others, who can re-use your trained model

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Write **fully custom models** with Python, run inside pure C++/Fortran engines

PyTorch

Metatensor based atomistic ML models

Exists

Planned

1

```
class MySuperModel(torch.nn.Module):
    def forward(self, ...):
        ...
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define required neighbors lists,
the engine will compute them

define possible outputs (energy, dipoles, …)
the engine will request them

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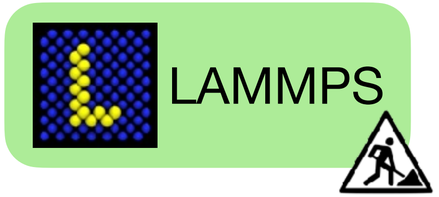
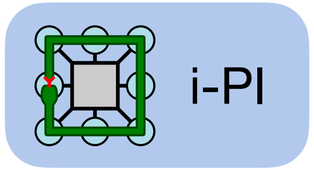
Metatensor-Engine interface, written once





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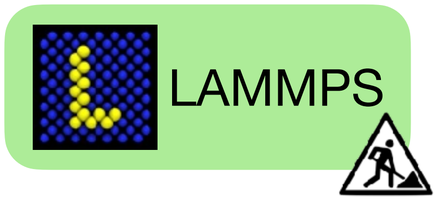

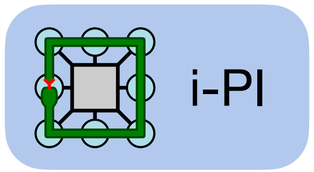

1 download pre-trained models

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pair_style metatensor my-model.pt
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run simulation && make paper
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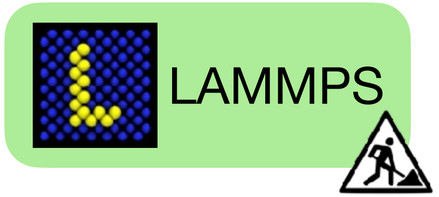
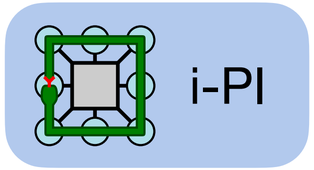




1 download pre-trained models

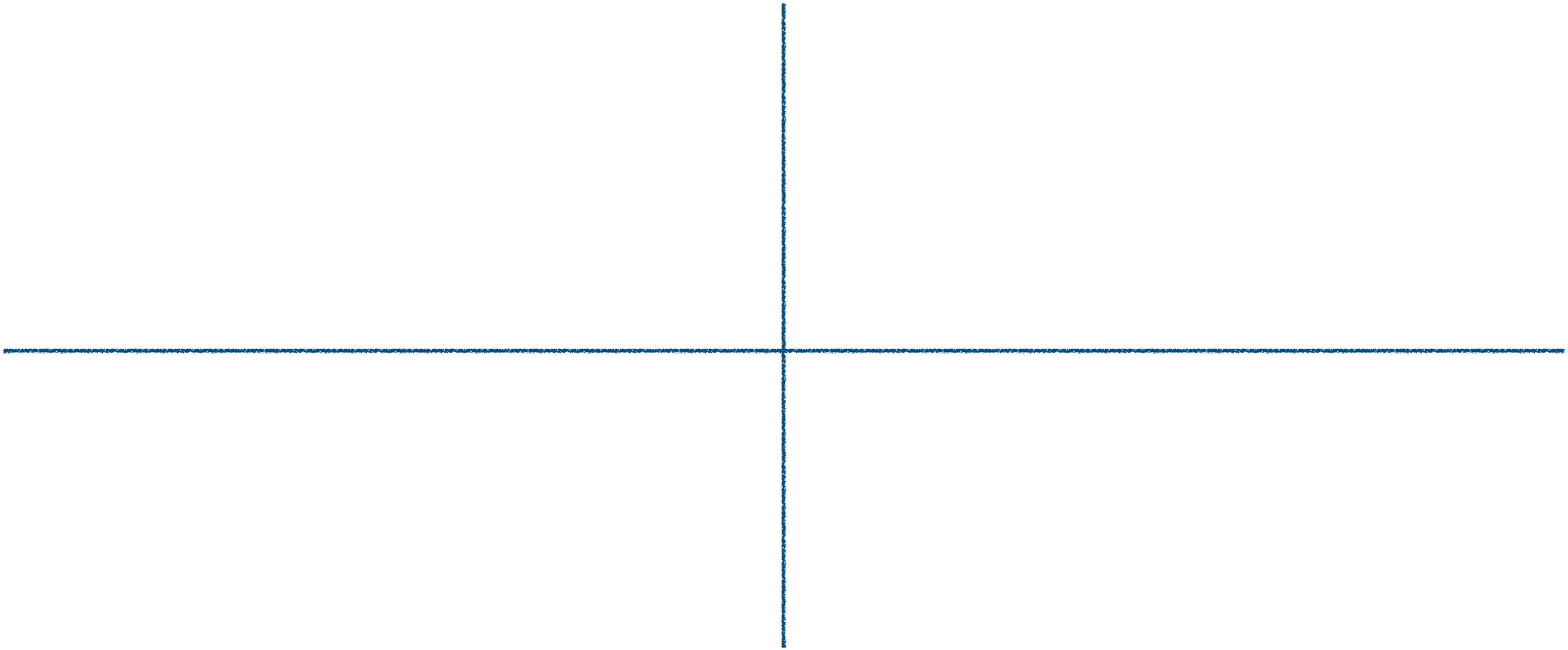
2 `pair_style metatensor my-model.pt`

3 `run simulation && make paper`

Tutorial later today: you'll write your own model and run MD using it in LAMMPS and ASE!

What do I gain?

You are …



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Make your architecture available to everyone immediately and with fewer efforts

Delegate work on simulation engine interface

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Check your model performance immediately with Python simulations, and then at scale

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Developing a simulation engine

Access the whole space of MLIP at once

Use ML surrogate for more than energy!

How can I adopt metatensor?

metatensor

lab-cosmo/metatensor

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Surface integration: wrap and unwrap, using metatensor at the boundaries

Very easy to get started **today**! Can be one of many option supported by the code

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No wrapping overhead, metadata helps debugging, helps staying in most memory efficient format

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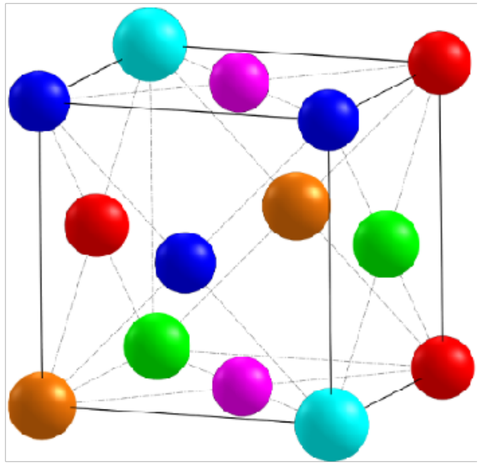
The code is in active development, we are taking feedback!

Cool science you can do with metatensor



High Entropy Alloys

Huge structure space, lot of complexity, hard to probe experimentally, tuneable properties

Very good system for atomistic simulations and MLIP

BUT: chemical complexity is hard to handle in MLIP

BASF

Natasha Lopanitsyna
Arslan Mazitov
Maximilian Springer
Sandip De
Michele Ceriotti

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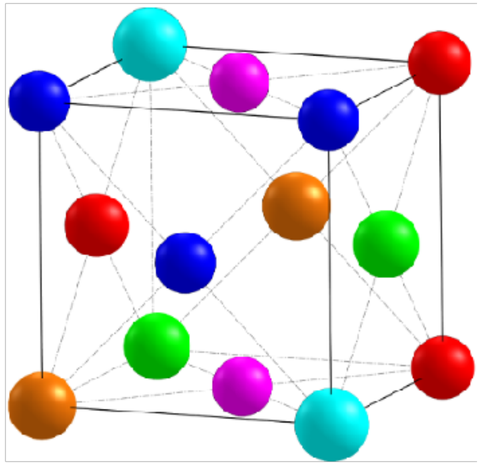

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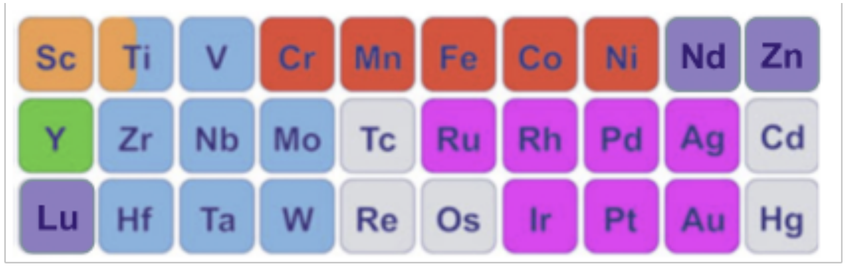
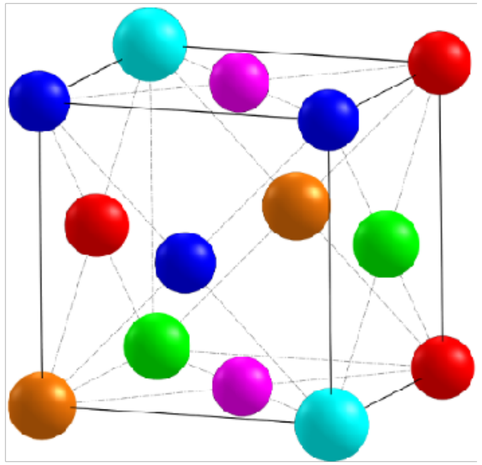


High Entropy Alloy dataset, 25 elements,
30k distorted bulk structures, DFT energies

Cool science you can do with metatensor



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BASF

Natasha Lopanitsyna
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Maximilian Springer
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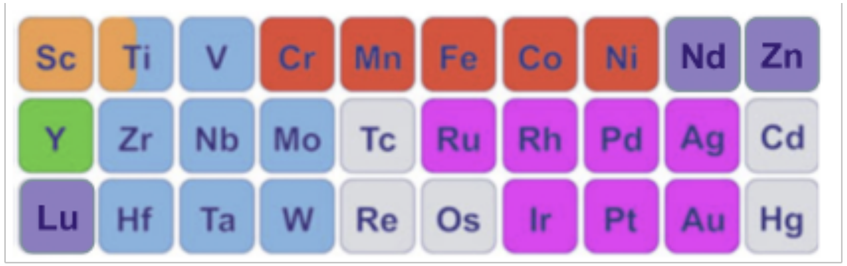
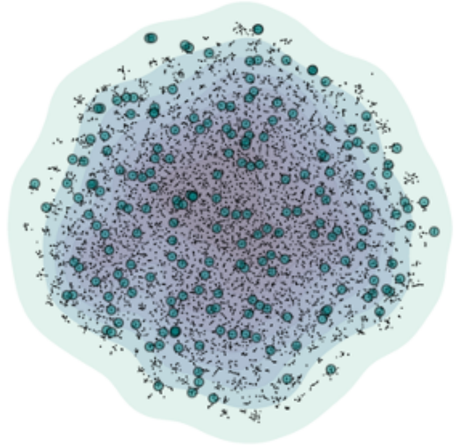


High Entropy Alloy dataset, 25 elements, 30k distorted bulk structures, DFT energies

Generate 1M random bulk structures, with random rattling. Higher energies than MD.

Subselect 30k covering most of the space (FPS) with radial descriptors



Exploiting atomic similarities in SOAP

$$\langle \alpha n \ \alpha' n' \ l \,|\, \rho_i^{\otimes 2} \rangle = \sum_m \langle \alpha n l m \,|\, \rho_i \rangle \otimes \langle \alpha' n' l m \,|\, \rho_i \rangle$$

SOAP power spectrum
(invariant)

Quadratic space scaling with number of species:
10 TiB of storage just for SOAP vectors (sparse!)

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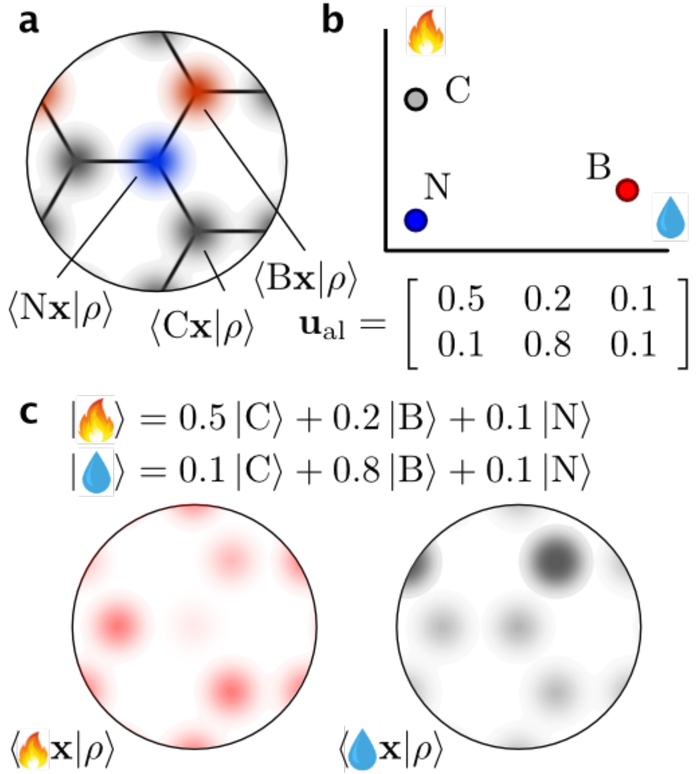
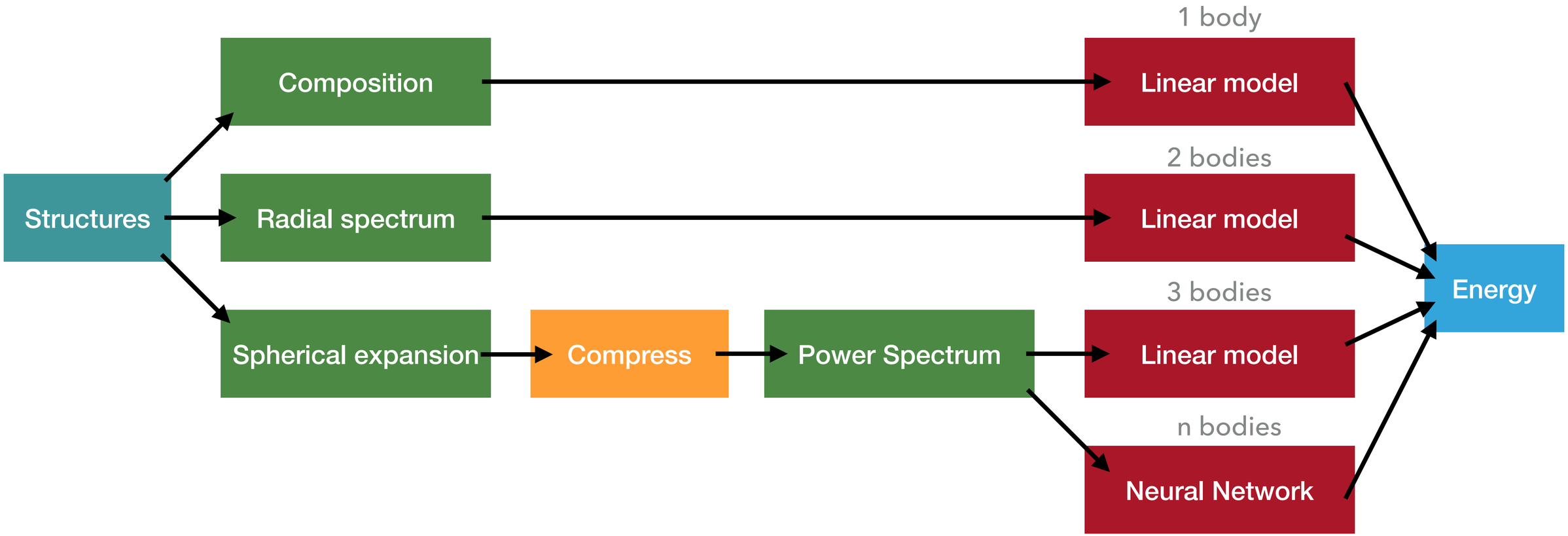
One solution: project real elements onto alchemical "*pseudo-elements*", optimizing the projection matrix in a data driven way

$$\langle \beta n l m \,|\, \rho_i \rangle = U_{\alpha\beta} \, \langle \alpha n l m \,|\, \rho_i \rangle$$

$$\langle \beta n \; \beta' n' \; l \,|\, \rho_i^{\otimes 2} \rangle = \sum_m \langle \beta n l m \,|\, \rho_i \rangle \otimes \langle \beta' n' l m \,|\, \rho_i \rangle$$



How to do this with metatensor?



Use Torch integration to learn both compression matrix & models weights simultaneously

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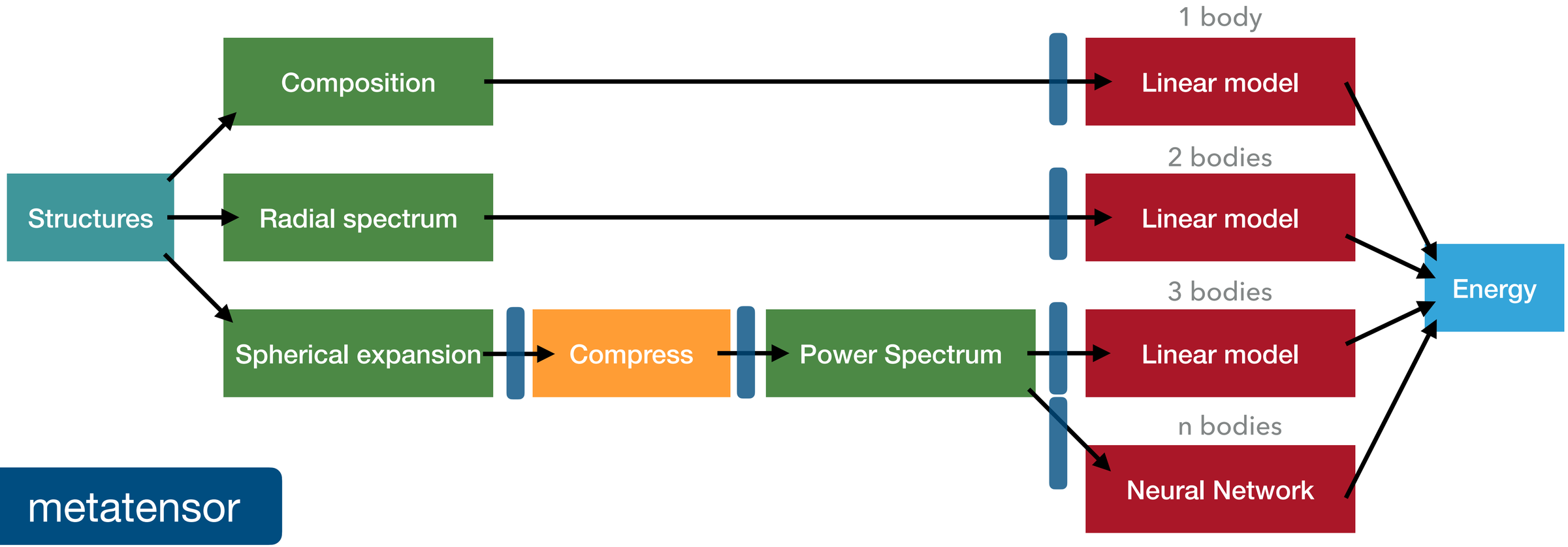

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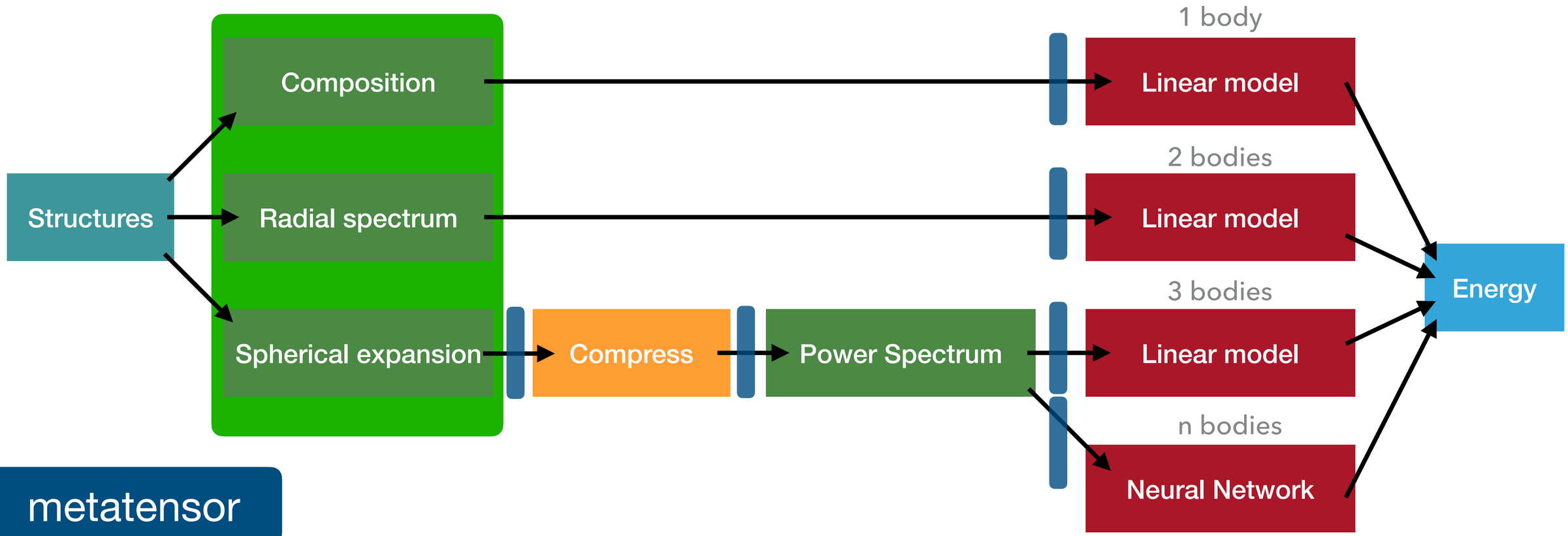

metatensor

rascaline

Use Torch integration to learn both compression matrix & models weights simultaneously

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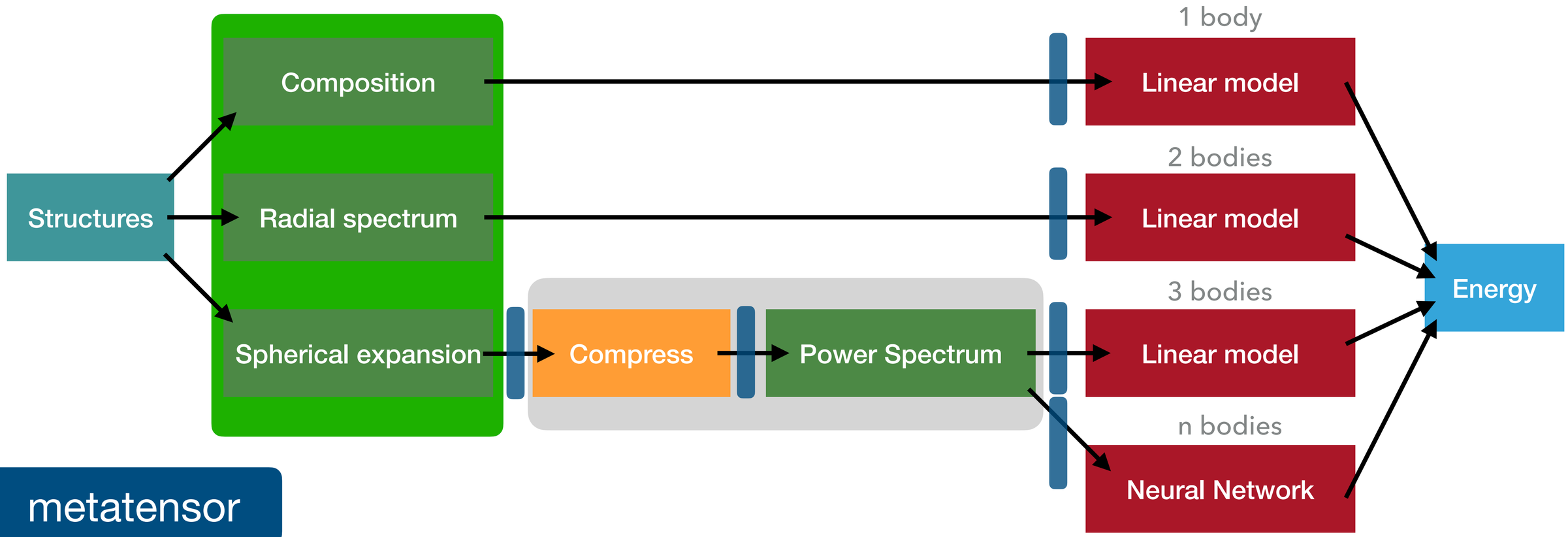

metatensor

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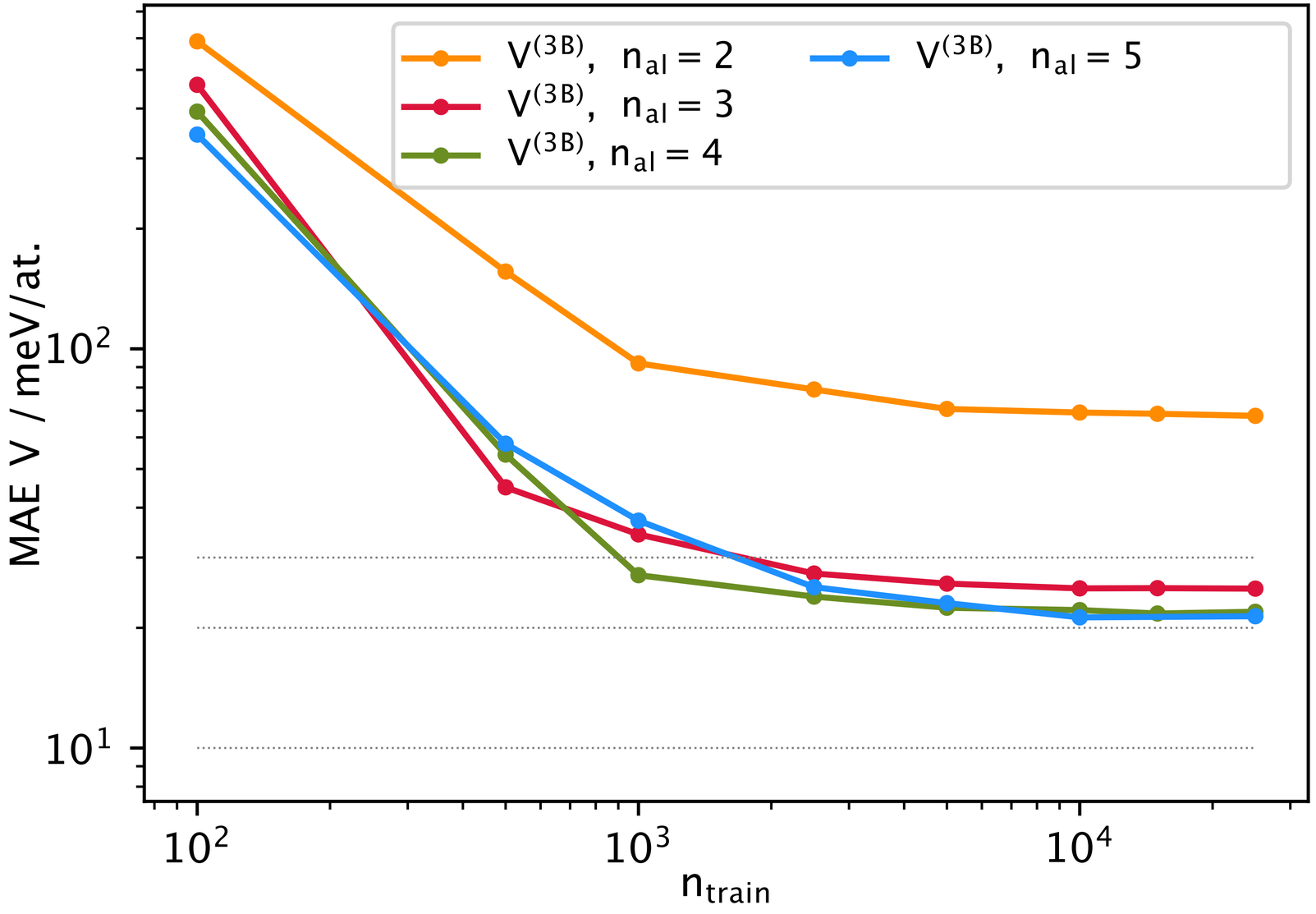
custom

Use Torch integration to learn both compression matrix & models weights simultaneously

Validating the architecture



4 pseudo-elements can capture all interactions

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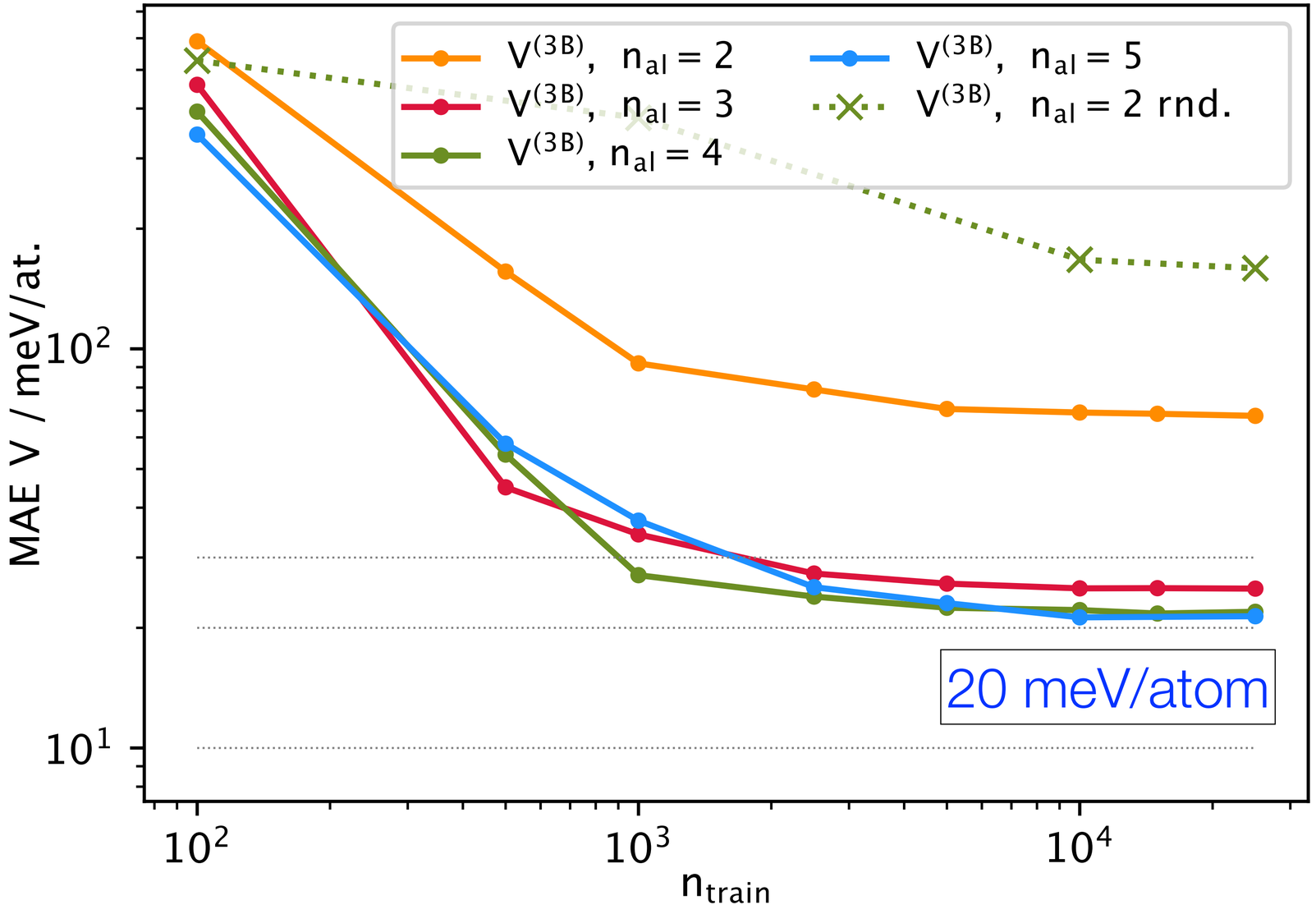

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Large improvement by optimising projection

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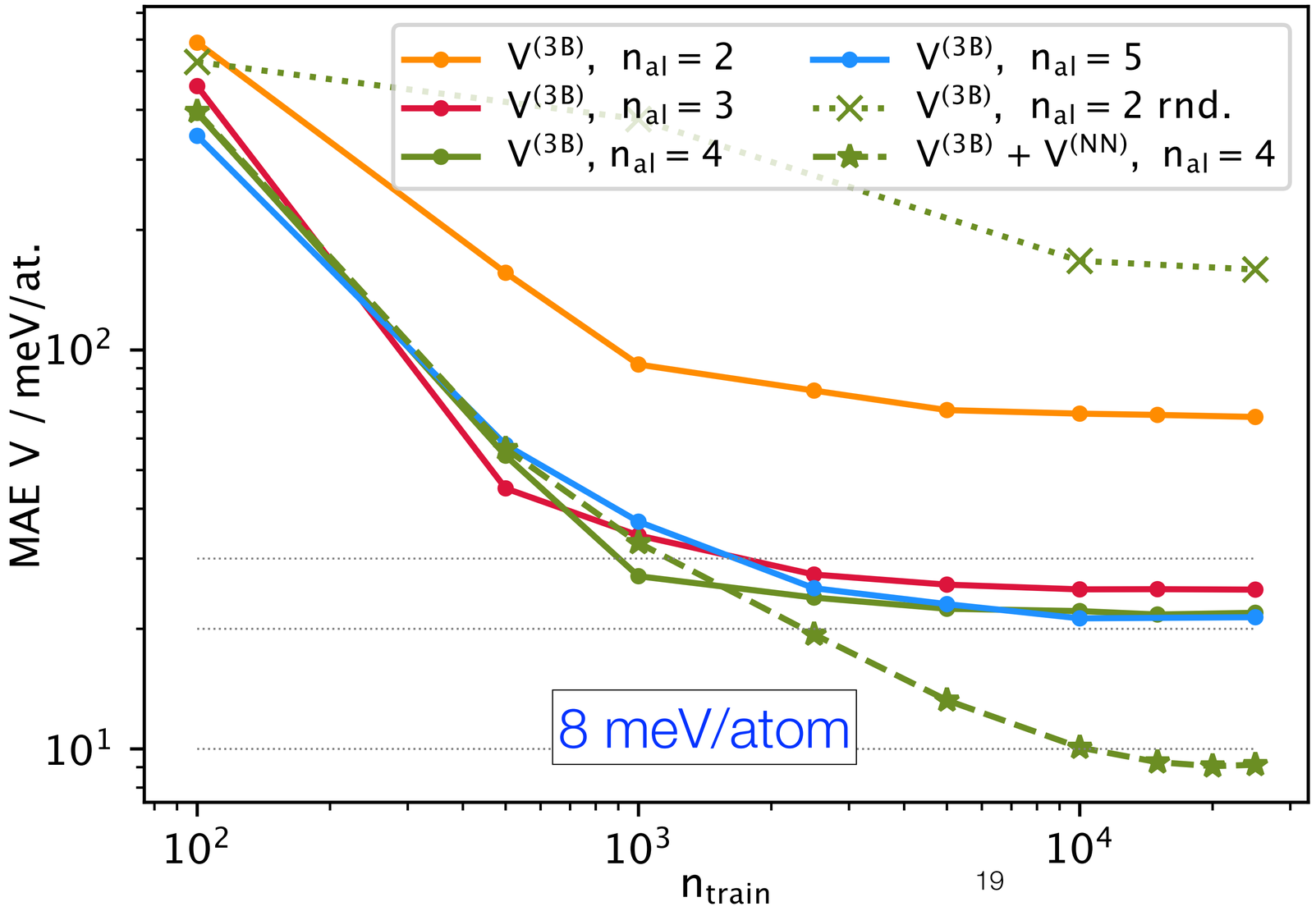

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Non-linearities to increase body-order

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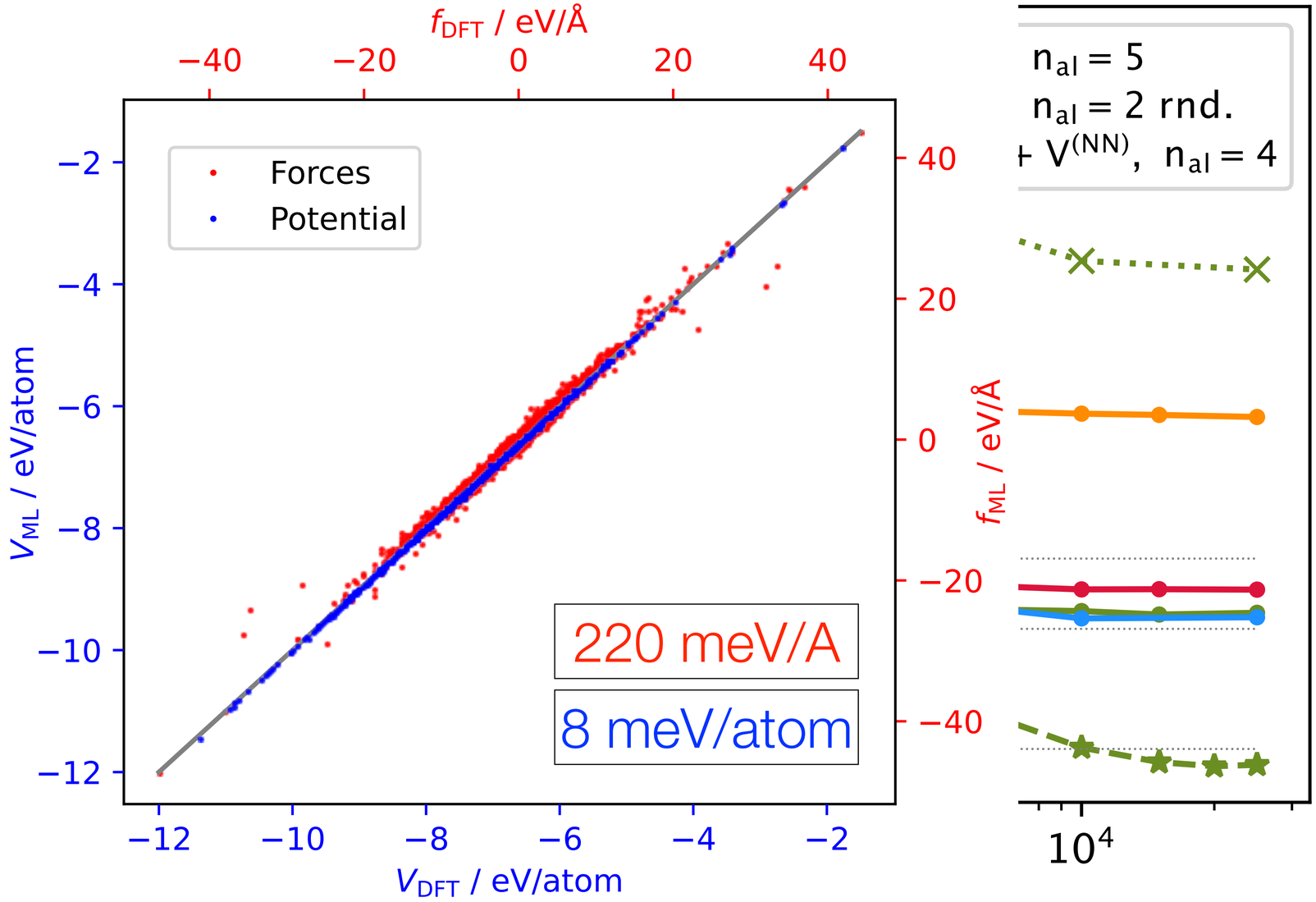

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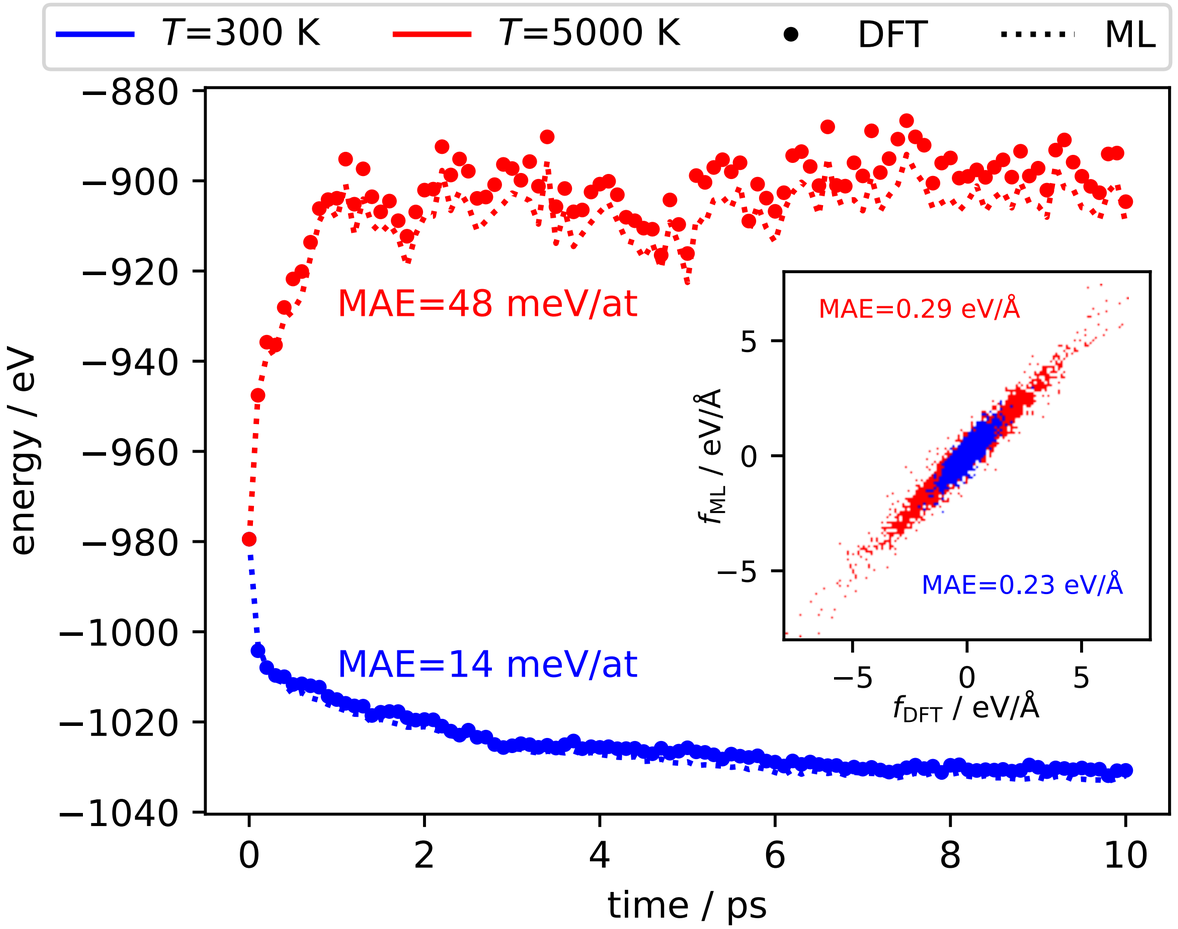
Validating the stability

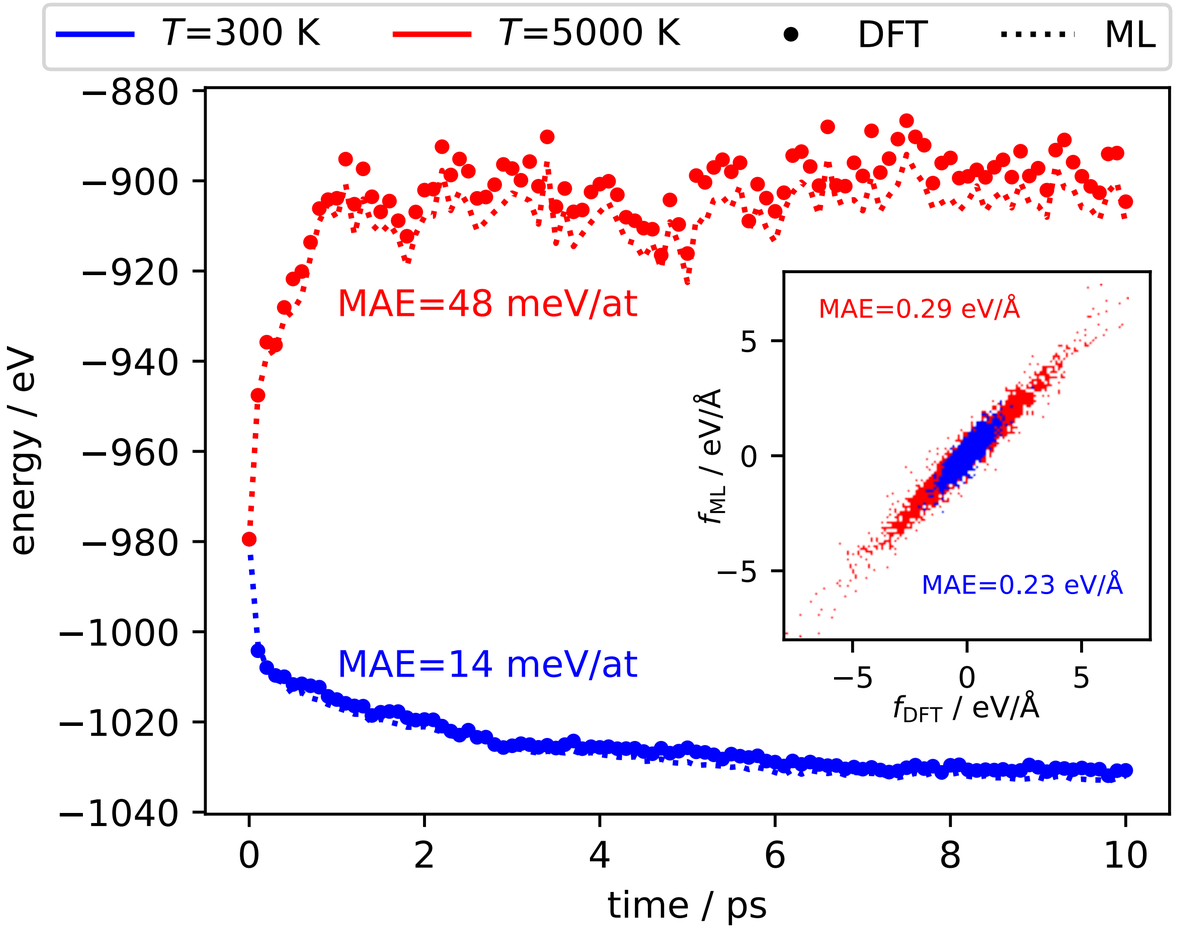


Extremely stable for bulk structures

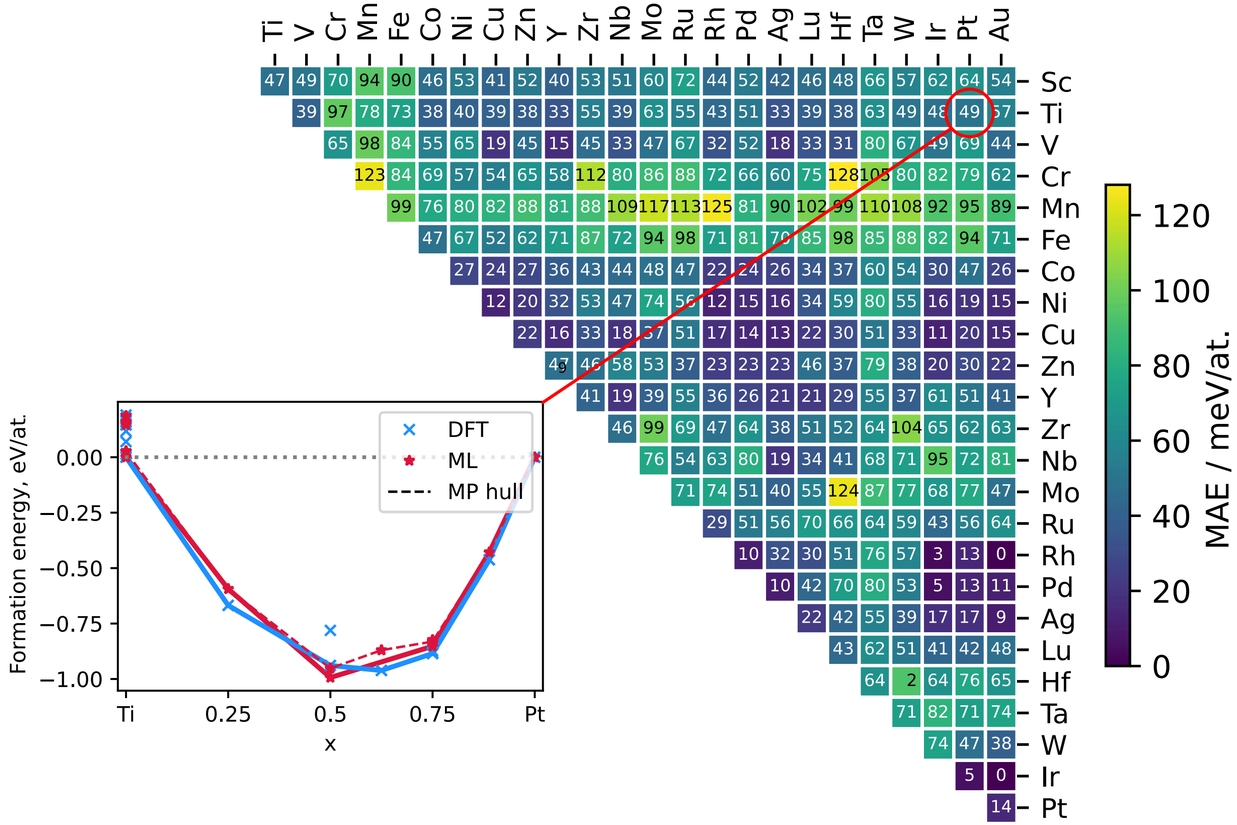
Able to run REMD, melted trajectories

Lopanitsyna, Fraux, Springer, De, Ceriotti, Phys. Rev. Mat. 2023

Validating the stability



Good extrapolation to data outside the training set



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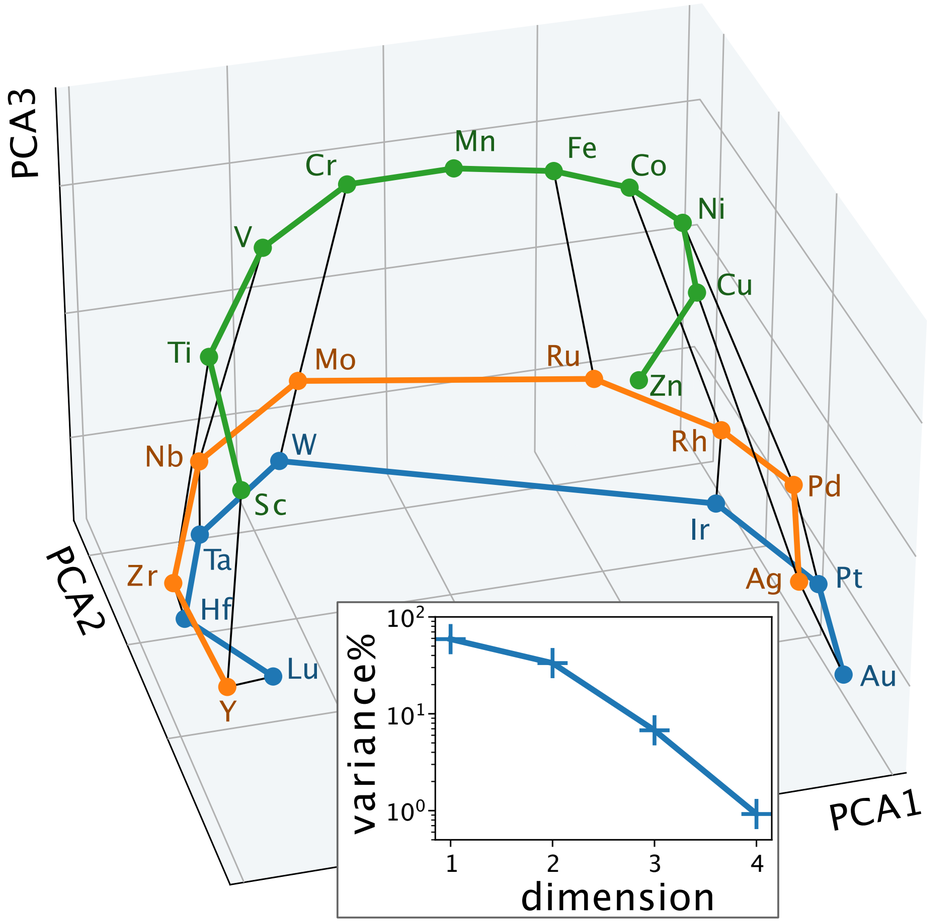
Data driven periodic table

4 pseudo-elements are enough to capture all the interactions



$$\langle \beta nlm \,|\, \rho_i \rangle = U_{\alpha\beta} \, \langle \alpha nlm \,|\, \rho_i \rangle$$

Data-driven periodic table structure

Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Nd	Zn
Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd
Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg

Lopanitsyna, Fraux, Springer, De, Ceriotti, Phys. Rev. Mat. 2023

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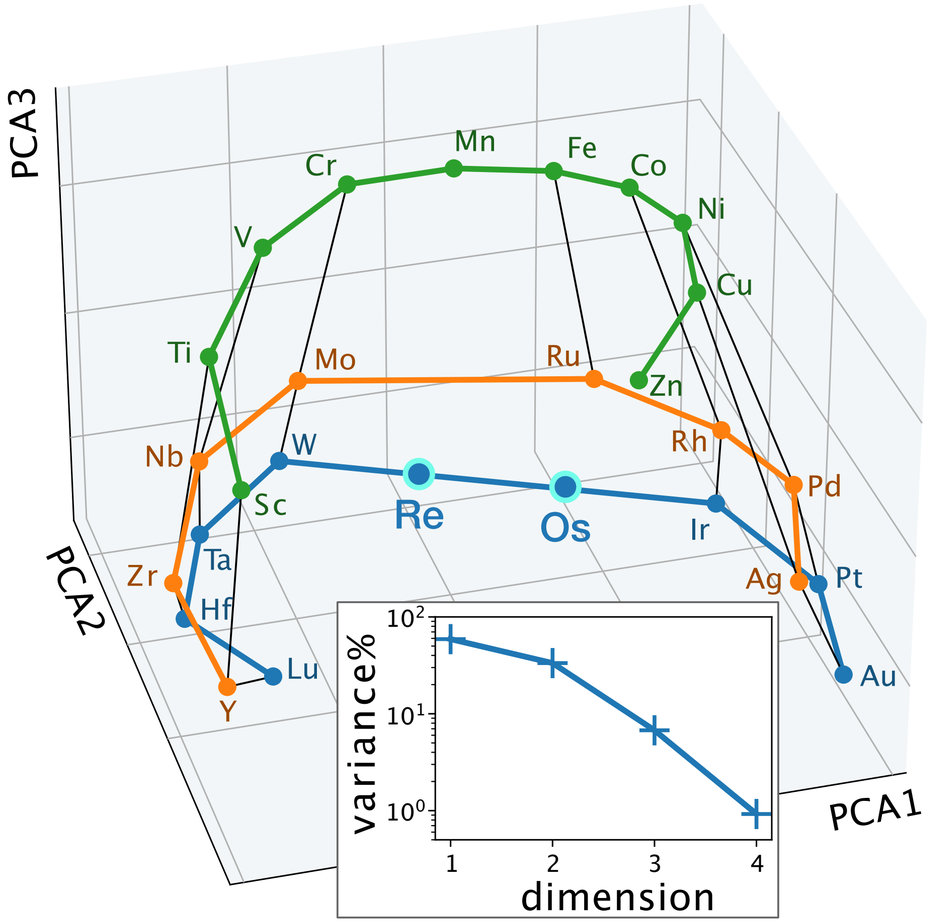

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Able to extrapolate to **new elements**!

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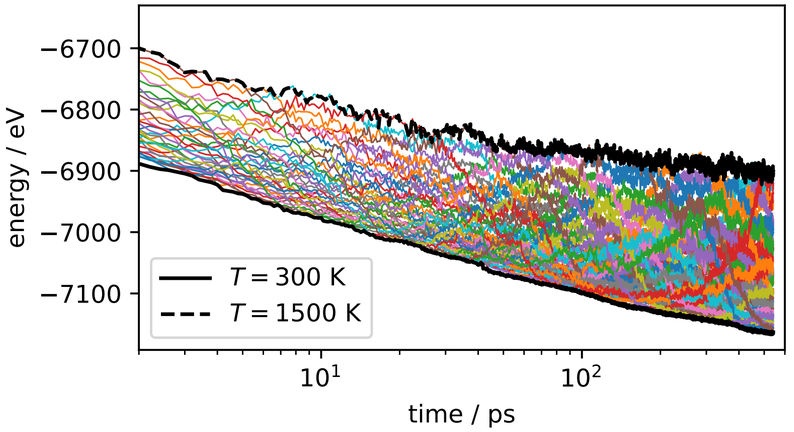
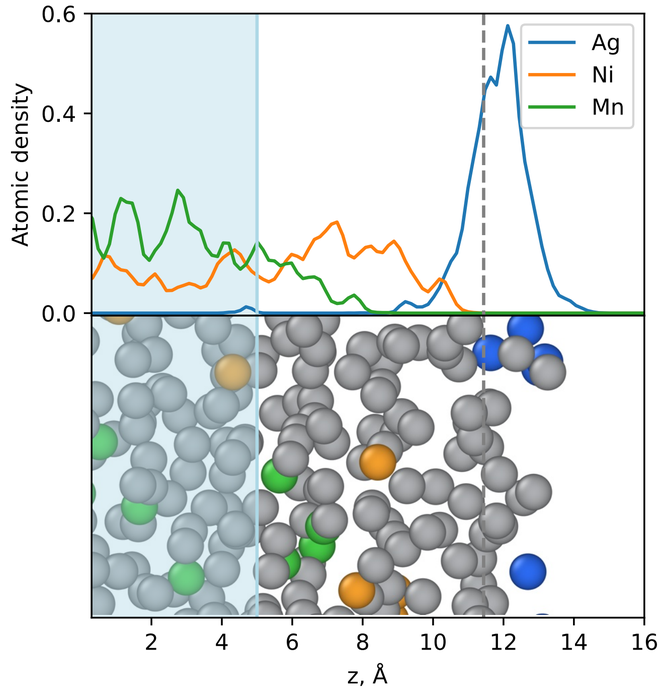
Surfaces segregation

Same element, add surfaces and melted structures

Identical compression weights

Get surfaces propensity from Replica-Exchange MD





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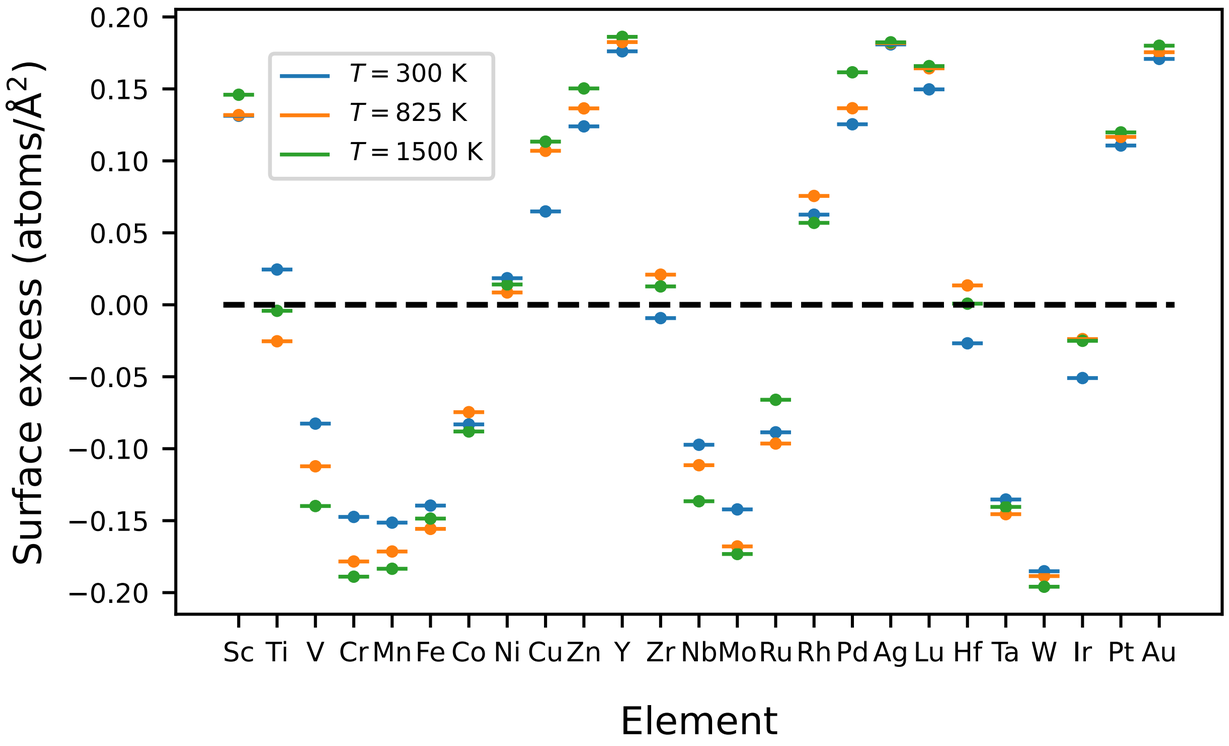
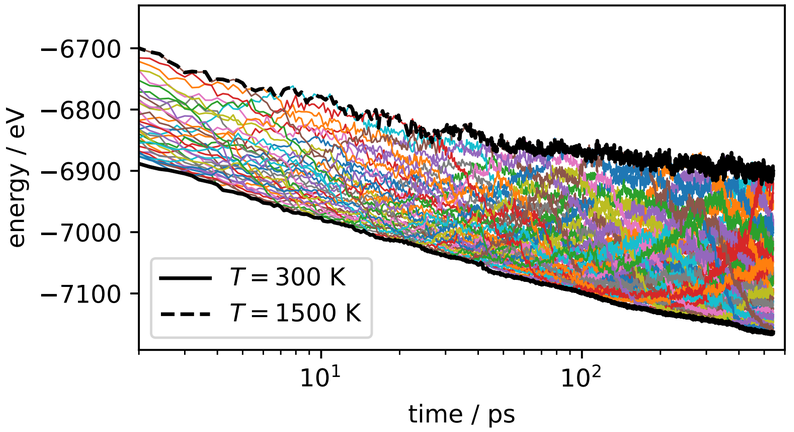
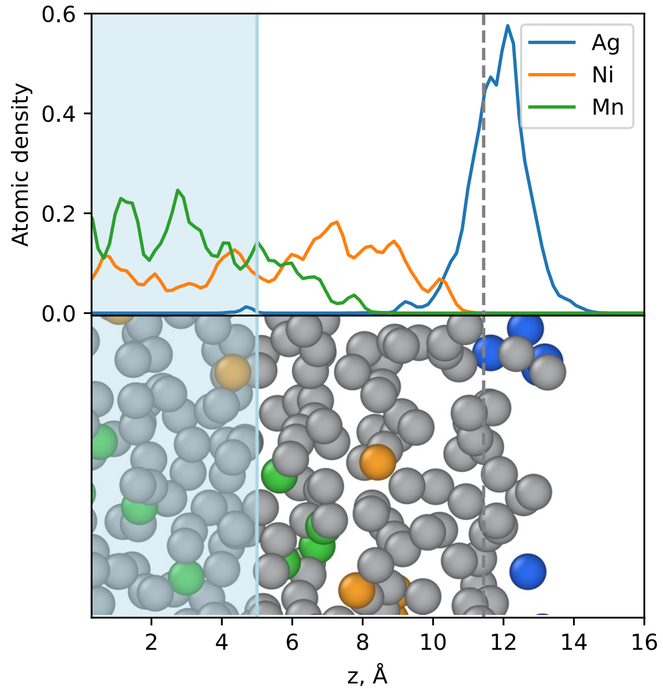
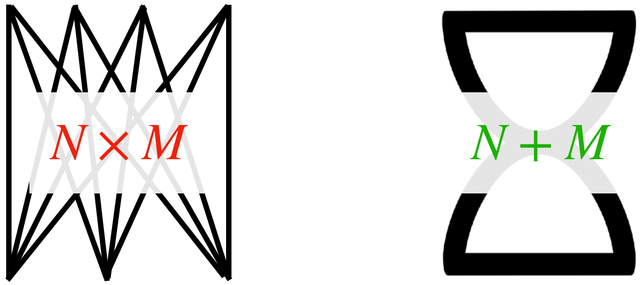




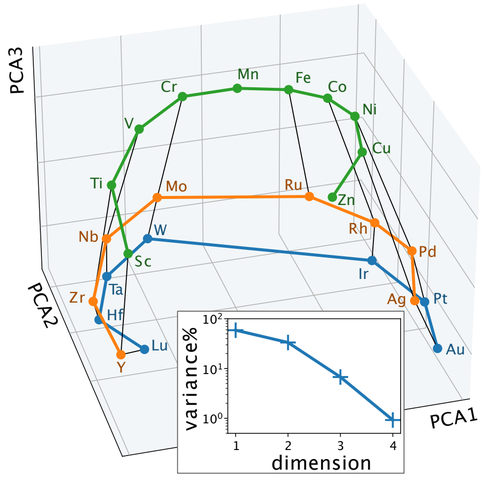


In summary

Sharing **data** for atomistic machine learning



Model for 25 elements,
with learned periodic table



Sharing **code** for atomistic machine learning

Tutorial later today: custom model,
ASE and LAMMPS simulations

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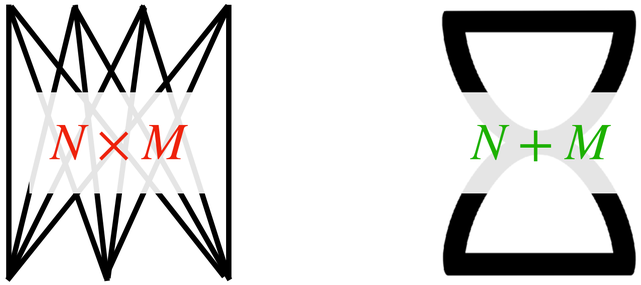

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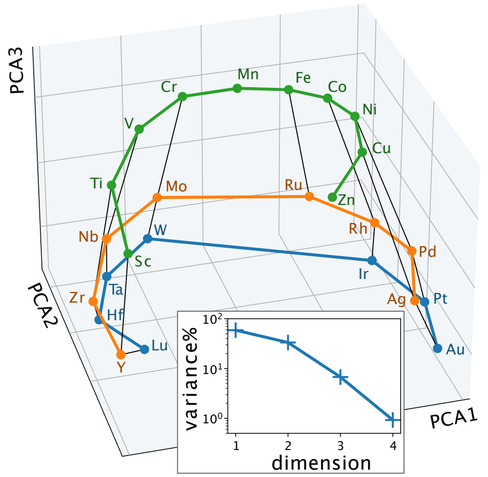

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Thank you for your attention!

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