psiflow

modular and scalable online learning for atomic simulations

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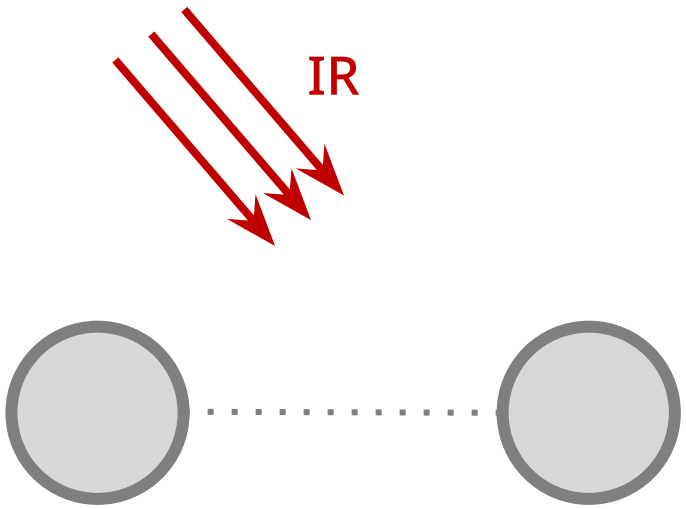
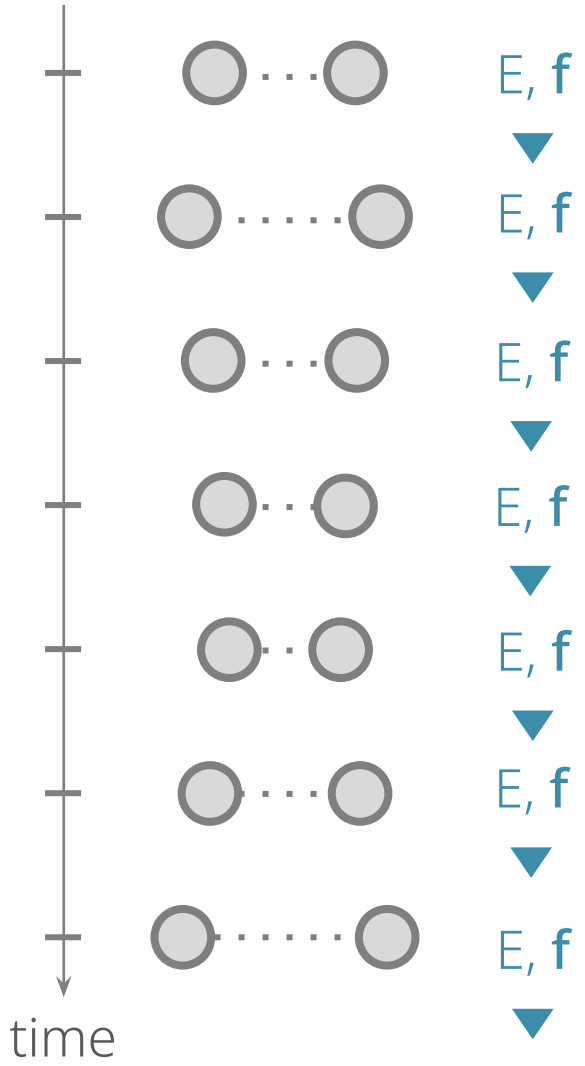
GHENT UNIVERSITY

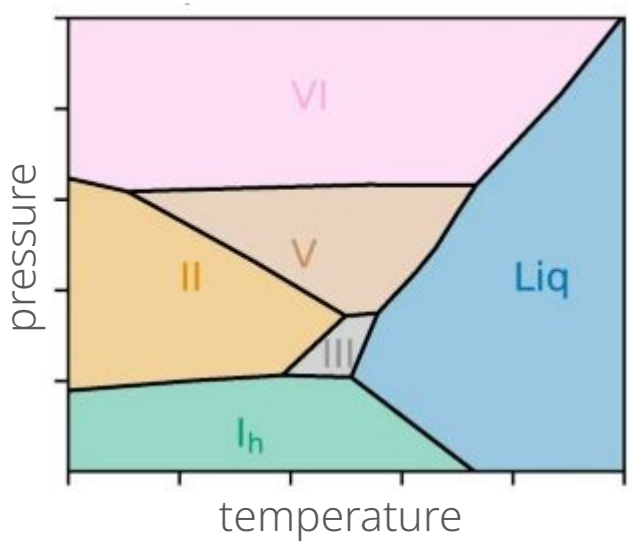
physical property



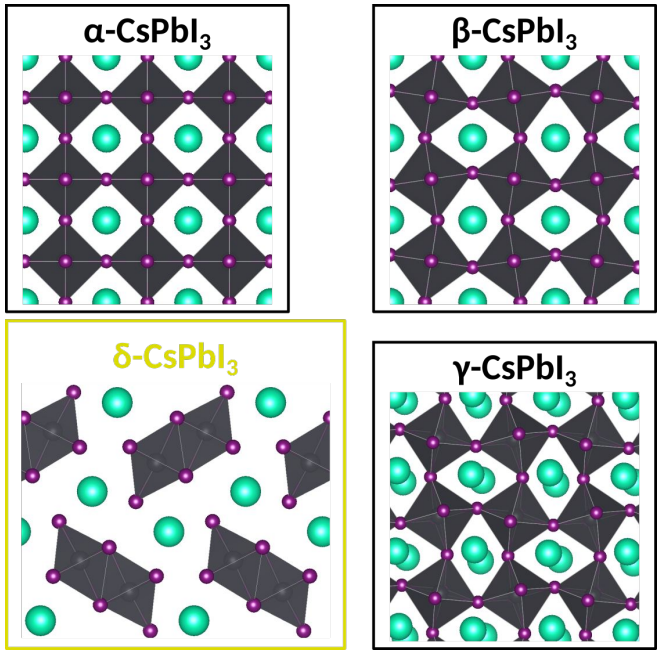
IR absorption in H_2



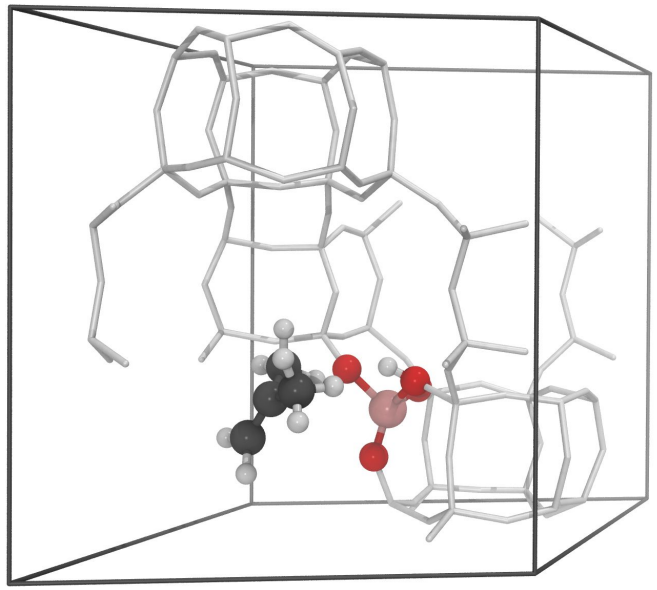
phase diagrams



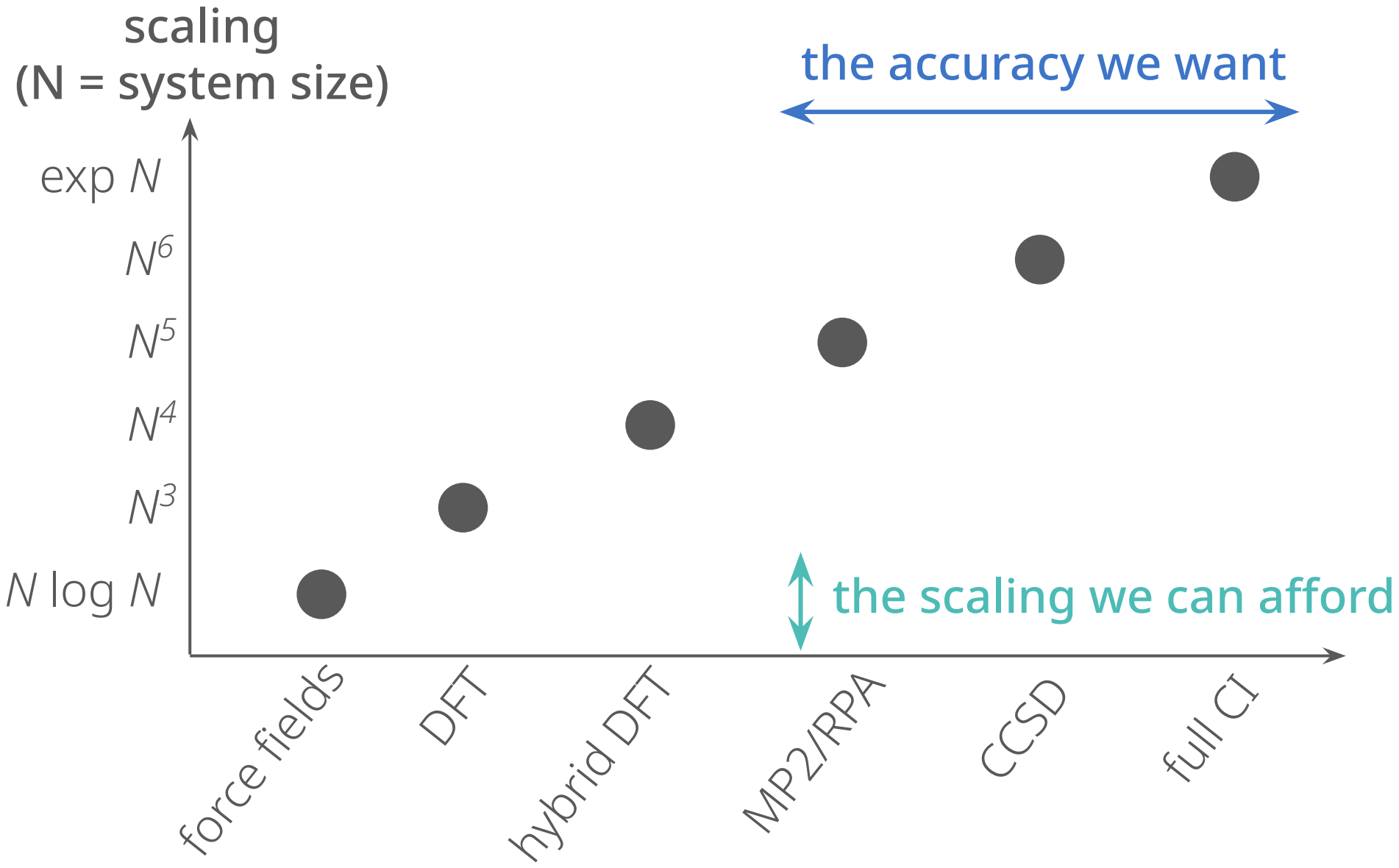
thermodynamic stability



chemical reactivity

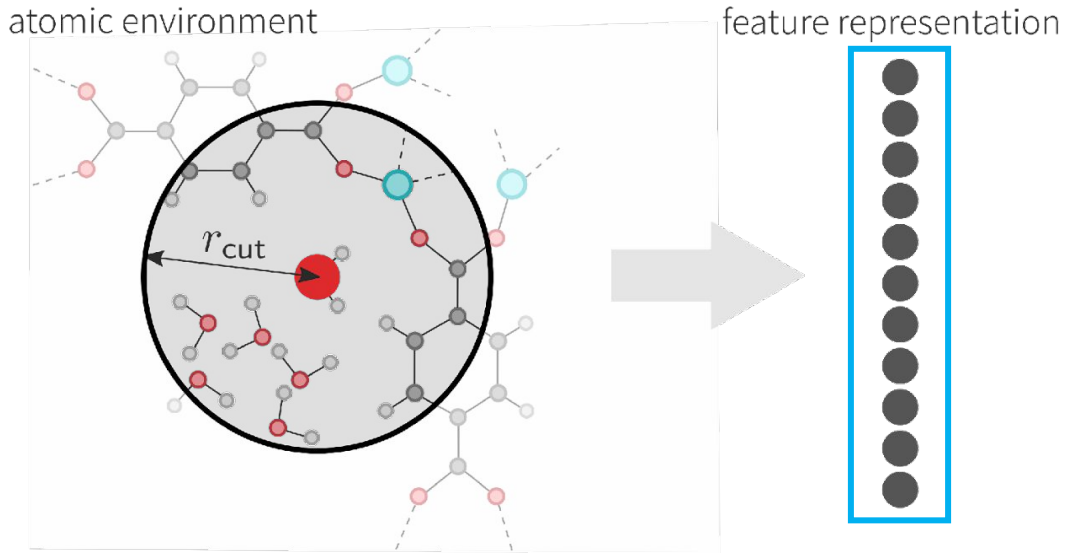


~~hundreds~~
~~thousands~~
millions/billions of E/**f** evaluations


scaling
(N = system size)
exp N
N^6
N^5
N^4
N^3
N log N
the accuracy we want
the scaling we can afford
force fields
DFT
hybrid DFT
MP2/RPA
CCSD
full CI

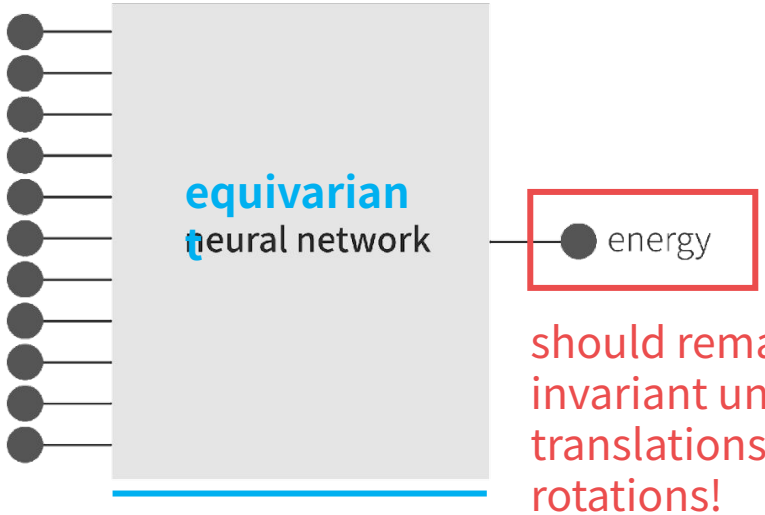
Use equivariant neural networks to learn E/f

STEP 1



use ‘equivariant’ features

STEP 2



should remain invariant under translations or rotations!

much less training data! (~100)

Tensor Field Networks: arXiv.1802.08219v2 **[cs.LG]**
Clebsch-Gordan Nets : arXiv.1806.09231v2 **[stat.ML]**

```
while error(model) is high:
    data = generate_atomic_data(model)     # CPU/
    data = evaluate_DFT_energy_forces(data)  # C
    model.train(data)                      # GPU
```

psiflow

average computational chemist is not very computational

- hide Parsl API as much as possible

enforce “write once, run anywhere”

- separate configuration from high-level workflow definition

WHAT?

high-level workflow definition using abstractions:

`Model`
`Dataset`
`Walker`
`Learning`
`...`

`run.py`

HOW?

run CP2K on N cores

train model for M minutes

Docker/Apptainer URIs

MPI/OpenMP

WHERE?

Parsl providers!

`lumi.py`
`frontier.py`

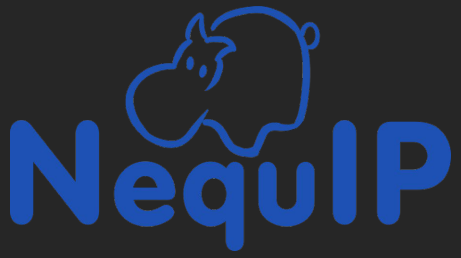
```
python run.py       # runs locally using ThreadPoolExecutors
python run.py --psiflow-config lumi.py   # on LUMI
```

```python
import psiflow
from psiflow.data import Dataset    # wraps around File/DataFuture
from psiflow.models import MACEModel   # wraps around File/DataFuture

psiflow.load()  # build and load Parsl config; ‘compile’ apps

train, valid = Dataset.load(‘dft.xyz’).split(0.9)
model = MACEModel()   # contains DataFuture of untrained model
model.train(train, valid)  # contains DataFuture of trained   model

errors = Dataset.get_errors(valid, model.evaluate(valid)) # Future
errors.result() # NumPy array of validation errors on energy/force
```

OpenMM

PyTorch

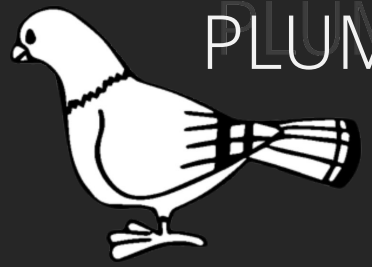
Weights & Biases



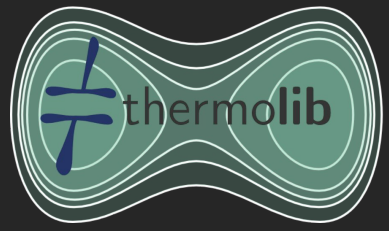
NWChem

Parsl

MACE



PLUMED



bundled in a Docker/Apptainer image → `ContainerizedLauncher`

Big workflows create huge amounts of files

- automatic tarring? Or even archived by default?

Big workflows require a lot of memory

- more extensive use of virtual, on-disk memory?

Debugging Parsl workflows is nontrivial

- lazy failure not always best option?

Veronique Van Speybroeck

Massimo Bocus
Tom Braeckevelt
Pieter Dobbelaere
& others

EuroHPC Joint Undertaking

LUMI

fwo Research Foundation Flanders
Opening new horizons

VLAAMS SUPERCOMPUTER CENTRUM

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