psiflow

modular and scalable online learning for atomic simulations

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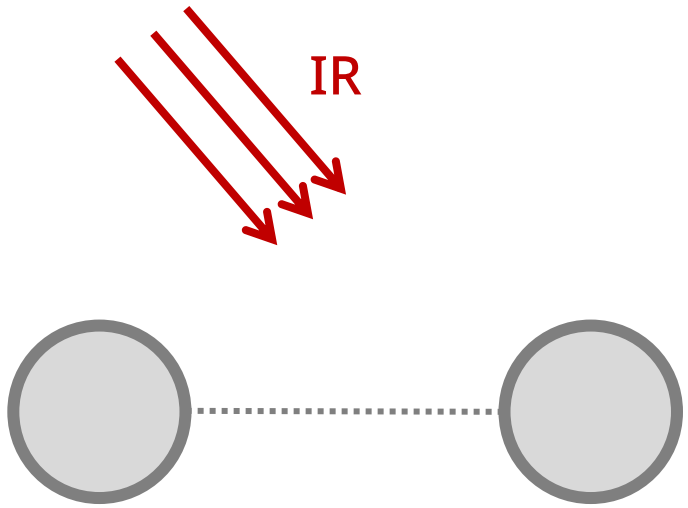
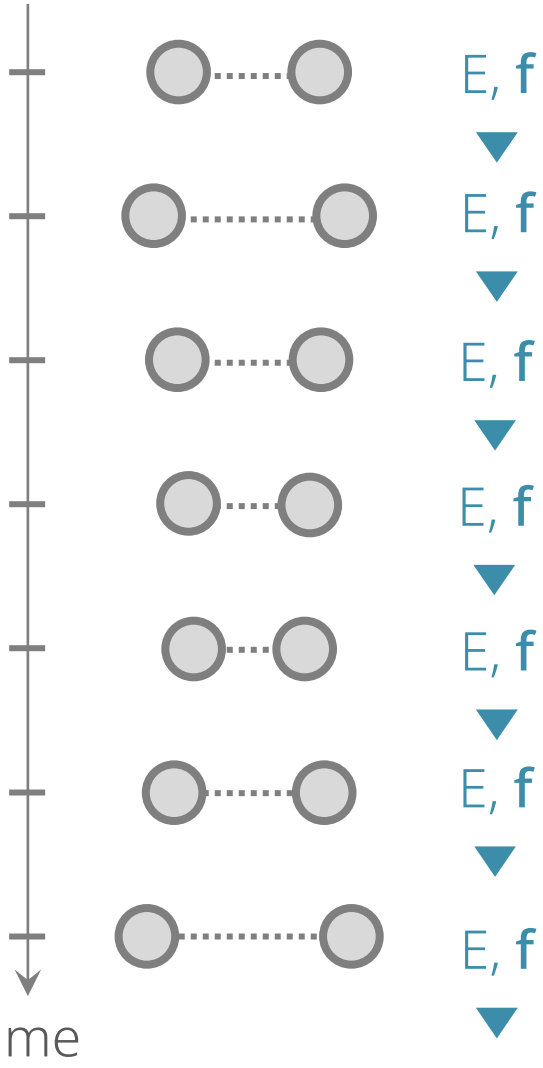
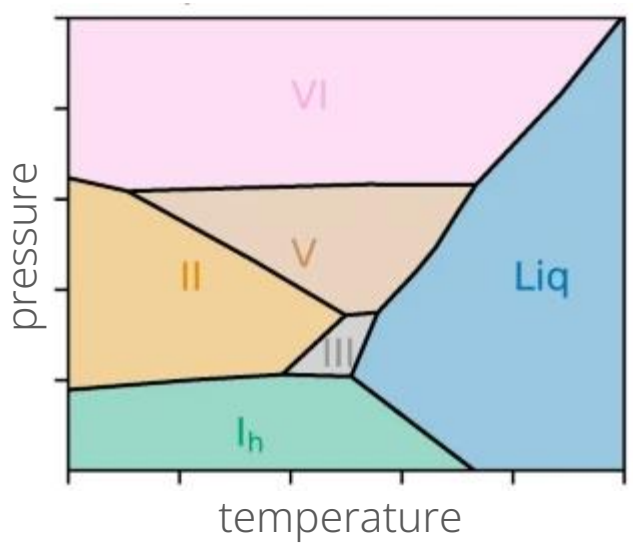
physical property



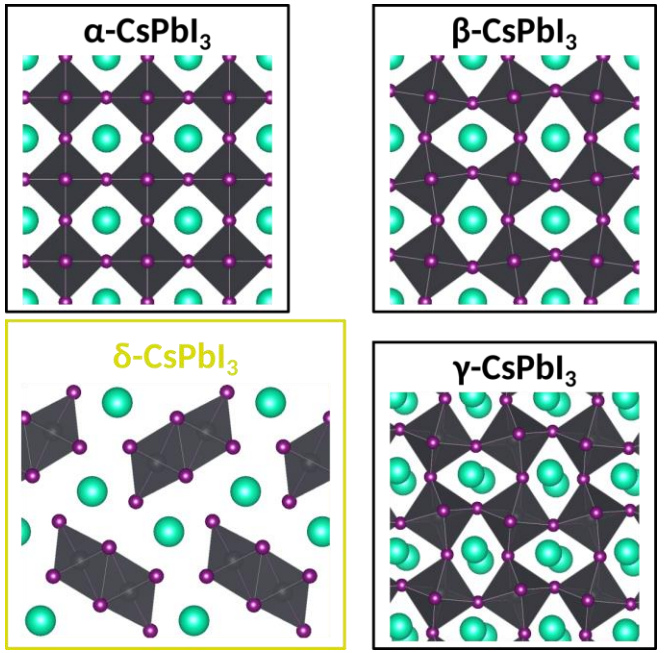
IR absorption in H_2



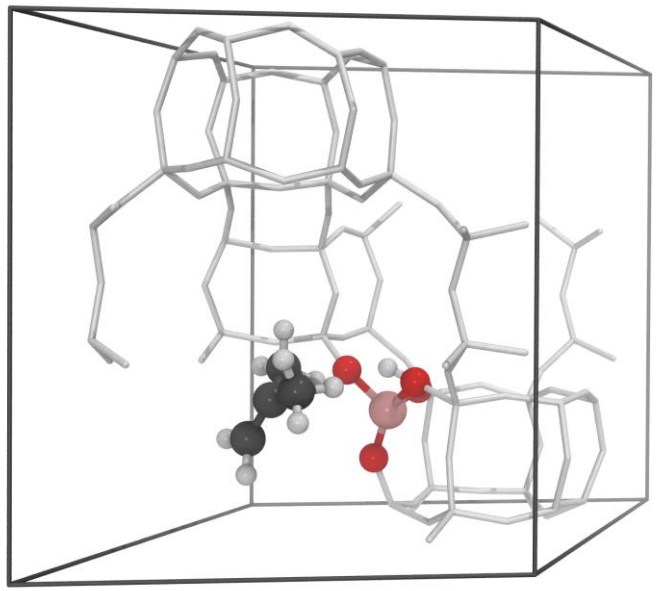
phase diagrams



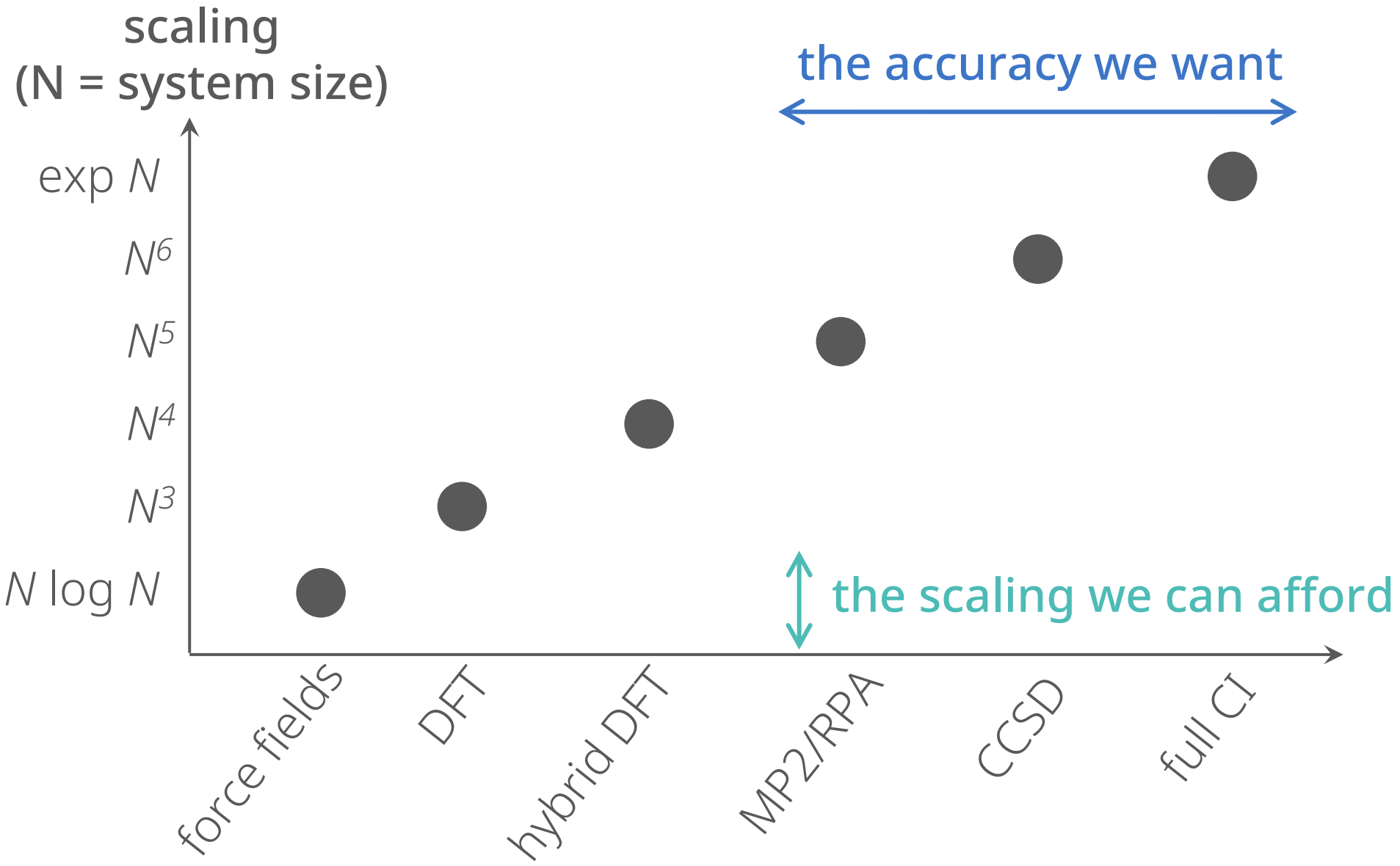
thermodynamic stability



chemical reactivity



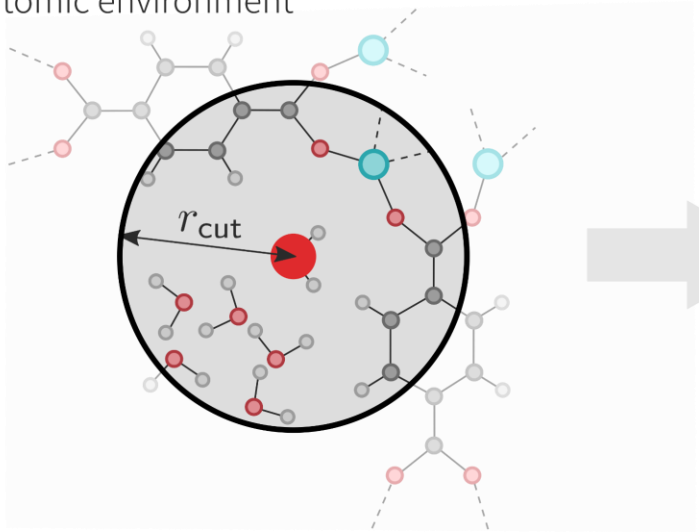
~~hundreds~~
~~thousands~~
millions/billions of E/**f** evaluations


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

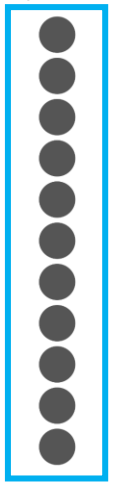
Use equivariant neural networks to learn E/f

STEP 1

atomic environment

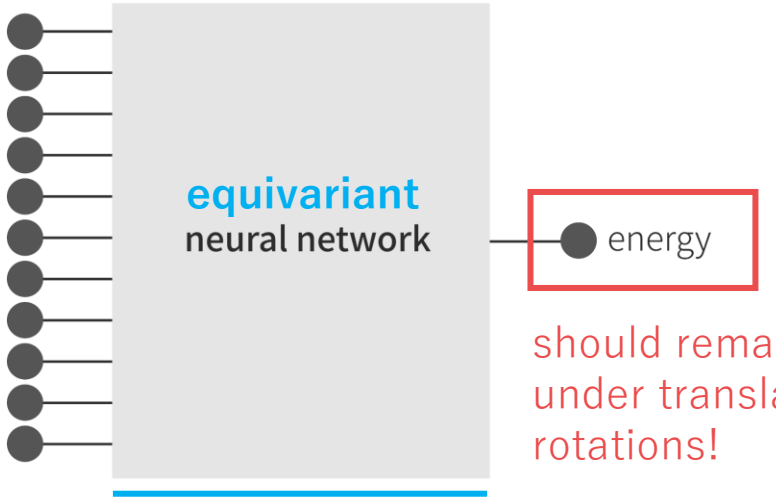


feature representation



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/GPU
      data = evaluate_DFT_energy_forces(data)     # CPU
      model.train(data)                           # GPU

evaluate_exact_groundstate_energy(data)     # large-memory CPU
model.train(data)                           # GPU
compute_free_energies(model)                # CPU/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`
`...`

HOW?

run CP2K on N cores

train model for M minutes

Docker/Apptainer URIs

MPI/OpenMP

WHERE?

Parsl providers!

`run.py`

`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

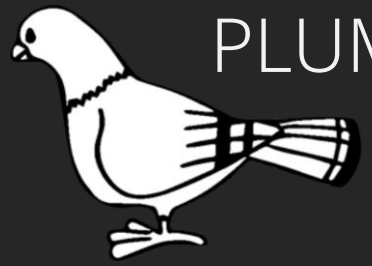
PyTorch

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

Vlaanderen is supercomputing

erc European Research Council