

# Adaptive-Precision Interatomic Potentials (APIP)

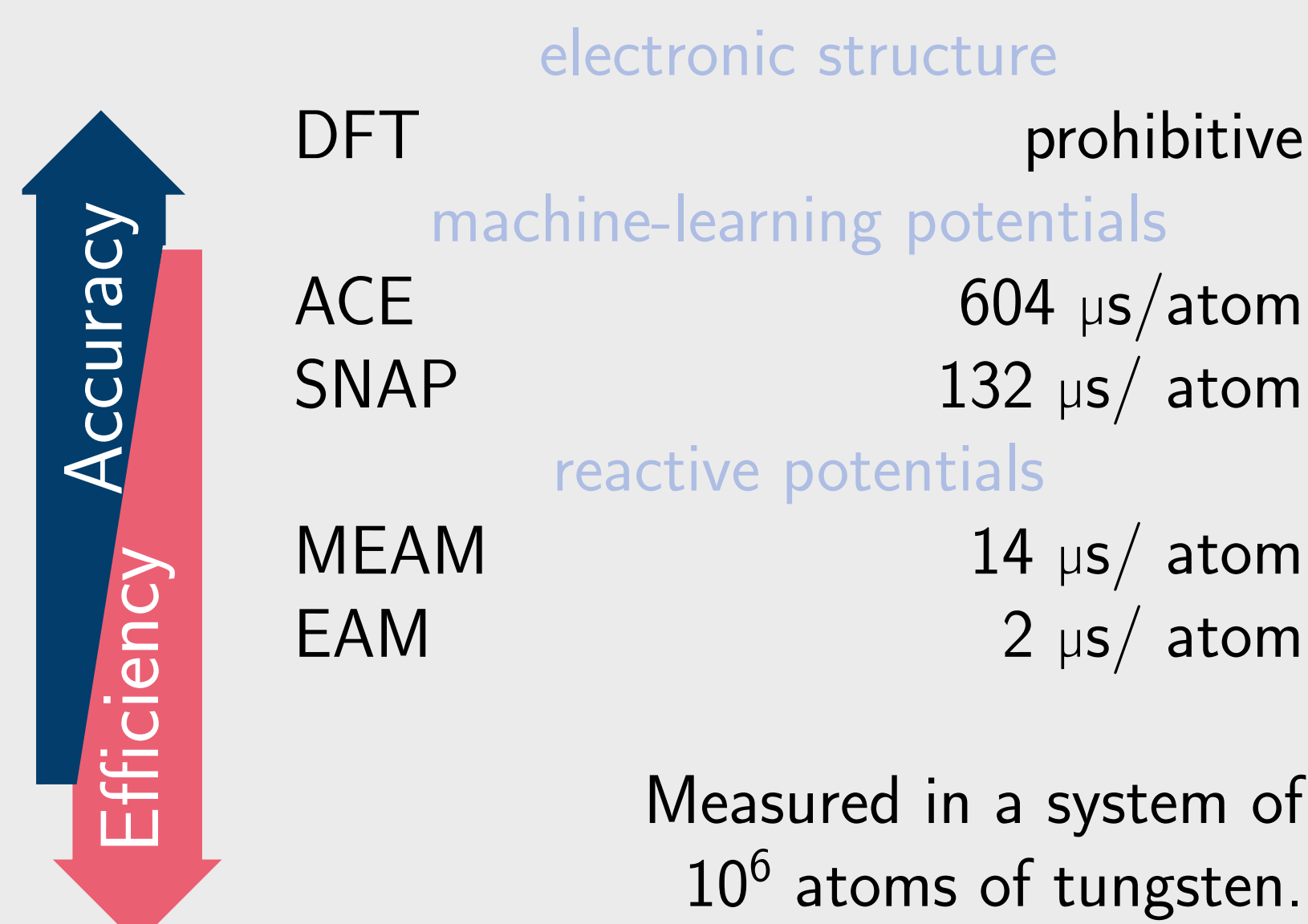
Atomistic simulations rely on interatomic potentials providing an efficient representation of atomic energies and forces. Modern machine learning (ML) potentials provide a density-functional theory-like accuracy, but are rarely used in large-scale simulations as

they remain orders of magnitude slower than simple empirical potentials. Often only a small number of atoms strongly influences the correct outcome of a simulation, while the majority of atoms forms a background. An APIP overcomes the performance gap between

the precise ML and the fast potentials for such simulations by combining two potentials of different accuracy and computational costs to an adaptive-precision description with an optimum of performance and precision in large complex atomistic systems.

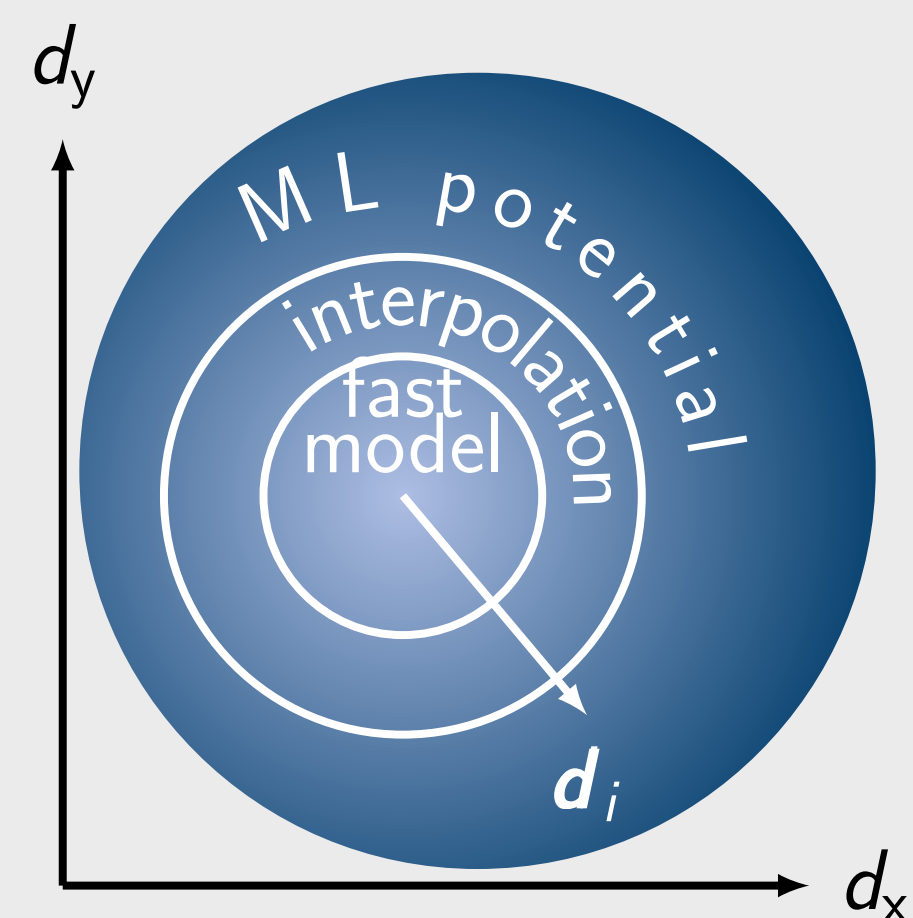
## Constant precision potentials

A potential can be either precise or efficient.



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## Atomistic precision switching



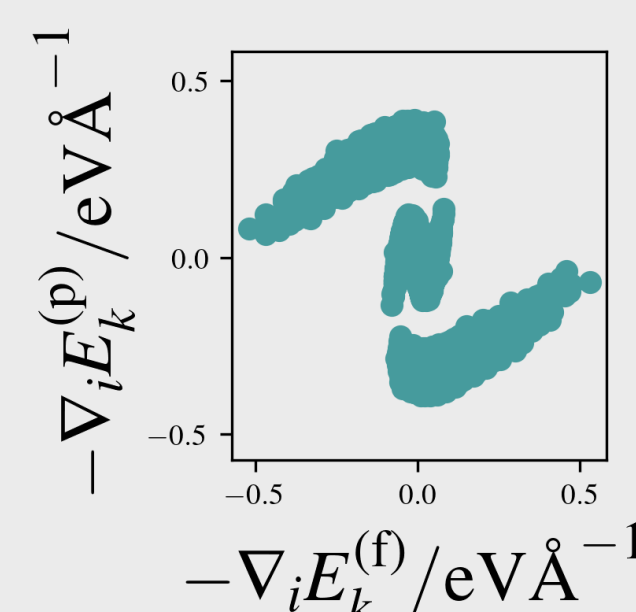
- A fast surrogate model ( $E_i^{(f)}$ ) reproduces the expensive ML potential ( $E_i^{(p)}$ ) in the vicinity of a reference environment.
- The descriptor  $d_i$  decides per atom  $i$  which model to use.

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## Adaptive-Precision Interatomic Potential

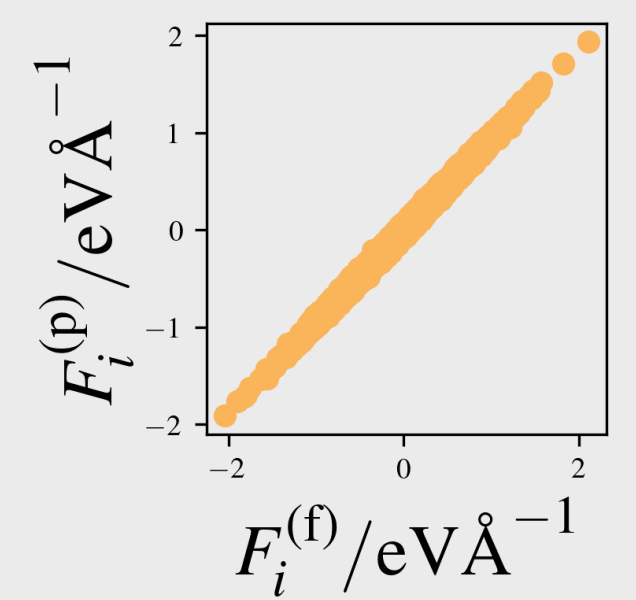
### energy-based

- $E_i = \lambda_i E_i^{(f)} + (1 - \lambda_i) E_i^{(p)}$
  - Provides precise potential energies.
  - $F_i = -\nabla_i \sum_k E_k$
- ⇒ Precise forces are challenging.



### force-based

- $F_i = \lambda_i F_i^{(f)} + (1 - \lambda_i) F_i^{(p)}$
- Provides precise forces.
- The potential energy is neither defined nor conserved.

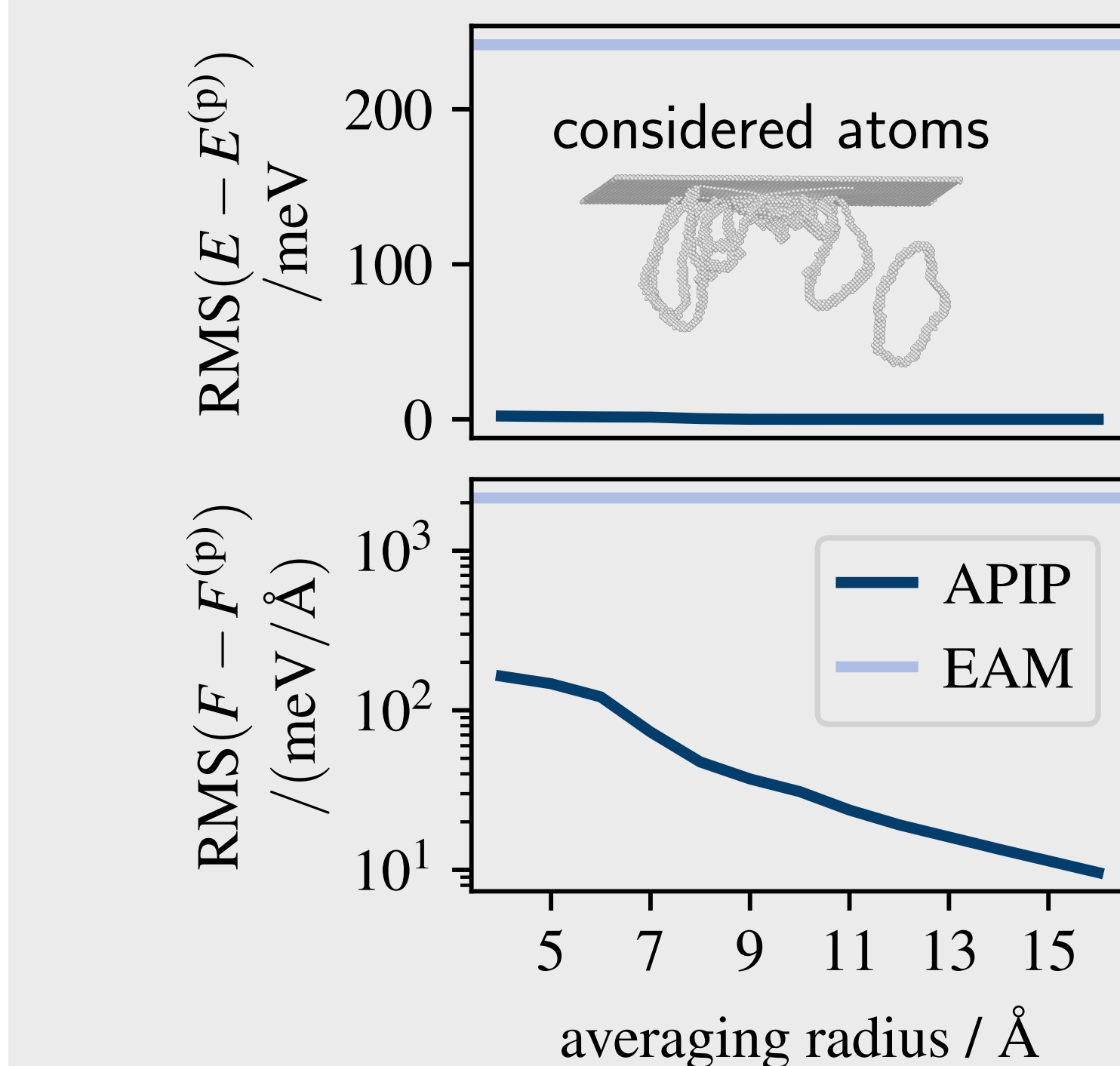


Plots from Ref. [1]

## Conservative APIP

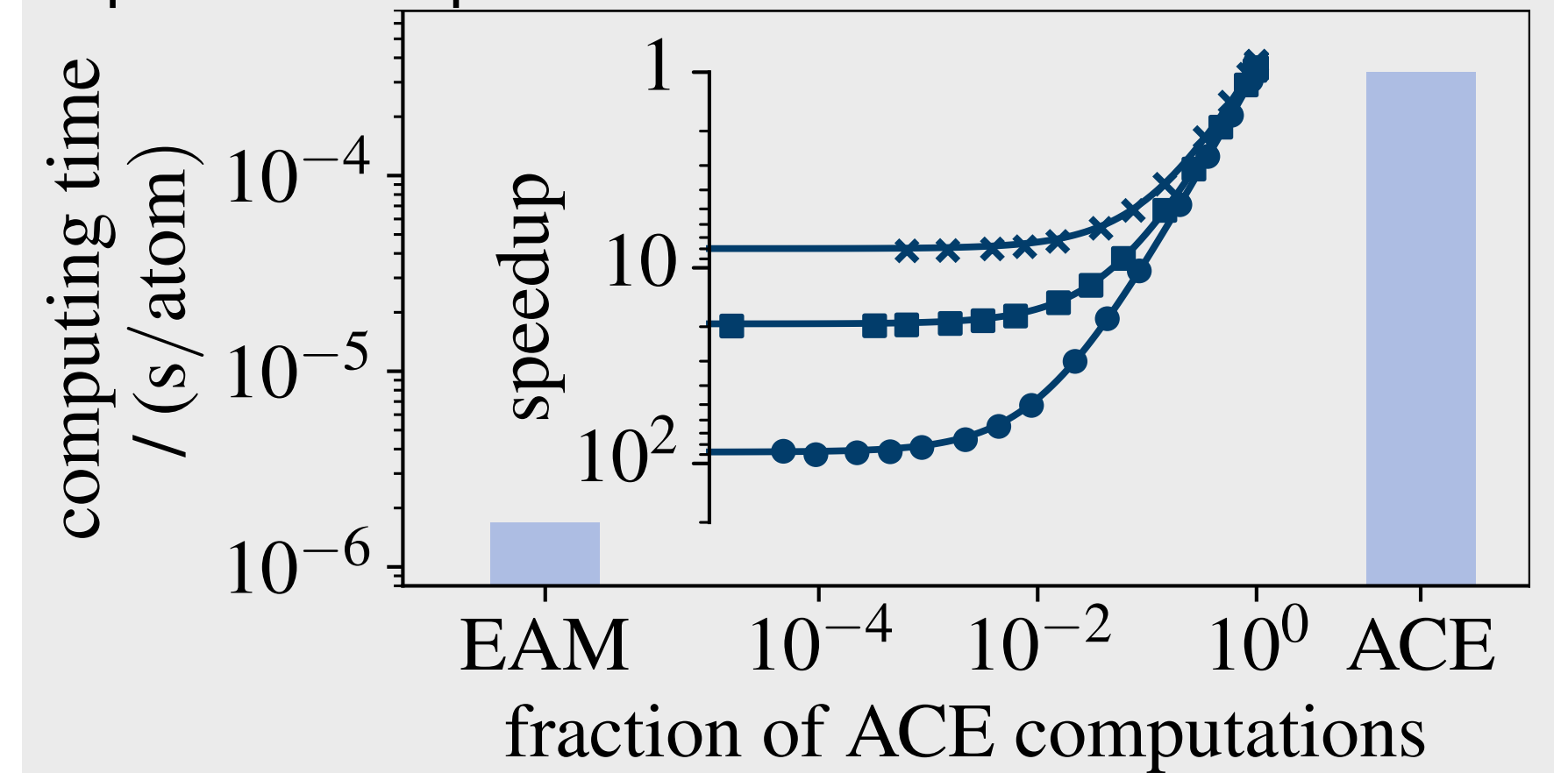
Local averaging for precise forces[2]

Thereby, one gets precise forces with an energy-based approach.

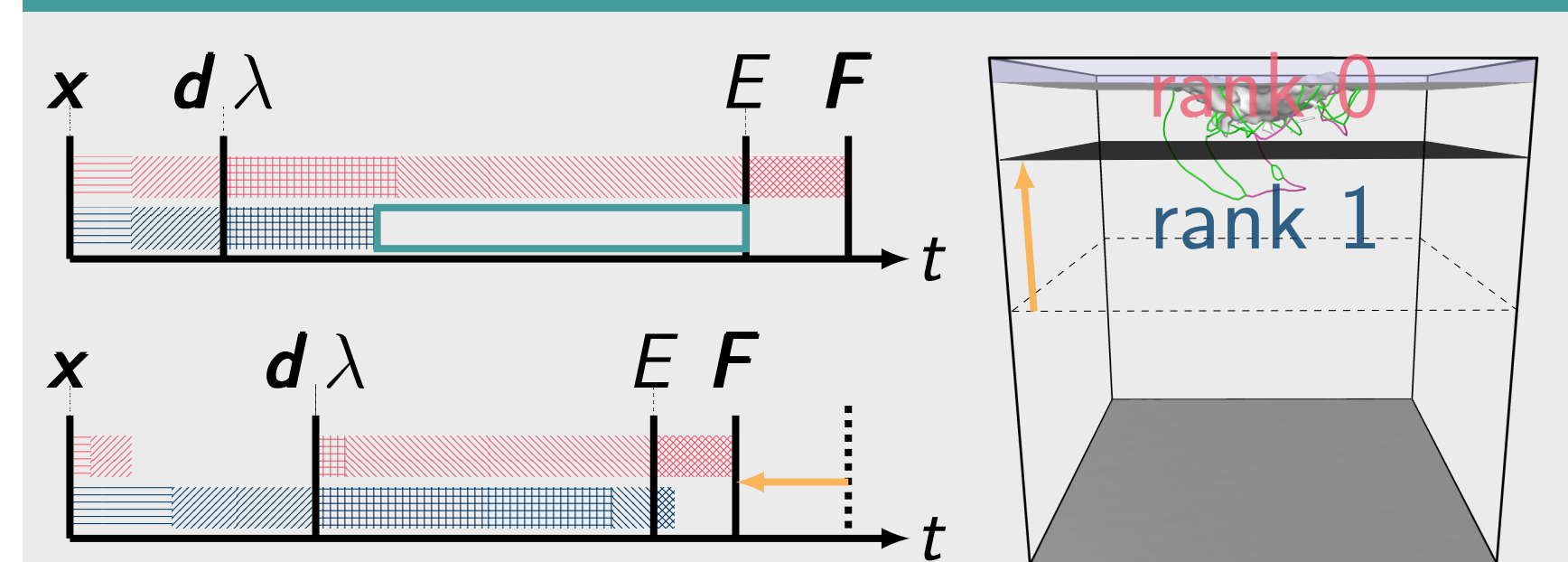


## Speedup[2]

APIP can be 1-2 orders of magnitude faster than a precise computation.



## Load balancing

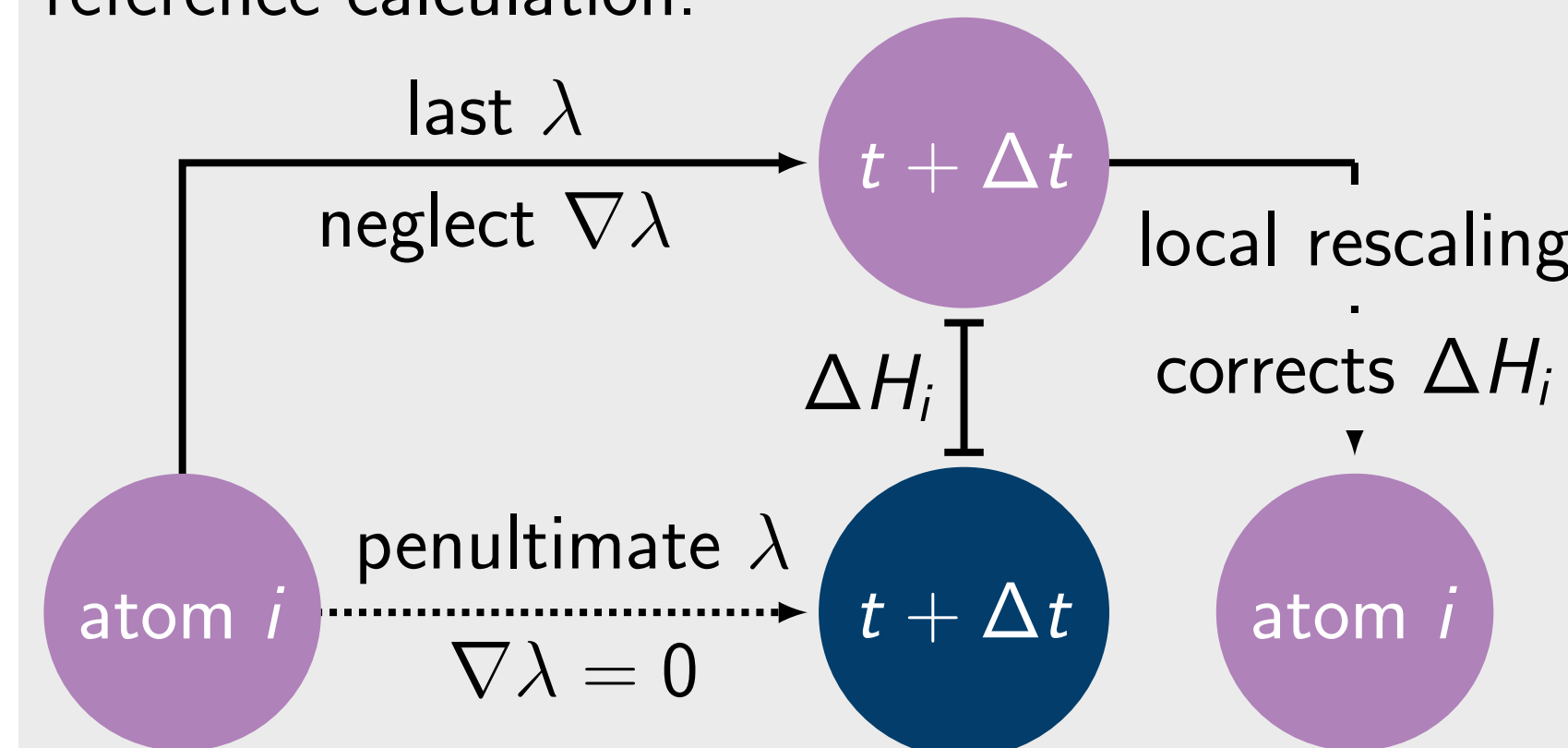


A processor (here 0 and 1) administers one domain. Dynamic load balancing shifts the domain boundaries to prevent idle time at communication steps ( $x, d, \lambda, E, F$ ).

## Efficient APIP

### Lambda thermostat[1]

Ensure energy conservation with conservative reference calculation.



### Load balancing[1]

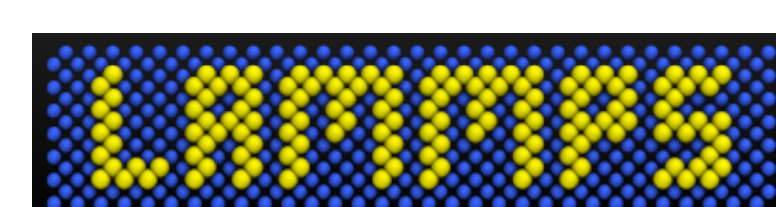
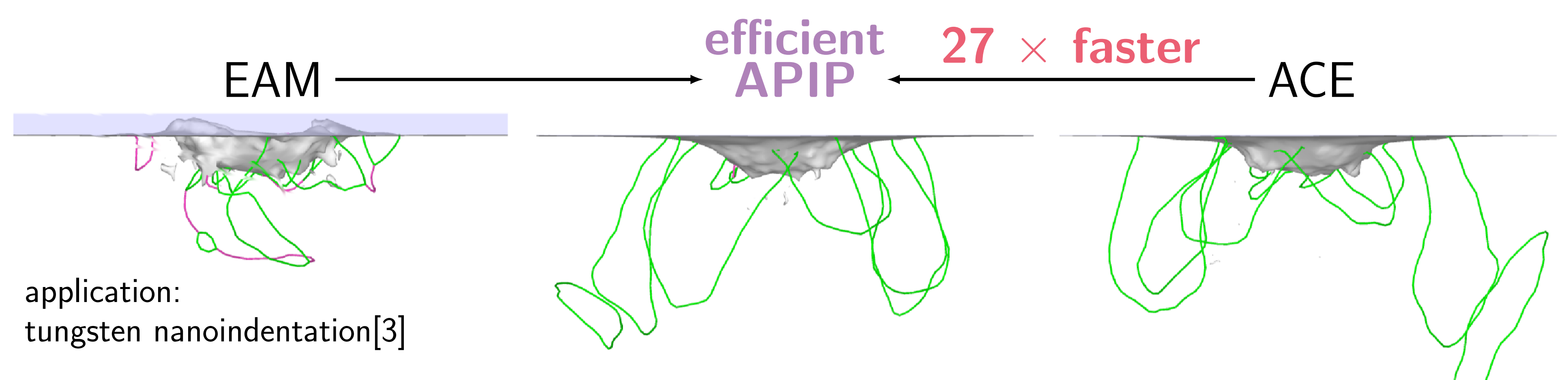
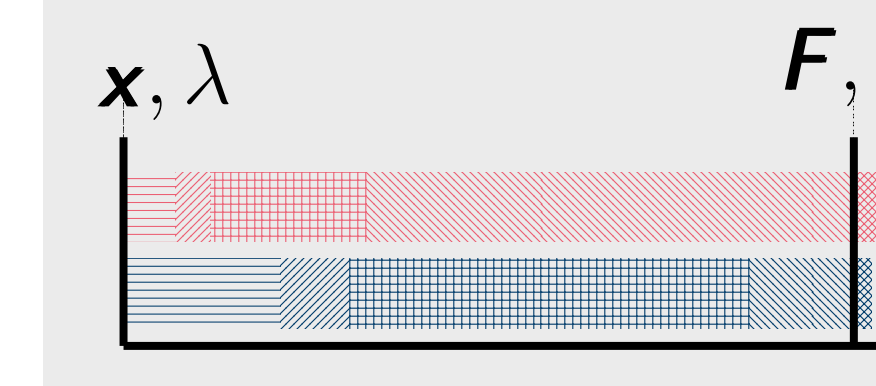
includes computation of

- descriptor
- switching parameter
- fast model
- precise model

$\lambda_i(t) \approx \lambda_i(t - \Delta t)$

use the last and penultimate  $\lambda_i$  for the lambda thermostat

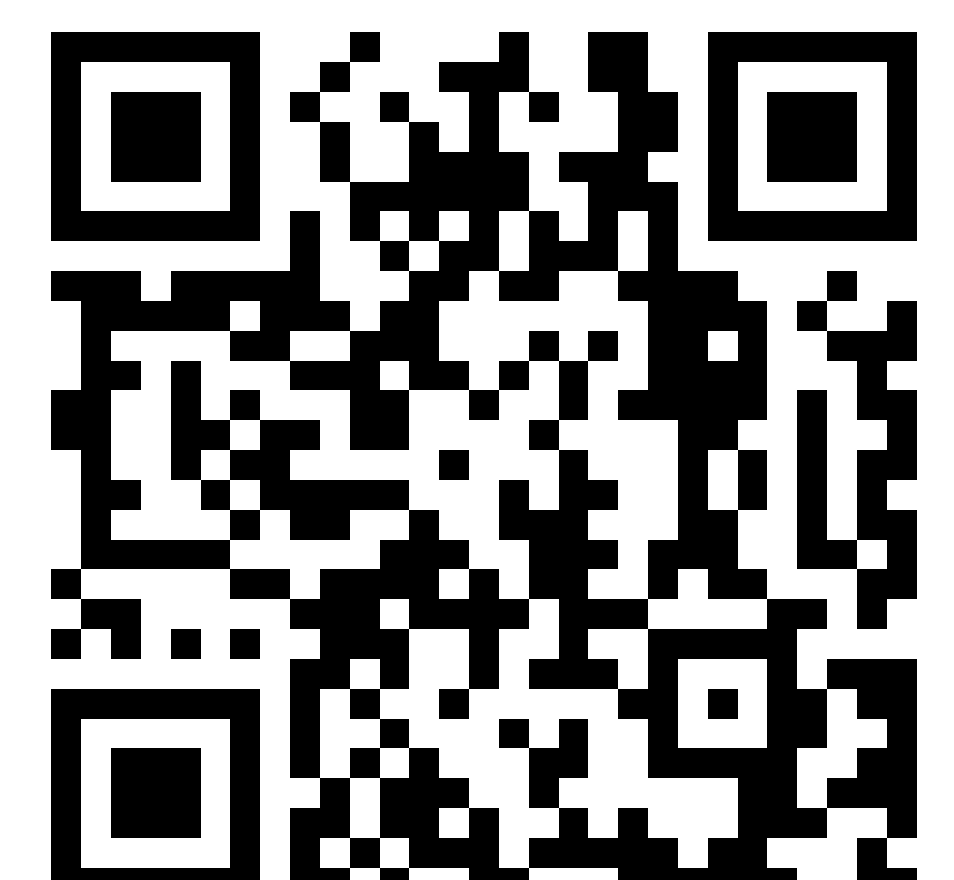
no additional communication steps



contains conservative APIP and efficient APIP

### code example (efficient APIP)

```
pair_style hybrid/overlay eam/fs/apip pace/precise/apip \
  lambda/input/csp/apip fcc cutoff 5.0 lambda/zone/apip 12.0
pair_coeff * * eam/fs/apip Cu.eam.fs Cu
pair_coeff * * pace/precise/apip Cu.yace Cu
pair_coeff * * lambda/input/csp/apip
pair_coeff * * lambda/zone/apip
fix 2 all lambda/apip 2.5 3.0 time averaged zone \
  4.0 12.0 110 110 min_delta_lambda 0.01
fix 3 all lambda_thermostat/apip N_rescaling 200
```



<sup>1</sup>D. Immel, R. Drautz, and G. Sutmann, "Adaptive-precision potentials for large-scale atomistic simulations", *The Journal of Chemical Physics* **162**, 114119 (2025).

<sup>2</sup>D. Immel, R. Drautz, and G. Sutmann, *Conservative adaptive-precision interatomic potentials*, arXiv:2512.07693, 2025.

<sup>3</sup>D. Immel, M. Mrovec, R. Drautz, and G. Sutmann, "Nanoindentation simulations for copper and tungsten with adaptive-precision potentials", *Phys. Rev. Mater.* **9**, 093805 (2025).