Building with Parsl: Molecular Simulation

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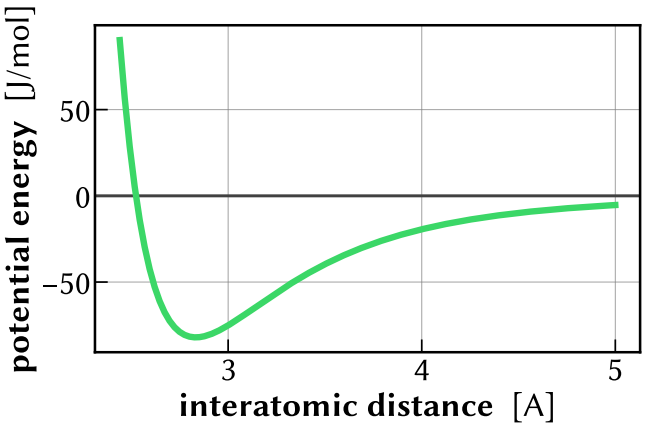
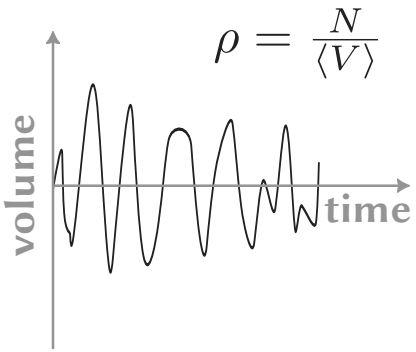
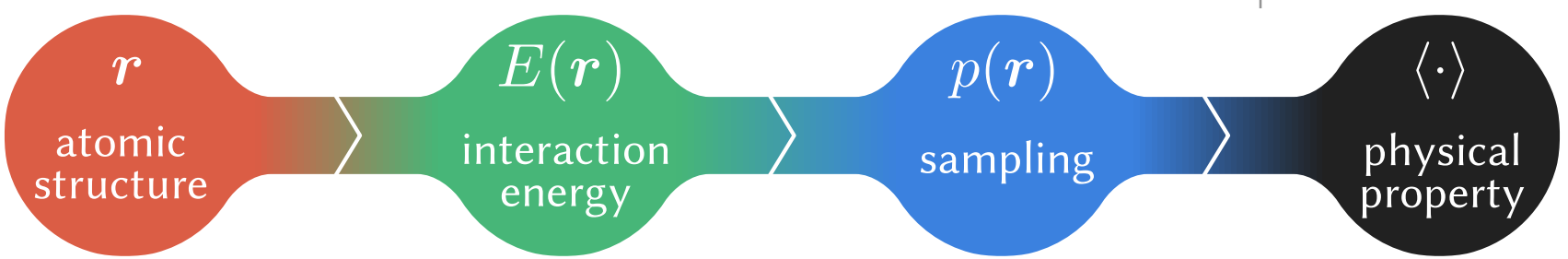
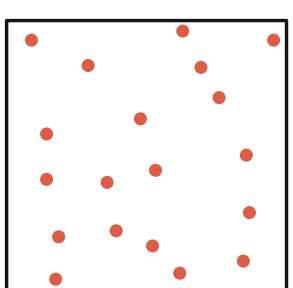






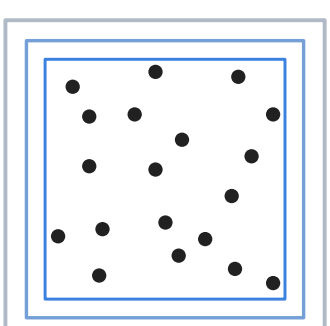


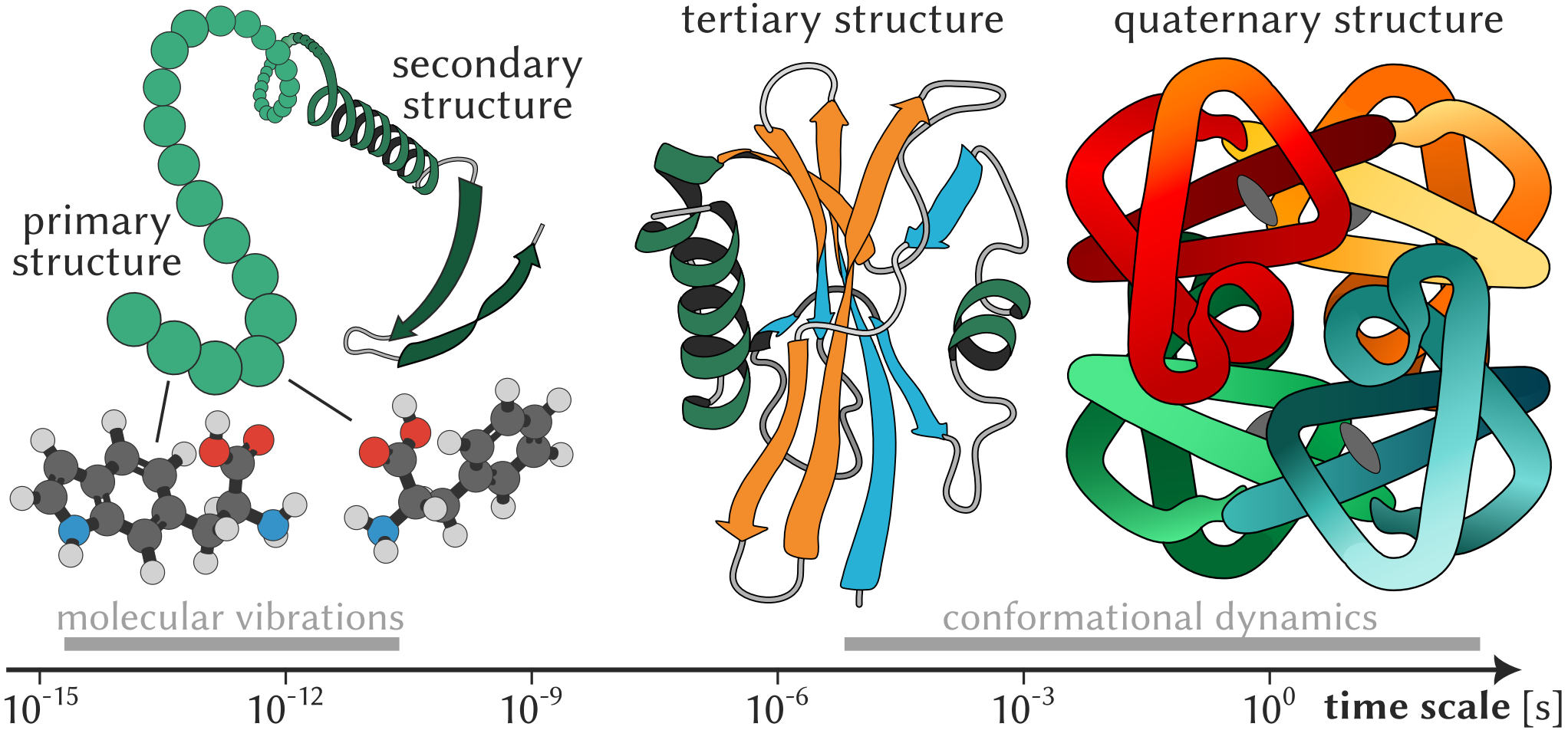
unit cell with N atoms

molecular dynamics

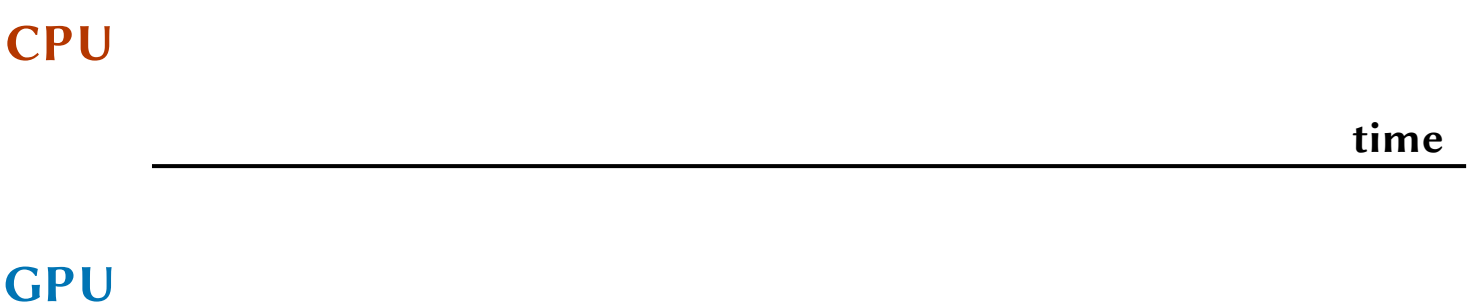
constant N, P, T

variable volume
variable energy




secondary structure
primary structure
tertiary structure
quaternary structure
molecular vibrations
conformational dynamics
10^{-15}
10^{-12}
10^{-9}
10^{-6}
10^{-3}
10^{0}
time scale [s]

Resource requirements: heterogeneous and unbalanced



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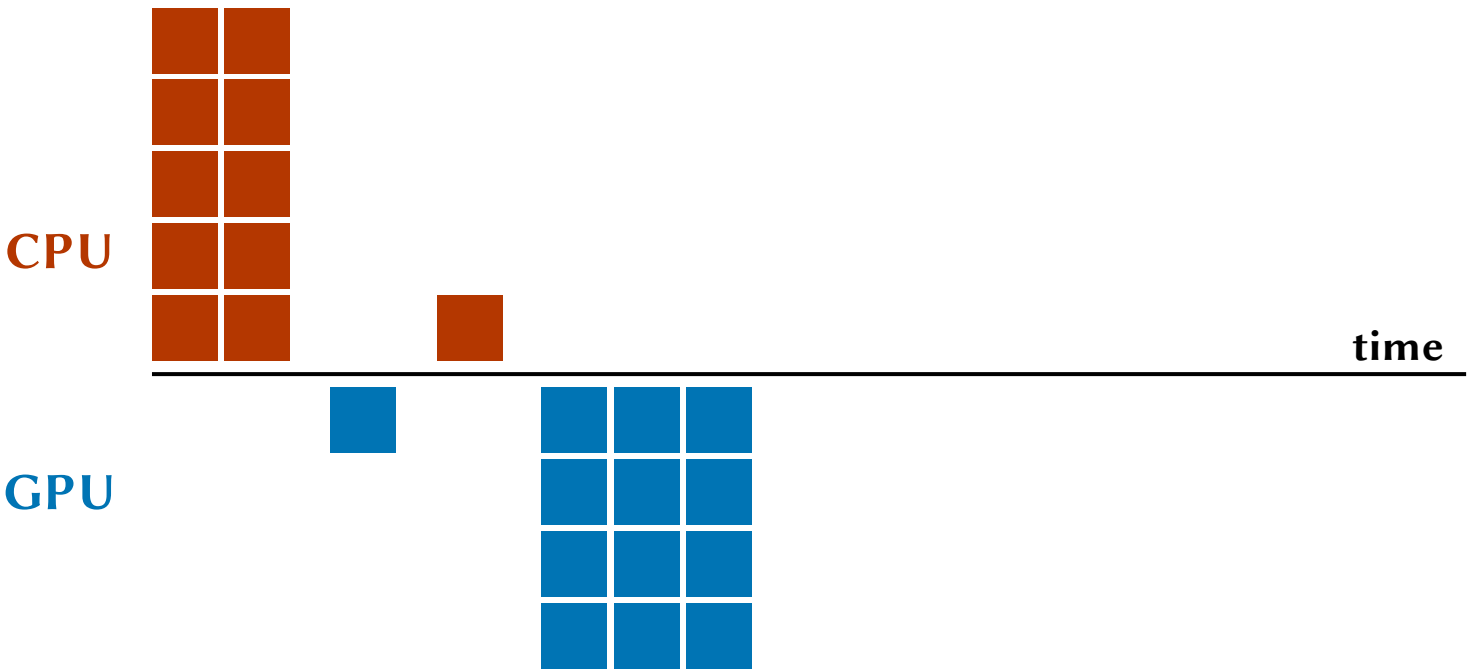

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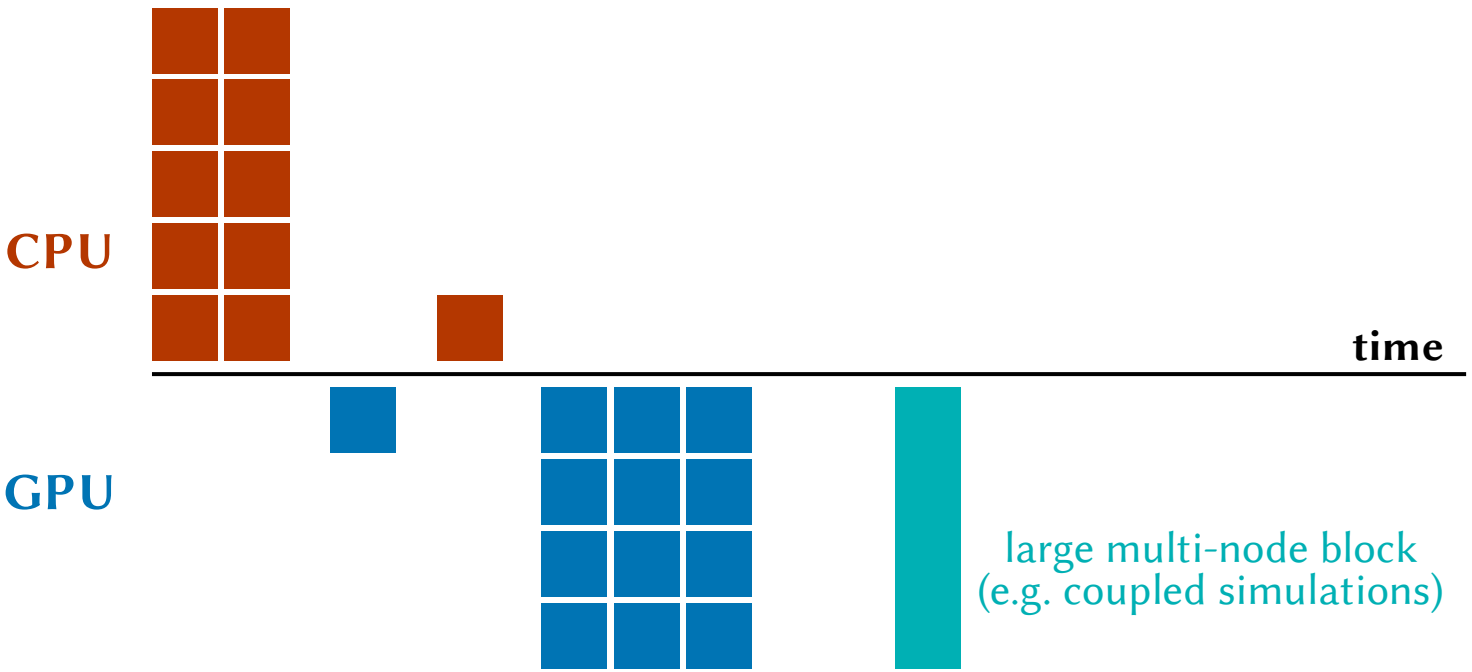

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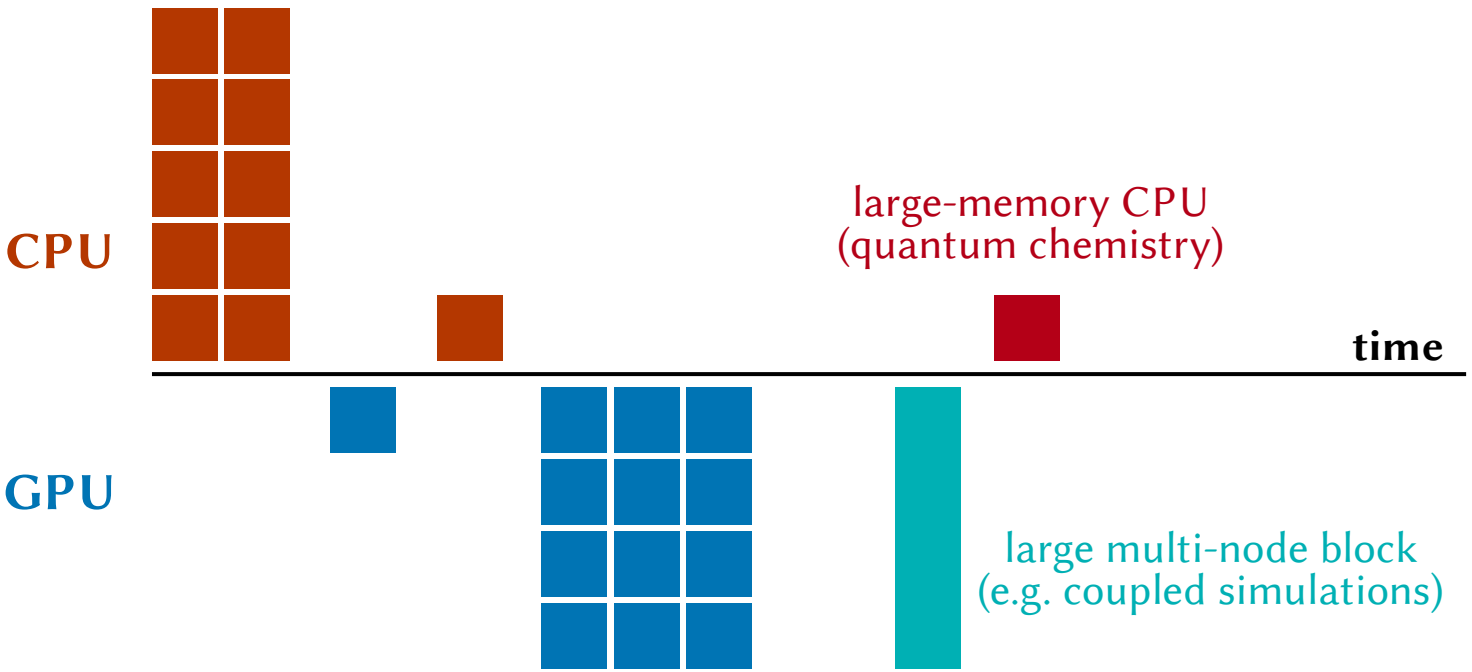

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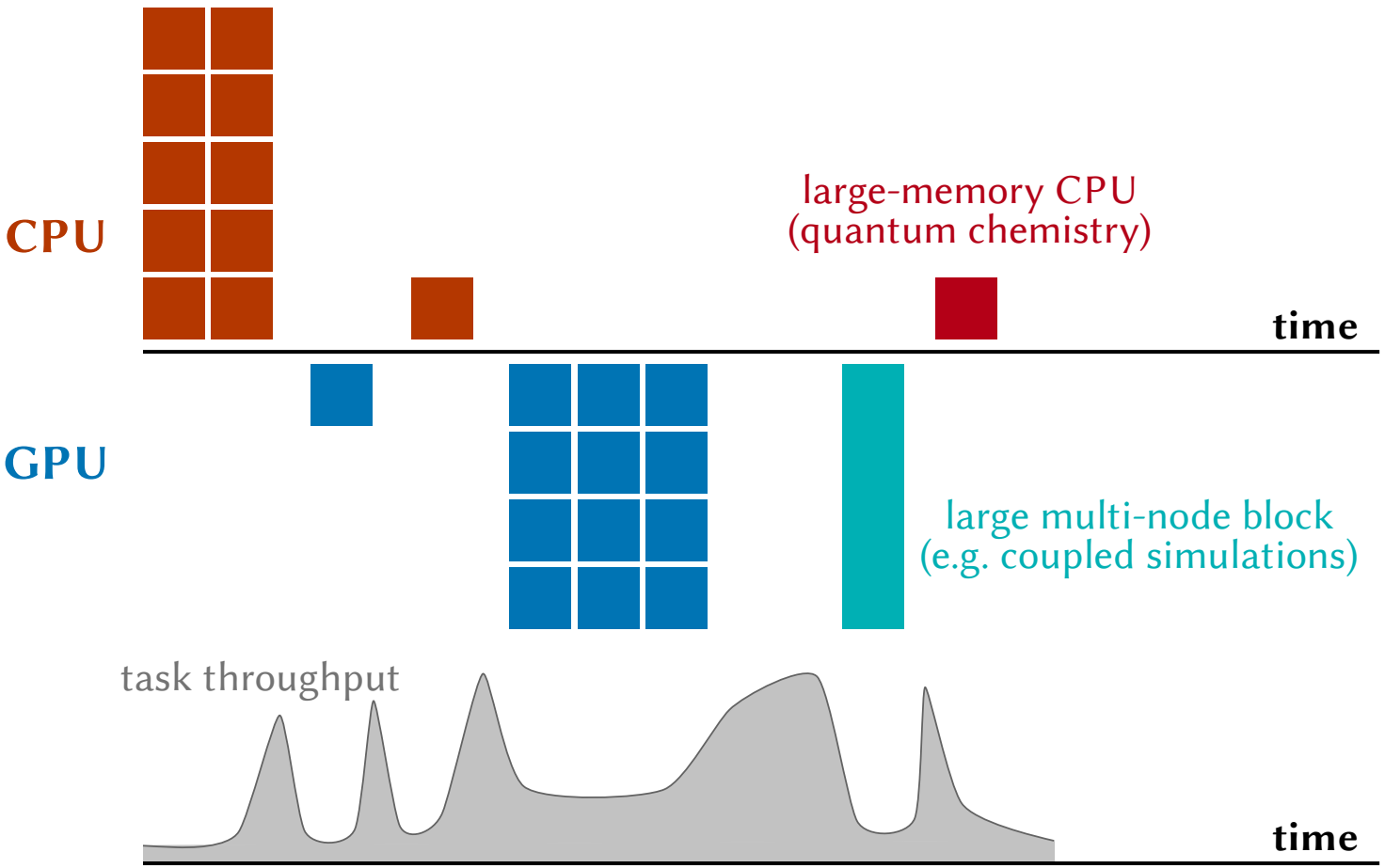

a Parsl-based library for molecular simulation

- **tasks**
  -
  -
- **resources**
  -
  -
- **user**
  -
  -

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  - heavy-lifting tasks with duration $\lesssim$ block walltime | task logs necessary
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  - dependencies? Python + Parsl, QM software, PyTorch (ROCm/CUDA)

How can users create a Parsl `config` if they don't know Parsl?

Force them into a **template** with `yaml` syntax

tasks in scientific workflow can be boiled down to a few 'types'. Let users define the `Provider` for each type.

dynamics **ML training** **QM calculations**

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dynamics ML training QM calculations

```yaml
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  slurm:
    account: "..."
    partition: "gpu"
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ML training

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ModelTraining:
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    account: "..."
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    nodes_per_block: 1
    ...
```

QM calculations

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QM calculations

```yaml
CP2K:
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  slurm:
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    partition: "cpu"
    nodes_per_block: 8
    ...
```

Launchers, Executors? Hardcoded!

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Dependencies? `Apptainer/Singularity` containers!

API: minimal interaction with Futures

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```
potential = MACEHamiltonian.mace_mp0()  # wraps a DataFuture (pytorch model)

walkers = Walker(start, potential, pressure=0).multiply(32)

outputs = sample(walkers, steps=10000)  # returns list of wrapped DataFutures

data = sum([o.trajectory for o in outputs])   # wraps a DataFuture
labeled = data.evaluate(CP2K(...))            # wraps a new DataFuture
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```
error = compute_rmse(   # THIS IS A FUTURE (of a numpy array)
        labeled.get('forces'),
        potential.compute(data, 'forces'),
)
```

github.com/molmod/psiflow