Parallelization of MDAnalysis

Egor Marin, Google Summer of Code contributor

marinegor@fastmail.com

Motivation

- `T(insight) = T(simulation) + T(analysis)`
- `pmda` : 30 ⭐, 21 🍴 (forks)
- all MDAnalysis instances are parallelizable (courtesy @yuxuanzhuang)

Goals

Change `AnalysisBase` in a way that...

1. Introduces multiple job support
   - local -- using multiprocessing?
   - non-local -- using dask?
2. Does not break existing code (subclasses, dependencies, etc)
3. Allows customization
   - add your own execution backend
   - write your own parallelizable classes

Sneak peak: results

```
>>> from MDAnalysis.analysis.rms import RMSD
>>> u, ref = ...

>>> % time long_run = RMSD(u, ref)
Wall time: 4 min

>>> % time long_run = RMSD(u, ref, backend='multiprocessing', n_workers=8)
Wall time: 50 sec
```

Sneak peak: results

```
>>> from MDAnalysis.analysis.rdf import InterRDF
>>> s1, s2 = ...

>>> % time long_run = InterRDF(s1, s2)
Wall time: 1 h

>>> % time long_run = InterRDF(s1, s2, backend='multiprocessing', n_workers=8)
Wall time: 8 min
```

Implementation

General `AnalysisBase.run()` protocol:

```
def run(self,
        start=None,
        stop=None,
        step=None,
        frames=None, ...):

  # prepare frames -- check boundaries, setup reader
  self._setup_frames(self._trajectory, start=start, stop=stop, step=step, frames=frames)

  # initialize attributes with intermediate results
  self._prepare()

  # go through trajectory
  for i, ts in enumerate(self._sliced_trajectory, ...):
    self._single_frame()

  # convert intermediate results into final ones
  self._conclude()
```

Implementation

split-apply-combine:

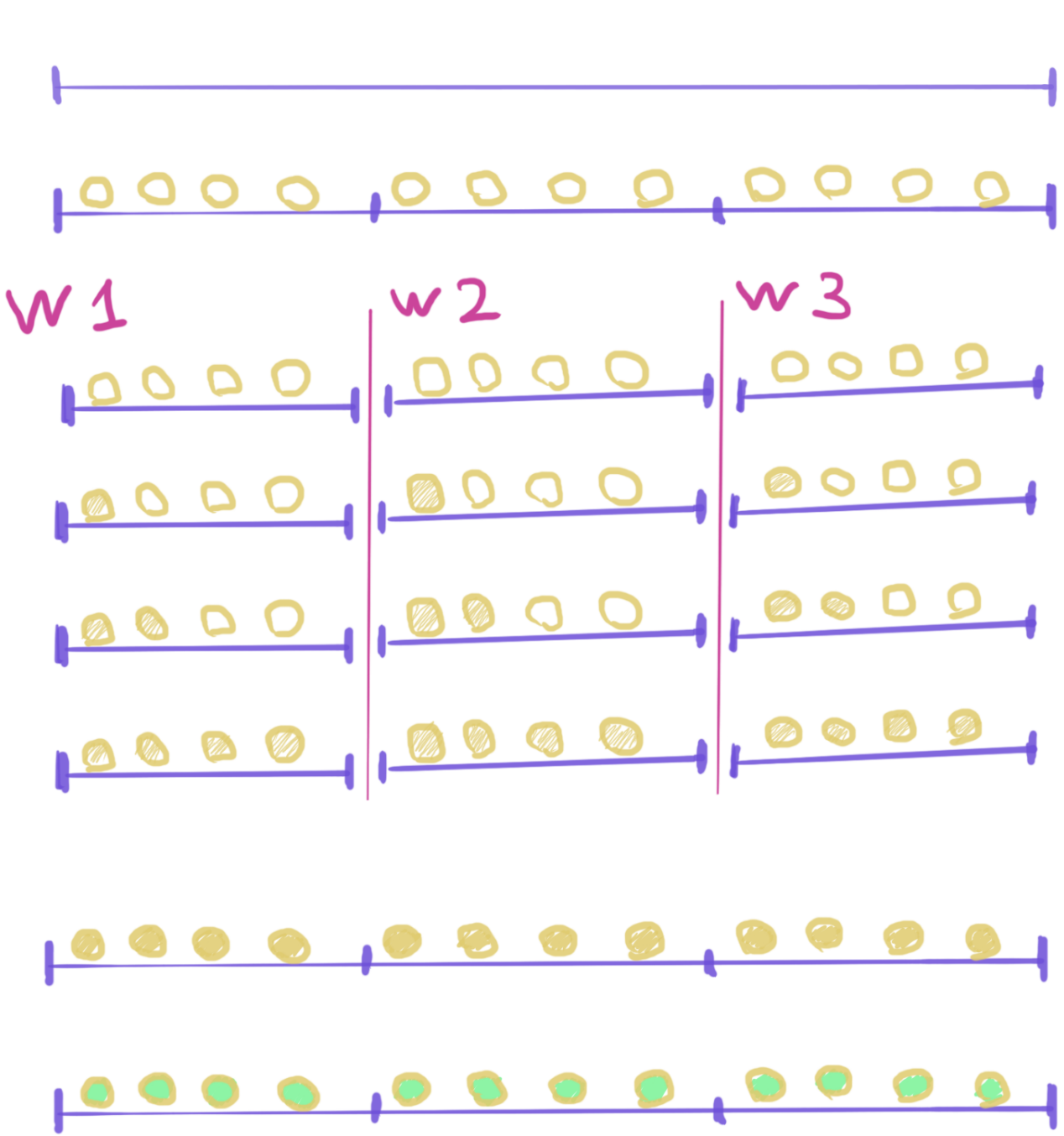
- split all frames into groups
- process each group independently
- combine results

Implementation

Additional methods of `AnalysisBase`:

- "split": `_setup_computation_groups()`
- "apply": `_compute`
- "combine": `_get_aggregator` & `ResultsGroup.merge()`
- housekeeping: `_configure_backend`

Implementation



_setup_frames

_prepare

_setup
_computation
_groups

W1: _compute(gr1)
W2: _compute(gr2)
W3: _compute(gr3)

ResultsGroup
.merge()

_conclude()

Implementation

Additional classes: `ResultsGroup`

```
class ResultsGroup:
  def __init__(self, lookup: dict[str, Callable]): ...
  def merge(self, objects: Sequence[Results],
            require_all_aggregators: bool = True) -> Results:
    ...
```

Implementation

Additional classes: `ResultsGroup`

```
>> from MDAnalysis.analysis.parallel import ResultsGroup, Results
>> group = ResultsGroup(lookup={'mass': lambda values: np.mean(values)}
>> obj1 = Results(mass=1)
>> obj2 = Results(mass=3)
>> group.merge([obj1, obj2])
{'mass': 2.0}
```

Implementation

Additional classes: `ResultsGroup`

```
# skip attributes you don't want to aggregate
>>> lookup = {'mass': ResultsGroup.float_mean, 'trajectory': Trajectory}
>>> group = ResultsGroup(lookup)
>>> objects = [Results(mass=1, trajectory=None), Results(mass=3, trajectory=Trajectory(...))]
>>> group.merge(objects, require_all_aggregators=False)
{'mass': 2.0}
```

Implementation

Additional classes: `BackendBase`

```
from MDAnalysis.parallel import BackendBase

class CustomBackend(BackendBase):
  def __init__(self, some_resource):
    self.some_resource = some_resource

  def apply(self,
            func: Callable[T, R],
            computations: list[T]) -> list[R]:
    results = [
      self.some_resource.do_compute(func, task)
      for task in computations]
    return results
```

Implementation

Additional classes: `BackendBase`

```
>>> backend_instance = CustomBackend(some_resource=...)
>>> my_run = RMSD(u, ref)
>>> my_run.run(backend=backend_instance, unsafe=True)
```

Implementation

Conditions for the `backend=...`

- `Subclass.is_parallelizable() == True`
- `backend: str|BackendBase`
  - if `str`, one of built-in backends (`multiprocessing` / `dask`)
  - if `BackendBase` subclass, explicitly say `unsafe=True`

Add to your subclass

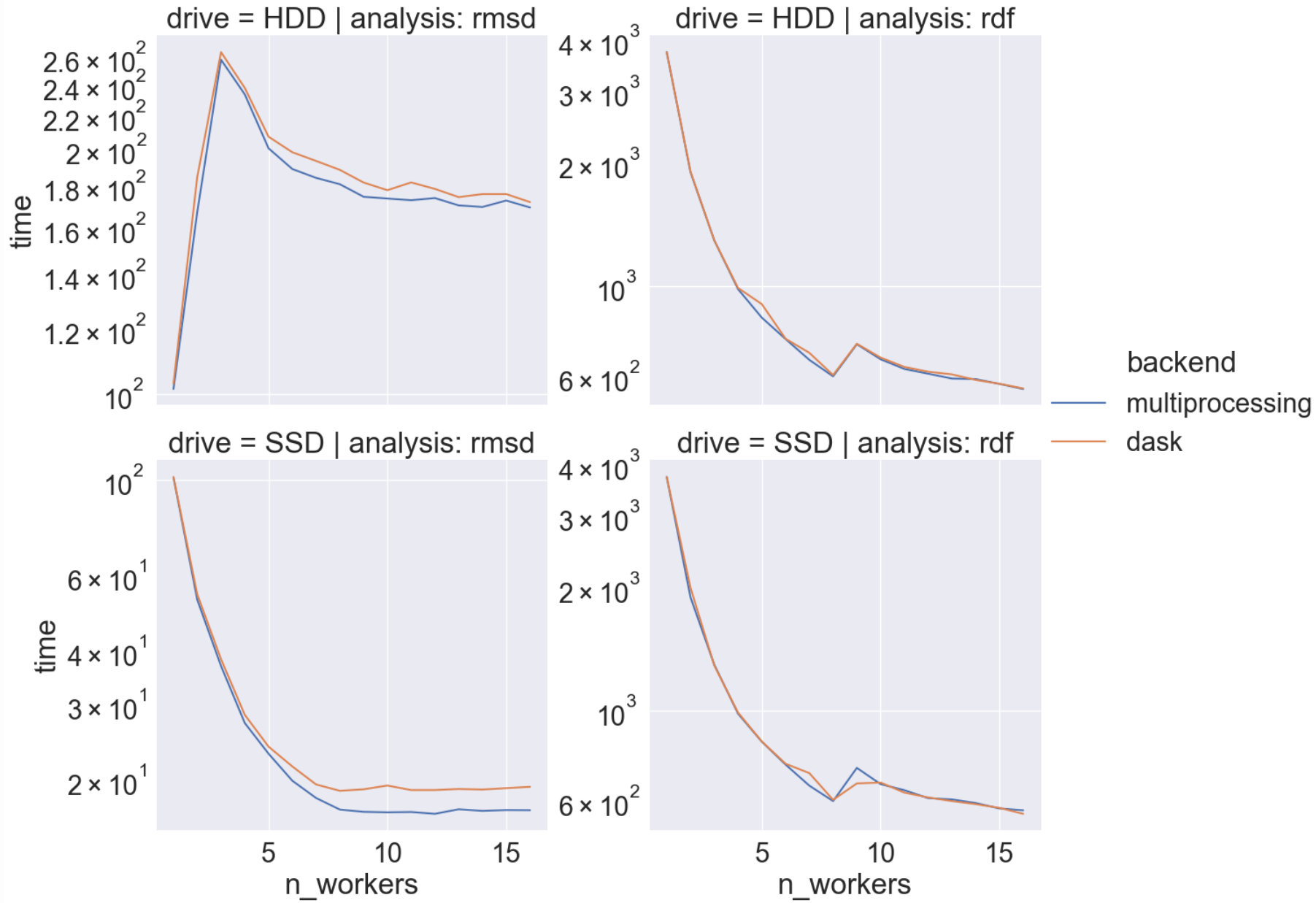
Example: `RMSD`

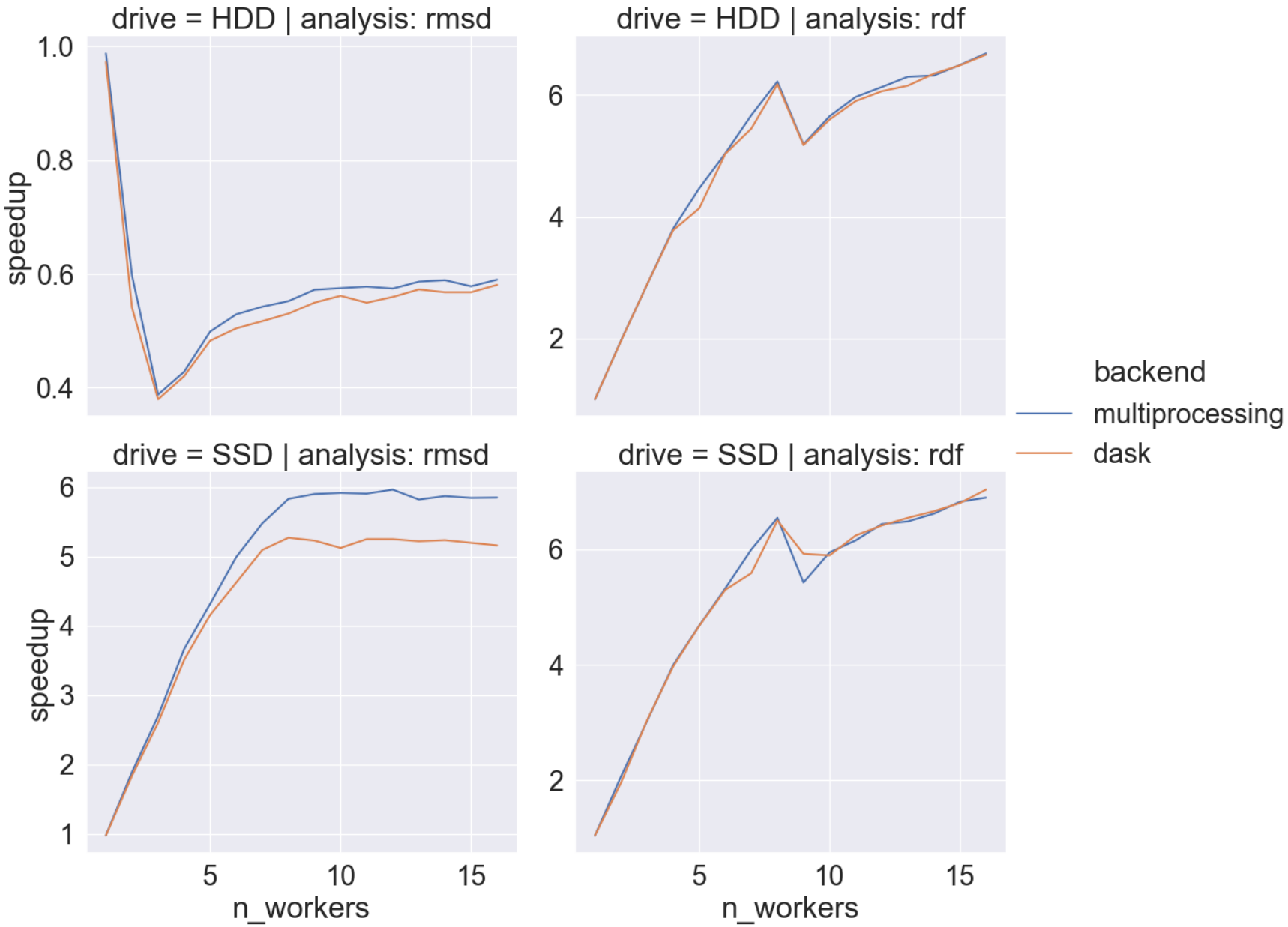
```
from MDAnalysis.analysis.parallel import ResultsGroup

class RMSD(AnalysisBase):
    @classmethod
    @property
    def available_backends(cls):
        return ('serial', 'multiprocessing', 'dask',)

    @classmethod
    @property
    def is_parallelizable(self):
      return True

    def _get_aggregator(self):
      return ResultsGroup(lookup={'rmsd': ResultsGroup.ndarray_vstack})
```

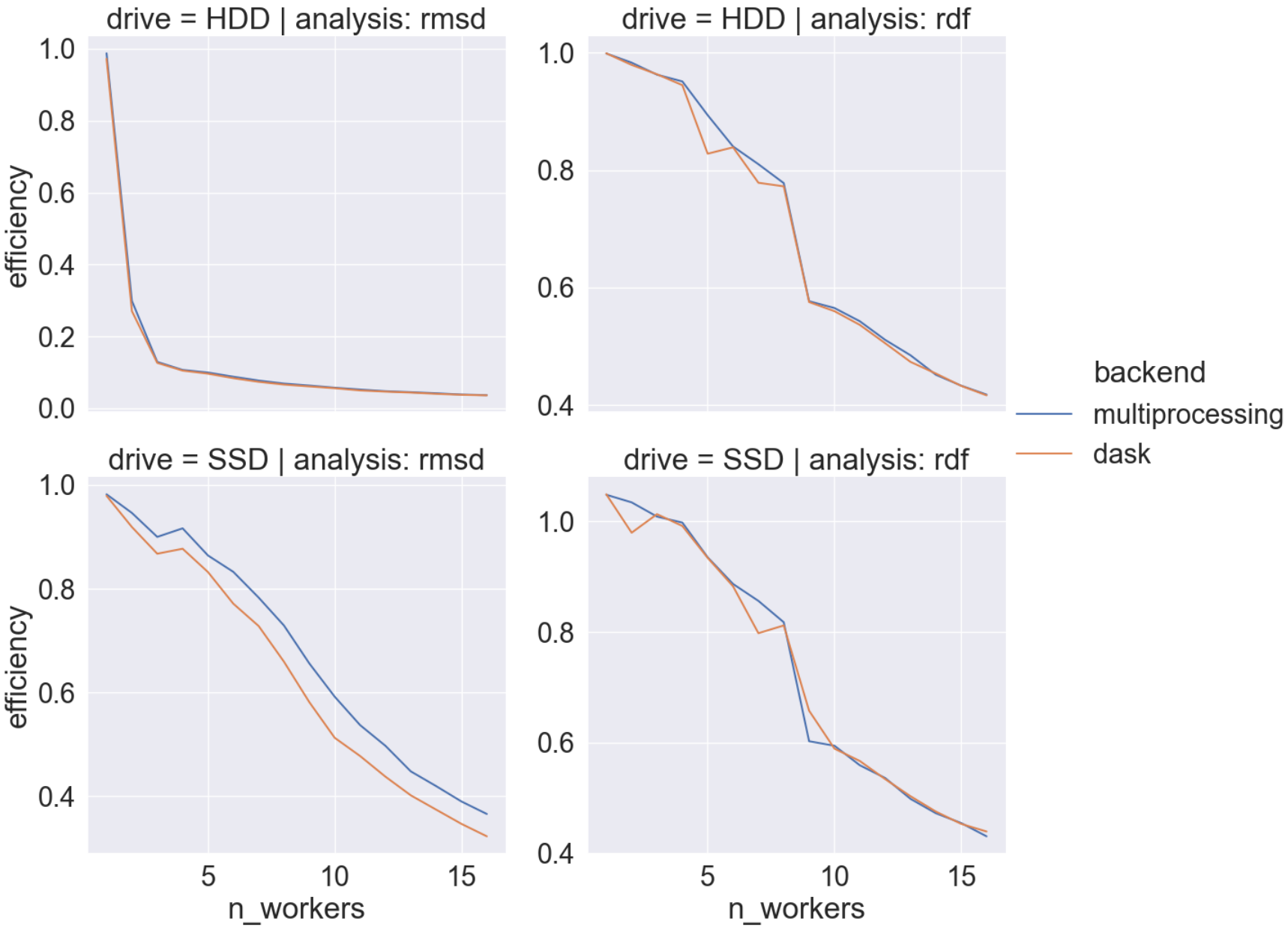
How fast

- full-atom `xtc` ("lysozyme in water")
- two different drives, `hdparm`:
  - HDD: 180 MB/sec
  - SSD: 460 MB/sec
- i9-9900K CPU @ 3.60GHz, 8 cores/socket

How fast


drive = HDD | analysis: rmsd
drive = HDD | analysis: rdf
drive = SSD | analysis: rmsd
drive = SSD | analysis: rdf
time
n_workers
backend
multiprocessing
dask

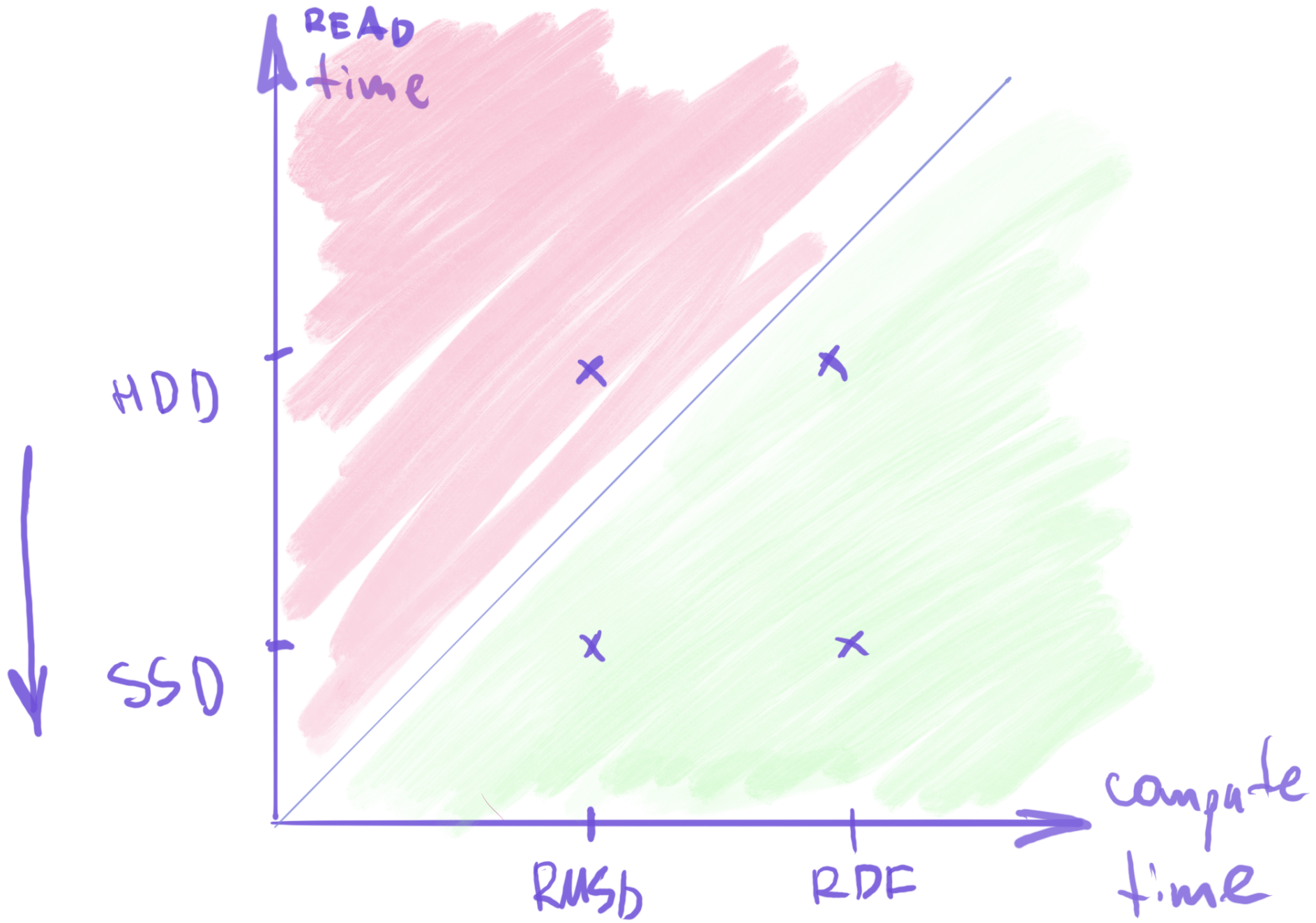

drive = HDD | analysis: rmsd
drive = HDD | analysis: rdf
drive = SSD | analysis: rmsd
drive = SSD | analysis: rdf
speedup
n_workers
backend
multiprocessing
dask


drive = HDD | analysis: rmsd
drive = HDD | analysis: rdf
drive = SSD | analysis: rmsd
drive = SSD | analysis: rdf
efficiency
n_workers
backend
multiprocessing
dask

When should I use it

Definitive answer: benchmark it yourself!

- `%%time` in jupyter notebook
- `step=MANY` or `start=0, stop=10_000` to achieve ~1-2 minute runtime with serial scheduler


READ
time
HDD
SSD
RMSD
RDF
compute
time

When should I use it

- `YourClass.is_parallelizable()` for your class
- `_single_frame()` slower than reading from disk

Future features

- ➡ SOON add to all subclasses
  - have separate issues for complicated ones?
- ➡ SOON add tutorials
  - how to use parallel backends
  - how to implement your own backend subclasses

Future features

- 🤔 add distributed support
  - rebrand `pmda` into MDAKit
  - focus on parallel filesystems, etc
- 🤔 add shareable memory trajectories
  - pre-load trajectory & analyze it
  - efficient for practically all subclasses
- 🤔 add `AnalysisCollection` (ht @PicoCentauri)
  - one frame read exactly once

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