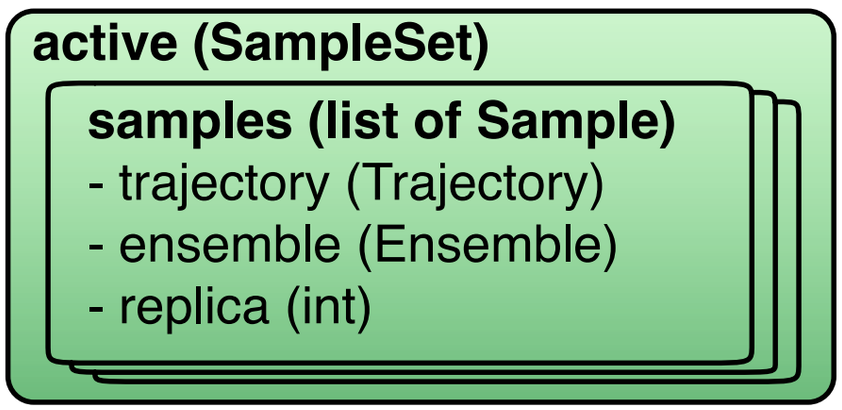
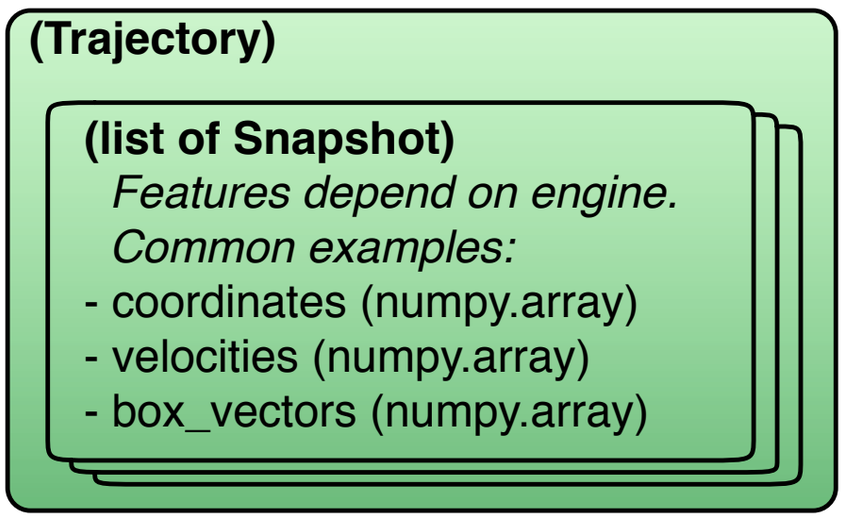
Analyzing *what* you sampled





Other “features”:

- masses
- instantaneous_temperature
- xyz (unitless coordinates)

“active”: state of the system after the step

```
sample = storage.steps[10].active[ensemble]
sample = storage.steps[10].active[0]  # replica ID
```

Analyze trajectory by accessing “features”:

```
# from a snapshot
trajectory[5].coordinates
# for the whole trajectory
trajectory.coordinates
```

Or, convert trajectory to MDTraj:

```
from openpathsampling.engines.openmm.tools \
    import trajectory_to_mdtraj

new_traj = trajectory_to_mdtraj(trajectory)
```

Analyzing *how* you sampled

PathMovers are part of a larger “move decision tree”

The entire progress through that “tree” is tracked with “move changes,” which often have “subchanges”

We also store additional details, which depend on the specific mover