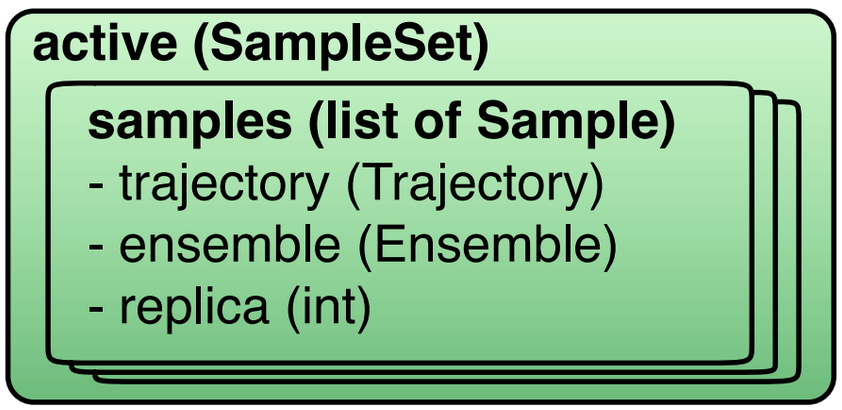
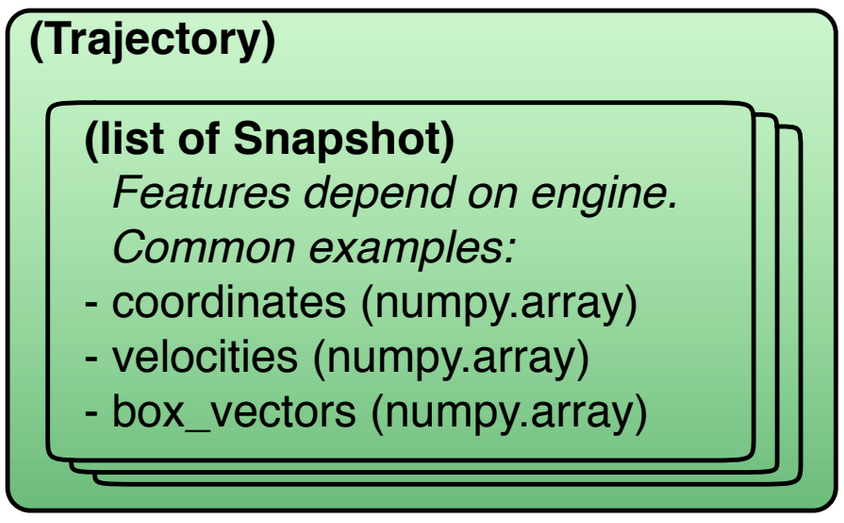
Analyzing *what* you sampled



"active": state of the system after the step

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



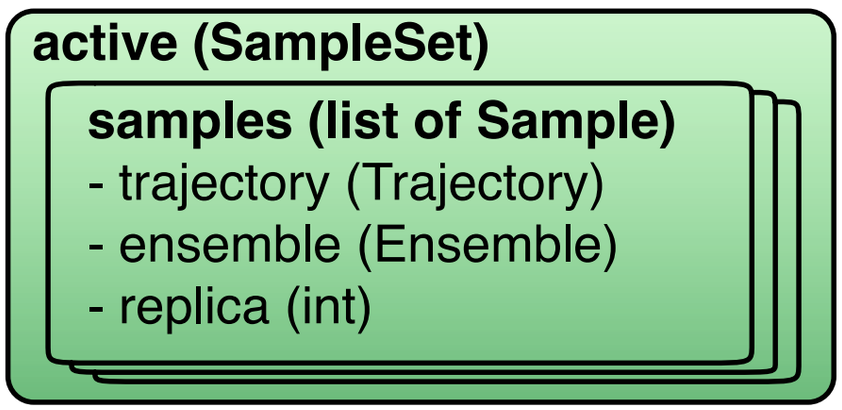
Analyze trajectory by accessing "features":

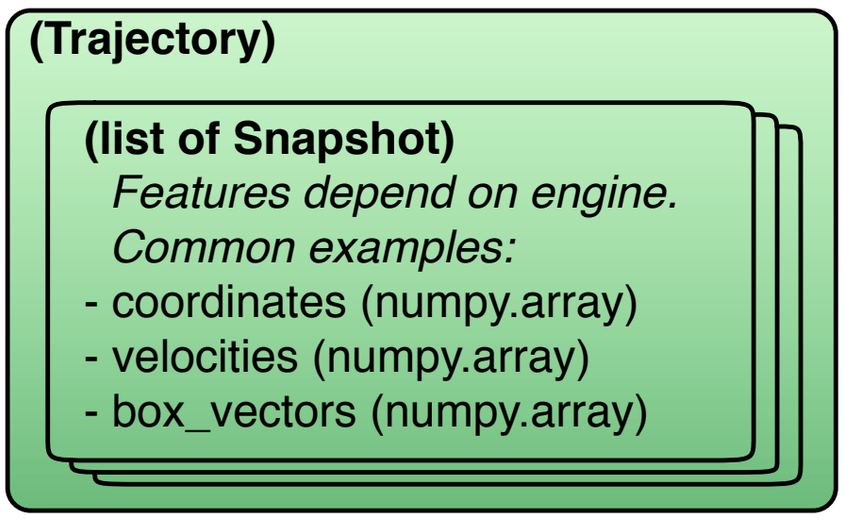
```
# from a snapshot
trajectory[5].coordinates
# for the whole trajectory
trajectory.coordinates
```

Other "features":

- masses
- instantaneous_temperature
- xyz (unitless coordinates)

Analyzing *what* you sampled





Other “features”:

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“active”: state of the system after the step

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```

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)
```