

Analyzing *what* you sampled

active (SampleSet)

samples (list of Sample)

- trajectory (Trajectory)
- ensemble (Ensemble)
- replica (int)

“active”: state of the system after the step

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

(Trajectory)

(list of Snapshot)

Features depend on engine.

Common examples:

- coordinates (numpy.array)
- velocities (numpy.array)
- box_vectors (numpy.array)

Analyze trajectory by accessing “features”:

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

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from a snapshot

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trajectory[5].coordinates
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for the whole trajectory

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trajectory.coordinates
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Other “features”:

- masses
- instantaneous_temperature
- xyz (unitless coordinates)