Simulation Steps

(MCStep)

active (SampleSet)

samples (list of Sample)
- trajectory (Trajectory)
- ensemble (Ensemble)
- replica (int)

change (MoveChange)
- subchanges (list of MoveChange)
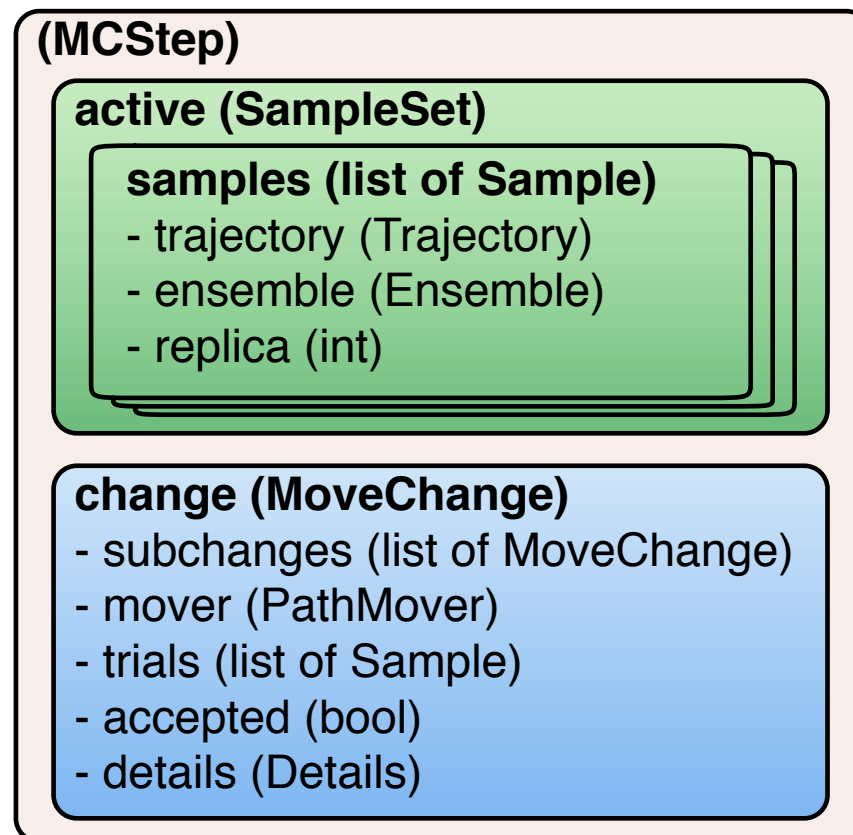- mover (PathMover)
- trials (list of Sample)
- accepted (bool)
- details (Details)

What you sampled

How you sampled it

You usually analyze results by
looping over the steps in a given file.

A list of steps will be the input for
most analysis functions.

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
```