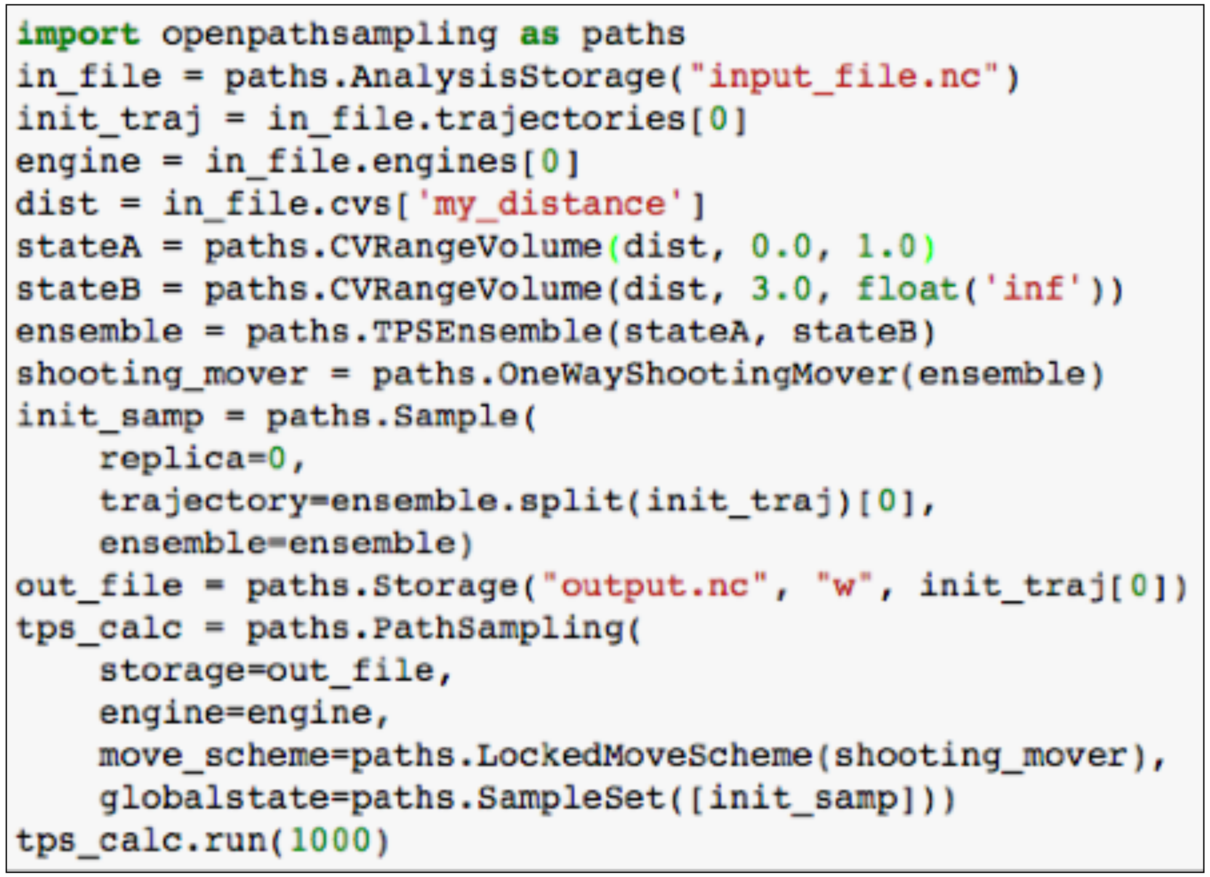
OpenPath Sampling

http://openpathsampling.org

Development at: http://github.org/choderalab/openpathsampling
Part of the Omnia consortium: http://omnia.md

A Python library for path sampling simulations

- ✓ **Easy to use**: Beginners can quickly learn to use it
- ✓ **Easy to extend**: Advanced users can use it to develop new methods
- ✓ **Independent of dynamics engine**: Useful in many fields and to the broadest audience



```python
import openpathsampling as paths
in_file = paths.AnalysisStorage("input_file.nc")
init_traj = in_file.trajectories[0]
engine = in_file.engines[0]
dist = in_file.cvs['my_distance']
stateA = paths.CVRangeVolume(dist, 0.0, 1.0)
stateB = paths.CVRangeVolume(dist, 3.0, float('inf'))
ensemble = paths.TPSEnsemble(stateA, stateB)
shooting_mover = paths.OneWayShootingMover(ensemble)
init_samp = paths.Sample(
    replica=0,
    trajectory=ensemble.split(init_traj)[0],
    ensemble=ensemble)
out_file = paths.Storage("output.nc", "w", init_traj[0])
tps_calc = paths.PathSampling(
    storage=out_file,
    engine=engine,
    move_scheme=paths.LockedMoveScheme(shooting_mover),
    globalstate=paths.SampleSet([init_samp]))
tps_calc.run(1000)
```

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Features

Methods implemented:

- Transition Path Sampling
- Transition Interface Sampling
- Replica Exchange TIS
- Multiple State TIS
- Multiple Interface Set TIS
- Single Replica TIS
- Adaptive Multiple Splitting
- Forward Flux Sampling

Engines supported:

- Toy Dynamics
- OpenMM
- LAMMPS
- Generic external engine

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Version 1.0: coming soon!

Additional features coming
late spring/early summer