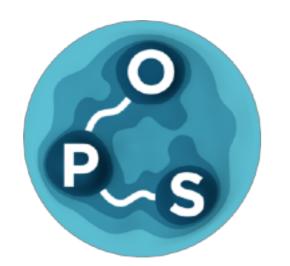
OpenPathSampling



http://openpathsampling.org

Twitter: @pathsampling

Development at: http://github.com/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

```
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)
```

Prinz, DWHS, Bolhuis, Chodera. In prep.

OPS Features

Methods implemented:

- Transition Path Sampling
- Transition Interface Sampling
- Replica Exchange TIS
- Multiple State TIS
- Multiple Interface Set TIS
- Single Replica TIS
- Committor Calculation
- Rates from direct MD

Engines supported:

- Toy Dynamics
- OpenMM
- Gromacs (mostly)
- LAMMPS (mostly)

Analysis tools:

- Rates (TIS)
- Path Densities
- Replica Travel
- Flux Calculation
- Channel analysis

... and much more!







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