

OpenPathSampling



<http://openpathsampling.org>

Twitter: @pathsampling

Development at: <http://github.org/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)
```

DWHS, Prinz, Noé, Bolhuis, Chodera. In prep.

[WIP] LAMMPS support #319



Open jhprinz wants to merge 24 commits into `openpathsampling:master` from `jhprinz:lamps`



Conversation 12

Commits

24



Checks 0



Files changed 7



jhprinz commented on Oct 5, 2015

Member



This is part of future stuff, but I thought to give it a little try. Apparently there is a python API for lammps that could make all of this extremely simple. [LAMMPS Python Docs](#)

So far no luck in installing LAMMPS but I will figure it out eventually...



jhprinz added this to the **Future** milestone on Oct 5, 2015



first lammps engine running

✗ d53d16d



jhprinz commented on Oct 7, 2015

Member



Woohoo... Created an engine today. Seems that it is not so difficult to use our framework at all...

I ran a 1000 steps trajectory of a simple LJ Fluid for testing. Still some subtleties to figure out, but we might interest a lot of people once lammps is supported. Not sure how to really test this since I have so clue on how to properly use lammps... Means we might need someone that has used lammps before.