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. bioRxiv 2018.

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!

Jan-Hendrik Prinz (Keylight GmbH)
Frank Noé (FU Berlin)
John Chodera (MSKCC)
Peter Bolhuis (UvA)