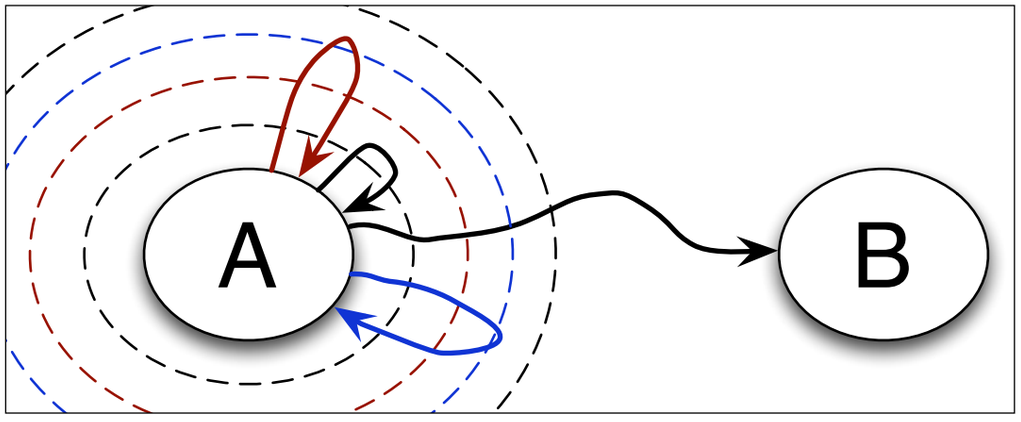
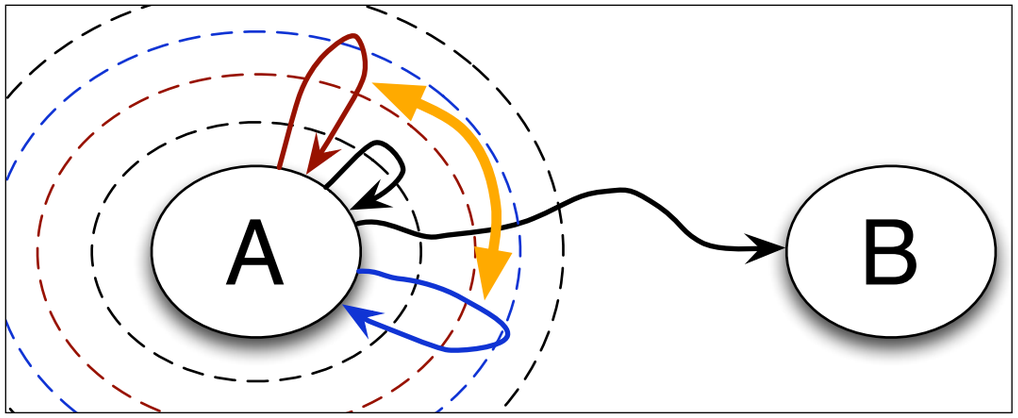
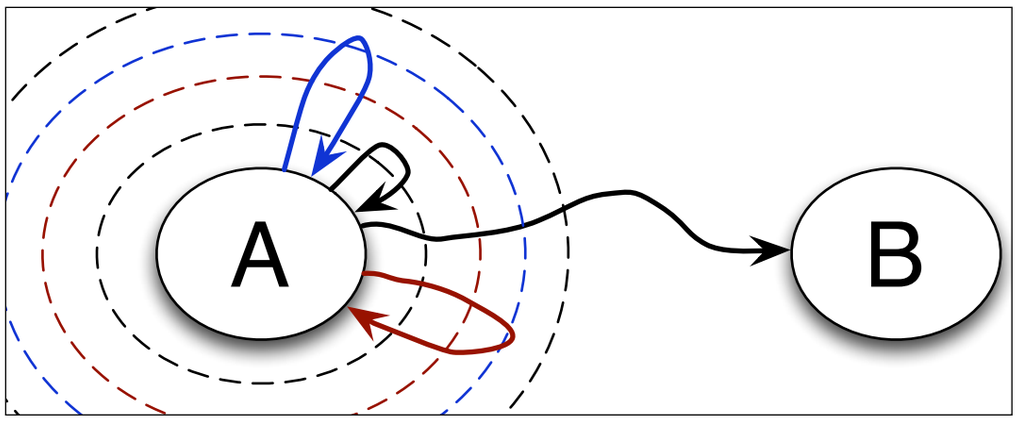
Replica Exchange TIS







Select paths associated with two interfaces. If each path satisfies the ensemble criteria for the other, swap which replica they're associated with.

RETIS allows switching between different reaction channels.

van Erp. PRL **98** 268301 (2007).

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. Submitted.