

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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