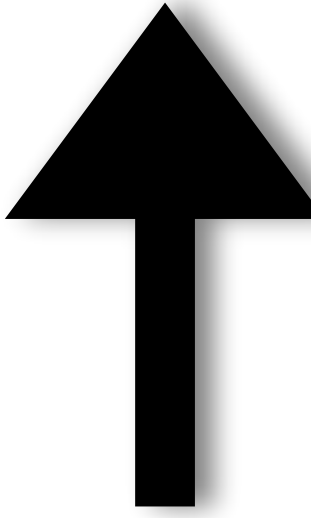
$$\mathcal{O}\left(N_{\mathrm{traj}}\, N_{\mathrm{ens}}\, N_{\mathrm{atom}}\, t\right)$$

Path Sampling:

More parallelization



this means that you sample multiple trajectories simultaneously: another parallelization level!

- TPS: 1 (times independent walkers)
- TIS: 10-100 (times independent walkers)
- Committor: 1000-10000 (or more!)

Coming soon! Running simultaneous trajectories

Simultaneous trajectories for various methods:

More parallelization

Path Sampling: $\mathcal{O}\left(N_{\mathrm{traj}}\, N_{\mathrm{ens}}\, N_{\mathrm{atom}}\, t\right)$

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Simultaneous trajectories for various methods:

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Conclusions

OpenPathSampling inherits its scaling from underlying engines

***Convergence* scales worse than linearly with number of atoms**

Future plans: Run multiple trajectories simultaneously