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- In (MS)TIS, so does number of ensembles, possibly number of trajectories
- Trade-off between number of defined states and trajectory time

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

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Molecular Dynamics:

Path Sampling:

But how long does it take to converge?

Computational Cost

Convergence scaling with number of atoms is unclear

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More parallelization

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

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