Lessons from Benchmarks

- In realistic simulations, the cost of the underlying dynamics dominates OpenPathSampling's performance

- The overhead from OpenPathSampling is less than the variance due to Gromacs's performance tuning

- Only large systems should be run on multiple GPUs with Gromacs

Computational Cost

Molecular Dynamics: $\mathcal{O}\left(N_{\mathrm{atom}}\, t\right)$

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