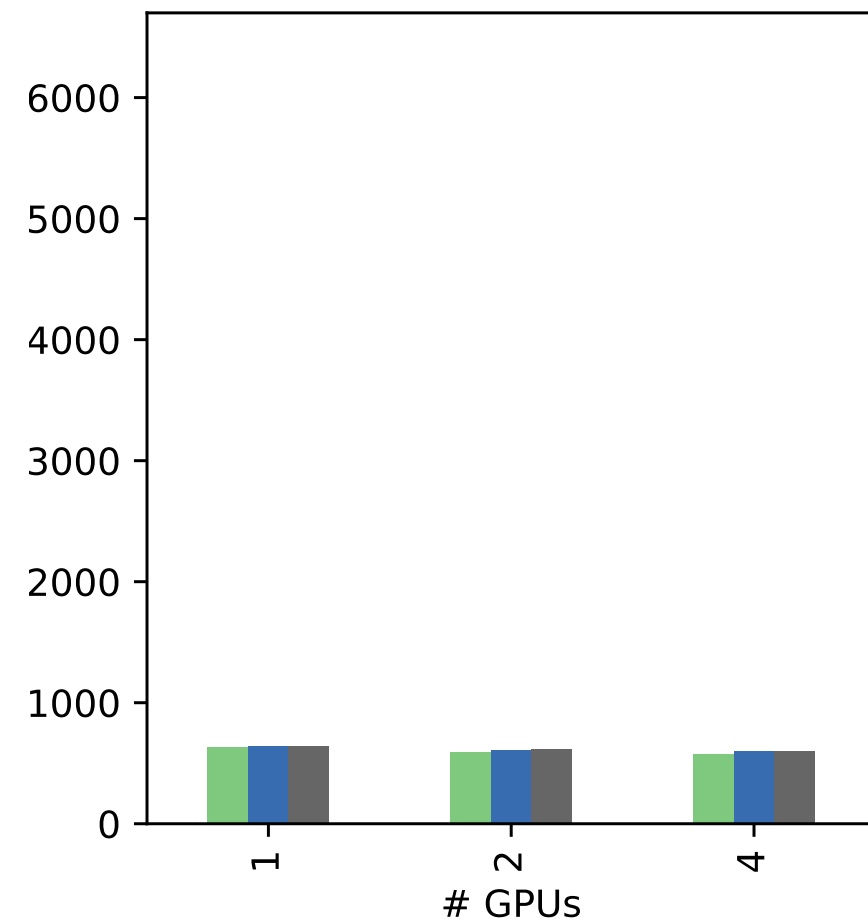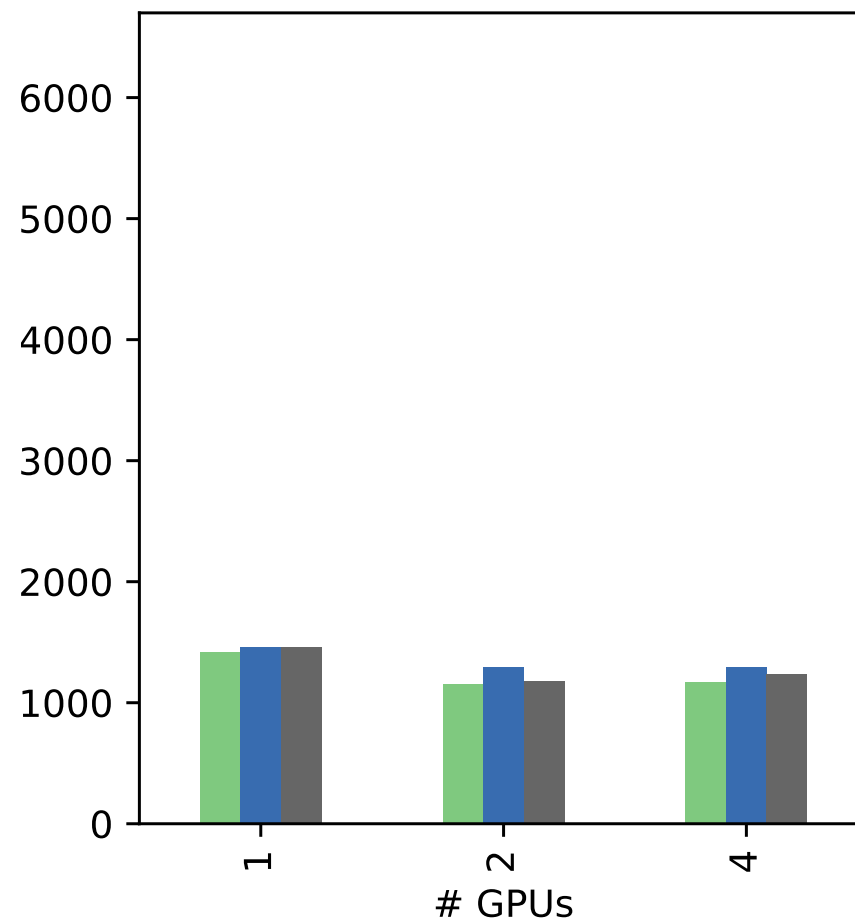# Quick & Dirty Benchmarks
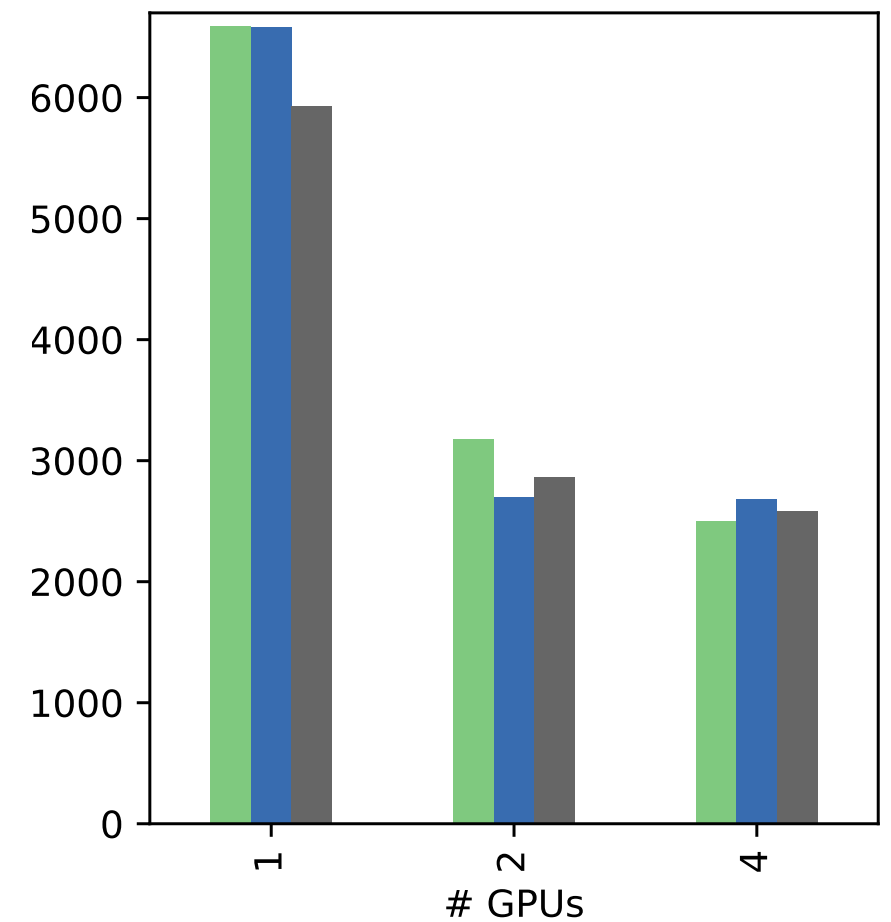

Gas hydrate (12288 atoms) · KRas (22561 atoms) · GSK3B & inhibitor (70996 atoms)

GPUs

Number of atoms matters a lot

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