

Path sampling: What's great

- Enables simulation of timescales not directly accessible
- Unbiased dynamics gives real mechanism, avoids problems of bad bias
- Data, once generated, can be re-analyzed with different CVs (because unbiased)
- Simultaneously obtain information about kinetics and thermodynamics

Path sampling: What's not great

- Still computationally intensive
 - 1000s of trajectories, ~ 10 -100 ns each (better than normal MD!)
 - multiple walker parallelization helps somewhat
- Set-up can be difficult
 - identifying metastable states
 - getting initial trajectory
- No widely-used software for path sampling