

Questions

- What are rare events, and why do we care?
- What is path sampling?
- What is OpenPathSampling (OPS)?
- What are some recent updates in OPS?
- How can your projects interface with OPS?
- What's coming soon?

Answers

- Rare events are ubiquitous in chemistry; any time there is a free energy barrier.
- Path sampling addresses rare events by doing Monte Carlo in trajectory space.
- OpenPathSampling is a modular package for path sampling.
- OPS now has a CLI, as well Gromacs and PLUMED support.
- It is easy to add new MD engines or CVs to OPS, and the CLI is also extensible.
- OPS 2.0 will feature new tools for parallelization and better performance and usability.