

LAMMPS support is **preliminary**

Although the LAMMPS engine for OPS can be used, it doesn't support all the features of other OPS engines. Some things that will help:

- should use integrators where velocities are reported at the same time as positions
- better understanding of the Python interface to LAMMPS (contact with devs?)
- beta testers!

Summary

- Rare events are a difficult, but important, challenge for molecular simulation
- Path sampling is a powerful tool for the study of rare events
- Path sampling gave us insight into why the Q61L mutant of K-Ras causes cancer
- LAMMPS users can use OpenPathSampling to perform path sampling simulations