Conclusions and Status

Replica Exchange Transition Interface Sampling can be parallelized using dask.distributed, a task-based programming framework

Still in development before release:

- Supports toy engine; needs further work to support OpenMM, LAMMPS, Gromacs

- Not fully integrated into the OPS path sampling "main" loop

Challenges we found:

- Serialization is either trivial or very difficult (nothing in between!)

- When the bottleneck is communication, that's always expensive

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