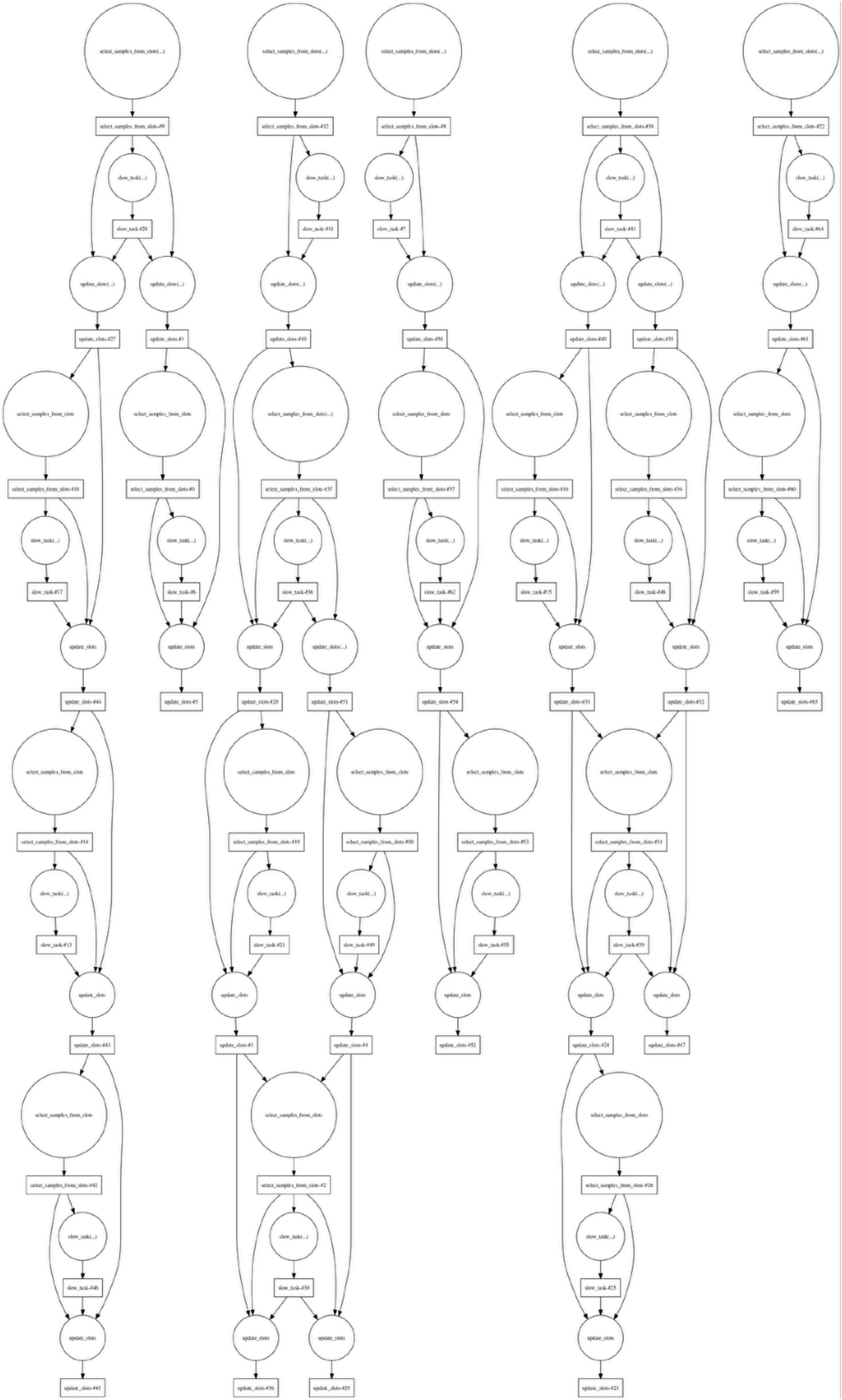


OPS TaskGraph: Full

20 MC moves (shooting and replica exchange)

9 ensembles



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