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Title: LAMMPS/Kokkos/HIPPYNN Sierra Timings

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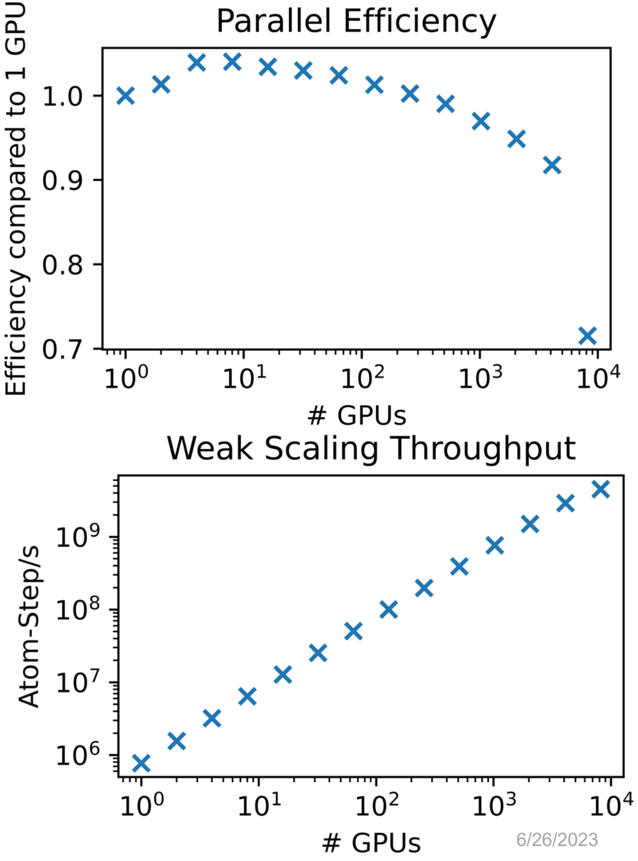
Molecular Dynamics Speeds

- Weak Scaling MD tests were run on an Ionic Liquid system
- Up to 2048 Sierra nodes were used
- The run on 2048 nodes failed when trying to write an output file. Unlike the other MD runs, the 2048 node MD test needed to use the first 750 time steps for timing, which results in poorer apparent performance (includes time associated with instantiating the MLIAP network)
- Otherwise, the code appears to scale well.



MPIIO Write speeds

- These tests attempted to use the MPIIO package for writing trajectory files.
- A ‘run’ without writing any files was compared in execution time to a run of the same length containing a write command.
- The linear scaling of the write time compared to the system size, suggests that MPIIO is not operating correctly.
- Writing a 1 billion atom trajectory frame will consume about 40Gb and tale 4 minutes.