LAMMPS with GPUs

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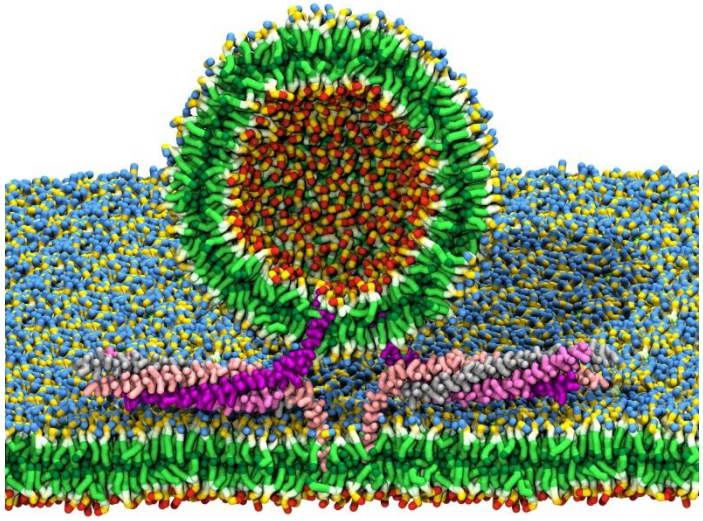
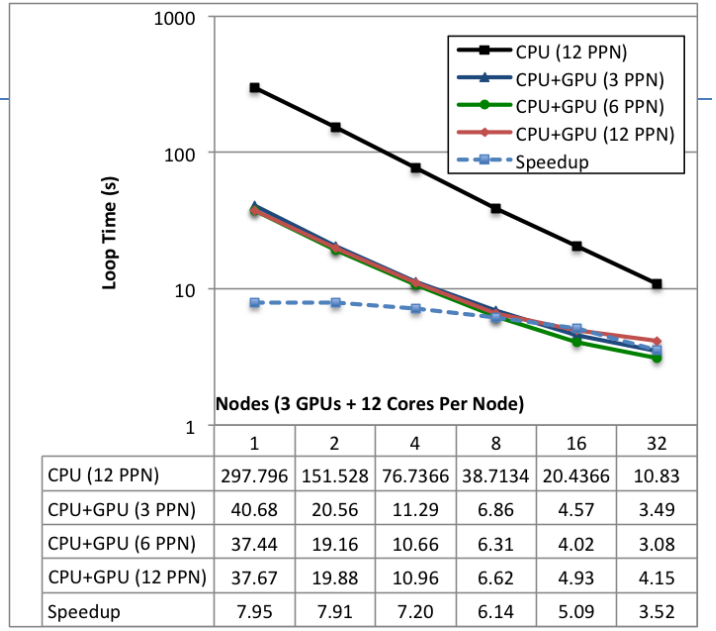
- Parallel Molecular Dynamics
  - http://lammps.sandia.gov
  - Classical Molecular Dynamics
  - Atomic models, Polymers, Metals, Bio-simulations, Coarse-grain (picture), Ellipsoids, etc.
  - Already good strong and weak scaling on CPUs via MPI

- Better performance on fewer nodes => larger problems faster
- Neighbor, non-bonded force, and long-range GPU acceleration
- Allows for CPU/GPU concurrency
- Implementation and benchmarks by W. Michael Brown, NCCS, ORNL





	1	2	4	8	16	32
CPU (12 PPN)	297.796	151.528	76.7366	38.7134	20.4366	10.83
CPU+GPU (3 PPN)	40.68	20.56	11.29	6.86	4.57	3.49
CPU+GPU (6 PPN)	37.44	19.16	10.66	6.31	4.02	3.08
CPU+GPU (12 PPN)	37.67	19.88	10.96	6.62	4.93	4.15
Speedup	7.95	7.91	7.20	6.14	5.09	3.52