Molecular Dynamics Studies on QueenBee

UPDATED BENCHMARKS ON QB2 Dec 2014

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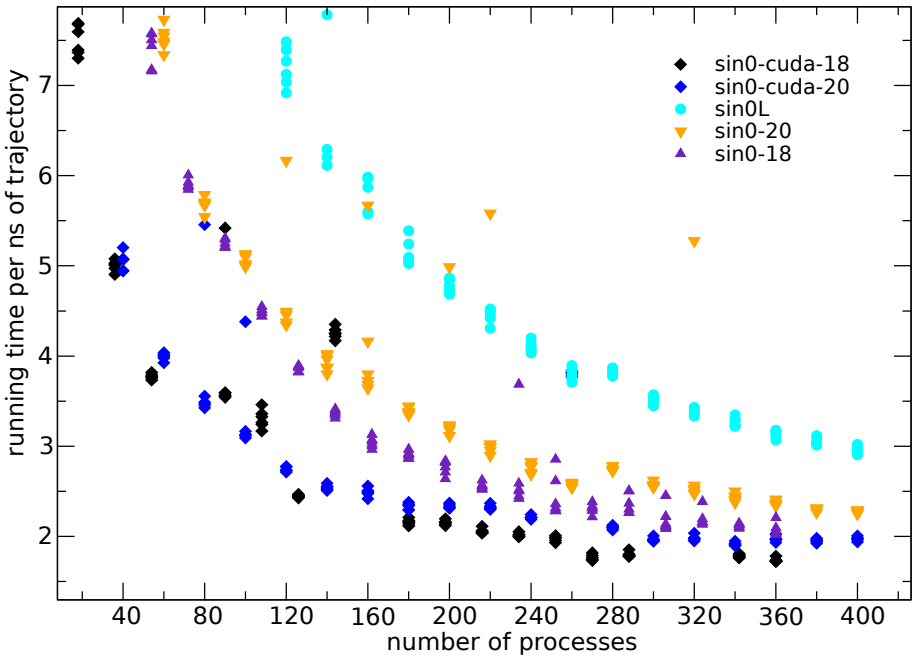

The figure above shows updated benchmarks for NAMD 2.10 running on QB2 using our "sin0" system (387,079 atoms). This system is nearly identical to the proposed simulations in both number of atoms, physical dimensions, and molecular contents. All benchmarks utilized NAMD2.10 with PME for long range electrostatics. The labels are such that "cuda" indicates GPU acceleration was utilized. The designation 18 or 20 indicates how many processes per node (20 core/node) were used for NAMD. Leaving one core per CPU inactive increases performance for NAMD when more than approximately 100 cores are utilized. The inactive core is free to handle communications. Sin0L is similar to sin0-20 but utilized a longer cut-off (12A vs 9A) for the direct summation electrostatics.

In summary NAMD2.10 cuda with one processor per CPU inactive allows us to achieve a throughput of more than 11ns per day per system with 180 processors (10 nodes and 432SU/ns) or 126 processors processors (7 nodes and 342SU/ns) is more efficient but falls short of our target of 10ns/day throughput.