

CPU-Performance scaling of the gromacs

Fully atomistic molecular dynamics (MD) trajectories will be generated with the GROMACS 5.0.6 MD computational packages.¹ . The software is open-source and is readily available (along with instructions and manual) in <http://www.gromacs.org>

The codes are industry standard, highly scalable programs on the number of average requested processors (16-128 cpus). The codes make extensive use of SIMD instruction sets, optimized interprocessor communication schemes using threading, and accurate single precision numerical techniques. Simulations will be performed in the *NPT* ensembles.

GROMACS scales quite favorably in parallel environments using both MPI and thread-based communications.^{1,2} Benchmark calculations were performed in a supercomputer with 1024 compute nodes and 64 I/O nodes. Each compute node contains two 8-core 2.6 GHz Intel EM64T Xeon E5 (Sandy Bridge) processors and 64 GB of DDR3-1333 memory. The I/O nodes each contain two 6-core 2.67 GHz Intel X5650 (Westmere) processors, 48 GB of DDR3-1333 memory, and sixteen 300 GB Intel 710 solid state drives. The network topology is a 4x4x4 3D torus with adjacent switches connected by three 4x QDR InfiniBand links (120 Gb/s). Compute nodes (16 per switch) and I/O nodes (1 per switch) are connected to the switches by 4x QDR (40 Gb/s).

Molecular dynamics simulation was performed in gromacs 5.0.6 with a 2 fs time-integration step on a representative system (see figure 1) comprising a lipid bilayer of 128 DPPG lipid molecules, 9 copies of β -peptides and 7000 water molecules (total number of particles 39000). As can be seen in Fig. 2, GROMACS has near ideal scaling up to 64 processors and excellent speed enhancement unto 128 processors.

TABLE I. Benchmark of Gromacs5.0.6 as provided by TCIS

number of cores	ns/day
16	17.853
32	29.869
64	59.243
128	109.974

¹ B. Hess, C. Kutzner, D. van der Spoel, and E. Lindahl, J. Chem. Theory Comput. **4**, 435 (2008).

² F. Affinito, A. Emerson, L. Litov, P. Petkov, R. A. L. Axner, B. Hess, E. Landahl, and M. F. Iozzi, "Performance analysis and petascaling enabling of gromacs," (2010).

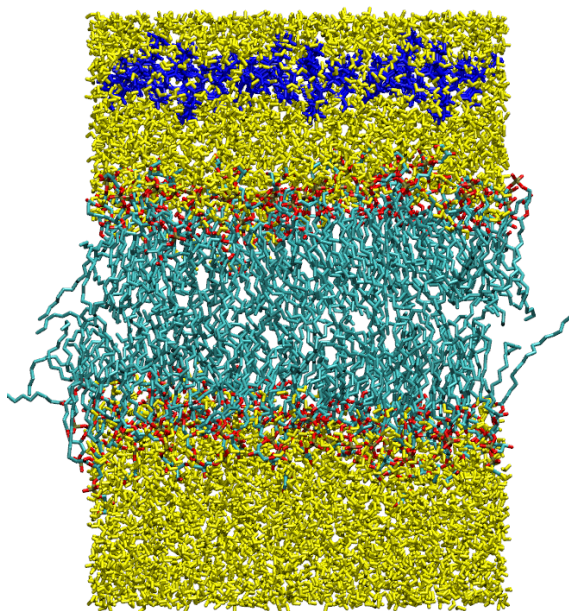


FIG. 1. Representative snapshots of a system of 9 copies of β -peptides and DPPG lipid bilayer and water (39,000 particles) The benchmark for this system were obtained in gordon using 2 fs time-integration time steps.

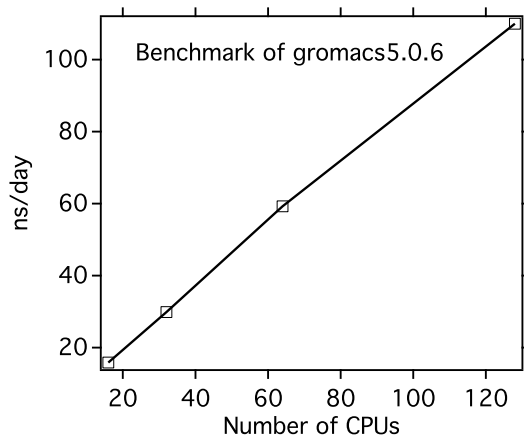


FIG. 2. Top: Computational speedup up to 128 processors for a system of 9 copies of β -peptides and DPPG lipid bilayer and water (39,000 particles) The benchmark were obtained in gordon using 2 fs time-integration time steps.