MD Benchmark studies using Gromacs on the Biblioteca Alexandrina Cluster

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We used Biblioteca Alexandrina, Sun Microsystems cluster, which has 130 eight-core compute nodes, each node equipped with 2 quad-core sockets of Intel Quad Xeon E5440 @ 2.83GHz to benchmark the scaling of Gromacs on a 200,000 atom-system. A more detailed description of the BA HPC facility can be found in: http://eniac.cyi.ac.cy/.

Molecular Dynamics simulations were carried out by using Gromacs 4.5.5 packages in double precision. The heterodimer PI3K alpha with 21806 atoms was solved in 57318 TIP3P water. The total number of the atoms in this system is 193761. The AMBER99SB-ILDN force field was used to model the protein interactions. The temperature was kept constant at 310 K, using the Nose-Hoover thermostat with a relaxation time of 1.0 ps. The pressure of the system was isotropically coupled and maintained at 1 bar using the Parrinello-Rahman barostat with a time constant of 5 ps and a compressibility of 4.5x 10^{-5} bar^{-1}. The nonbonded potential energy functions were cut off and shifted at 10 Å, with forces smoothly decaying between 8 and 10 Å. The particle-mesh Ewald method (PME) was employed to calculate long-range electrostatic interactions with a grid spacing of 0.11 nm. The simulations were run using a 2-fs integration time step and a total number of 1000 time steps.

Simulations were performed by 8, 16, 32, 64, 80, 88, 96, 104, 112, 120 and 128 cores. The results from our study are presented in the following. Output/input files, etc, are available upon request.

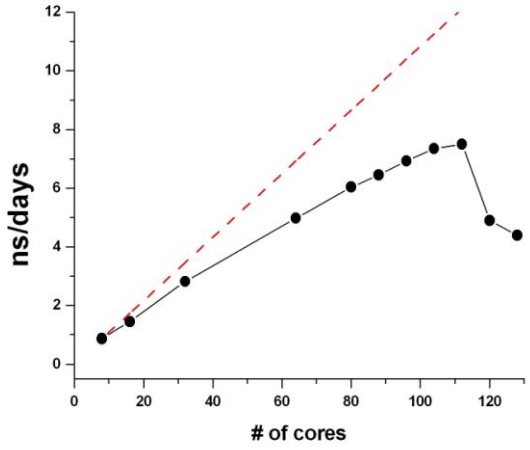

Figure: GROMACS performance on the BA_cluster. The red line represents the ideal scaling and the black line our scaling results.

Table. *Performance of Gromacs on the BA_cluster*

# of cores	8	16	32	64	80	88	96	104	112	120	128
ns/day	0.866	1.443	2.817	4.976	6.039	6.451	6.927	7.357	7.51	4.902	4.39

Our results show that the MD calculation performance increases almost linearly with increasing core number 8 - 112. The performance is decreased when using more than 120 cores.