

GROMACS Benchmark

1. Compilation of GROMACS 4.6.3

- Visit: <http://www.gromacs.org/Downloads> for download of GROMACS 4.6.3.
- Specify the operating system (version number) on which GROMACS 4.6.3 will be compiled.
- Specify environmental variables used during the start and/or process of compilation.
- Specify all options used with every command used in compilation.
- Specify the cmake version used (CMAKE version 2.8.11.x is required)
- Specify the libraries and compilers with respective version numbers used for compilation. (Any additional options used also should be mentioned).
- Examples of libraries and compilers (Intel MKL Math library, FFTW library, openMPI, Intel compilers)

Important: mdrun executables (created from compilation) for running benchmarks for each run should be double precision.

2. Benchmarks should be done using CPU cores and software on the proposed solution:

Information and instructions:

- Benchmark system contains DPPC + water = 121856 atoms.
- A twin-range group based cut-off is used, 1.8 nm for electrostatics and 1.0 nm for Lennard-Jones interactions.
- Input files can be downloaded from:
http://www.gromacs.org/About_Gromacs/Benchmarks (DPPC zip file contains 3 input files)
- To run simulation runs: first change the value of nsteps in .mdp input file to 150000
- No other change in input files are permitted.
- Please provide the output files for each simulation run.
- Using the information from your output files of each simulation run, complete the following table:

3. You have to provide following information in addition to whatever asked in EOI

Number of Nodes	CPU cores	Number of nanoseconds/day	TFlops
1			
2			
4			
8			
16			
32			
50			

For any clarification regarding GROMACS benchmarking, the bidders are advised to contact

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