

GROMACS Best Practices for Intel® Cluster Ready



BEST PRACTICES

1. Introduction

The following best practices document is provided as courtesy of the HPC Advisory Council.

2. Application Description

GROMACS stands for GROMACS (GROningen Machine for Chemical Simulation). It is a molecular dynamics simulation package, primarily designed for biochemical molecules like proteins, lipids and nucleic acids. Many algorithmic optimizations have been introduced in the code. It is extremely fast at calculating the nonbonded interactions. There is ongoing development to extend GROMACS with interfaces to Quantum Chemistry and Bioinformatics/databases. GROMACS is an open source software released under the GPL.

3. Version Information

The version of GROMACS being used is: 4.5.4

4. Prerequisites

The instructions from this best practice have been tested with the following configuration:

Hardware Used:

The instructions from this best practice have been tested on the HPC Advisory Council, Dell PowerEdge M610 blade server based cluster.

- Dell PowerEdge M610 38-node cluster
- Intel Xeon X5670 CPUs @ 2.93 MHz, Intel Xeon X5675 CPUs @ 3.06 MHz
- Memory: 24GB per node @ 1333MHz
- Mellanox ConnectX-2 QDR InfiniBand Adapters
- Mellanox QDR InfiniBand Switch

Software Used:

- Intel® Cluster Ready running RHEL 5.5
- Mellanox OFED 1.5.2 InfiniBand Software Stack
- Compilers: Intel Composer XE 2011 for Linux
- Math Libraries: MKL 10.3 Update 5
- MPI: Intel MPI 4 Update 2, Open MPI 1.5.4 with KNEM 0.9.7, Platform MPI 8.1.1

- Application: GROMACS 4.5.4
- Benchmark workload: Kinesin Dimer docked to the MicroTubule (309,453 atoms, 20000 steps, 80.0 ps)

5. Getting GROMACS

You can download GROMACS at:

<http://www.gromacs.org/Downloads>

Download the list of tests for GROMACS from:

<http://www.gromacs.org/Downloads/Test-Set>

http://www.gromacs.org/About_Gromacs/Benchmarks

After downloading the GROMACS source code and test dataset, extract them in a directory:

```
$ cd ~
```

```
$ tar xzf gromacs-4.5.4.tar.gz
```

Instructions for building GROMACS and additional guidelines are located on the GROMACS website:

http://www.gromacs.org/Downloads/Installation_Instructions

6. Compile using Make

```
$ cd gromacs-4.5.4
```

```
$ ../configure --enable-sse --enable-mpi --with-fft=mkl
```

```
$ mkdir config-dir
```

```
$ cd config-dir
```

```
$ ../configure --enable-mpi --with-fft=mkl CC=icc F77=ifort CXX=icpc
```

```
$ make -j 4
```

You can modify the Makefile for the optimization CFLAGS flag for GROMACS. Such as using "-xSSE4.2".

7. Running GROMACS

There is a load distribution (for example: `-dlb yes -dd 16 8 1 -npme 64`). The `-npme` specifies the number of PME nodes. The `-dd` parameter specifies the grid configuration. When you multiply these numbers, you get the number of non-PME nodes.

Running with Intel MPI

```
$ mpdboot --parallel-startup -r ssh -f <PATH_TO_
HOSTFILE> -n 16

$ mpiexec -ppn 12 -np 192 -IB <GROMACS_ROOT>/
build-4.5.4-intel-ompi/src/kernel/mdrun_mpi -dd 16 8 1
-npme 64 -dlb yes -s topology.tpr

$ mpdallexit
```

Running with Platform MPI

```
$ mpirun -np 192 -IBV -prot -hostfile <PATH_TO_
HOSTFILE> <GROMACS_ROOT>/build-4.5.4-intel-
pmpi/src/kernel/mdrun_mpi -dd 16 8 1 -npme 64 -dlb
yes -s topology.tpr
```

Running with Open MPI

```
$ mpirun -np 192 -hostfile <PATH_TO_HOSTFILE>
-mca btl self,sm,openib -mca btl_sm_use_knem 1
-mca mpi_paffinity_alone 1 <GROMACS_ROOT>/
build-4.5.4-intel-ompi/src/kernel/mdrun_mpi -dd 16 8 1
-npme 64 -dlb yes -s topology.tpr
```

