GROMACS on HPC Systems

Description of the LRZ specific usage of GROMACS on the Linux Cluster HPC Systems.

Introductory Remarks

What is GROMACS?

GROMACS is a versatile package to perform molecular dynamics, i.e. simulate the Newtonian equations of motion for systems with hundreds to millions of particles.

It is primarily designed for biochemical molecules like proteins and lipids that have a lot of complicated bonded interactions, but since GROMACS is extremely fast at calculating the nonbonded interactions (that usually dominate simulations) many groups are also using it for research on non-biological systems, e.g. polymers.

GROMACS is licensed and redistributed under the GPL.

Please consult the GROMACS web site for further information on this package.

The xdrfile library facility for I/O to xtc, edr and trr files is also available.

Authors

GROMACS was first developed in Herman Berendsens group, department of Biophysical Chemistry of Groningen University. It is a team effort, with contributions from several current and former developers all over world.

Available Versions at LRZ

Use module avail gromacs to find the available versions of GROMACS installations at LRZ including the default versions.

Please consult the example batch scripts below for how to use the MPI parallel versions. The single precision builds typically show larger numerical instabilities than the double precision builds. Furthermore, the GROMACS executables always have the same name (no additional _d suffix for the double precision version) with exception of the MPI parallel mdrun_xxx binaries.

Please note:

Starting with version 5.0 all Gromacs executables are collected in the ‘gmx’ utility (see http://manual.gromacs.org/programs/byname.html)

Usage

Access to the binaries, libraries, and data files are provided through the gromacs module. This module sets up environmental variables which point to these locations and updates the required paths.

module load gromacs

- On all systems, the single precision version will be loaded by default. To use the double precision builds, please issue e.g.,
  module load gromacs/5.1d
  (the version number with the attached "d" indicates double precision).
- You can list the names of the available gromacs modules using: module avail gromacs
- Note that in the GROMACS path there are automatic shell completion files available (completion.$SHELL) which add all GROMACS file extensions if you source them into your shell.

Setting up batch jobs

Gromacs on the Linux Cluster systems:

For long production runs, a SLURM batch job should be used to run the program. The example batch scripts provided in this section require the input files speptide.top, after_pr.gro and full.mdp, all contained in the example archive, to be placed in ~/mydir before the run.

Further notes:

- to run in batch mode, submit the script using the sbatch command. To run small test cases interactively, first log in to SLURM cells and reserve the needed resources.
- for batch jobs, the nice switch is set to 0 for mdrun. Please omit this switch when running interactively, otherwise your job will be forcibly removed from the system after some time.
- please do not forget to replace the dummy e-Mail address and the input folder ‘mydirctory’ in the example scripts by your own.
Gromacs on SuperMUC:

A LoadLeveler job script must be generated and submitted. An example is given at the end of the table below.

<table>
<thead>
<tr>
<th>Linux-Cluster with SLURM</th>
<th>SuperMUC Phase2 with Loadleveler</th>
</tr>
</thead>
<tbody>
<tr>
<td>gromacs/4.6</td>
<td>gromacs/5.1</td>
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```bash
#!/bin/bash
#SBATCH -o /home/cluster/<group>/<user>/mydir/gromacs.%j.out
#SBATCH -D /home/cluster/<group>/<user>/mydir
#SBATCH --job-name
#SBATCH --get-user-env
#SBATCH --clusters=mpp1
#SBATCH --ntasks=32
#SBATCH --mail-type=end
#SBATCH --mail-user=<email_address>@<domain>
#SBATCH --export=NONE
#SBATCH --time=24:00:00
source /etc/profile.d/modules.sh
cd mydirectory
module load gromacs/4.6

#generate .tpr file
grompp -v -f full -o full -c after_pr -p speptide

# start mdrun
mdrun -v -nice 0 -s full -e full -o full -c after_full -g flog
# or
srun_ps -n 64 $(which mdrun_mpi) -s inputfile.tpr -resethway
```

```bash
#!/bin/bash
#SBATCH -o /home/cluster/<group>/<user>/mydir/gromacs.%j.out
#SBATCH -D /home/cluster/<group>/<user>/mydir
#SBATCH --job-name
#SBATCH --get-user-env
#SBATCH --clusters=mpp1
#SBATCH --ntasks=32
#SBATCH --mail-type=end
#SBATCH --mail-user=<email_address>@<domain>
#SBATCH --export=NONE
#SBATCH --time=24:00:00
source /etc/profile.d/modules.sh
cd mydirectory
module load gromacs/5.1

# to use grompp on the command line
# gmx grompp ...

# start mdrun with the 5.1 gmx executable
mpiexec -n 56 gmx mdrun -s input_file.tpr -mconfout -resethway
```

Documentation

After loading the environment module, the `$GROMACS_DOC` variable points to a directory containing documentation and tutorials.

For further information (including the man pages for all GROMACS subcommands), please refer to the GROMACS web site.