About

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, lipids and nucleic acids 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.

More information: [http://www.gromacs.org](http://www.gromacs.org)

Using Gromacs on Magnus/Galaxy and Zeus

Gromacs is compiled with GNU programming environment on Magnus/Galaxy and Zeus.

To use Gromacs on Magnus/Galaxy load an appropriate module:

```
$ module swap PrgEnv-cray PrgEnv-gnu
$ module load gromacs
```

To use Gromacs on Zeus load an appropriate module:

```
$ module load gromacs
```

Note that for most modules both the single and double precision of GROMACS has been installed. The double precision executables have the default _d suffix, e.g. "mdrun_mpi_d" is compiled with MPI and double precision.

Example: running Gromacs on Magnus

An example Gromacs job queueing script for Magnus:

```bash
#!/bin/bash --login
#SBATCH --nodes=1
#SBATCH --time=00:05:00
#SBATCH --account=[your-project]
#SBATCH --export=NONE

module swap PrgEnv-cray PrgEnv-gnu
module load gromacs
export OMP_NUM_THREADS=1
srun --export=all -N 1 -n 24 mdrun_mpi -s ion_channel.tpr -maxh 0.50 -resethway -noconfout -nsteps 10000 -g logile
```

(example above uses the Gromacs Test Case A available within the Unified European Applications Benchmark Suite here: [http://www.prace-ri.eu/ueabs](http://www.prace-ri.eu/ueabs))
Example: running Gromacs on Zeus

An example Gromacs job queueing script for Zeus:

```bash
#!/bin/bash --login
#SBATCH --nodes=1
#SBATCH --ntasks=28
#SBATCH --account=[your-project]
#SBATCH --export=NONE

module load gromacs
export OMP_NUM_THREADS=1
srun --export=all -N 1 -n 28 mdrun_mpi -s ion_channel.tpr -maxh 0.50 -resethway -noconfout -nsteps 10000 -g logile
```

(example above uses the Gromacs Test Case A available within the Unified European Applications Benchmark Suite here: http://www.prace-ri.eu/ueabs/GROMACS)

Installing Gromacs with Maali

Users can install their own version of Gromacs with the use of Maali Build Tool, e.g.:

```bash
$ module load maali
$ maali -t gromacs -v 5.1.3
```

Since the build process for all available compiler versions and architectures available on Magnus/Galaxy/Zeus might be time consuming it is worthwhile to consider building Gromacs within a batch SLURM job.

Note that without the `-g` option, Maali builds modules in

```
/group/$PAWSEY_PROJECT/$USERNAME/software/$PAWSEY_OS
```

but with it, it builds in

```
/group/$PAWSEY_PROJECT/software/$PAWSEY_OS
```

which could be useful if the module is to be shared among the group.