# GROMACS

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

## Description

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

Read more on the GROMACS home page.

For a manual consult the the GROMACS home page.

## Modules

| Version | Installation Path | modulefile | compiler | comment |
|---|---|---|---|---|
| 2018.4 | `/sw/chem/gromacs/2018.4/skl/impi` | gromacs/2018.4 | intelmpi | |
| 2018.4 | `/sw/chem/gromacs/2018.4/skl/impi-plumed` | gromacs/2018.4-plumed | intelmpi | with plumed |
| 2019.6 | `/sw/chem/gromacs/2019.6/skl/impi` | gromacs/2019.6 | intelmpi | |
| 2019.6 | `/sw/chem/gromacs/2019.6/skl/impi-plumed` | gromacs/2019.6-plumed | intelmpi | with plumed |
| 2021.2 | `/sw/chem/gromacs/2021.2/skl/impi` | gromacs/2021.2 | intelmpi | |
| 2021.2 | `/sw/chem/gromacs/2021.2/skl/impi-plumed` | gromacs/2021.2-plumed | intelmpi | with plumed |

## Usage

Load the necessary modulefiles. Note that Intel MPI module file should be loaded first

```
module load impi/2019.5 gromacs/2019.6
```

This provides access to the binary **gmx_mpi** wich can be used to run simulations with sub-commands as **gmx_mpi mdrun**

In order to run simulations MPI runner should be used:

```
mpirun gmx_mpi mdrun MDRUNARGUMENTS
```

## Job Script Examples

1. A simple case of a GROMACS job using a total of 640 CPU cores for 12 hours. The requested amount of cores in the example does not include all available cores on the allocated nodes. The job will execute 92 ranks on 3 nodes + 91 ranks on 4 nodes. You can use this example if you know the exact amount of required ranks you want to use.

   ```
   #!/bin/bash
   #SBATCH -t 12:00:00
   #SBATCH -p standard96
   #SBATCH -n 640

   export SLURM_CPU_BIND=none

   module load impi/2019.5
   module load gromacs/2019.6

   mpirun gmx_mpi mdrun MDRUNARGUMENTS
   ```

2. In case you want to use all cores on the allocated nodes, there are another options of the batch system to request the amount of nodes and number of tasks. The example below will result in running 672 ranks.

```
#!/bin/bash
#SBATCH -t 12:00:00
#SBATCH -p standard96
#SBATCH -N 7
#SBATCH --tasks-per-node 96

export SLURM_CPU_BIND=none

module load impi/2019.5
module load gromacs/2019.6

mpirun gmx_mpi mdrun MDRUNARGUMENTS
```