Gromacs

Purpose: Molecular Dynamics
Latest version: 2021.3
License: Free of use
GNU LGPL _ext-link
Website: *http://www.gromacs.org/ _ext-link*

Gromacs is a program for general molecular dynamics, notable for its fast computation of 1-4 interactions.

It can implement regular molecular dynamics simulations using a variety of integrators, Langevin dynamics, energy minimisation, test-particle insertion, etc. It implements a variety of methods to calculate electrostatics and Van der Waals interactions, thermostats and barostats, 2- and 3-dimensional periodic boundary conditions, etc.

SLURM Submit script example

More information about the submit script can be found using the ***Job Script Generator***.

⚠ For optimal performance, before a long production run, you are advised to experiment with different thread allocations to PME and DD tasks, using mdrun options. Please refer to the ***Gromacs documentationext-link*** for more details.

Sbatch options:

The options shown in the example are detailed below. For more information and a more comprehensive list of available options, see the ***sbatch command page***.

- **-J**: Name for the job's allocation.
- **-e**: Name of the sterr redirection filename.
- **-o**: Name of the stdout redirection filename.
- **-p**: Name of the partition (queue) where the job will be submited.

gromacs_example.slm

```
#!/bin/bash
#SBATCH -J gromacs_example
#SBATCH -e gromacs_example.err
#SBATCH -o gromacs_example.out
#SBATCH -p std
#SBATCH --ntasks=24

module load apps/gromacs/2019.1

##
#  Modify the input and output files!
cp -r ${SLURM_SUBMIT_DIR}/*.trp ${SCRATCH}
cd ${SCRATCH}

srun gmx_mpi mdrun \
  -s gromacs_example.tpr \
  -g gromacs_example.log \
  -o gromacs_example.trr \
  -c gromacs_example.gro \
  -e gromacs_example.edr

cp ./{*.log,*.cpt,*.gro,*.edr}
${SLURM_SUBMIT_DIR}
```

- **-n**: Number of tasks.
- **-t**: Set the job's time limit. If the job don't finish before the time runs out, it will be killed.

Software execution information:

The ***mdrun*** program is the main program of Gromacs. It can perform Molecular Dynamics, Stochastic Dynamics, Energy Minimisation, test particle insertion or (re) calculation of energies.

- **-s:** Input file (.tpr .tpb .tpa).
  - Contains the **topology** of the system.
- **-g:** Output log file.
- **-o:** Output trajectory file (.trr .cpt .trj . tng). Use **.trr** for full-precision data.
  - Contains **coordinates**, **velocities** and, optionally, **forces**.
- **-c:** Output structure file (.gro .g96 .pdb . brk .ent .esp).
  - Contains the coordinates and velocities of last step.
- **-e:** Output energy file (.edr).
  - Contains energies, temperature, pressure, etc.

Tutorial

You can follow ***this tutorial*** about a protein's simulation using Gromacs to get hands-on with the program.