Gromacs on HPC

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 and is a **community-driven project**.

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 and fluid dynamics.[Source]

Links:

Official Website

Documentation

Versions Available:

The following versions are available on the cluster:

- physical/gromacs/5.0.7
- physical/gromacs/2020.2_deepMD
- physical/gromacs/2021.1
- physical/gromacs/2021.1_gpu
- physical/gromacs/2022.1_CP2Kv9.1

How to load Gromacs?

To load software, use the following commands:

```
#Load the Gromacs module
module load physical/gromacs/2022.1_CP2Kv9.1
```

To verify if the module and dependencies are loaded correctly, use the following command.

```
#Show all the modules loaded
module list
```

This should list all the dependencies that are loaded. In this case, python, openmpi and gcc compiler should be loaded along with gromacs.

How to use Gromacs?

The main executable of gromacs is **gmx_mpi_d**. See the usage by using help command,

```
#See all commands
gmx_mpi_d help commands
```

For this tutorial, use the following tutorial to run gromacs:

Tutorial

```
# Download PDB file
wget https://files.rcsb.org/download/1AKI.pdb


#Jump to compute node
srun -p main --qos main -n 1 -c 16  --mem 16G --pty bash
```

```
#Clean the pdb file
grep -v HOH 1AKI.pdb > 1AKI_clean.pdb
```

```
#Execute gmx | choose the 15-force field
gmx_mpi_d pdb2gmx -f 1AKI_clean.pdb -o 1AKI_processed.gro -water spce
```

This should result in three processed files - .gro, .itp, and .top.

```
#Define a box
gmx editconf -f 1AKI_processed.gro -o 1AKI_newbox.gro -c -d 1.0 -bt
cubic
#Fill with water
gmx solvate -cp 1AKI_newbox.gro -cs spc216.gro -o 1AKI_solv.gro -p
topol.top
```

Download the mdb file to run energy simulations,

```
wget http://www.mdtutorials.com/gmx/lysozyme/Files/ions.mdp
```

Assemble the .tpr file,

```
gmx_mpi_d grompp -f ions.mdp -c 1AKI_solv.gro -p topol.top -o ions.tpr
```

Run genion,

```
gmx_mpi_d genion -s ions.tpr -o 1AKI_solv_ions.gro -p topol.top -pname
NA -nname CL -neutral
```

Assemble the binary input,

```
wget http://www.mdtutorials.com/gmx/lysozyme/Files/minim.mdp
gmx mdrun -v -deffnm em
gmx energy -f em.edr -o potential.xvg
```

To see more tutorials, visit the documentation of gromacs. These all command to can be wrapped in slurm script. See some of the sample slurm scripts for gromacs in here,

Sample GPU script

Sample CPU Script

User may need to edit these scripts to run gromacs. However, slurm directive used above should be useful.

Where to find help?

If you are stuck on some part or need help at any point, please contact OIT at the following address.

https://ua-app01.ua.edu/researchComputingPortal/public/oitHelp