How to run Gromacs

A number of Gromacs versions are available at our machines. You can see a list of available versions with:

```
module av apps/gromacs
```

Some of them are patched with PLUMED for free energy calculations, enhanced-sampling methods, etc. These are marked as ***XXXX.X-plumed***.

If you need a different version, please let us know and we will install it for you.

Running Gromacs with GPU

Gromacs benefits greatly from GPU acceleration for non-bonding interactions. Considering requesting access to our GPU nodes (*How to request GPUs*) in order to accelerate your computations.