

# Gromacs Server

## GROMACS Server

### Official Documentation:

<https://manual.gromacs.org/current/user-guide/index.html>

### Gromacs Server and Environment:

Gromacs is pre-installed on a Levich server and user accounts are initialized to include Gromacs path.

In case you want to see how the Gromacs environment was set, Here it is:

In file ~/.profile, the last line points to gromacs environment initialization:

```
source /usr/local/gromacs/bin/GMXRC
```

**Users are expected to install their own Python and Python modules.**

Install Conda Python and Python modules:

```
wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh
```

```
chmod +x Miniconda3-latest-Linux-x86_64.sh
```

```
./Miniconda3-latest-Linux-x86_64.sh (answer yes to initialize Minicoda3)
```

Logout and back in to have conda environment, then run:

```
conda install numpy scipy matplotlib pandas
```

Conda can be deactivated or reactivated by command:

```
conda deactivate
```

```
conda activate
```

# Gromacs Command

Main Command: `gmk`

## Examples:

`gmx -h`

(print help)

`gmk -v`

(show version)

`gmx help [module]`

(documentation of a module)

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