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 initilized 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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