Python for HPC

Which versions of python are installed at LRZ?

We provide several versions of python at LRZ which have different levels of customization by the user:

OS installed python

/usr/bin/python: this is the version of python that comes preinstalled by the OS. It is rather old, but stable. **DON'T USE!**

LRZ python module

python via the module system gives you only outdated version python2.7

$ module load python

We provide python 2.7 which is already outdated. To use the latest version of python and additional libraries you have to use conda.

Installing python packages using conda

You can download the latest packages via conda. For that you have to generate your own environment by

$ module load python
$ conda create -n py38 python=3.8
$ source activate py38
(py38) $ conda install numpy

then you can load numpy into python.

For additional libraries search the internet for "conda install mylib" and then use the conda command to install the library (e.g. jupyter or pandas)

(py38) $ python
Python 3.8.0 (default, Nov 6 2019, 21:49:08)
[GCC 7.3.0] :: Anaconda, Inc. on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import numpy

Python on SuperMUC-NG

SuperMUC-NG does not allow for outgoing internet connections and therefore conda does not work out of the box (same for pip or R-CRAN) and you have to use a tunnel or use conda pack.

Please consult our FAQ section.

Using other linux distributions at LRZ

Due to the requirements of stability the operating system used on the LRZ server is not the latest version and might be already several years old. However, there are several linux distributions that provide binary versions of python and additional modules which are cutting edge and we understand that our users would like to use them. Unfortunately this is not possible at LRZ and we can only hint at a workaround if a user really needs the latest version of a tools.

Please install the tool locally on you own machine and then use sshfs to mount the LRZ filesystems in order to obtain access to the data. Even though this might in some cases slow down the working speed it is the only possibility as we cannot and will not install cutting edge unstable operating systems.