Python for HPC

At LRZ python is provided by the operating system itself. You can find it under /usr/bin/python on all machines. In order to provide additional libraries for python, LRZ also provides a module which loads a python interpreter into the $PATH. The current version of python can be loaded by:

$ module load python

We provide python 2.7 and python 3.6.

together with the basic python interpreter several additional libraries are installed on an experimental basis and might or might not work on the chosen LRZ machine, due to incompatibilities in operating system version and libraries (MKL, MPI, tcl/tk). We try to provide all the libraries for the state of the art machines (SuperMUC, CoolMUC) but can not guarantee that all libraries are fully functional. Please consider this installation as work in progress.

In case a user needs an additional package not provided in the module it is possible to install the package in his own HOME directory. We are always pleased to help our users in case of any problems.

The idea behind the home scheme is that you build and maintain a personal stash of Python modules. This scheme's name is derived from the idea of a home directory on Unix, since it's not unusual for a Unix user to make their home directory have a layout similar to /usr/ or /usr/local/. This scheme can be used by anyone, regardless of the operating system they are installing for.

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 my_python
$ source activate my_python

(my_python) $ conda install numpy

then you can load numpy into python

(my_python) $ python
Python 2.7.13 |Anaconda 4.3.1 (64-bit)| (default, Dec 20 2016, 23:09:15)
[GCC 4.4.7 20120313 (Red Hat 4.4.7-1)] on linux2
Type "help", "copyright", "credits" or "license" for more information.
Anaconda is brought to you by Continuum Analytics.
Please check out: http://continuum.io/thanks and https://anaconda.org
>>> 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). 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 your 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.