Using Python @ NSC

Warning: Python bites can be very painful

OS Python

- NSC's clusters have the CentOS standard Python 2.7.5 and Python 3.4.10 installed.

```
[x_abcde@tetralith]$ module purge
[x_abcde@tetralith]$ which python
/usr/bin/python
[x_abcde@tetralith]$ which python3
/usr/bin/python3
```

- Recommendation: don’t use them

Python modules

Python modules

- Python modules provide access to a recent version of Python + scientific libraries: e.g. NumPy, SciPy, Matplotlib, Pandas etc

```
[x_abcde@tetralith]$ module avail Python/
 . . .
Python/recommendation                (D)
Python/2.7.14-anaconda-5.0.1-nsc1
Python/2.7.14-nsc1-gcc-2018a-eb
 . . .
Python/3.6.3-anaconda-5.0.1-nsc1
Python/3.6.4-nsc1-intel-2018a-eb
 . . .
```

Python modules

- After loading a Python module, you will have a new Python installation in your PATH
- A range of scientific packages are also made available e.g. NumPy

```
[x_abcde@tetralith]$ module load Python/3.7.0-anaconda-5.3.0-extras-nsc1
$ python
Python 3.7.0 (default, Jun 28 2018, 13:15:42)
[GCC 7.2.0] :: Anaconda, Inc. on linux
Type "help", "copyright", "credits" or "license" for more information.

>>> import numpy
>>> numpy.linspace(0, 2, 9)
array([0.  , 0.25, 0.5 , 0.75, 1.  , 1.25, 1.5 , 1.75, 2.  ])
```

Python modules

Three flavors of Python module

1. Python/x.y.z-nscX-toolchain
2. Python/x.y.z-env-nscX-toolchain
3. Python/x.y.z-anaconda-....

Some guidelines to help you choose a module:

A. There are generally more packages included in the Anaconda installations
B. If there are modules that only differ in the -nsc build/installation tag, then choose the one with the highest integer (e.g. nsc2 rather than nsc1)

Python modules

Check available packages in a module: Anaconda modules

To list the installed packages in an Anaconda Python installation, simply load the module and run: `conda list`.

If you are looking for a specific package, then pipe the output from `conda list` to `grep`:

```
[x_abcde@tetralith]$ module load Python/3.6.3-anaconda-5.0.1-nsc1
[x_abcde@tetralith]$ conda list | grep -i scipy
scipy                     0.19.1           py36h9976243_3
```

Python modules

Check available packages in a module: NSC build modules

To list the installed packages in a NSC build installation, simply load the module and run: `pip list`.

If you are looking for a specific package, then pipe the output from `pip list` to `grep`:

```
[x_abcde@tetralith]$ module load Python/3.6.4-nsc2-intel-2018a-eb
[x_abcde@tetralith]$ pip list --format=legacy | grep -i scipy
scipy (1.0.0)
```

Managing your python environment

Managing your python environment

- Python modules provide a set of common python packages.
- For technical reasons, we cannot install all the packages that everyone needs in the same module installation.
- Instead, we recommend that you install extra packages in your own user space using a **managed environment**.
- We support two options:
  1. anaconda
  2. virtualenv

Managing your python environment: conda

- Use an **Anaconda** module for managing your conda environments (NOT `Python/x.y.z-anaconda-...`)

```
[x_abcde@tetralith]$ module load Anaconda/2021.05-nsc1
[x_abcde@tetralith]$ conda create -n myownenv python=3.8 pandas seaborn
[x_abcde@tetralith]$ conda activate myownenv
(myownenv)[x_abcde@tetralith]$ which python
     ~/.conda/envs/myownenv/bin/python
(myownenv)[x_abcde@tetralith]$ python
     Python 3.8.13 | packaged by conda-forge | (default, Mar 25 2022, 06:04:18)
     [GCC 10.3.0] on linux
     Type "help", "copyright", "credits" or "license" for more information.
     >>> import pandas
     >>> pandas.__version__
     '1.4.2'
```

Managing your python environment: conda

- If you need to use the conda command for anything other than `conda list`, use an **Anaconda** module to create your own local conda environment.

- By default, your conda environments are installed in `${HOME}/.conda`. If you have multiple conda environments here there is a risk of filling up your `${HOME}` space.
  - There are ways to install conda environments outside `${HOME}`, see https://www.nsc.liu.se/software/python/
- If you need to install a python package that requires **compiling**, then you should NOT use a conda environment! (try virtualenv instead).

Managing your python environment: virtualenv

- Use any of the **Python/x.y.z** modules for managing environments using virtualenv

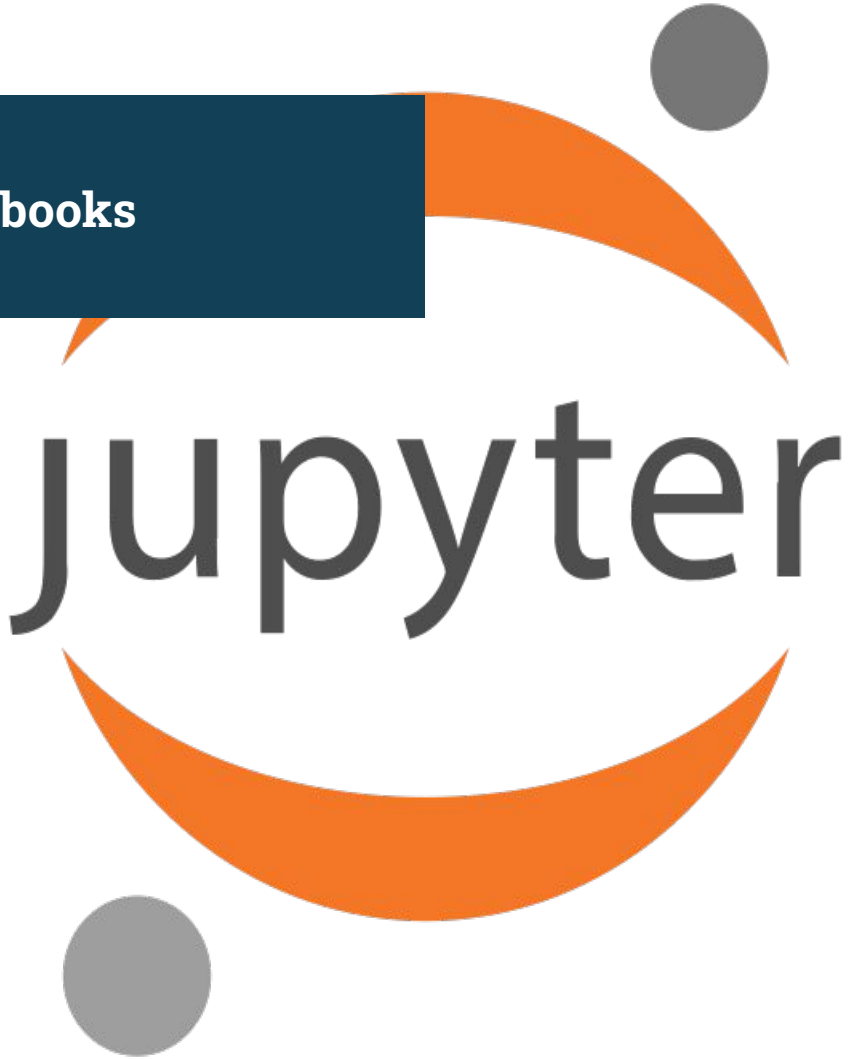
```
[x_abcde@tetralith]$ module load Python/3.6.7-env-nsc1-gcc-2018a-eb
[x_abcde@tetralith]$ virtualenv --system-site-packages myownvirtualenv
[x_abcde@tetralith]$ source myownvirtualenv/bin/activate
(myownvirtualenv)[x_abcde@tetralith]$ pip install python-hostlist
(myownvirtualenv)[x_abcde@tetralith]$ python
     Python 3.6.7 (default, Nov 26 2018, 16:42:15)
     [GCC 6.4.0] on linux
     Type "help", "copyright", "credits" or "license" for more information.
     >>> import hostlist
     >>> hostlist.__file__
     '/home/x_abcde/myownvirtualenv/lib/python3.6/site-packages/hostlist.py'
```

Installing packages that require compiling

- Start from the gcc or intel Python and corresponding buildenv modules
- Create a virtual environment for building and adding packages using pip.

```
[x_abcde@tetralith]$ module load Python/3.6.7-env-nsc1-gcc-2018a-eb
[x_abcde@tetralith]$ module load buildenv-gcc/2018a-eb
[x_abcde@tetralith]$ virtualenv --system-site-packages myownvirtualenv
[x_abcde@tetralith]$ source myownvirtualenv/bin/activate
(myownvirtualenv)[x_abcde@tetralith]$ …
```

jupyter notebooks



Jupyter notebooks

- Jupyter notebooks can be run on with the login nodes or compute nodes.
- Jupyter packages are included in the `Python/x.y.z-anaconda-...-extras-nsc1` modules

```
[x_abcde@tetralith]$ module load Python/3.8.3-anaconda-2020.07-extras-nsc1
[x_abcde@tetralith]$ conda list | grep jupyter
…
```

- (or you can create and manage your own python environment that includes juypyter)

Jupyter notebooks

- Recommendation: Use jupyter in combination with thinlinc.
  - E.g. on a login node, in a thinlnc terminal:

```
[x_abcde@tetralith]$ module load Python/3.8.3-anaconda-2020.07-extras-nsc1
[x_abcde@tetralith]$ jupyter-notebook
[x_abcde@tetralith]$ …
```

- Jupyter notebooks can also be used via an ssh tunnel

mpi4py

mpi4py

- Python scripts that use mpi4py are now supported by the latest version of NSC's mpi launcher (`mpprun/4.3.0`).
  - E.g. interactive:

```
[x_abcde@tetralith]$ module load mpprun/4.3.0
[x_abcde@tetralith]$ module load Python/3.6.7-env-nsc1-gcc-2018a-eb
[x_abcde@tetralith]$ interactive -n 4 -A <my-project> -t 01:00:00
…
[x_abcde@n1234]$ mpprun python mpi4py-pythonscript-py
…
```

- where `mpi4py-pythonscript.py` includes, e.g.:

```
import mpi4py as MPI
```

mpi4py

- You can also run in batch mode using a script something like:

```
#!/bin/bash
#SBATCH -A snic2022-x-yyy
#SBATCH -n 4
#SBATCH -t 01:00:00
#SBATCH -J jobname

module load mpprun/4.3.0
module load Python/3.6.7-env-nsc1-gcc-2018a-eb
mpprun python mpi4py-pythonscript.py
```

Final recommendations:

- Maintain separate python environments for separate work tasks
- Do NOT use `pip install -local`
- Remove `conda init` from your `.bashrc` (and try to keep changes to `.bashrc` to a minimum)
- …