# Using Python @ NSC

# OS Python

- NSC's clusters have the Rocky 9 standard Python installed.

```
[x_abcde@tetralith]$ module purge
[x_abcde@tetralith]$ which python
    /usr/bin/python
[x_abcde@tetralith]$ python --version
    Python 3.9.21
```

- Recommendation:
  - don’t use it
  - okej, maybe use it for simple python tasks that do not have any difficult dependencies.

# Python 2: please try to upgrade

# Python modules

# Python modules: 3 flavors

1. Python/<version>-**env**-hpcX-<toolchain>
2. Python/<version>-**bare**-hpcX-<toolchain>
3. “Miniforge/<version>-hpcX”

```
[x_abcde@tetralith2 ~]$ module avail python/

-------------------- /software/sse2/tetralith_el9/modules  -----------------------------------
Python/recommendation                (D)    Python/3.10.4-bare-hpc1-gcc-2022a-eb
Python/2.7.18-bare-hpc1-gcc-2022a-eb        Python/3.10.4-env-hpc1-gcc-2022a-eb
Python/3.10.4-env-hpc2-gcc-2022a-eb         Python/3.11.5-bare-hpc1-gcc-2023b-eb
Python/3.11.5-env-hpc1-gcc-2023b-eb

  Where:
   D:  Default Module
```

# Python/<version>-env-hpcX-<toolchain>-eb

- After loading a Python module, you will have a new Python installation in your PATH
- Provides a specific python version and a fairly extensive range of scientific packages e.g. NumPy, SciPy, Matplotlib, Pandas, etc.

```
[x_abcde@tetralith]$ module load Python/3.11.5-env-hpc1-gcc-2023b-eb
[x_abcde@tetralith]$ which python
/software/sse2/tetralith_el9/easybuild/pure/software/Python/3.11.5-GCCcore-13.2.0/bin/python
[x_abcde@tetralith]$ python
     Python 3.11.5 (main, Nov 18 2024, 16:41:22) [GCC 13.2.0] 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/<version>-env-hpcX-<toolchain>-eb

- Useful for python scripts that need extra packages but are not picky with the precise versions.
- Use “pip list” to give a listing of the installed packages (including versions)

```
[x_abcde@tetralith]$ module load Python/3.11.5-env-hpc1-gcc-2023b-eb
[x_abcde@tetralith]$ pip list --format=columns | grep -i scipy
    SciPy                           1.11.4

    [notice] A new release of pip is available: 23.2.1 -> 25.0.1
    [notice] To update, run: pip install --upgrade pip
```

# Managing your python environment

# Managing your python environment

- Python **env** 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. Virtualenv
  2. Miniforge

# Managing your python environment: virtualenv

- Recommend using e.g. **Python/3.11.5-bare-hpc1-gcc-2023b-eb** for managing environments using virtualenv

```
[x_abcde@tetralith]$ module load Python/3.11.5-bare-hpc1-gcc-2023b-eb
[x_abcde@tetralith]$ python -m venv myownvirtualenv
[x_abcde@tetralith]$ source myownvirtualenv/bin/activate
(myownvirtualenv)[x_abcde@tetralith]$ python -m pip install python-hostlist
…
(myownvirtualenv)[x_abcde@tetralith]$ python
     Python 3.11.5 (main, Nov 18 2024, 16:41:22) [GCC 13.2.0] on linux
     Type "help", "copyright", "credits" or "license" for more information.
     >>> import hostlist
     >>> hostlist.__file__
     '/home/x_abcde/myownvirtualenv/lib/python3.11/site-packages/hostlist.py'
```

# Python/<version>-bare-hpcX-<toolchain>-eb

- Provide a specific python version without any preinstalled packages
- “bare” modules are primarily for use with Python venvs, so you can install packages using the pip command. This allows requesting precise versions of desired package(s).

```
[x_abcde@tetralith]$ module load Python/3.11.5-bare-hpc1-gcc-2023b-eb
[x_abcde@tetralith]$ python -m venv numpyscipy.venv
[x_abcde@tetralith]$ source numpyscipy.venv/bin/activate
(numpyscipy.venv) [x_abcde@tetralith]$ python -m pip install numpy==1.26.4 scipy==1.11.4
…
Installing collected packages: numpy, scipy
Successfully installed numpy-1.26.4 scipy-1.11.4
(numpyscipy.venv) [x_abcde@tetralith]$
```

# Installing packages that require compiling

- If you need to install a pip package that requires **compiling** , then we strongly recommend using a virtualenv.
- Load the corresponding buildenv module (e.g. buildenv-gcc/2023b-eb)
- Create a virtual environment for building and adding packages.

```
[x_abcde@tetralith]$ module load Python/3.11.5-bare-hpc1-gcc-2023b-eb
[x_abcde@tetralith]$ module load buildenv-gcc/2023b-eb
[x_abcde@tetralith]$ python -m venv myownvirtualenv
[x_abcde@tetralith]$ source myownvirtualenv/bin/activate
(myownvirtualenv)[x_abcde@tetralith]$ …
```

- For more details (section “Pip packages that require compilation”)

# Managing your python environment: conda/Miniforge

- Use a Miniforge module for managing your conda environments

```
[x_abcde@tetralith]$ module load Miniforge/24.7.1-2-hpc1
[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 3.8.20 | packaged by conda-forge | (default, Sep 30 2024, 17:52:49)
     [GCC 13.3.0] on linux
     Type "help", "copyright", "credits" or "license" for more information.
     >>> import pandas
     >>> pandas.__version__
     '2.0.3'
```

# Managing your python environment: conda/Miniforge

- Miniforge modules are available as a “drop-in” replacement for Anaconda.
- The `mamba` command can be used in place of `conda` (and in general performs better)
- By default, miniforge uses the `conda-forge` community-driven library of packages instead of channels offered by the Anaconda company
- 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: Python @ NSC
- More detailed information: Anaconda @ NSC

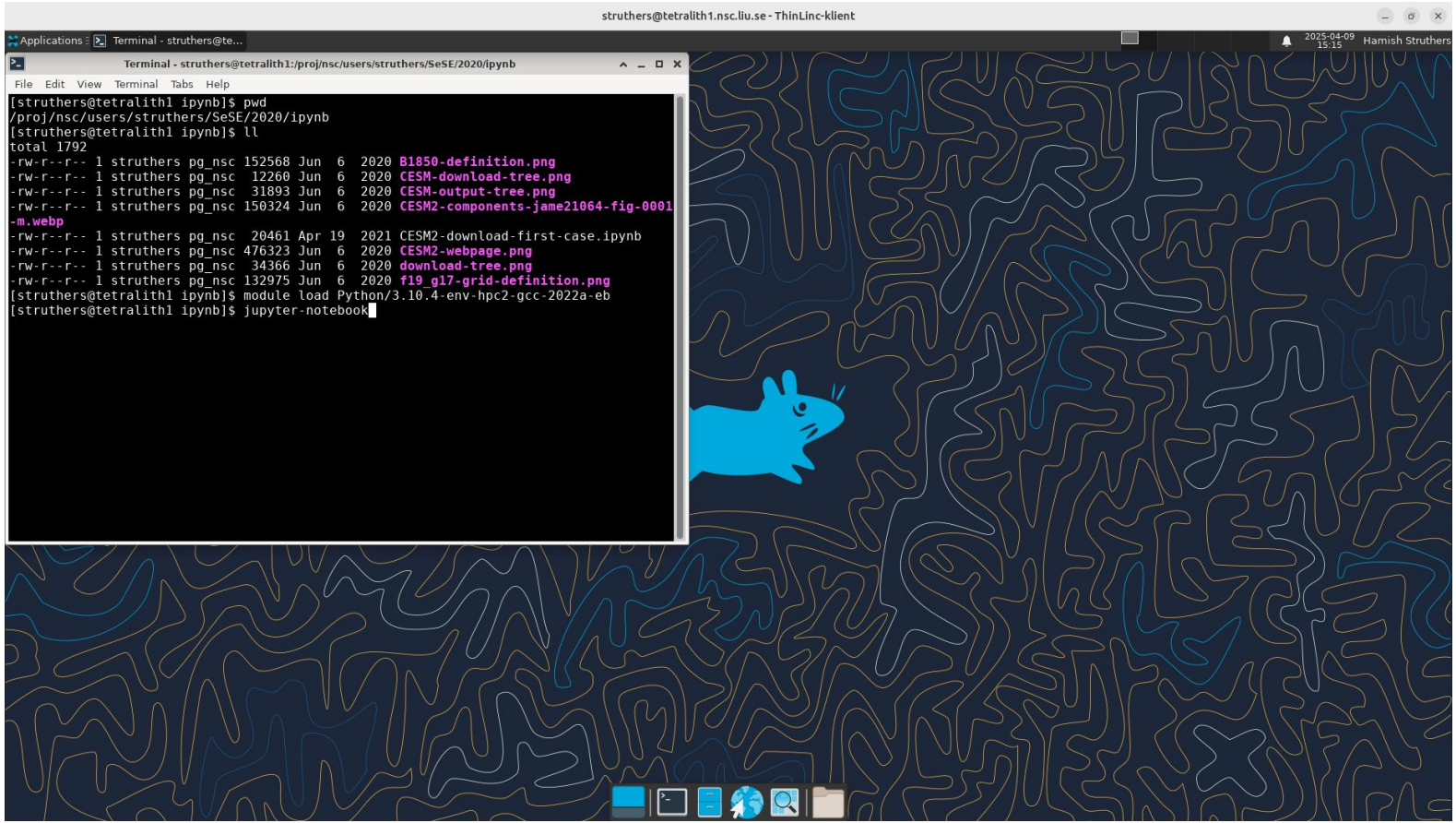
# jupyter notebooks

# Jupyter notebooks

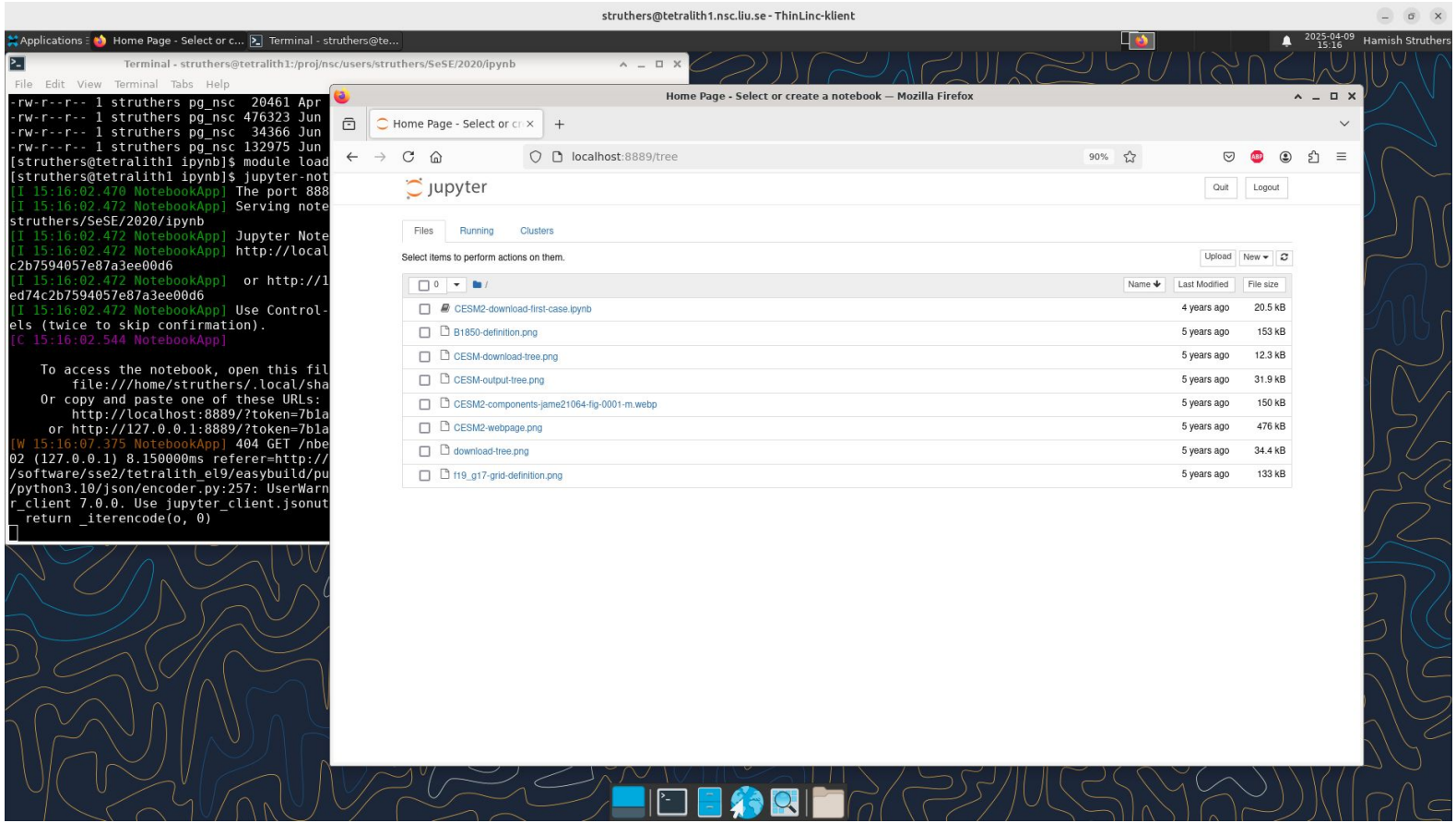
- Jupyter notebooks can be run on with the login nodes or compute nodes.
- Jupyter packages are included in the `Python/3.11.5-env-hpc1-gcc-2023b-eb` module

```
[x_abcde@tetralith]$ module load Python/3.11.5-env-hpc1-gcc-2023b-eb
[x_abcde@tetralith]$ pip list | grep jupyter
…
```

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




For light calculations, use jupyter in combination with thinlinc (on a login node).




For light calculations, use jupyter in combination with thinlinc (on a login node).

# Jupyter notebooks

- For more heavy jupyter notebook calculations: recommend using jupyter on a compute node (interactive session) and connecting via an ssh tunnel

# mpi4py

- Python scripts that use mpi4py are supported by NSC's mpi launcher `mpprun`.
  - E.g. interactive:

```
[x_abcde@tetralith]$ module load  Python/3.11.5-env-hpc1-gcc-2023b-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 naiss2025-x-yyy
#SBATCH -n 4
#SBATCH -t 01:00:00
#SBATCH -J jobname

module load Python/3.11.5-env-hpc1-gcc-2023b-eb
mpprun python mpi4py-pythonscript.py
```

# Final notes:

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