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Working with Python at CHPC

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Working with python

- From the command line (via ssh or FastX) or within a SLURM script:

```
$ module load python/3.7.3  
$ python my_script_name.py ...
```

- From a jupyter notebook:

- <https://ondemand.chcp.utah.edu> -> Interactive Apps

- From within a workflow manager like snakemake

```
$ module load snakemake/5.6.0  
$ snakemake -s my_workflow.snakefile
```

Which distribution / version of python to use?

- CHPC-installed “standard” distributions

```
$ module spider python          # This will list the available versions  
$ module load python/3.6.3  
$ which python  
/uufs/chpc.utah.edu/sys/installldir/python/3.6.3/bin/python
```

- CHPC-installed anaconda distributions

```
$ module spider anaconda3  
$ module load anaconda3/2019.03  
$ which python  
/uufs/chpc.utah.edu/sys/installldir/anaconda3/2019.03/bin/python
```

- Self-installed anaconda

- <https://www.chpc.utah.edu/documentation/software/python-anaconda.php>

- Jupyter notebook will use the version of python that you have loaded
- We discourage use of the operating system's python (/usr/bin/python)

Using Python libraries

- A library you need may already be installed – try to import it:

```
>>> import sklearn  
>>> sklearn.__file__  
/uufs/chpc.utah.edu/sys/installdir/anaconda3/2019.03/lib/python3.7/...
```

- You can install your own using “`pip install --user package_name`”
 - This installs under your home directory in `$HOME/.local/lib/version/...`
- Within a self-installed anaconda:

```
$ conda install -c channel_name package_name
```

- <https://www.chpc.utah.edu/documentation/software/python-anaconda.php>



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Python example...

- Serial python example
 - in a job script
 - in a jupyter notebook
- Martin will discuss parallelization...