

Introduction to pythonTM

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- **Target audience**

- Basic understanding and experiences with programming languages
- Zero or little experiences with Python

- **What to expect**

- √ Basic knowledge of Python
- × Advanced programming

1. About Python

- 1) What is Python
- 2) Pros & Cons

2. Running Python on Clusters

- 1) Load Python
- 2) Ways to run Python on clusters

3. Python 101 (in Google Colab)

- 1) Variables and operators
- 2) Data types
- 3) File I/O
- 4) Control structures and functions
- 5) Python modules

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1) What is Python

- **Guido van Rossum @ 2/20/1991**
- **High-level & general-purpose**
- **Intuitive & minimal** coding
- **Interpreted**, not compiled
- **Dynamic typing**
 - No type declarations, data type tracked at runtime
- **Automatic** memory management
- Blocks defined by **indentation**



```
void ExceptionHandling()
{
    try
    {
    }
    catch (const Foo &f)
    {
        throw Foo();
    }
    catch (const Bar)
    {
        throw Bar();
    }
    catch (...)
    {
        throw FooBar();
    }
}
```

C++

```
def ExceptionHandling(self):
    try:
        pass
    except Foo as f:
        raise Foo()
    except Bar:
        raise Bar()
    except:
        raise FooBar()
```

Python

2) Pros & Cons

- **Pros:**

- Ease of programming
- Minimal time to develop and maintain codes
- Modular and object-oriented
- Large standard and user-contributed libraries
- Large user community

- **Cons:**

- Interpreted → slower
- Not great for 3D graphic applications requiring intensive computations

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- **Running on local machine?**
 - a) Terminal (command-line)
 - b) GUI (Spyder)
 - c) Jupyter Notebook (web-interface)
 - d) ...

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1) Load python

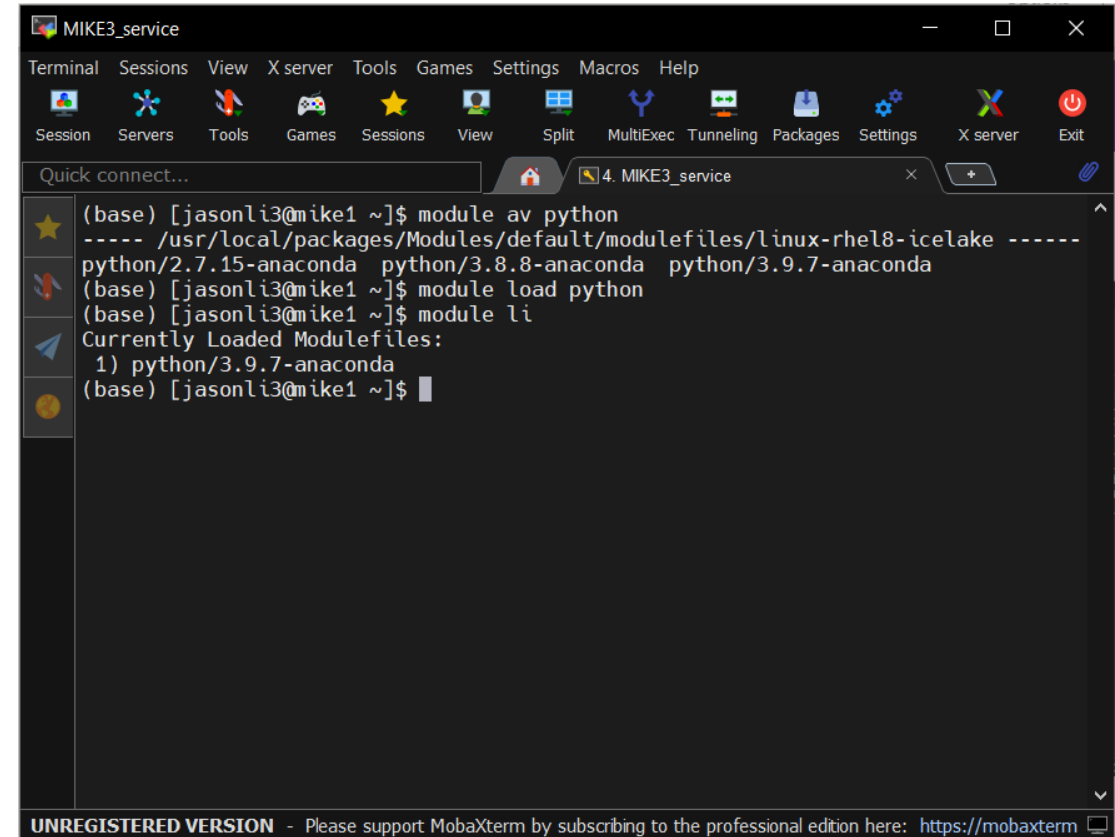
- Python installation on HPC clusters

- ☐ Modules

- Check availability: `module av python`
- Load: `module load python/...`
- Auto-loading: `~/.modules`

- ☐ Customized version: Conda virtual environment

- See: <https://youtu.be/tl3vSxZZr-c>



```
MIKE3_service
Terminal Sessions View X server Tools Games Settings Macros Help
Session Servers Tools Games Sessions View Split MultiExec Tunneling Packages Settings X server Exit
Quick connect... 4. MIKE3_service
(base) [jasonli3@mike1 ~]$ module av python
----- /usr/local/packages/Modules/default/modulefiles/linux-rhel8-icelake -----
python/2.7.15-anaconda python/3.8.8-anaconda python/3.9.7-anaconda
(base) [jasonli3@mike1 ~]$ module load python
(base) [jasonli3@mike1 ~]$ module li
Currently Loaded Modulefiles:
  1) python/3.9.7-anaconda
(base) [jasonli3@mike1 ~]$
```

2) Ways to run Python on clusters

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2) Ways to run Python on clusters

- Main difference from using your local machine:

Must submit a job!!!

2) Ways to run Python on clusters

a) Interactively

- * Must submit an **interactive job**
- * Make sure you are **NOT** running on head node!

```
MIKE3_service
Terminal Sessions View X server Tools Games Settings Macros Help
Session Servers Tools Games Sessions View Split MultiExec Tunneling Packages Settings X server Exit
Quick connect... 4. MIKE3_service
(base) [jasonli3@mike1 ~]$ srun --pty bash
srun: Job is in held state, pending scheduler
srun: job 15381 queued and waiting for resources
Interactive job 15381 waiting:
srun: job 15381 has been allocated resources
(base) [jasonli3@mike060 ~]$ module load python
(base) [jasonli3@mike060 ~]$ which python
/usr/local/packages/python/3.9.7-anaconda/bin/python
(base) [jasonli3@mike060 ~]$ python
Python 3.9.7 (default, Sep 16 2021 13:09:58)
[GCC 7.5.0] :: Anaconda, Inc. on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> print("Hello Python!")
Hello Python!
>>>
```

i. Submit an interactive job

ii. Load python module

iii. Run command "python"

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2) Ways to run Python on clusters

b) Python script

- * Must submit a **batch job**

```
(base) [jasonli3@mike4 ~]$ cat test.py
import sys
print("Hello Python!\n")
(base) [jasonli3@mike4 ~]$ cat test.sbatch
#!/bin/bash
#SBATCH -N 1
#SBATCH -n 1
#SBATCH -t 1:00:00
#SBATCH -p single

module load python
cd $SLURM_SUBMIT_DIR
python test.py
exit 0
(base) [jasonli3@mike4 ~]$ sbatch test.sbatch
Submitted batch job 15385 estimates 1 SUS from alloc
ed remaining SUSs: 353087
JOBID      NAME                PARTITION  TIME_LIMIT  ST  NODES  REASON
15385      test.sbatch         single     1:00:00     PD   1      None

(base) [jasonli3@mike4 ~]$ ls
CATSettings R setenv.sh slurm-15385.out test.py test.sbatch
(base) [jasonli3@mike4 ~]$ cat slurm-15385.out
Hello Python!
(base) [jasonli3@mike4 ~]$
```

i. Python script

ii. Batch job submission script

iii. Submit batch job

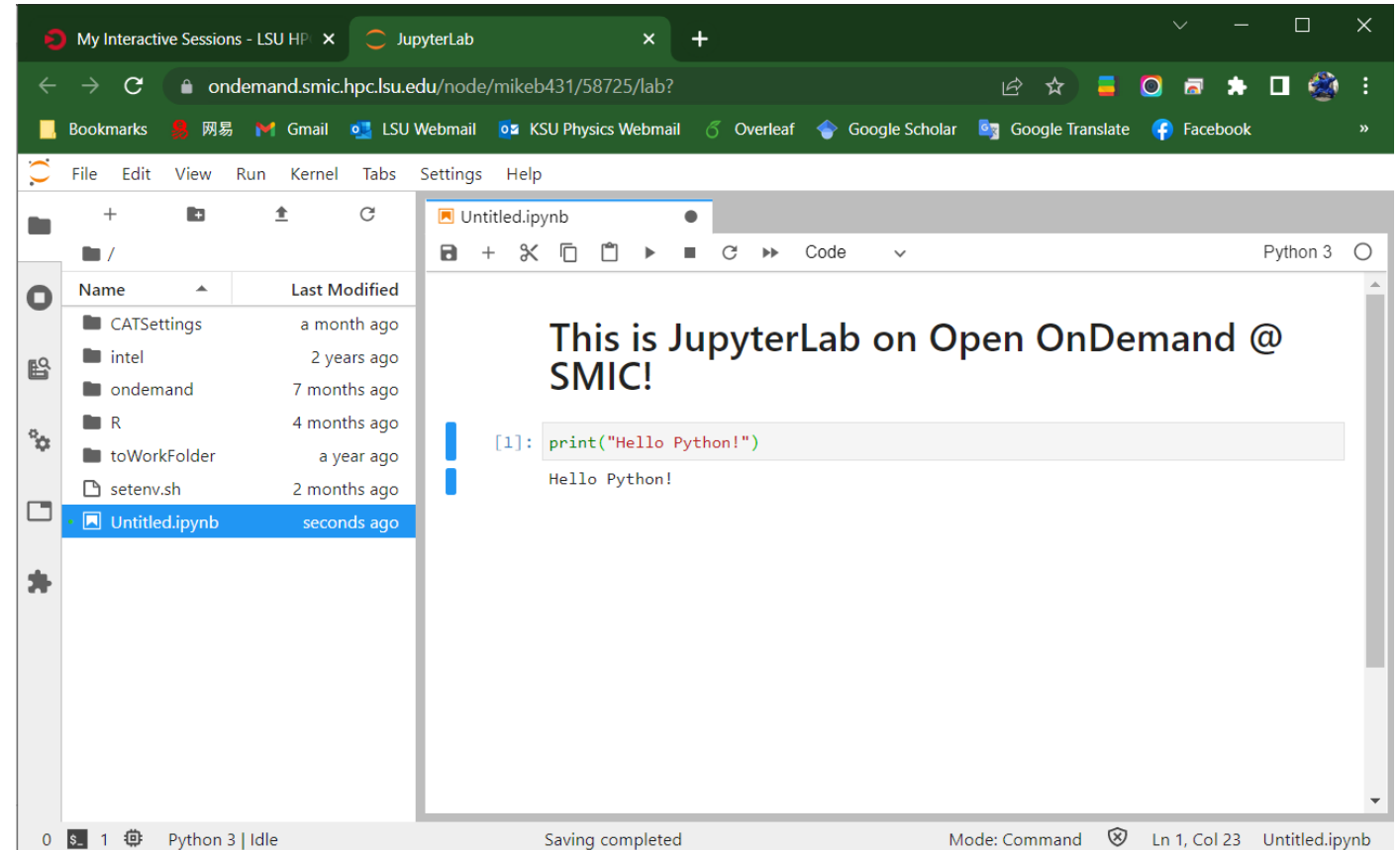
iv. Results

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2) Ways to run Python on clusters

c) Jupyter Notebook / JupyterLab

- * Must use **Open OnDemand** via web browser
- * Currently only available on SMIC: <https://ondemand.smic.hpc.lsu.edu/>



[1] <http://www.hpc.lsu.edu/training/archive/tutorials.php>



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