

# Introduction to python<sup>TM</sup>

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# About this training

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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

# 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

# 1) What is Python language?

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A set of rules and grammar that define a python code.

# 1) Why Python?

Free and open source

Modular

Easy to learn

Multi-purpose

# 1) Applications

Data analysis

Web applications

Machine learning

Mobile applications

Desktop applications

Automatic scripts

# 1) Python versions

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Python 2.x

Python 3.x

# 1) Python reference



<http://python.org>

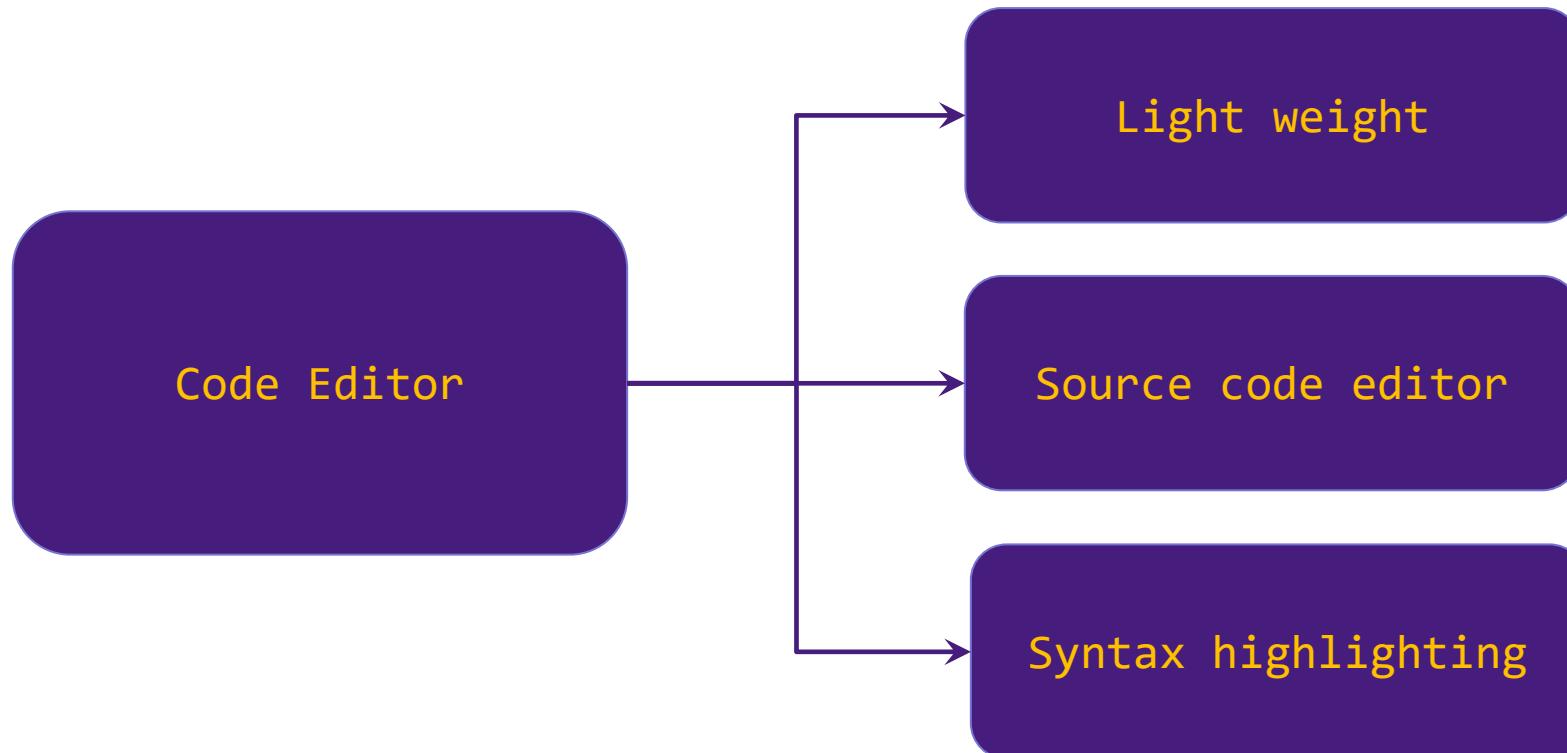
# 1) Programming tools

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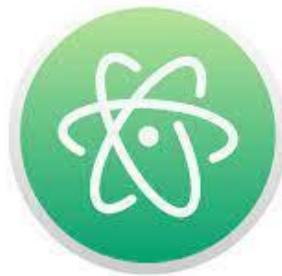
Code Editor

Integrated  
Development  
Environment  
(IDE)

# 1) What is the Code Editor



# 1) Code editors



Atom



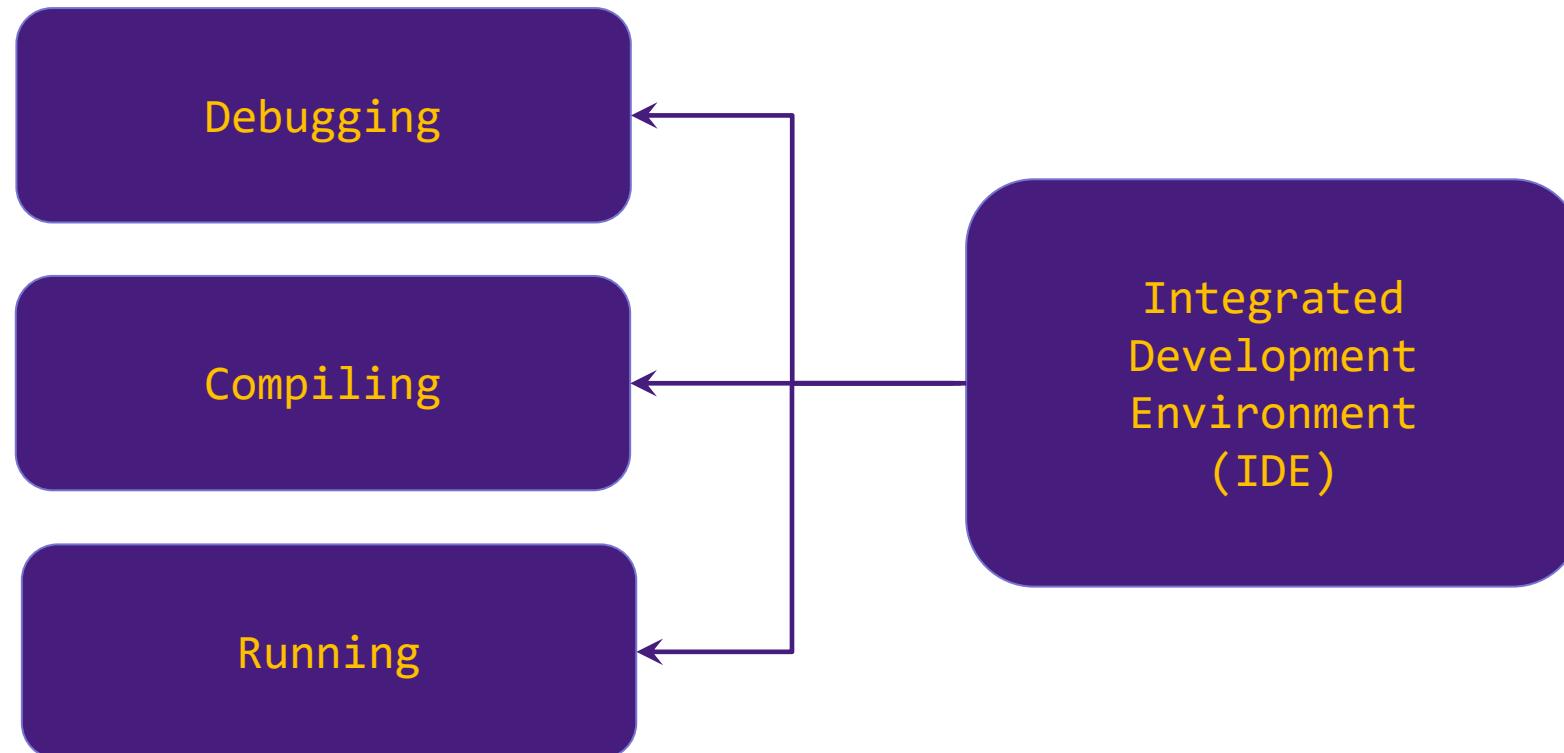
Sublime Text



VS Code

# 1) What is the Integrated Development Environment

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# 1) Integrated Development Environment Features

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Linting

Autocompletion

Debugging

Unit Testing

Code Formatting

Code Snippets

# 1) Integrated Development Environment

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IDLE



PyCharm IDE



Spyder

# 1) Integrated Development Environment

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## 2) Pros & Cons

- **Pros:**

- Python is free, it is ease to obtain and to install
- It is easy
- 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

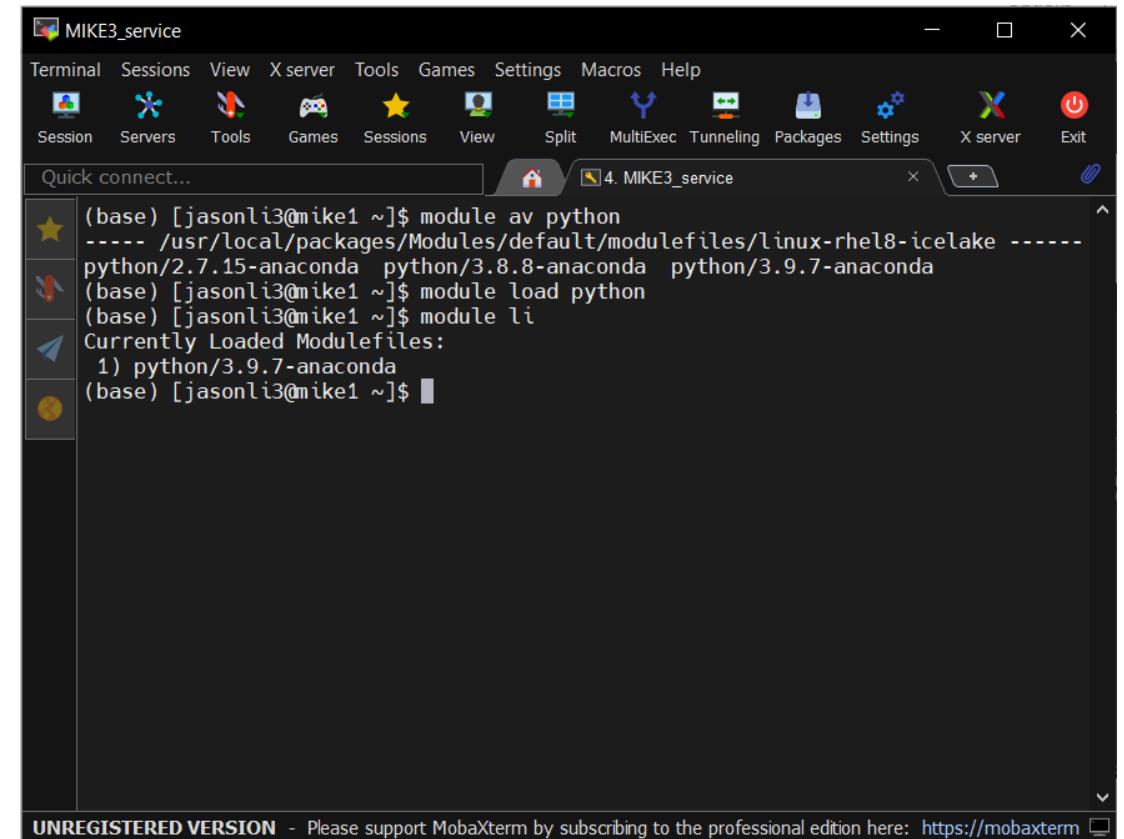
- **Python installation on HPC clusters**

- Modules

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

- Customized version: Conda virtual environment

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



The screenshot shows a terminal window titled "MIKE3\_service". The window has a dark theme with various icons in the toolbar. The terminal itself displays the following text:

```
(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 ~]$
```

At the bottom of the terminal, there is a watermark that reads "UNREGISTERED VERSION - Please support MobaXterm by subscribing to the professional edition here: https://mobaxterm.com".

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



## 2) Ways to run Python on clusters

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## 2) Ways to run Python on clusters



- Unlike using your local machine:

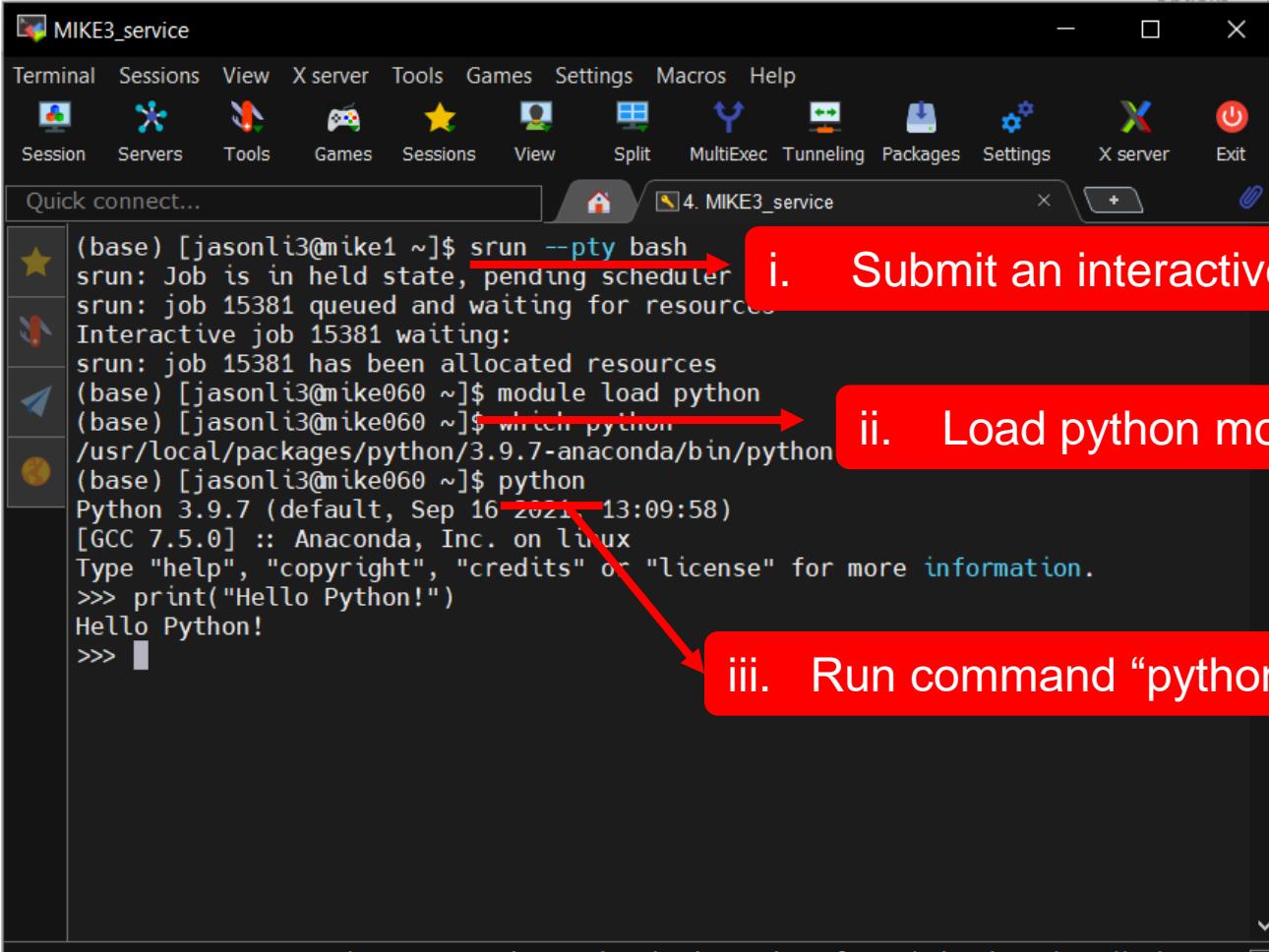
Must submit a job!!!

## 2) Ways to run Python on clusters

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### a) Interactively

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



The screenshot shows a terminal window titled "MIKE3\_service" with a dark theme. The window has a toolbar with icons for Session, Servers, Tools, Games, Sessions, View, Split, MultiExec, Tunneling, Packages, Settings, X server, and Exit. A red box highlights the "Sessions" icon. Below the toolbar is a "Quick connect..." search bar and a tab labeled "4. MIKE3\_service". The terminal window displays the following command sequence:

```
(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!  
>>> █
```

Three red arrows point from the right side of the slide to specific parts of the terminal output:

- Submit an interactive job
- Load python module
- Run command "python"

At the bottom of the terminal window, a message reads: "UNREGISTERED VERSION - Please support MobaXterm by subscribing to the professional edition here: <https://mobaxterm.com>".

## 2) Ways to run Python on clusters

### b) Python script

- \* Must submit a **batch job**

The screenshot shows a terminal window titled "MIKE3\_service" in MobaXterm. The terminal session is labeled "4. MIKE3\_ser". The user has run several commands:

- i. Python script: The user runs `cat test.py`, which contains the code 

```
import sys
print("Hello Python!\n")
```
- ii. Batch job submission script: The user runs `cat test.sbatch`, which contains the Slurm batch script:

```
#!/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
```
- iii. Submit batch job: The user runs `sbatch test.sbatch`, which submits the job and displays its ID:

```
(base) [jasonli3@mike4 ~]$ sbatch test.sbatch
Submitted batch job 15385
```

JOBID	NAME	PARTITION	TIME_LIMIT	ST	NODES	REASON
15385	test.sbatch	single	1:00:00	PD	1	None
- iv. Results: The user runs `ls` to see the job output files, then `cat slurm-15385.out` to view the results:

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

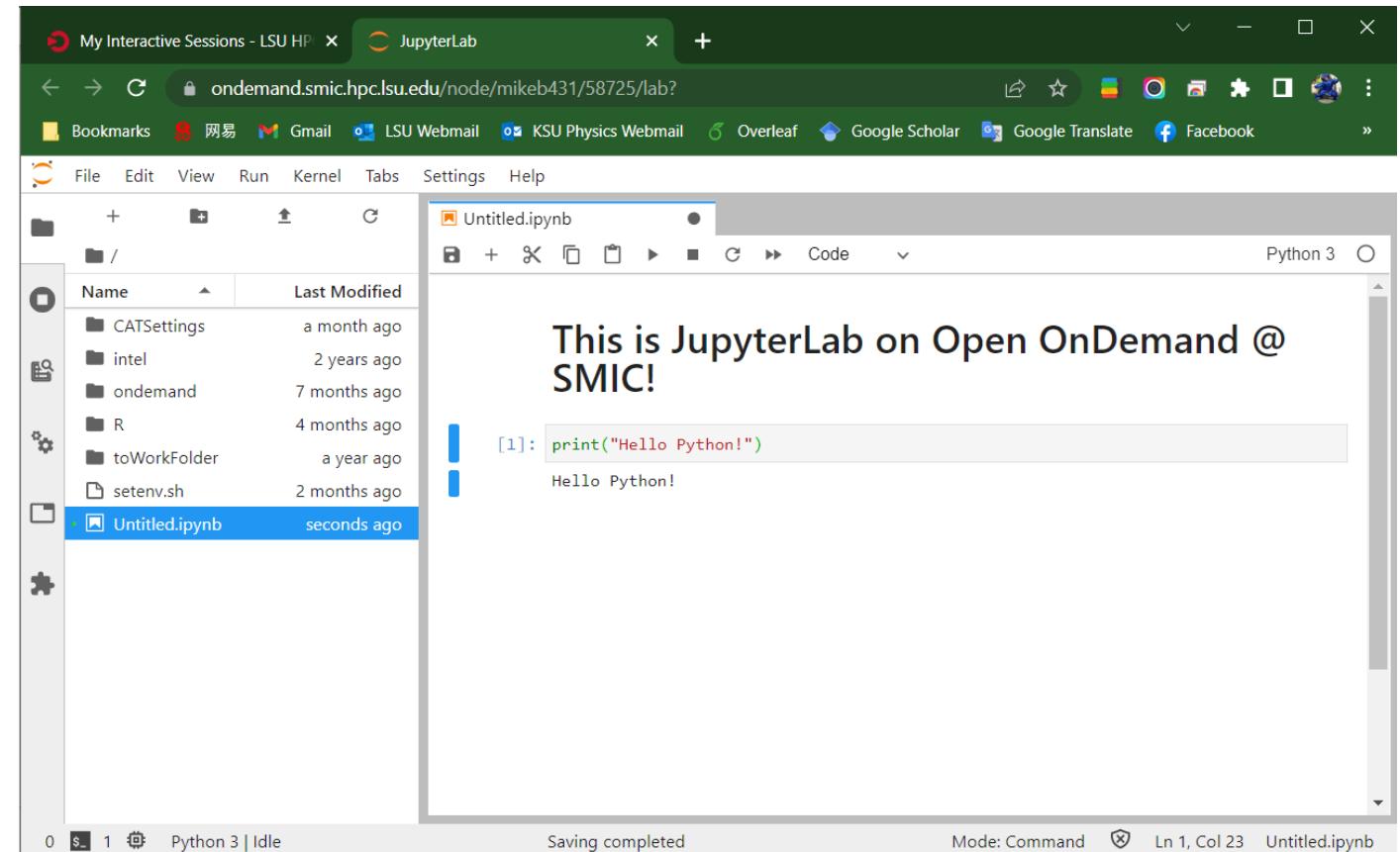
At the bottom of the terminal window, it says "UNREGISTERED VERSION - Please support MobaXterm by subscribing to the professional edition here: <https://mobaxterm.com>".

## 2) Ways to run Python on clusters

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### c) Jupyter Notebook / JupyterLab

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



The screenshot shows a web browser window titled "JupyterLab" with the URL "ondemand.smic.hpc.lsu.edu/node/mikeb431/58725/lab?". The browser toolbar includes links for Bookmarks, LSU Webmail, KSU Physics Webmail, Overleaf, Google Scholar, Google Translate, and Facebook. The JupyterLab interface has a sidebar showing a file tree with folders like CATSettings, intel, ondemand, R, toWorkFolder, and setenv.sh, and a file named "Untitled.ipynb" which was saved "seconds ago". The main area displays a code cell with the Python command `print("Hello Python!")`, which has been executed and printed the output "Hello Python!". A message in the center of the interface reads "This is JupyterLab on Open OnDemand @ SMIC!". The status bar at the bottom indicates "Saving completed", "Mode: Command", "Ln 1, Col 23", and "Untitled.ipynb".

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



## 2) Ways to run Python on clusters

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- a) Interactively (submit an **interactive job**)
- b) Python script (submit a **batch job**)
- c) Jupyter Notebook / JupyterLab (**Open OnDemand**)

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<https://github.com/qmpotential/Python101/blob/main/Python101.ipynb>