

Introduction to python™

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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?

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

Python 2.x

Python 3.x

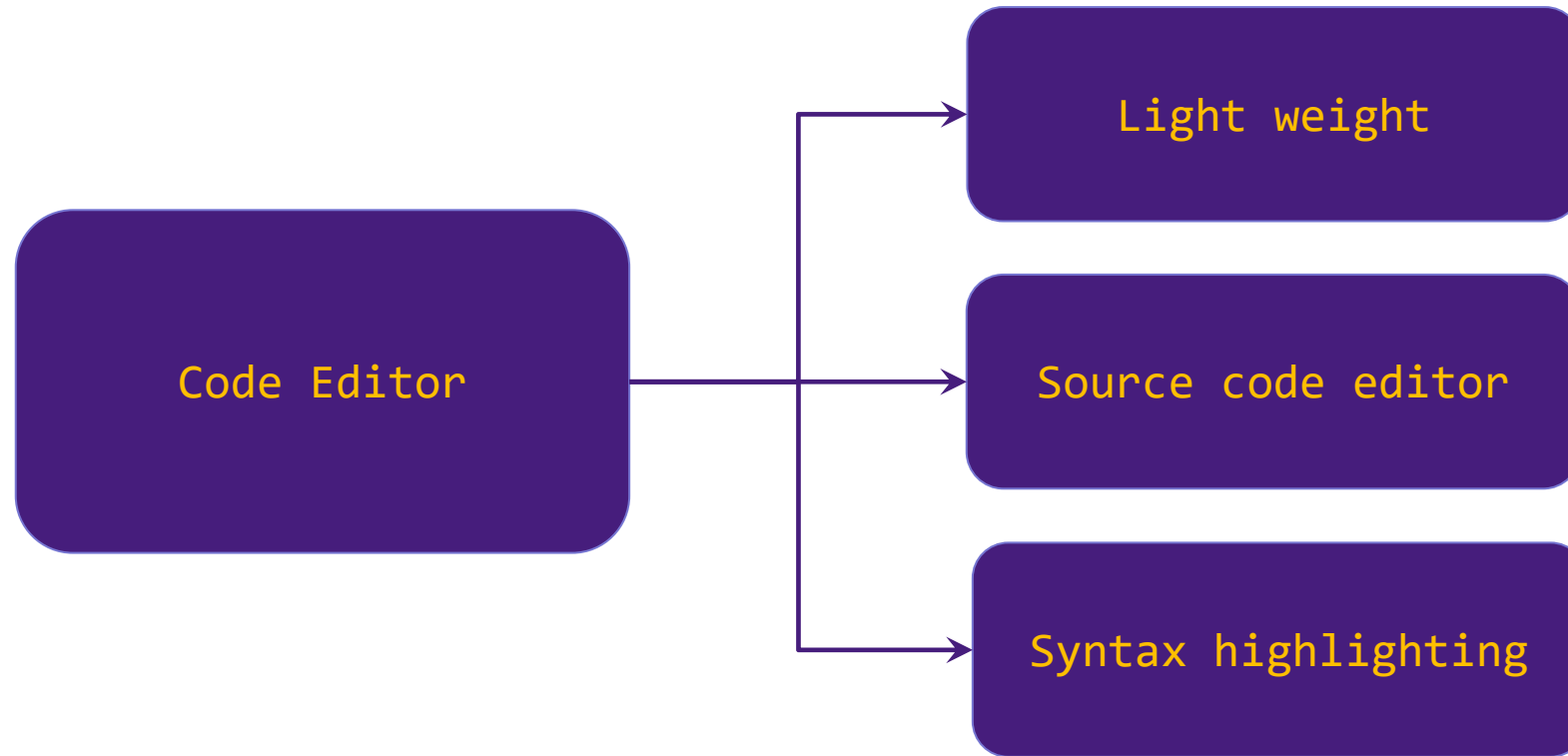
<http://python.org>

1) Programming tools

Code Editor

Integrated
Development
Environment
(IDE)

1) What is the Code Editor





Atom

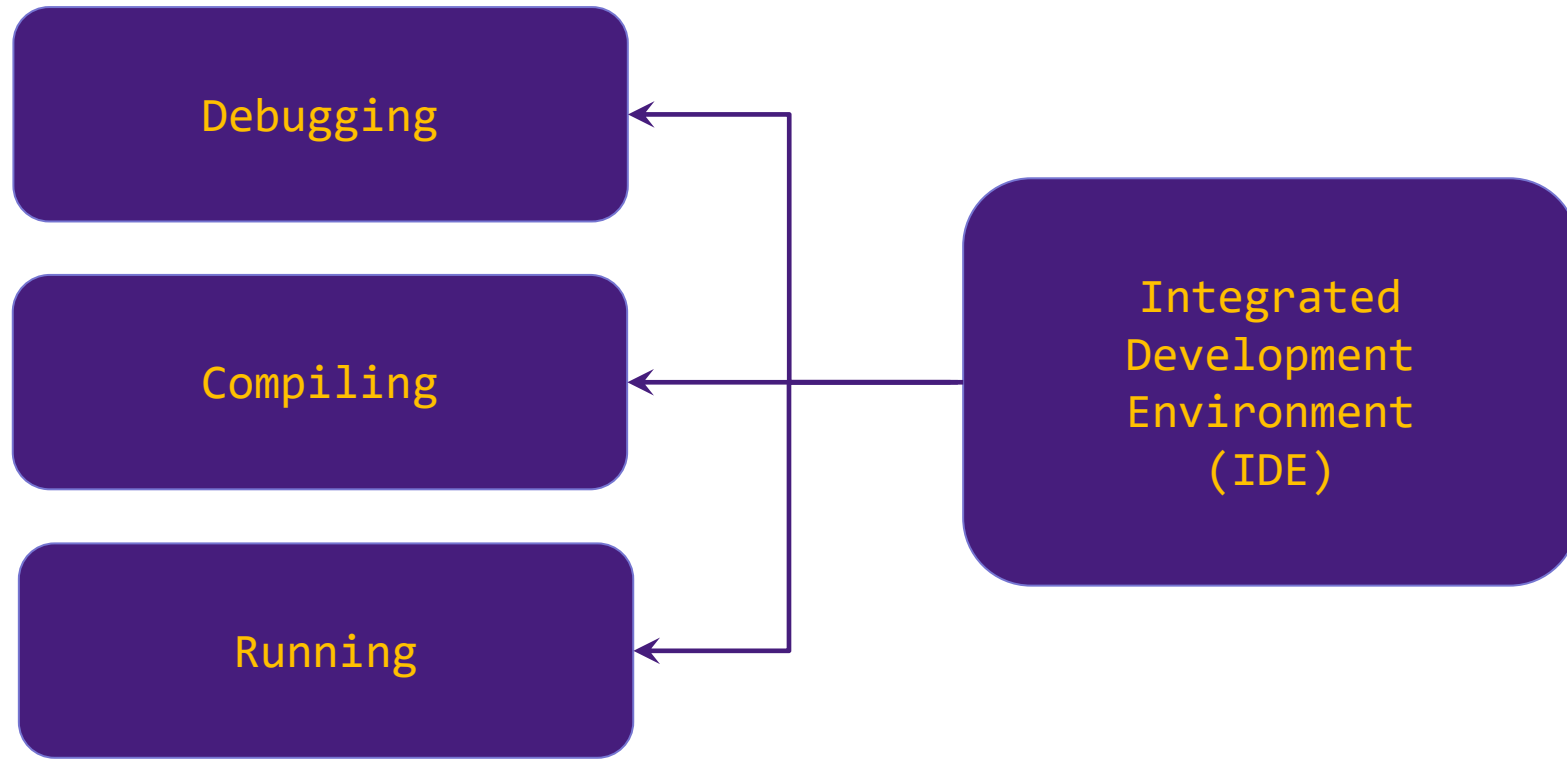


Sublime Text



VS Code

1) What is the Integrated Development Environment



1) Integrated Development Environment Features

Linting

Autocompletion

Debugging

Unit Testing

Code Formatting

Code Snippets

1) Integrated Development Environment



IDLE



PyCharm IDE



Spyder



- **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

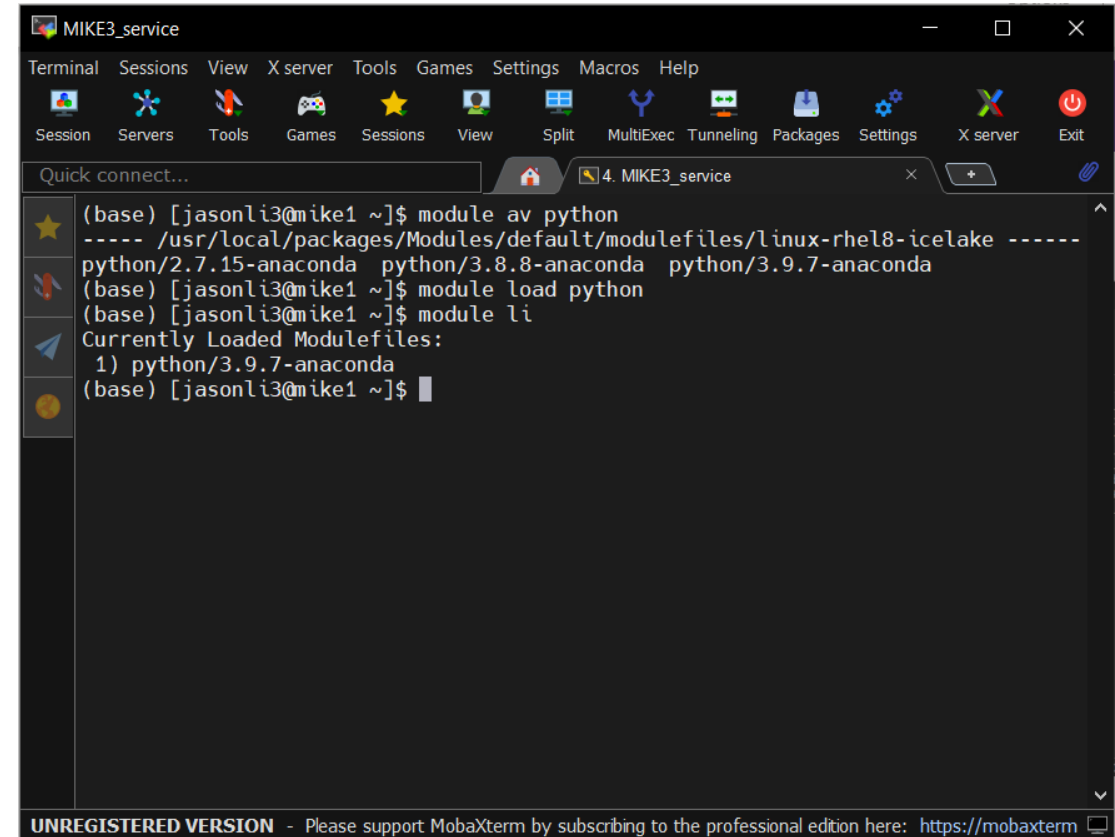
- Python installation on HPC clusters

- ❑ Modules

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

- ❑ Customized version: Conda virtual environment

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



```
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 ~]$
```

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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

a) Interactively

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

```
(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 SUs: 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

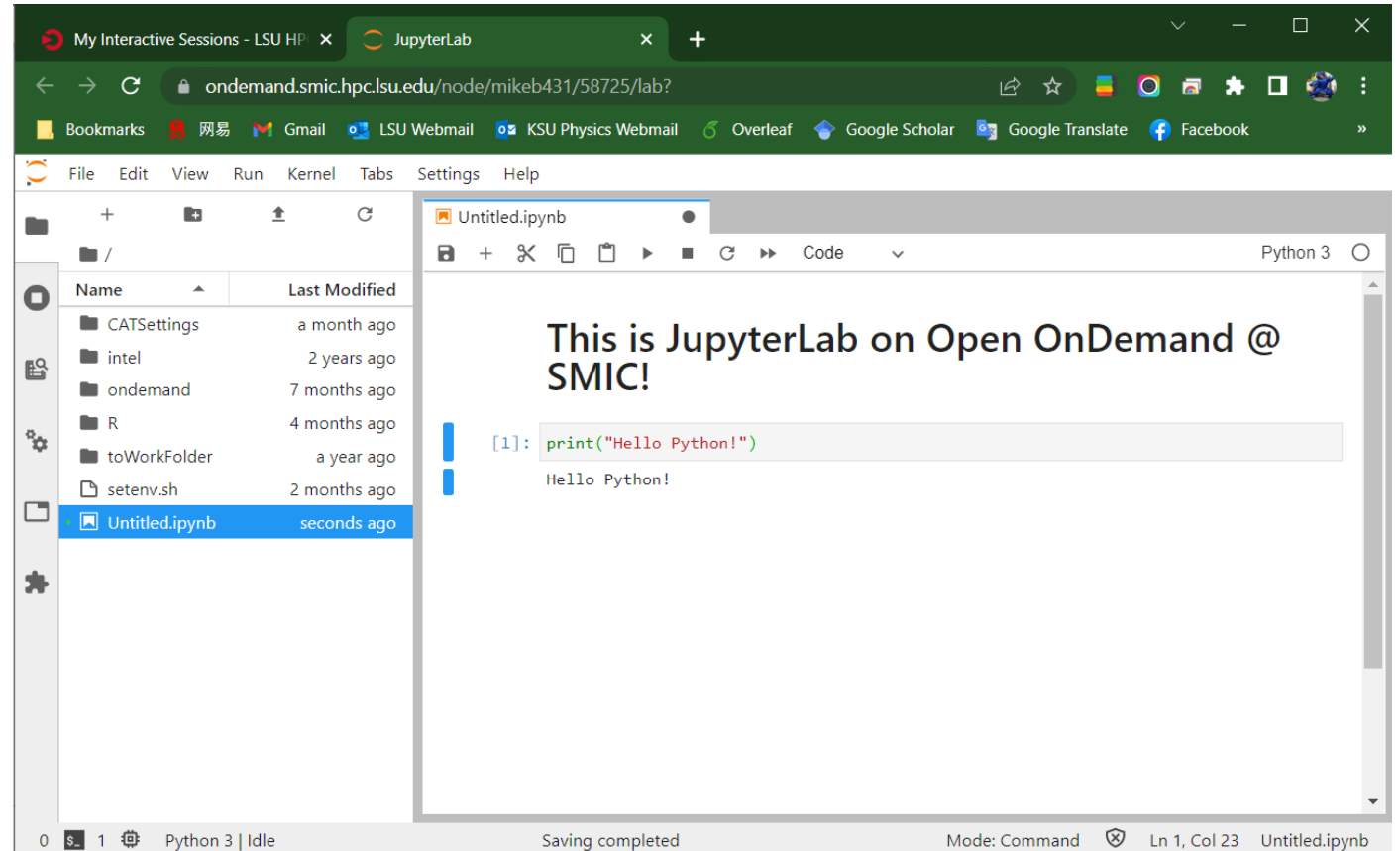
iii. Submit batch job

iv. Results

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>



2) Ways to run Python on clusters

- 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>