Introduction to python™

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About this training

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

- **What to expect**
  - √ Basic knowledge of Python
  - × Advanced programming

Outline

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

Machine learning

Desktop applications

Web applications

Mobile applications

Automatic scripts

1) Python versions

Python 2.x

Python 3.x

1) Python reference

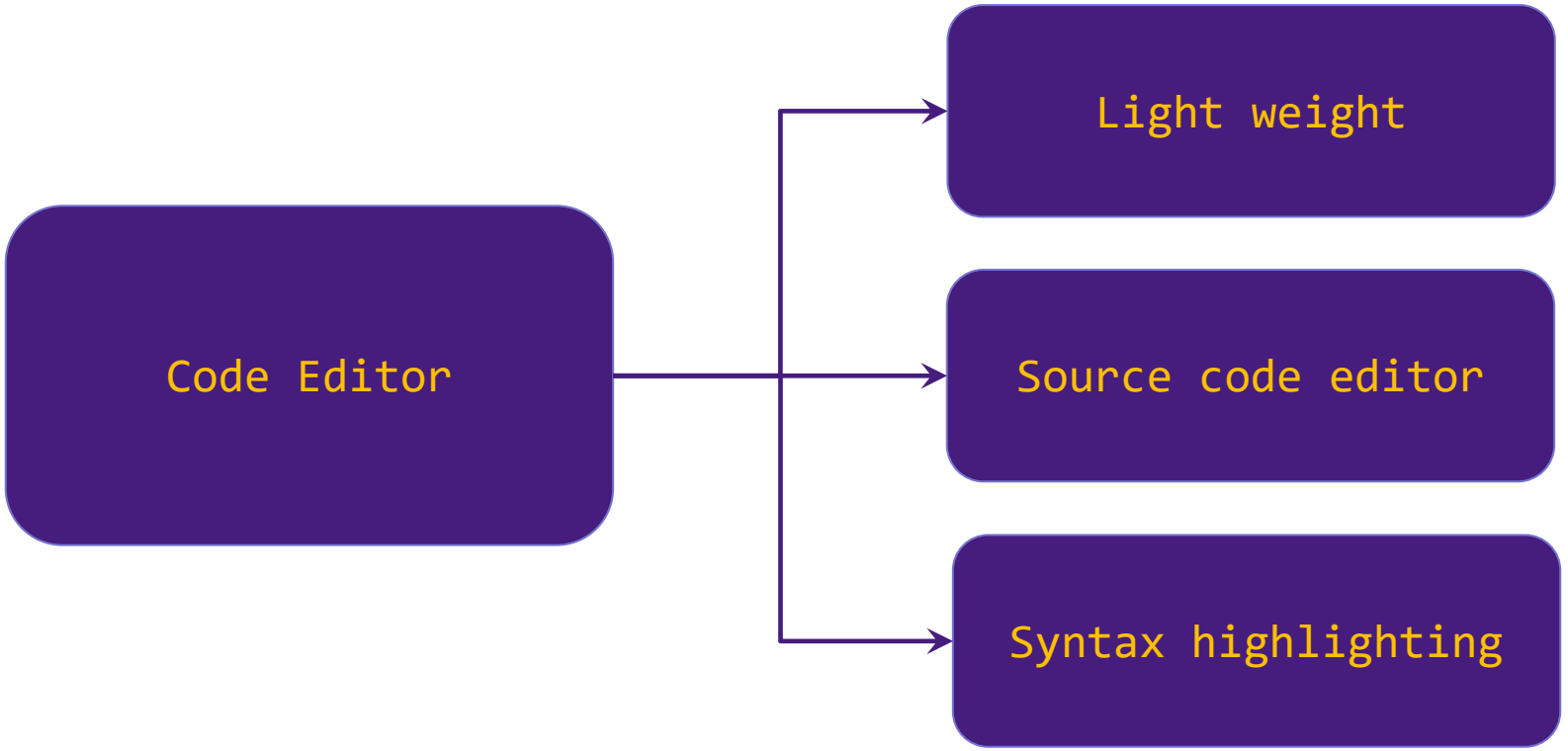
http://python.org

1) Programming tools

Code Editor

Integrated Development Environment (IDE)

1) What is the Code Editor



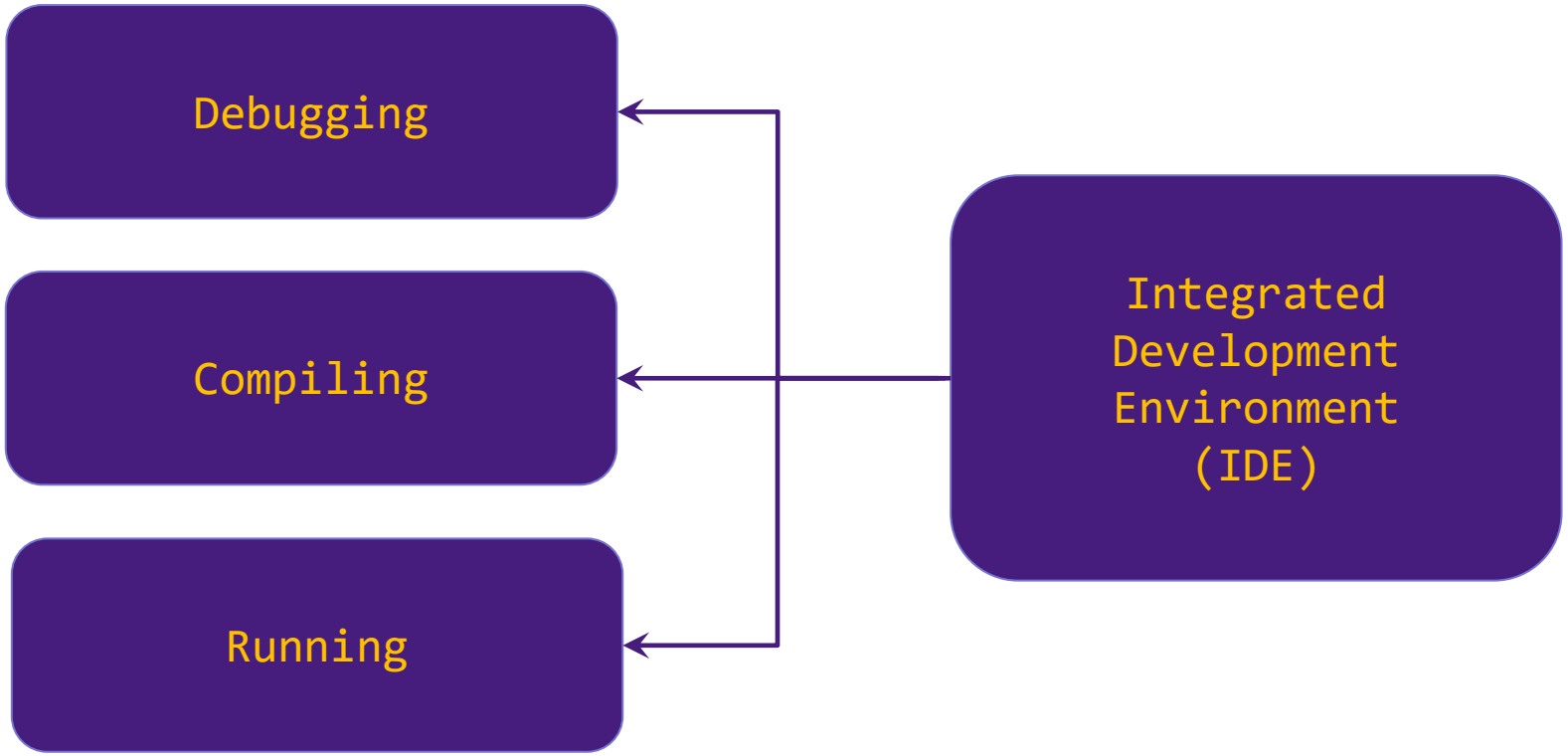
1) Code editors

Atom

Sublime Text

VS Code

1) What is the Integrated Development Environment



1) Integrated Development Environment Features

- Linting
- Autocompletion
- Debugging
- Unit Testing
- Code Formatting
- Code Snippets

1) Integrated Development Environment

IDLE

PyCharm IDE

Spyder

1) Integrated Development Environment

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 Python

- **Running on local machine?**

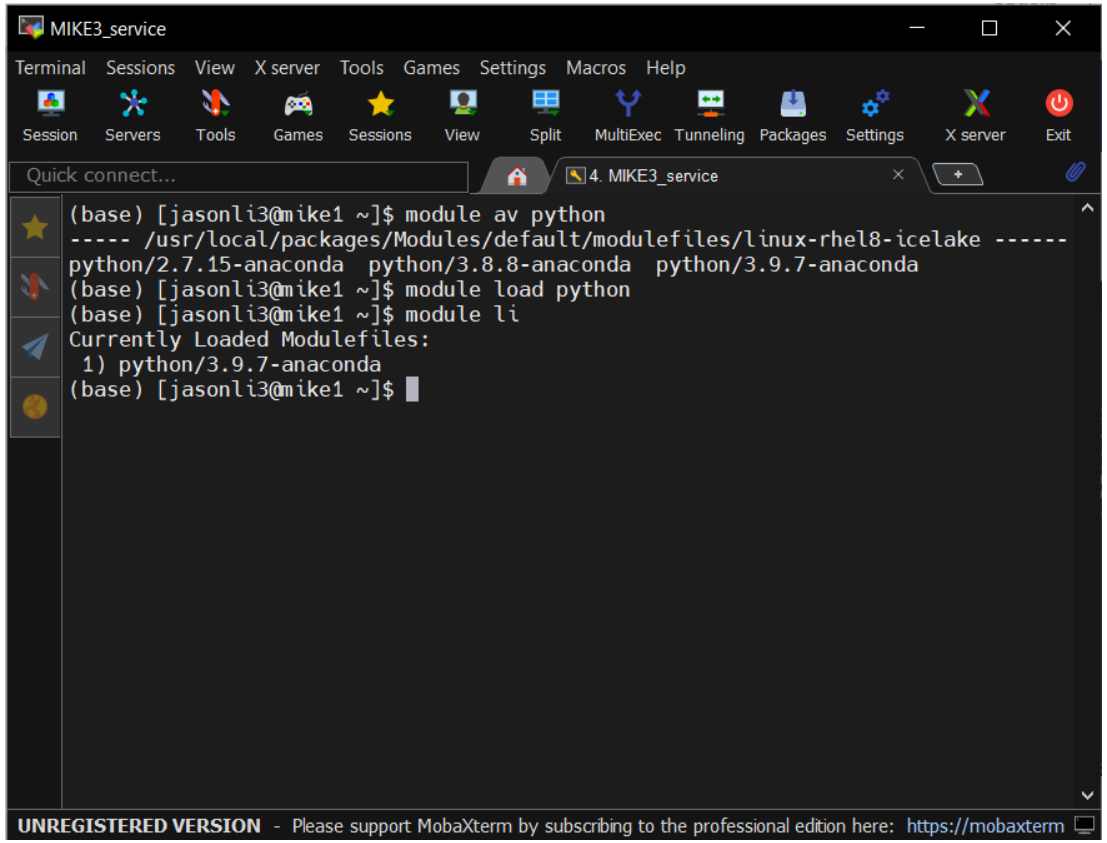
  a) Terminal (command-line)
  b) GUI (Spyder)
  c) Jupyter Notebook (web-interface)
  d) …

1) Load python

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



[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

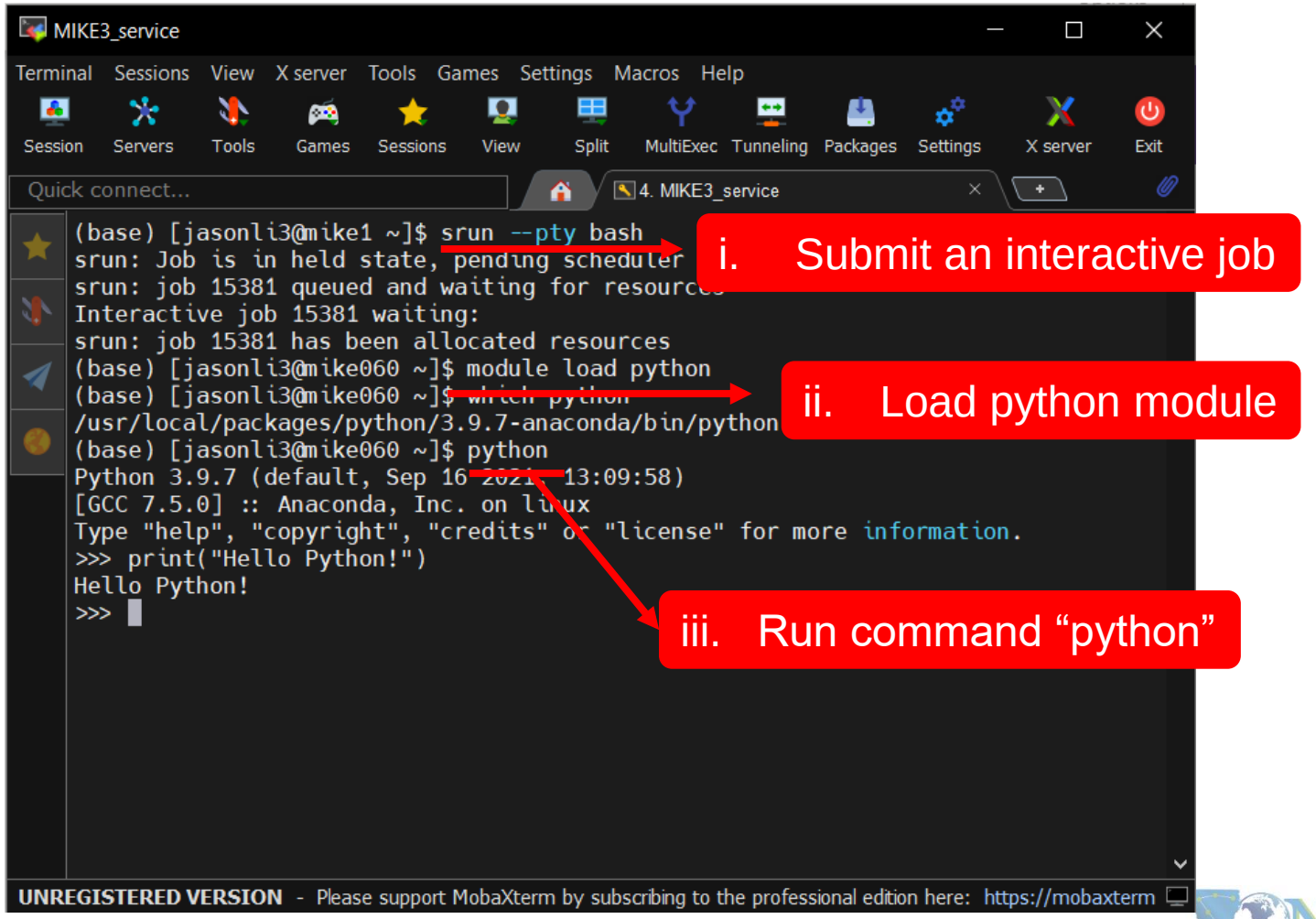
- **Unlike using your local machine:**

Must submit a job!!!

2) Ways to run Python on clusters

a) Interactively

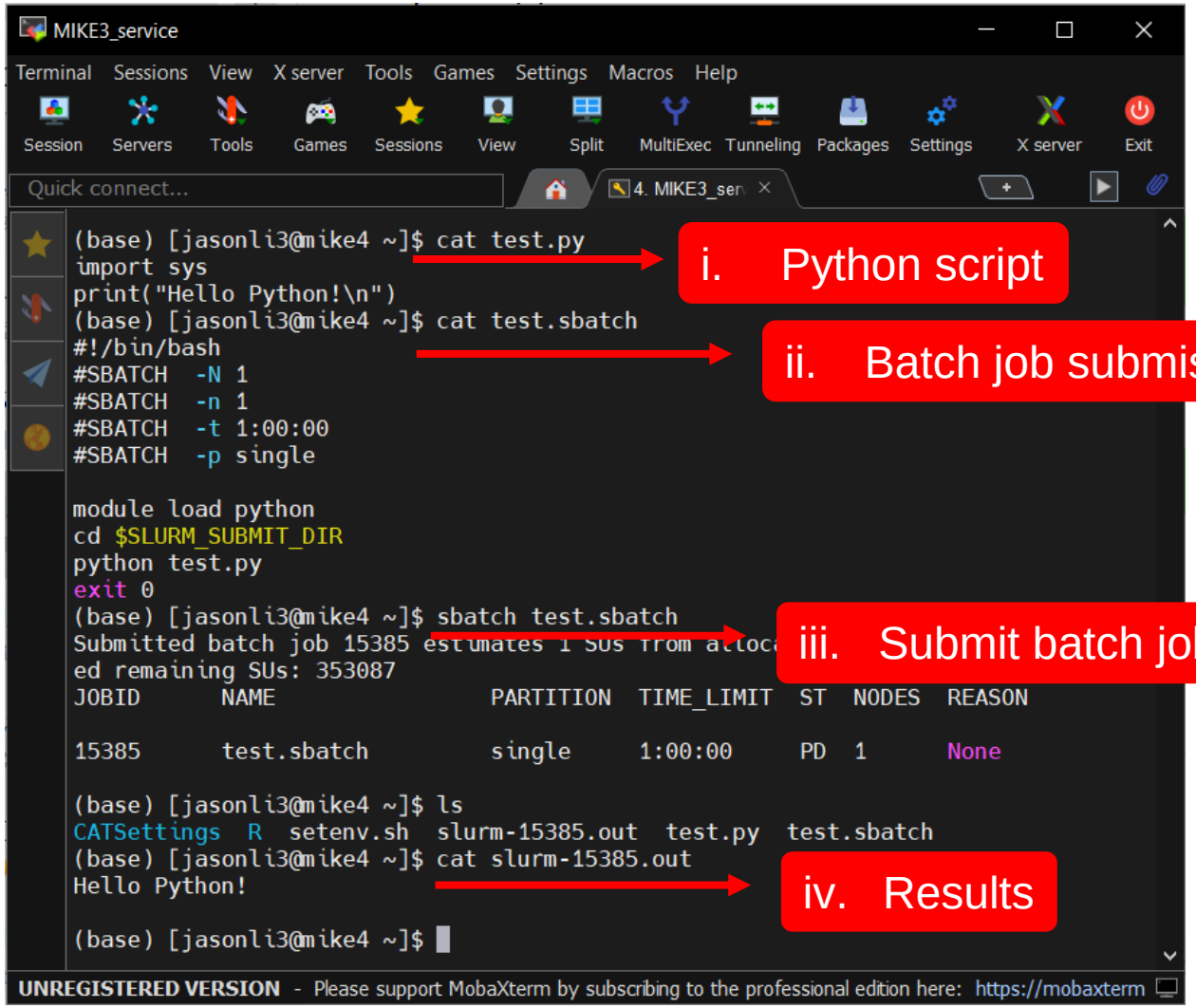
* Must submit an **interactive job**
* Make sure you are **NOT** running on head node!



2) Ways to run Python on clusters

b) Python script

* Must submit a **batch job**

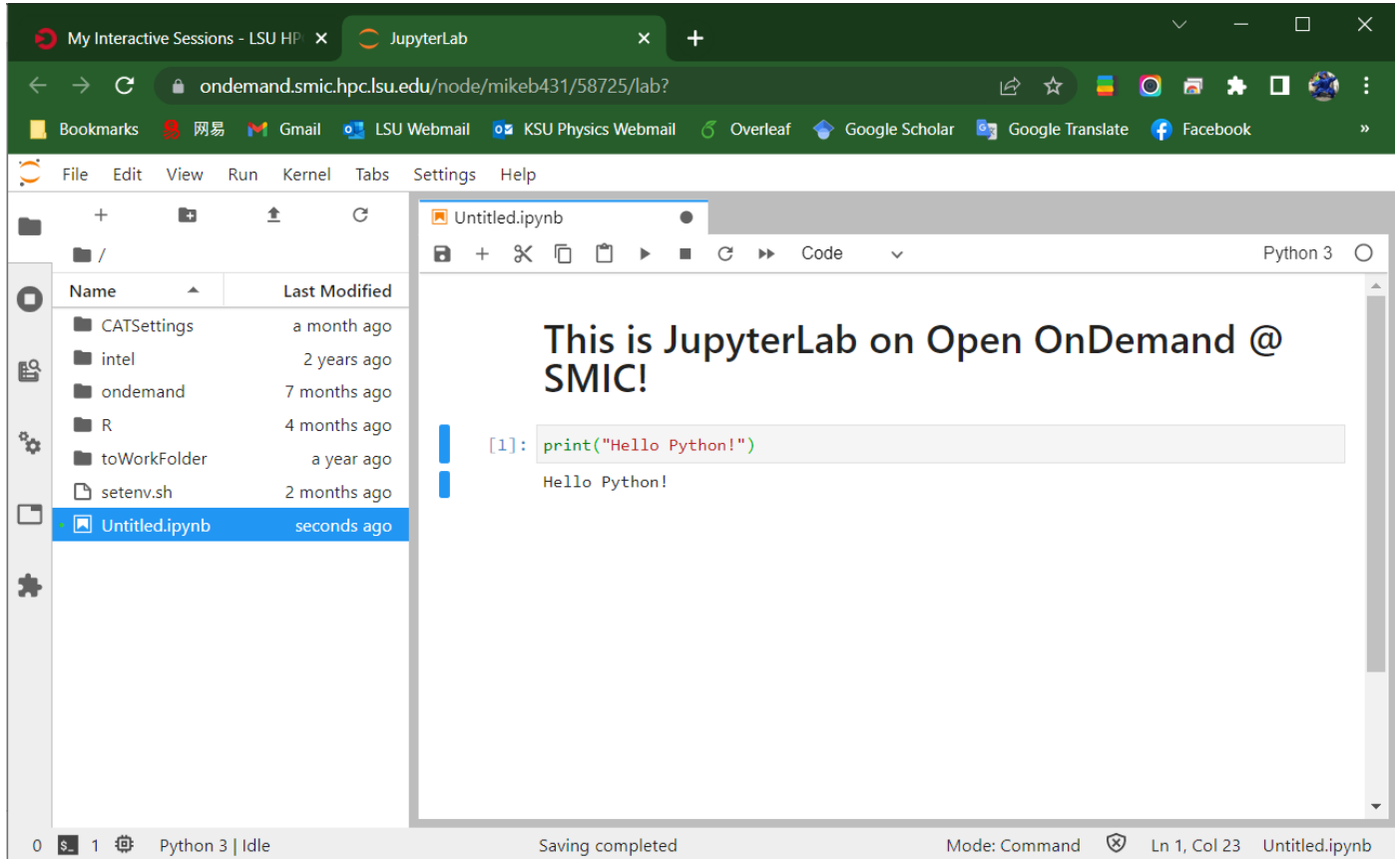


2) Ways to run Python on clusters

c) Jupyter Notebook / JupyterLab

* Must use **Open OnDemand** via web browser

* Currently only available on SMIC: https://ondemand.smic.hpc.lsu.edu/



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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