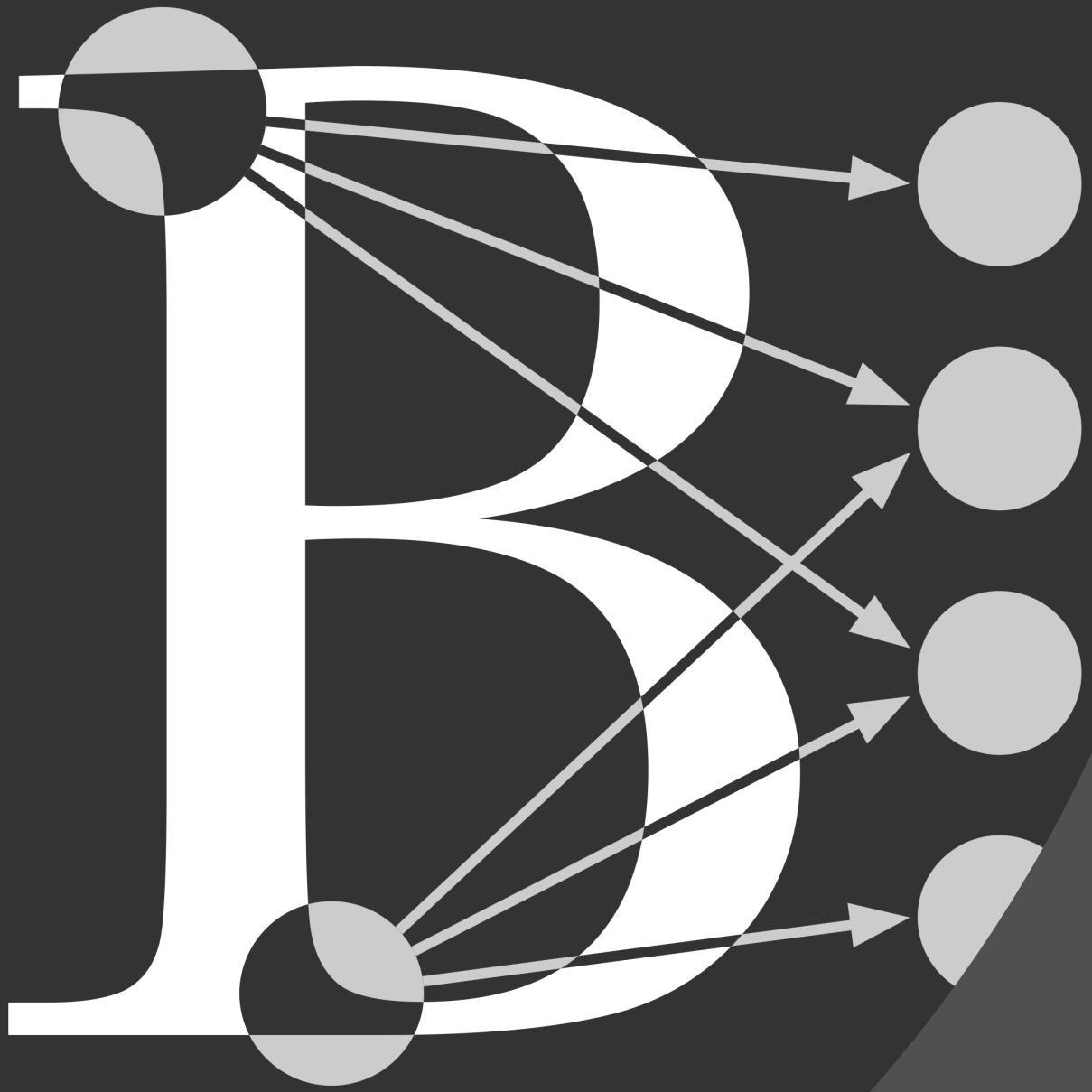


Baskerville Portal

EPSRC Tier 2 HPC System

University of Birmingham

Overview

1. What is Baskerville Portal?
2. Connect and Configure Baskerville Portal
3. JupyterLab
    a) Module Loading
    b) Conda Environments
4. Final Task: Build PyTorch in a Conda Environment

1. What is Baskerville Portal?

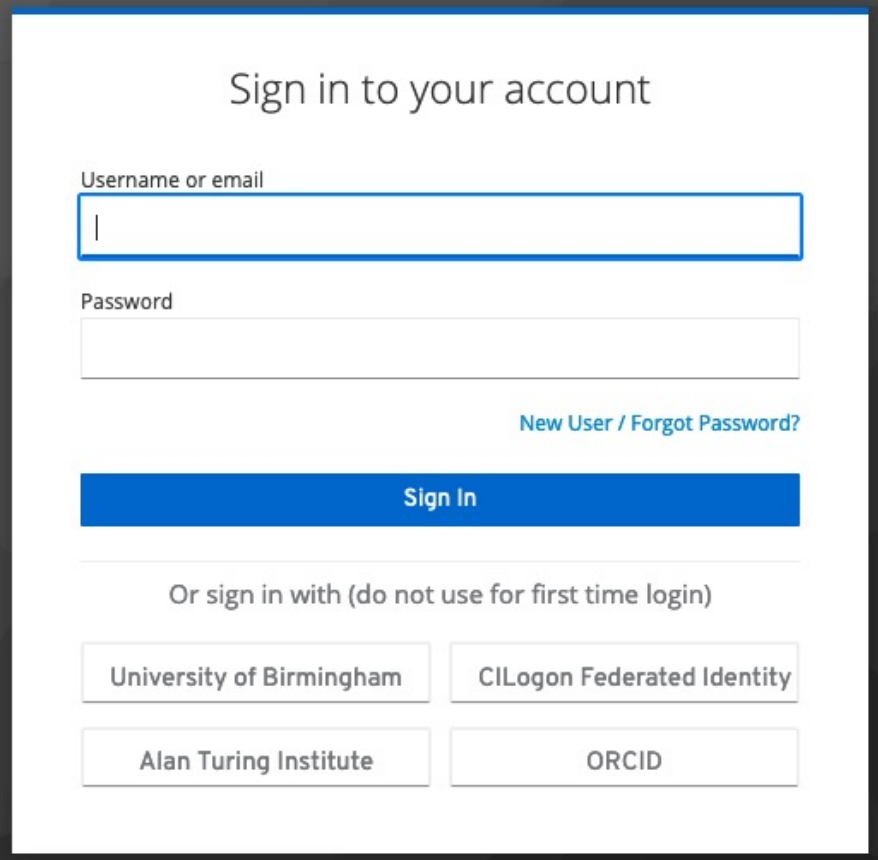
The Baskerville portal provides web-based access to the Baskerville Tier 2 system

This service is operated by Advanced Research Computing at the University of Birmingham and is funded by EPSRC Grant EP/T022221/1

portal.baskerville.ac.uk/

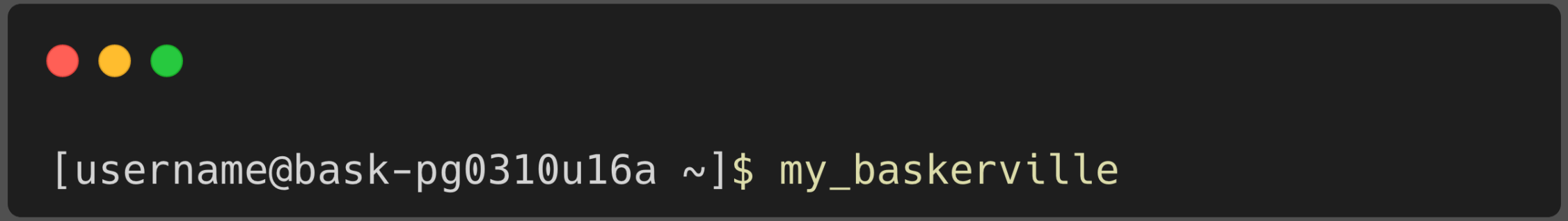
2. Connect and Configure Baskerville Portal

BASKERVILLE



Open a Terminal

Click Clusters > Baskerville Tier 2 HPC Shell Access, enter your Password and OTP to access a Terminal.



to see information about your Baskerville projects and available QoS.

This information is also available at **admin.baskerville.ac.uk/.**

Note: OTP – One Time Passcode, QoS – Quality of Service/Queue

Your home folder | 20GB

```
[username@bask-pg0310u16a ~]$ pwd
/bask/homes/u/username
[username@bask-pg0310u16a ~]$ my_quota
Your home directory on Baskerville (/bask/homes
/u/username):
You are using 97.30 percent ( 19.48 GB ) of your total
quota 20.02 GB
```

Your project folder | 1TB

```
[username@bask-pg0310u16a ~]$ cd /bask/projects/m/myproject
[username@bask-pg0310u16a myproject]$ df -h .
Filesystem      Size  Used Avail Use% Mounted on
bask            1.0T   64M  1.0T   1% /bask
```

Symlink your home and project folder

- For JupyterLab, only the home folder is accessible from the GUI
- Solution - Access data in your project folder from your home folder via a symbolic link. Configure this with:

```
[username@bask-pg0310u16a ~]$ ln -s /bask/projects
/m/myproject ~/myproject
```

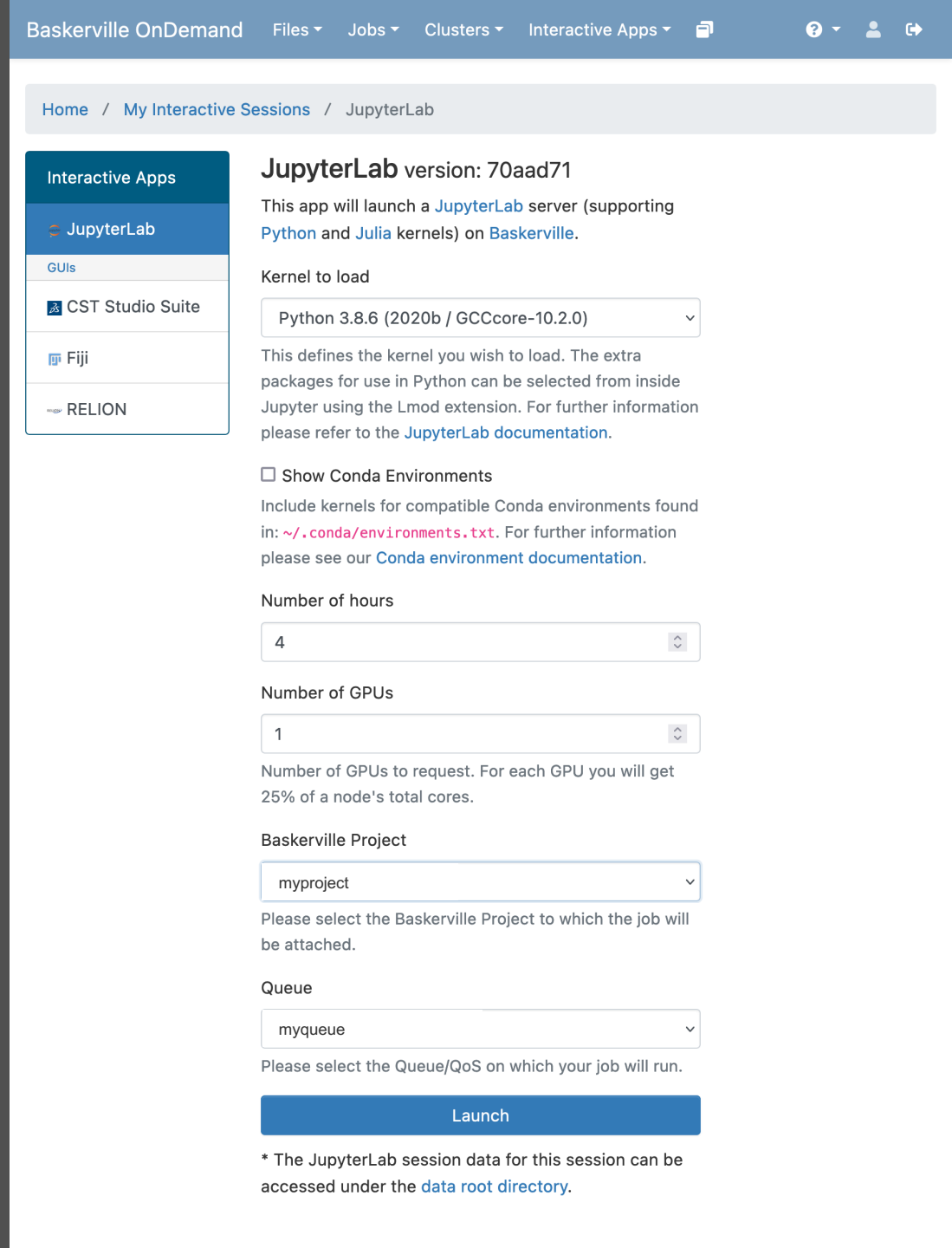
baskstatus - Query Available GPUs

```
username@bask-pg0310u16a myproject]$ baskstatus
Current Baskerville GPU availability:
 * 1 node with 3 x A100-40 available
 * 10 nodes with 1 x A100-40 available
 * 2 nodes with 4 x A100-80 available
 * 1 node with 2 x A100-80 available
```

3. JupyterLab

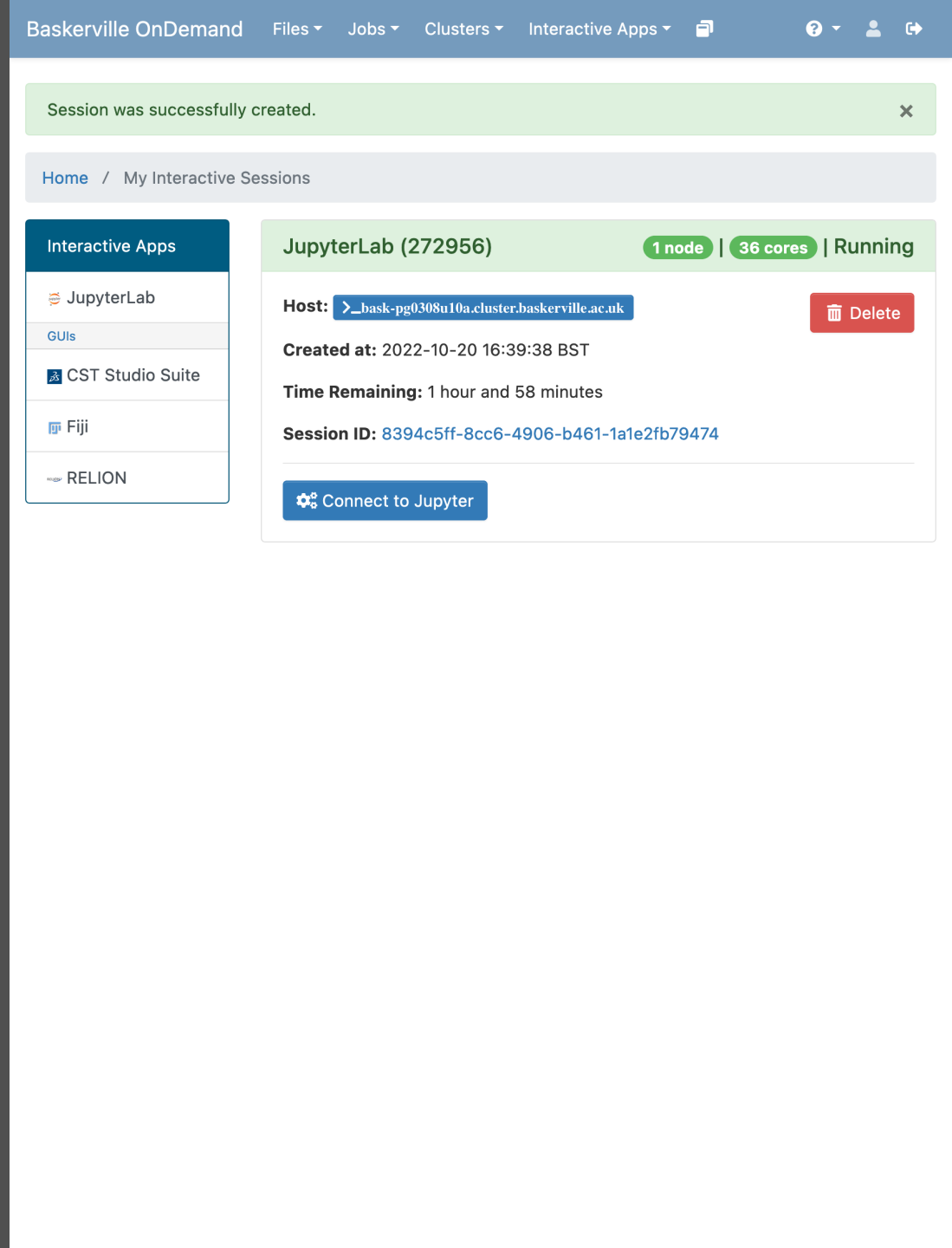
Launch a JupyterLab server

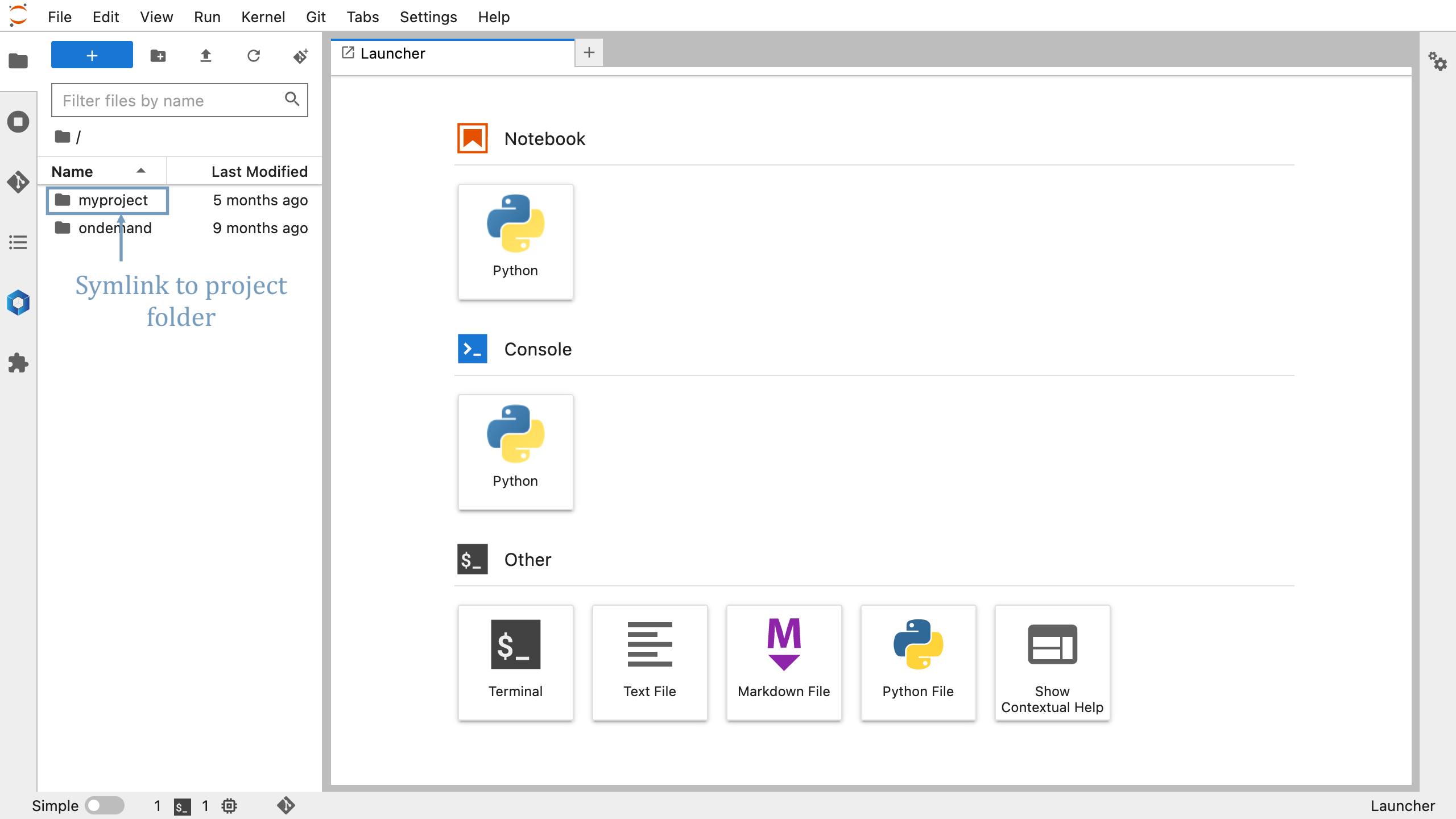
- Click Interactive Apps > JupyterLab
- Load Python kernel
- Request Resources - number of hours and number of GPUs
- Select Project and Queue
- Click Launch to launch JupyterLab server

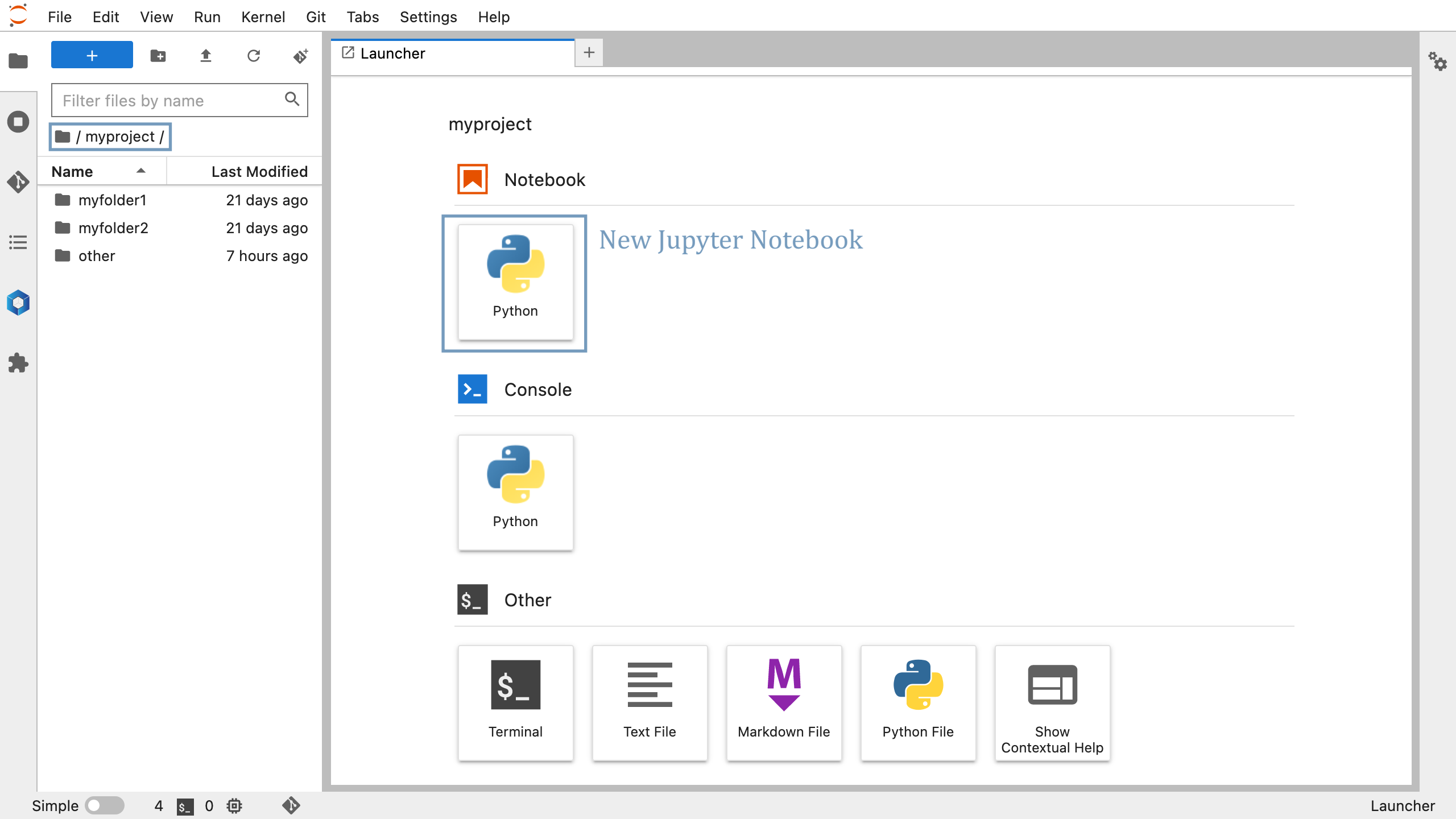


Launch a JupyterLab server

- Wait time depends on number of GPUs requested and time requested
- Each node has 4 GPUs available, with 36 CPU cores per GPU
- Once loaded, click Connect to Jupyter




File
Edit
View
Run
Kernel
Git
Tabs
Settings
Help
Launcher
Filter files by name
/
Name
Last Modified
myproject
5 months ago
ondemand
9 months ago
Symlink to project folder
Notebook
Python
Console
Python
Other
Terminal
Text File
Markdown File
Python File
Show Contextual Help
Simple
1
1
Launcher


File
Edit
View
Run
Kernel
Git
Tabs
Settings
Help
Launcher
Filter files by name
/ myproject /
Name
Last Modified
myfolder1
21 days ago
myfolder2
21 days ago
other
7 hours ago
myproject
Notebook
Python
New Jupyter Notebook
Console
Python
Other
Terminal
Text File
Markdown File
Python File
Show Contextual Help
Simple
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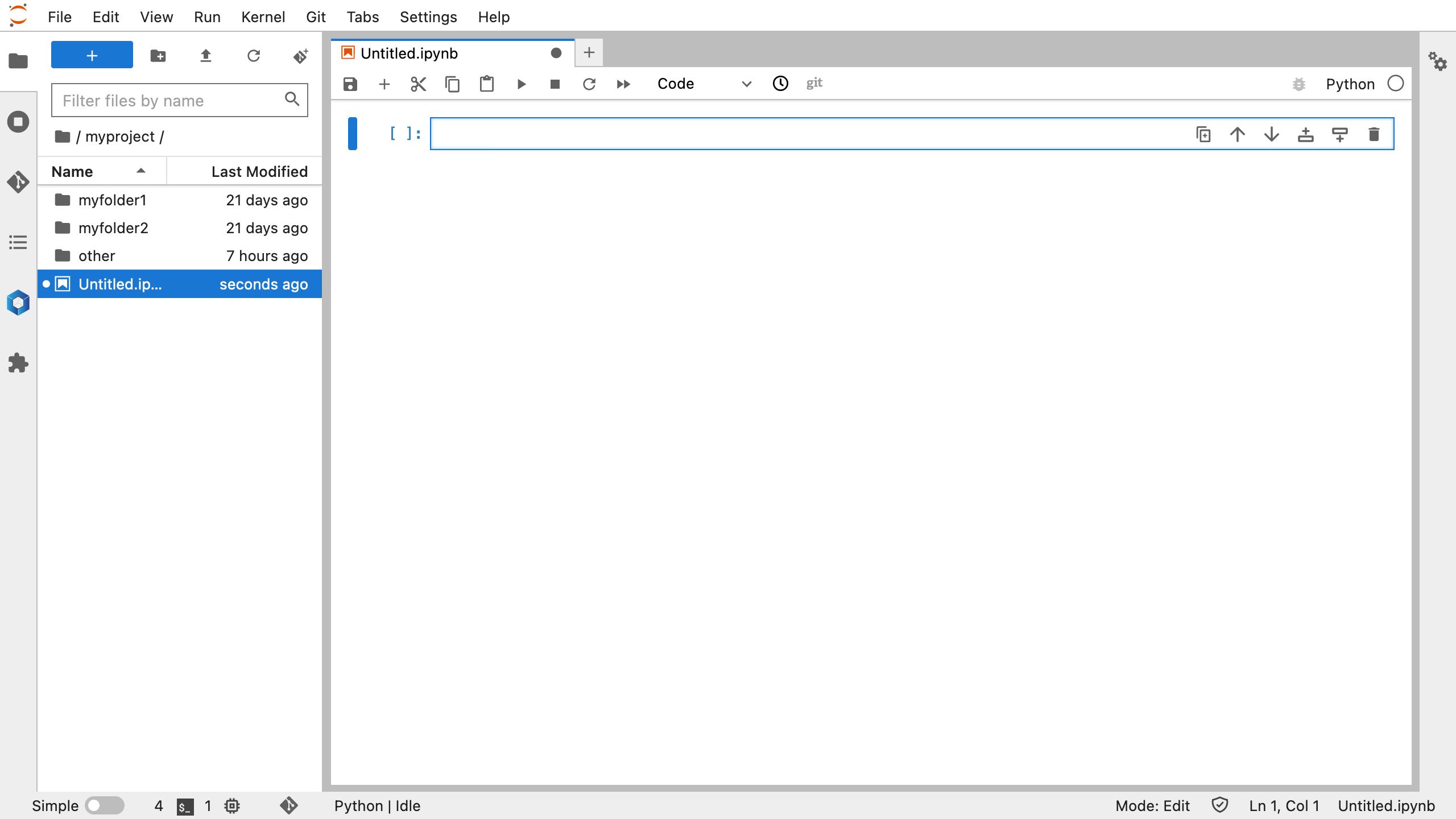
0
Launcher


File
Edit
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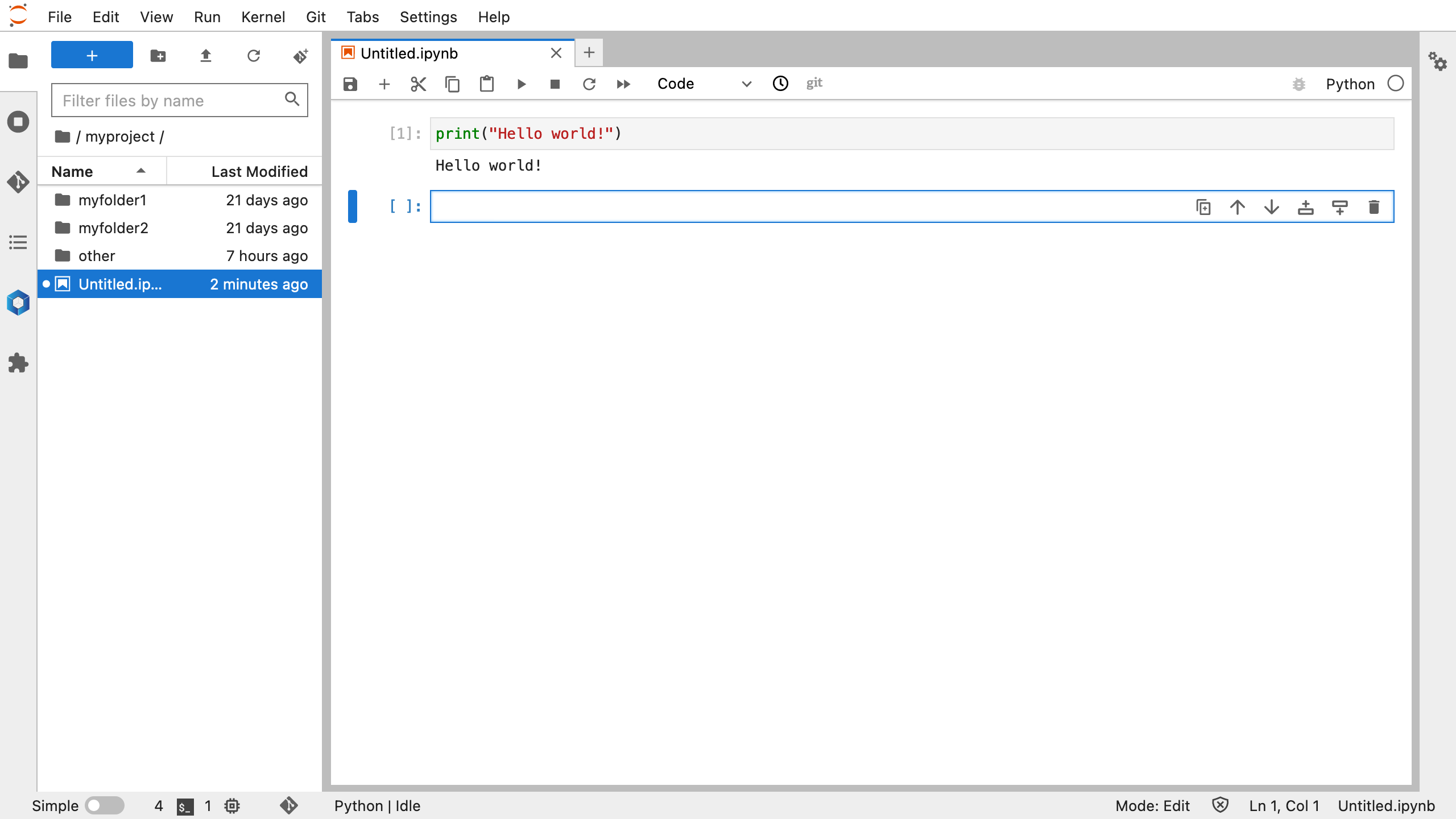
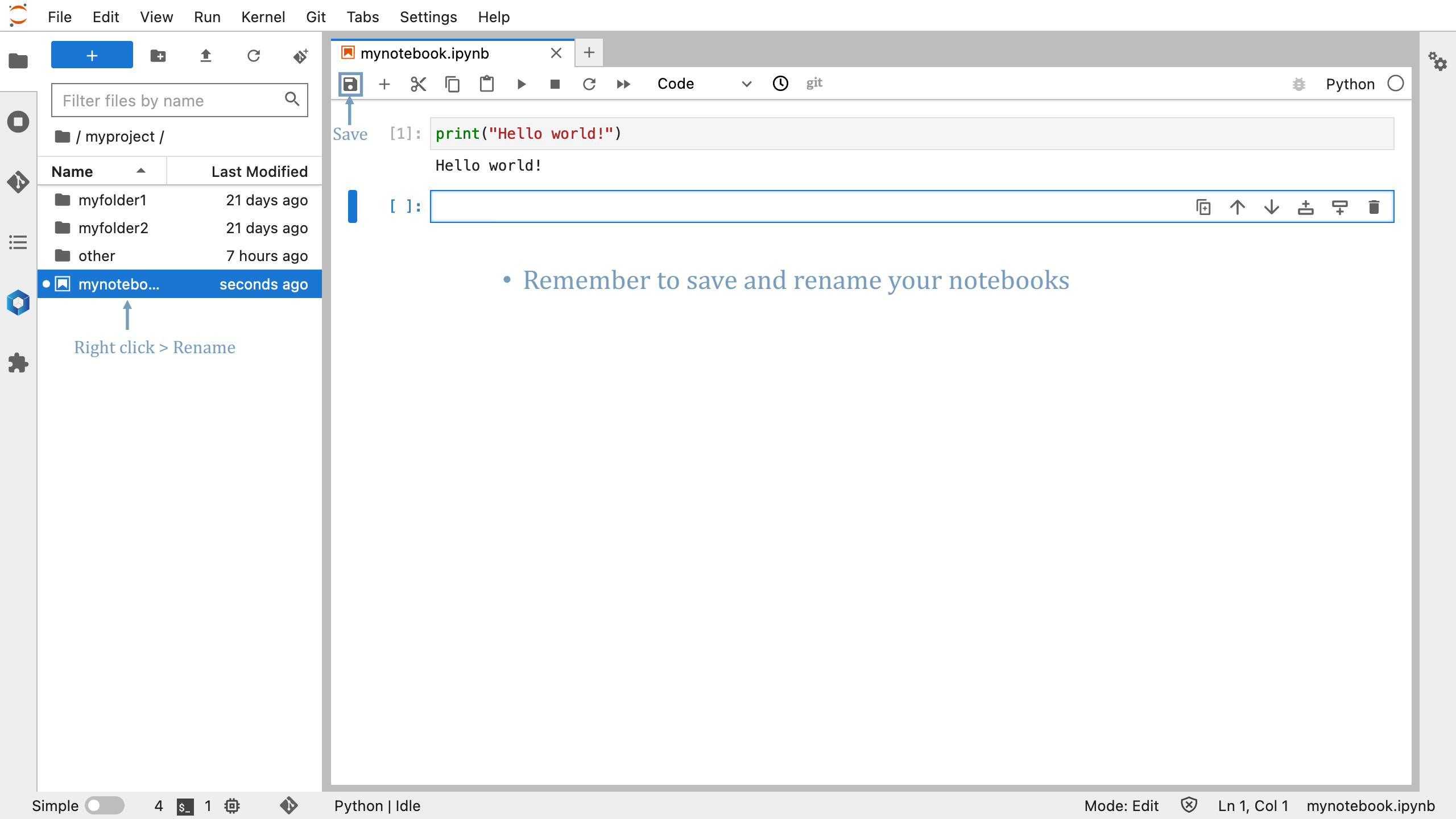
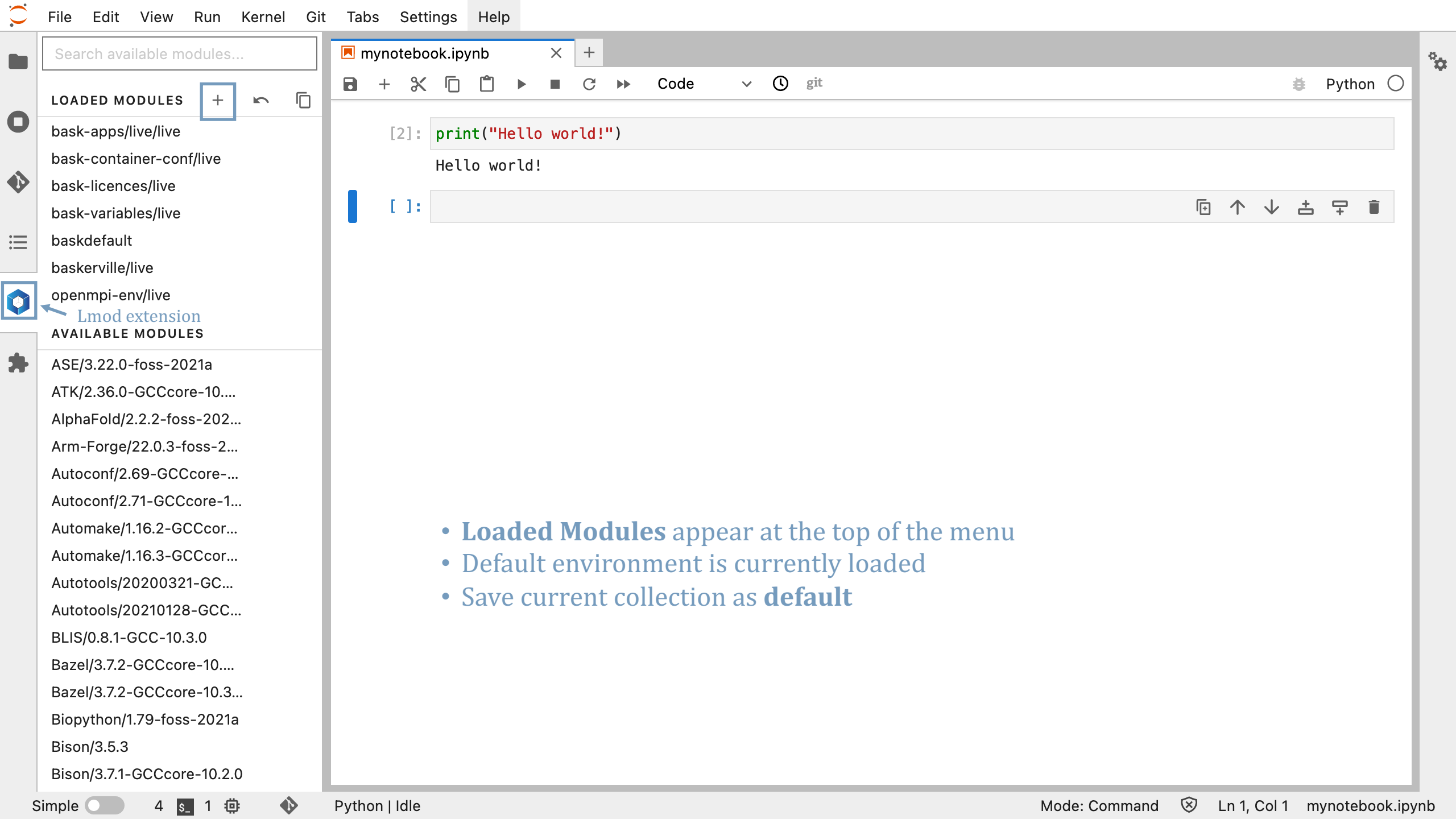
Kernel
Git
Tabs
Settings
Help
Filter files by name
/ myproject /
Name
Last Modified
myfolder1
21 days ago
myfolder2
21 days ago
other
7 hours ago
Untitled.ip...
seconds ago
Untitled.ipynb
Code
git
Python
[ ]:
Simple
4
1
Python | Idle
Mode: Edit
Ln 1, Col 1
Untitled.ipynb


File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
myfolder1 21 days ago
myfolder2 21 days ago
other 7 hours ago
Untitled.ip... 2 minutes ago
Untitled.ipynb
Code
git
Python
[1]: print("Hello world!")
Hello world!
[ ]:
Simple 4 1 Python | Idle Mode: Edit Ln 1, Col 1 Untitled.ipynb


File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
myfolder1 21 days ago
myfolder2 21 days ago
other 7 hours ago
mynotebo... seconds ago
Right click > Rename
mynotebook.ipynb
Code
git
Python
Save
[1]:
print("Hello world!")
Hello world!
[ ]:
• Remember to save and rename your notebooks
Simple
4
1
Python | Idle
Mode: Edit
Ln 1, Col 1
mynotebook.ipynb

a) Module Loading

- Module applications available include
    - PyTorch
    - TensorFlow
    - Keras
    - Dask
    - … and many more!
- See **apps.baskerville.ac.uk/applications/** for a complete list


File
Edit
View
Run
Kernel
Git
Tabs
Settings
Help
Search available modules...
LOADED MODULES
bask-apps/live/live
bask-container-conf/live
bask-licences/live
bask-variables/live
baskdefault
baskerville/live
openmpi-env/live
Lmod extension
AVAILABLE MODULES
ASE/3.22.0-foss-2021a
ATK/2.36.0-GCCcore-10....
AlphaFold/2.2.2-foss-202...
Arm-Forge/22.0.3-foss-2...
Autoconf/2.69-GCCcore-...
Autoconf/2.71-GCCcore-1...
Automake/1.16.2-GCCcor...
Automake/1.16.3-GCCcor...
Autotools/20200321-GC...
Autotools/20210128-GCC...
BLIS/0.8.1-GCC-10.3.0
Bazel/3.7.2-GCCcore-10....
Bazel/3.7.2-GCCcore-10.3...
Biopython/1.79-foss-2021a
Bison/3.5.3
Bison/3.7.1-GCCcore-10.2.0
mynotebook.ipynb
Code
git
Python
[2]:
print("Hello world!")
Hello world!
[ ]:
• Loaded Modules appear at the top of the menu
• Default environment is currently loaded
• Save current collection as default
Simple
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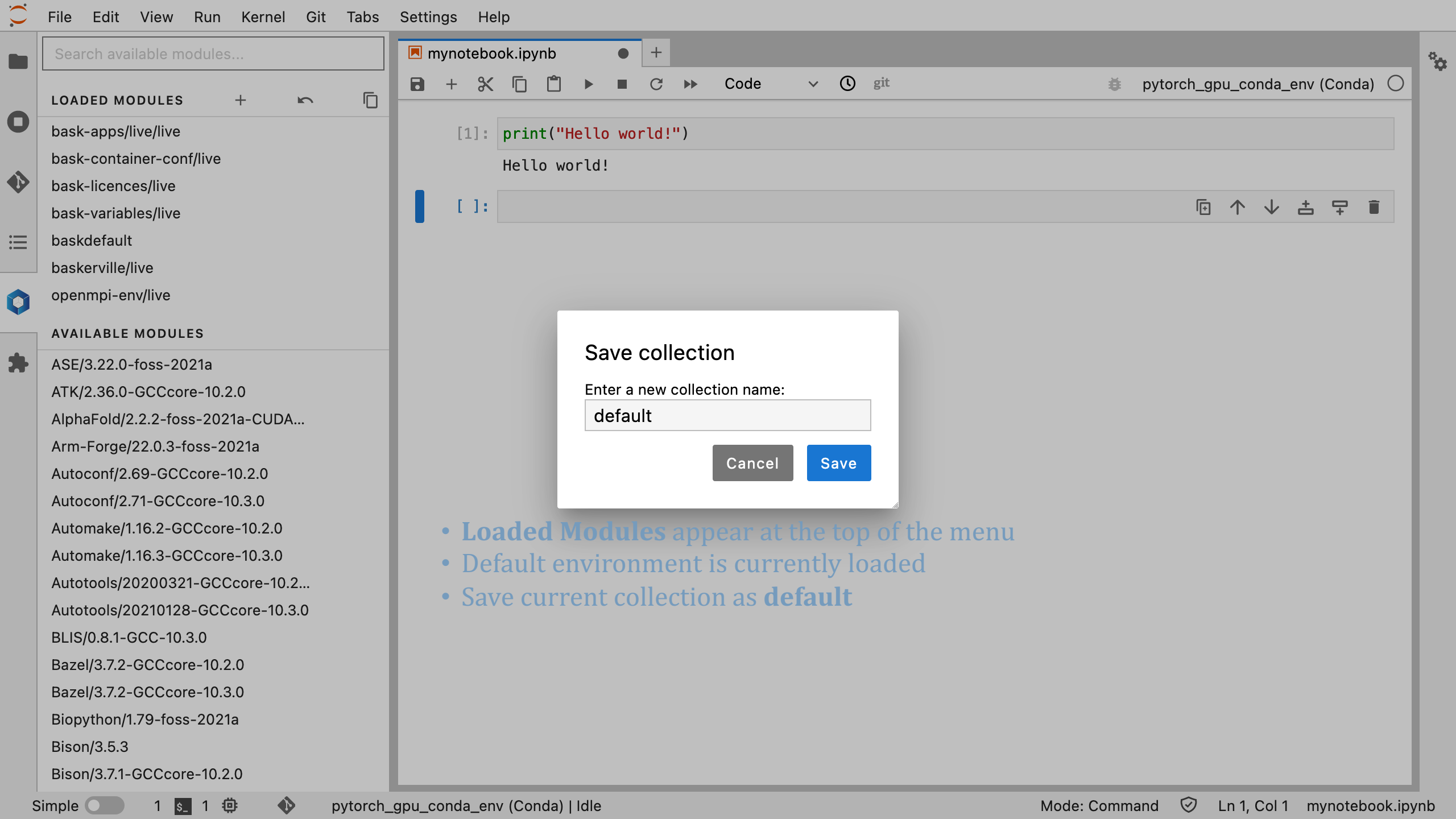
Python | Idle
Mode: Command
Ln 1, Col 1
mynotebook.ipynb


File Edit View Run Kernel Git Tabs Settings Help
Search available modules...
LOADED MODULES
bask-apps/live/live
bask-container-conf/live
bask-licences/live
bask-variables/live
baskdefault
baskerville/live
openmpi-env/live
AVAILABLE MODULES
ASE/3.22.0-foss-2021a
ATK/2.36.0-GCCcore-10.2.0
AlphaFold/2.2.2-foss-2021a-CUDA...
Arm-Forge/22.0.3-foss-2021a
Autoconf/2.69-GCCcore-10.2.0
Autoconf/2.71-GCCcore-10.3.0
Automake/1.16.2-GCCcore-10.2.0
Automake/1.16.3-GCCcore-10.3.0
Autotools/20200321-GCCcore-10.2...
Autotools/20210128-GCCcore-10.3.0
BLIS/0.8.1-GCC-10.3.0
Bazel/3.7.2-GCCcore-10.2.0
Bazel/3.7.2-GCCcore-10.3.0
Biopython/1.79-foss-2021a
Bison/3.5.3
Bison/3.7.1-GCCcore-10.2.0
mynotebook.ipynb
Code
git
pytorch_gpu_conda_env (Conda)
[1]: print("Hello world!")
Hello world!
[ ]:
Save collection
Enter a new collection name:
default
Cancel
Save
• Loaded Modules appear at the top of the menu
• Default environment is currently loaded
• Save current collection as default
Simple
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pytorch_gpu_conda_env (Conda) | Idle
Mode: Command
Ln 1, Col 1
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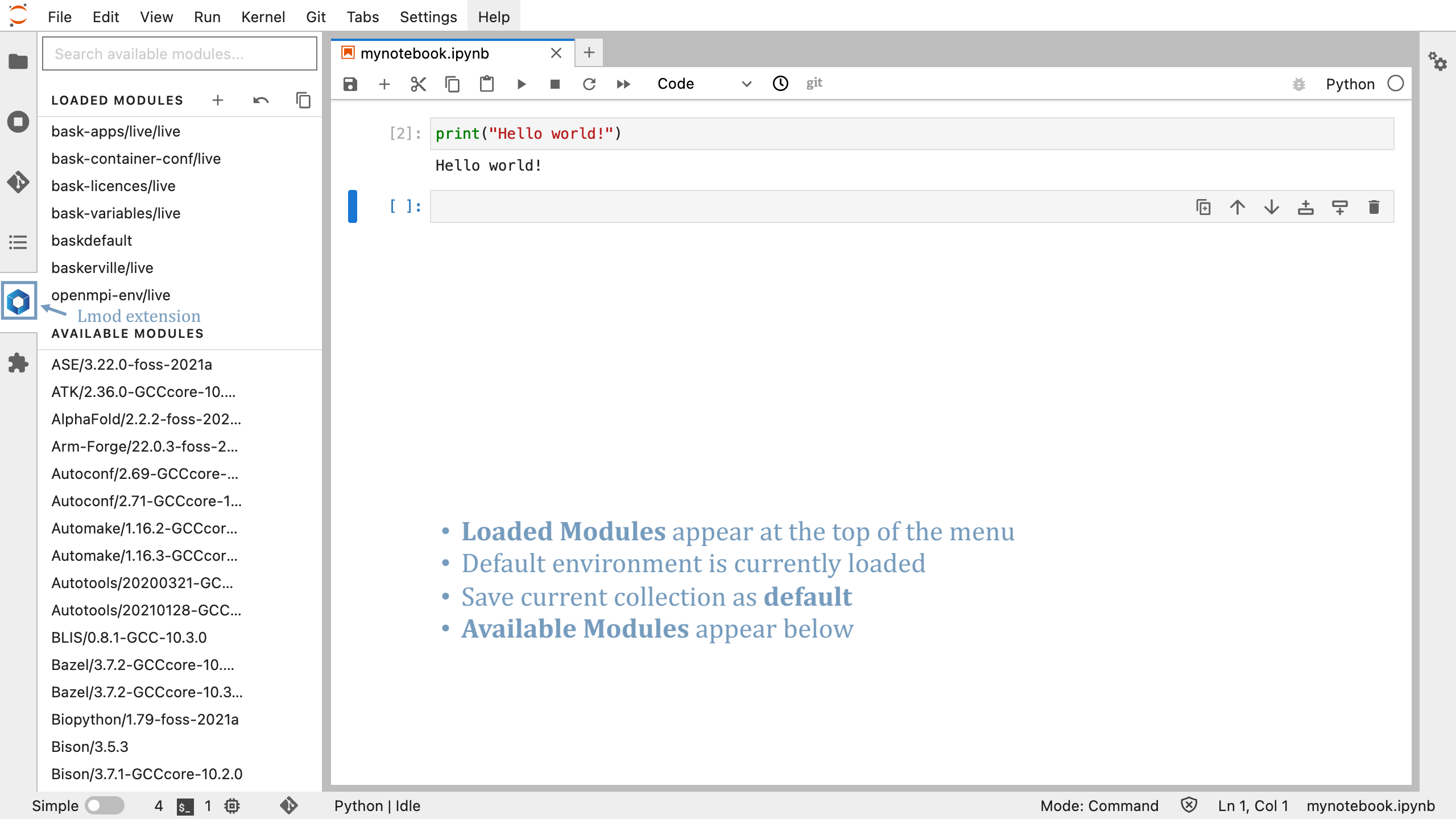
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Tabs
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Search available modules...
LOADED MODULES
bask-apps/live/live
bask-container-conf/live
bask-licences/live
bask-variables/live
baskdefault
baskerville/live
openmpi-env/live
Lmod extension
AVAILABLE MODULES
ASE/3.22.0-foss-2021a
ATK/2.36.0-GCCcore-10....
AlphaFold/2.2.2-foss-202...
Arm-Forge/22.0.3-foss-2...
Autoconf/2.69-GCCcore-...
Autoconf/2.71-GCCcore-1...
Automake/1.16.2-GCCcor...
Automake/1.16.3-GCCcor...
Autotools/20200321-GC...
Autotools/20210128-GCC...
BLIS/0.8.1-GCC-10.3.0
Bazel/3.7.2-GCCcore-10....
Bazel/3.7.2-GCCcore-10.3...
Biopython/1.79-foss-2021a
Bison/3.5.3
Bison/3.7.1-GCCcore-10.2.0
mynotebook.ipynb
Code
git
Python
[2]:
print("Hello world!")
Hello world!
[ ]:
• Loaded Modules appear at the top of the menu
• Default environment is currently loaded
• Save current collection as default
• Available Modules appear below
Simple
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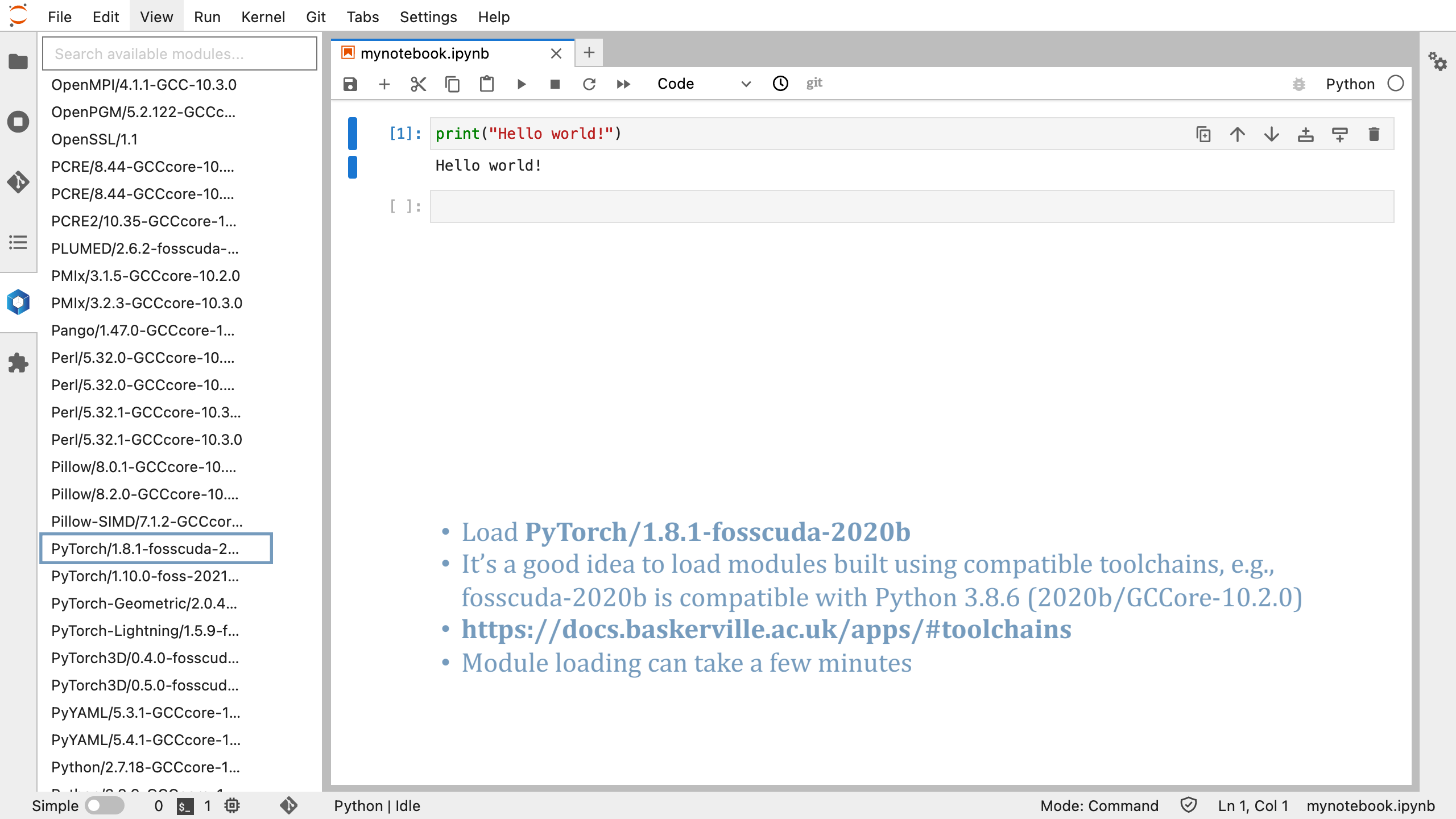
Python | Idle
Mode: Command
Ln 1, Col 1
mynotebook.ipynb


File
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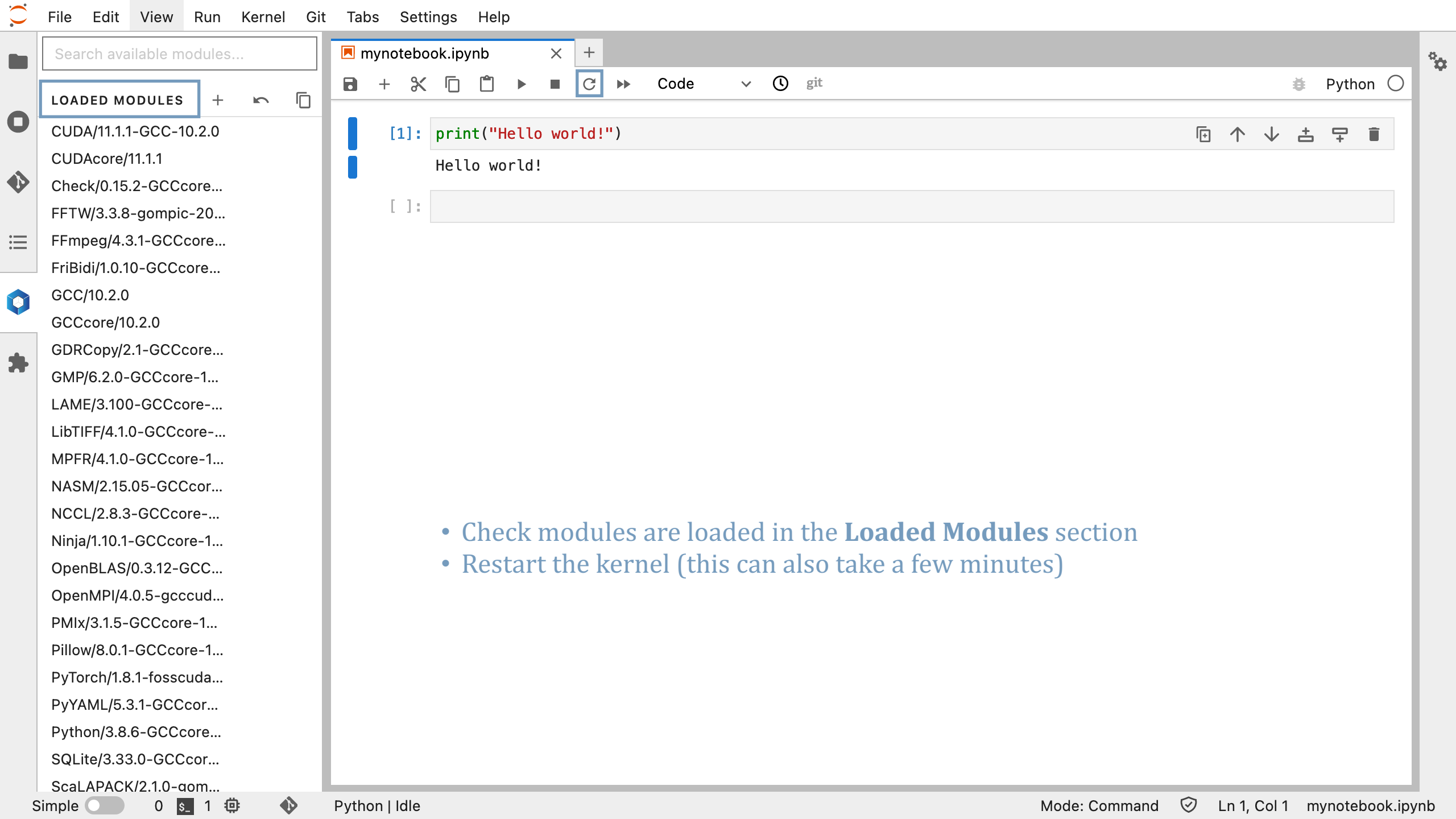
Kernel
Git
Tabs
Settings
Help
Search available modules...
OpenMPI/4.1.1-GCC-10.3.0
OpenPGM/5.2.122-GCCc...
OpenSSL/1.1
PCRE/8.44-GCCcore-10....
PCRE/8.44-GCCcore-10....
PCRE2/10.35-GCCcore-1...
PLUMED/2.6.2-fosscuda-...
PMIx/3.1.5-GCCcore-10.2.0
PMIx/3.2.3-GCCcore-10.3.0
Pango/1.47.0-GCCcore-1...
Perl/5.32.0-GCCcore-10....
Perl/5.32.0-GCCcore-10....
Perl/5.32.1-GCCcore-10.3...
Perl/5.32.1-GCCcore-10.3.0
Pillow/8.0.1-GCCcore-10....
Pillow/8.2.0-GCCcore-10....
Pillow-SIMD/7.1.2-GCCcor...
PyTorch/1.8.1-fosscuda-2...
PyTorch/1.10.0-foss-2021...
PyTorch-Geometric/2.0.4...
PyTorch-Lightning/1.5.9-f...
PyTorch3D/0.4.0-fosscud...
PyTorch3D/0.5.0-fosscud...
PyYAML/5.3.1-GCCcore-1...
PyYAML/5.4.1-GCCcore-1...
Python/2.7.18-GCCcore-1...
mynotebook.ipynb
Code
git
Python
[1]:
print("Hello world!")
Hello world!
[ ]:
• Load PyTorch/1.8.1-fosscuda-2020b
• It's a good idea to load modules built using compatible toolchains, e.g., fosscuda-2020b is compatible with Python 3.8.6 (2020b/GCCore-10.2.0)
• https://docs.baskerville.ac.uk/apps/#toolchains
• Module loading can take a few minutes
Simple
0
1
Python | Idle
Mode: Command
Ln 1, Col 1
mynotebook.ipynb


File
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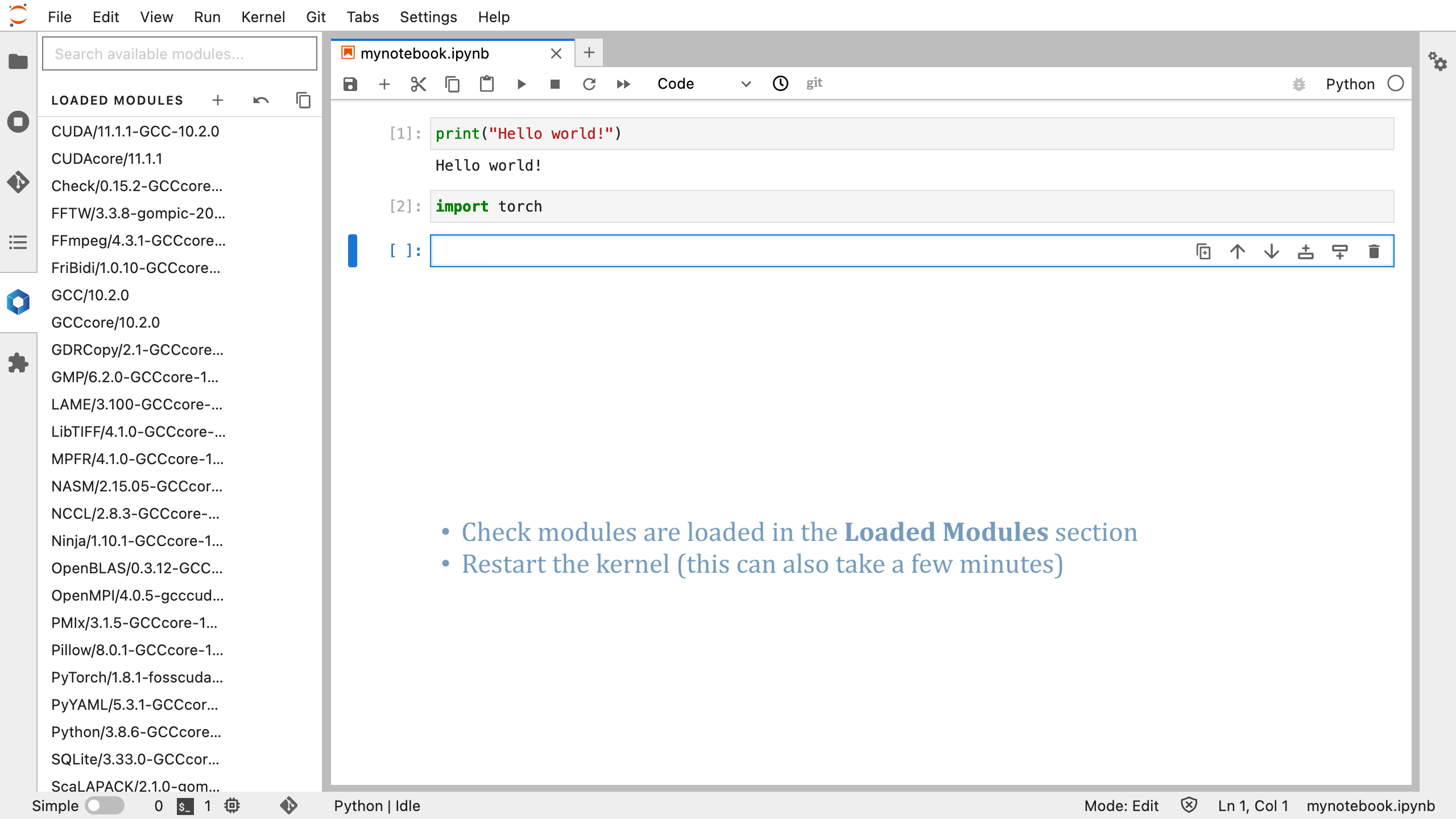
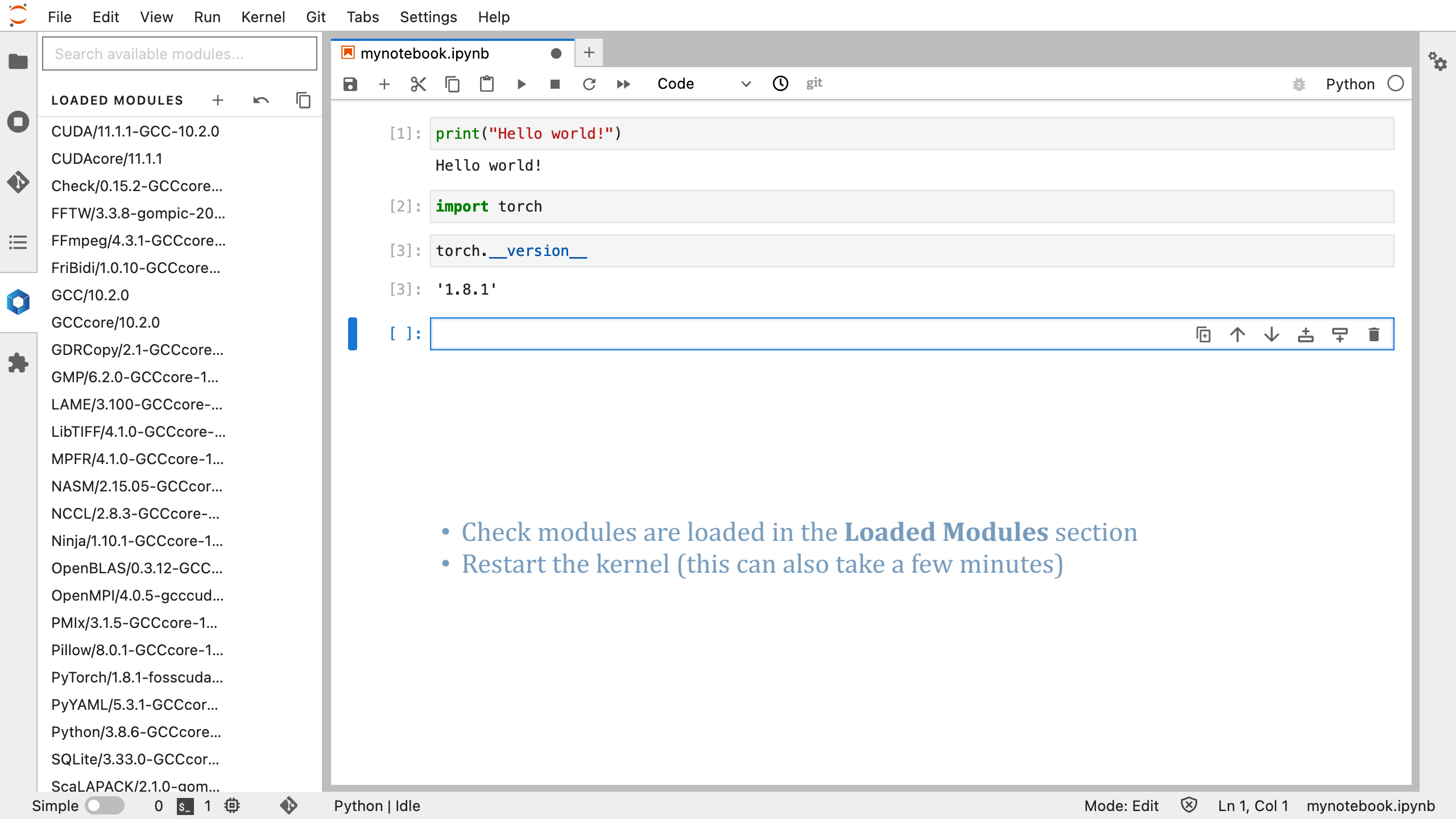
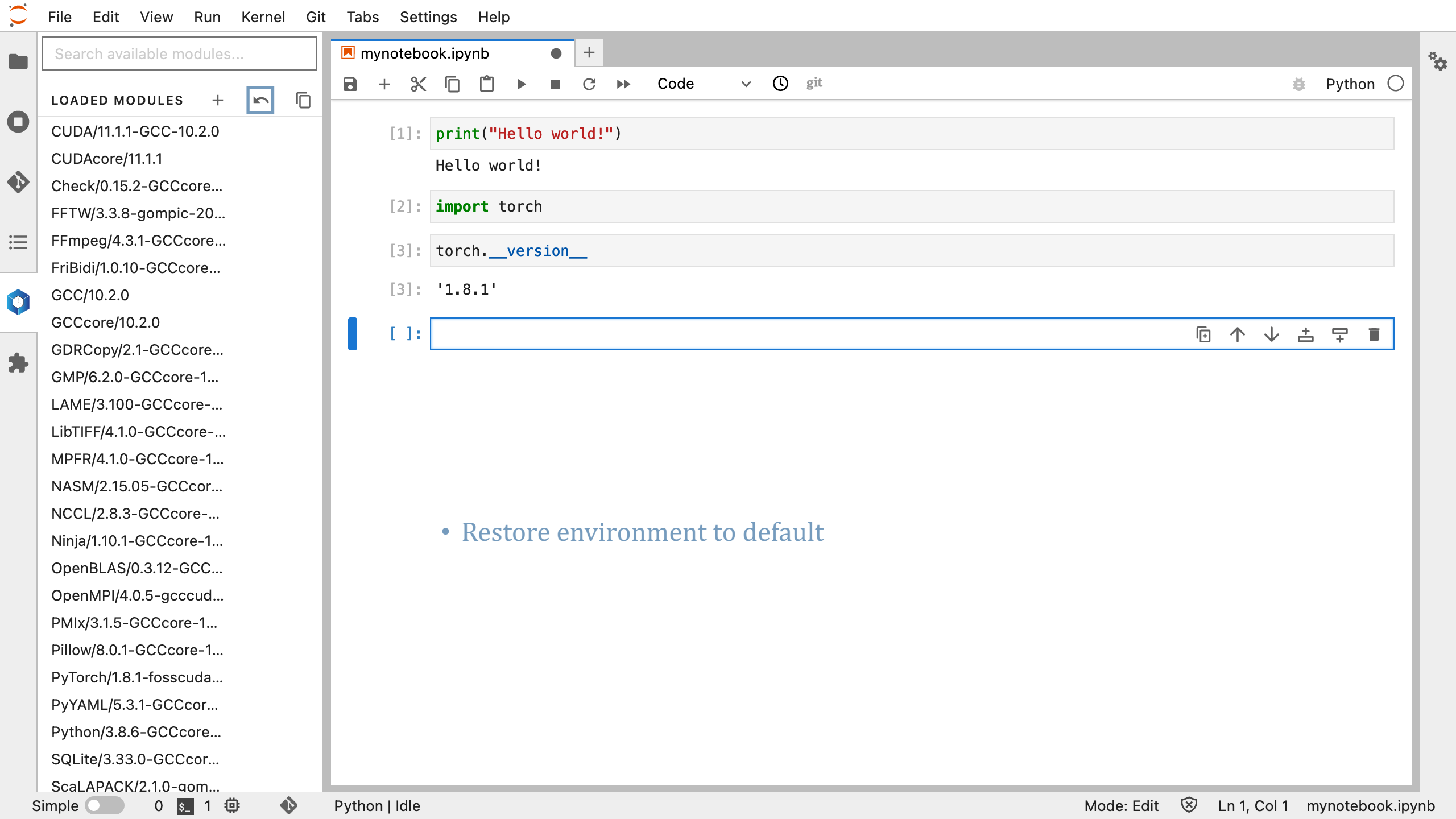
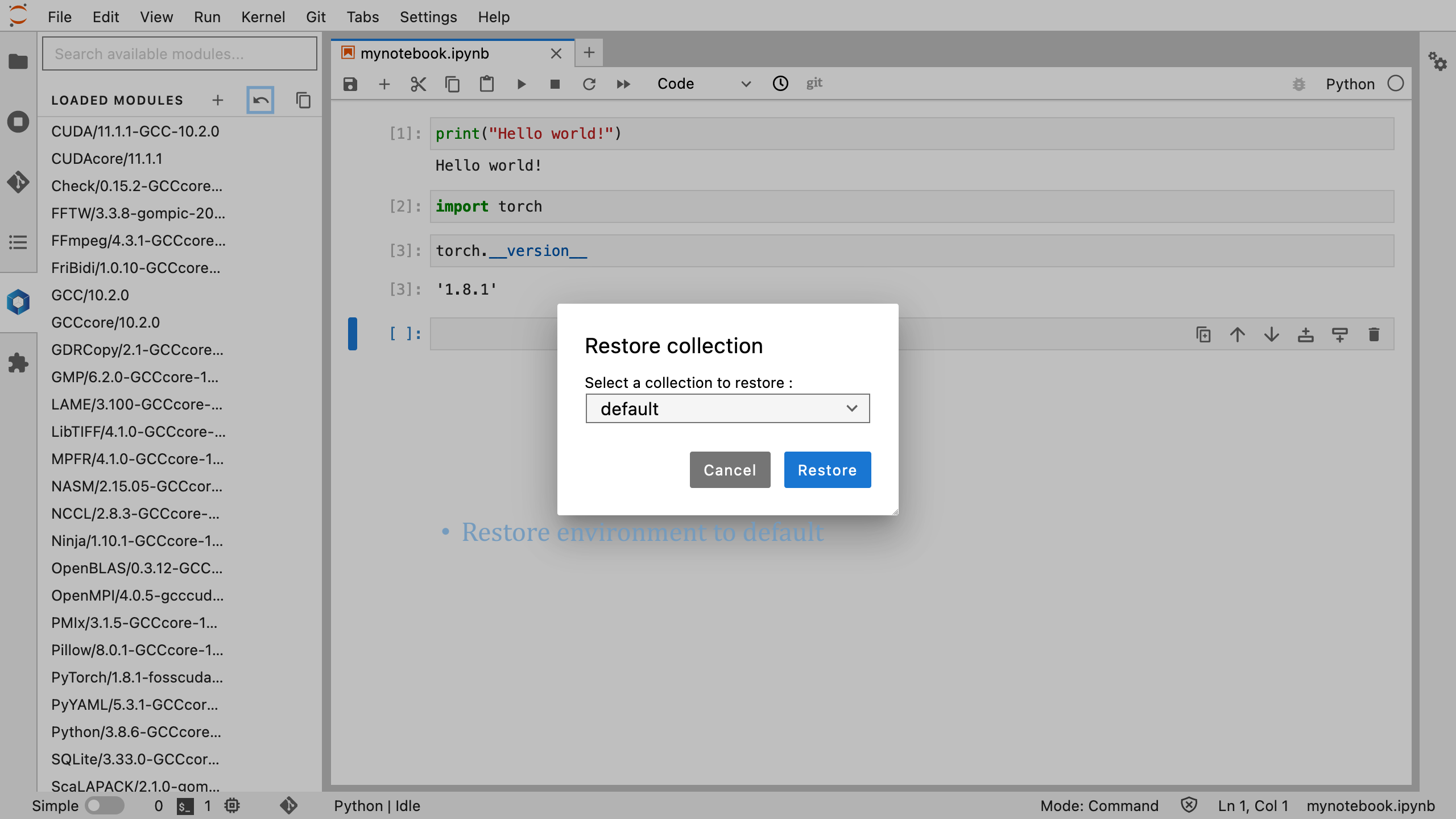
View
Run
Kernel
Git
Tabs
Settings
Help
Search available modules...
LOADED MODULES
CUDA/11.1.1-GCC-10.2.0
CUDAcore/11.1.1
Check/0.15.2-GCCcore...
FFTW/3.3.8-gompic-20...
FFmpeg/4.3.1-GCCcore...
FriBidi/1.0.10-GCCcore...
GCC/10.2.0
GCCcore/10.2.0
GDRCopy/2.1-GCCcore...
GMP/6.2.0-GCCcore-1...
LAME/3.100-GCCcore-...
LibTIFF/4.1.0-GCCcore-...
MPFR/4.1.0-GCCcore-1...
NASM/2.15.05-GCCcor...
NCCL/2.8.3-GCCcore-...
Ninja/1.10.1-GCCcore-1...
OpenBLAS/0.3.12-GCC...
OpenMPI/4.0.5-gcccud...
PMIx/3.1.5-GCCcore-1...
Pillow/8.0.1-GCCcore-1...
PyTorch/1.8.1-fosscuda...
PyYAML/5.3.1-GCCcor...
Python/3.8.6-GCCcore...
SQLite/3.33.0-GCCcor...
ScaLAPACK/2.1.0-gom...
mynotebook.ipynb
Code
git
Python
[1]:
print("Hello world!")
Hello world!
[ ]:
• Check modules are loaded in the Loaded Modules section
• Restart the kernel (this can also take a few minutes)
Simple
0
1
Python | Idle
Mode: Command
Ln 1, Col 1
mynotebook.ipynb


File Edit View Run Kernel Git Tabs Settings Help
Search available modules...
LOADED MODULES
CUDA/11.1.1-GCC-10.2.0
CUDAcore/11.1.1
Check/0.15.2-GCCcore...
FFTW/3.3.8-gompic-20...
FFmpeg/4.3.1-GCCcore...
FriBidi/1.0.10-GCCcore...
GCC/10.2.0
GCCcore/10.2.0
GDRCopy/2.1-GCCcore...
GMP/6.2.0-GCCcore-1...
LAME/3.100-GCCcore-...
LibTIFF/4.1.0-GCCcore-...
MPFR/4.1.0-GCCcore-1...
NASM/2.15.05-GCCcor...
NCCL/2.8.3-GCCcore-...
Ninja/1.10.1-GCCcore-1...
OpenBLAS/0.3.12-GCC...
OpenMPI/4.0.5-gcccud...
PMIx/3.1.5-GCCcore-1...
Pillow/8.0.1-GCCcore-1...
PyTorch/1.8.1-fosscuda...
PyYAML/5.3.1-GCCcor...
Python/3.8.6-GCCcore...
SQLite/3.33.0-GCCcor...
ScaLAPACK/2.1.0-gom...
mynotebook.ipynb
Code
git
Python
[1]: print("Hello world!")
Hello world!
[2]: import torch
[ ]:
• Check modules are loaded in the Loaded Modules section
• Restart the kernel (this can also take a few minutes)
Simple 0 1
Python | Idle
Mode: Edit
Ln 1, Col 1
mynotebook.ipynb


File Edit View Run Kernel Git Tabs Settings Help
Search available modules...
LOADED MODULES
CUDA/11.1.1-GCC-10.2.0
CUDAcore/11.1.1
Check/0.15.2-GCCcore...
FFTW/3.3.8-gompic-20...
FFmpeg/4.3.1-GCCcore...
FriBidi/1.0.10-GCCcore...
GCC/10.2.0
GCCcore/10.2.0
GDRCopy/2.1-GCCcore...
GMP/6.2.0-GCCcore-1...
LAME/3.100-GCCcore-...
LibTIFF/4.1.0-GCCcore-...
MPFR/4.1.0-GCCcore-1...
NASM/2.15.05-GCCcor...
NCCL/2.8.3-GCCcore-...
Ninja/1.10.1-GCCcore-1...
OpenBLAS/0.3.12-GCC...
OpenMPI/4.0.5-gcccud...
PMIx/3.1.5-GCCcore-1...
Pillow/8.0.1-GCCcore-1...
PyTorch/1.8.1-fosscuda...
PyYAML/5.3.1-GCCcor...
Python/3.8.6-GCCcore...
SQLite/3.33.0-GCCcor...
ScaLAPACK/2.1.0-gom...
mynotebook.ipynb
Code
git
Python
[1]: print("Hello world!")
Hello world!
[2]: import torch
[3]: torch.__version__
[3]: '1.8.1'
[ ]:
• Check modules are loaded in the Loaded Modules section
• Restart the kernel (this can also take a few minutes)
Simple 0 1
Python | Idle
Mode: Edit
Ln 1, Col 1
mynotebook.ipynb


File Edit View Run Kernel Git Tabs Settings Help
Search available modules...
LOADED MODULES
CUDA/11.1.1-GCC-10.2.0
CUDAcore/11.1.1
Check/0.15.2-GCCcore...
FFTW/3.3.8-gompic-20...
FFmpeg/4.3.1-GCCcore...
FriBidi/1.0.10-GCCcore...
GCC/10.2.0
GCCcore/10.2.0
GDRCopy/2.1-GCCcore...
GMP/6.2.0-GCCcore-1...
LAME/3.100-GCCcore-...
LibTIFF/4.1.0-GCCcore-...
MPFR/4.1.0-GCCcore-1...
NASM/2.15.05-GCCcor...
NCCL/2.8.3-GCCcore-...
Ninja/1.10.1-GCCcore-1...
OpenBLAS/0.3.12-GCC...
OpenMPI/4.0.5-gcccud...
PMIx/3.1.5-GCCcore-1...
Pillow/8.0.1-GCCcore-1...
PyTorch/1.8.1-fosscuda...
PyYAML/5.3.1-GCCcor...
Python/3.8.6-GCCcore...
SQLite/3.33.0-GCCcor...
ScaLAPACK/2.1.0-gom...
mynotebook.ipynb
Code
git
Python
[1]: print("Hello world!")
Hello world!
[2]: import torch
[3]: torch.__version__
[3]: '1.8.1'
[ ]:
• Restore environment to default
Simple 0 1
Python | Idle
Mode: Edit
Ln 1, Col 1
mynotebook.ipynb

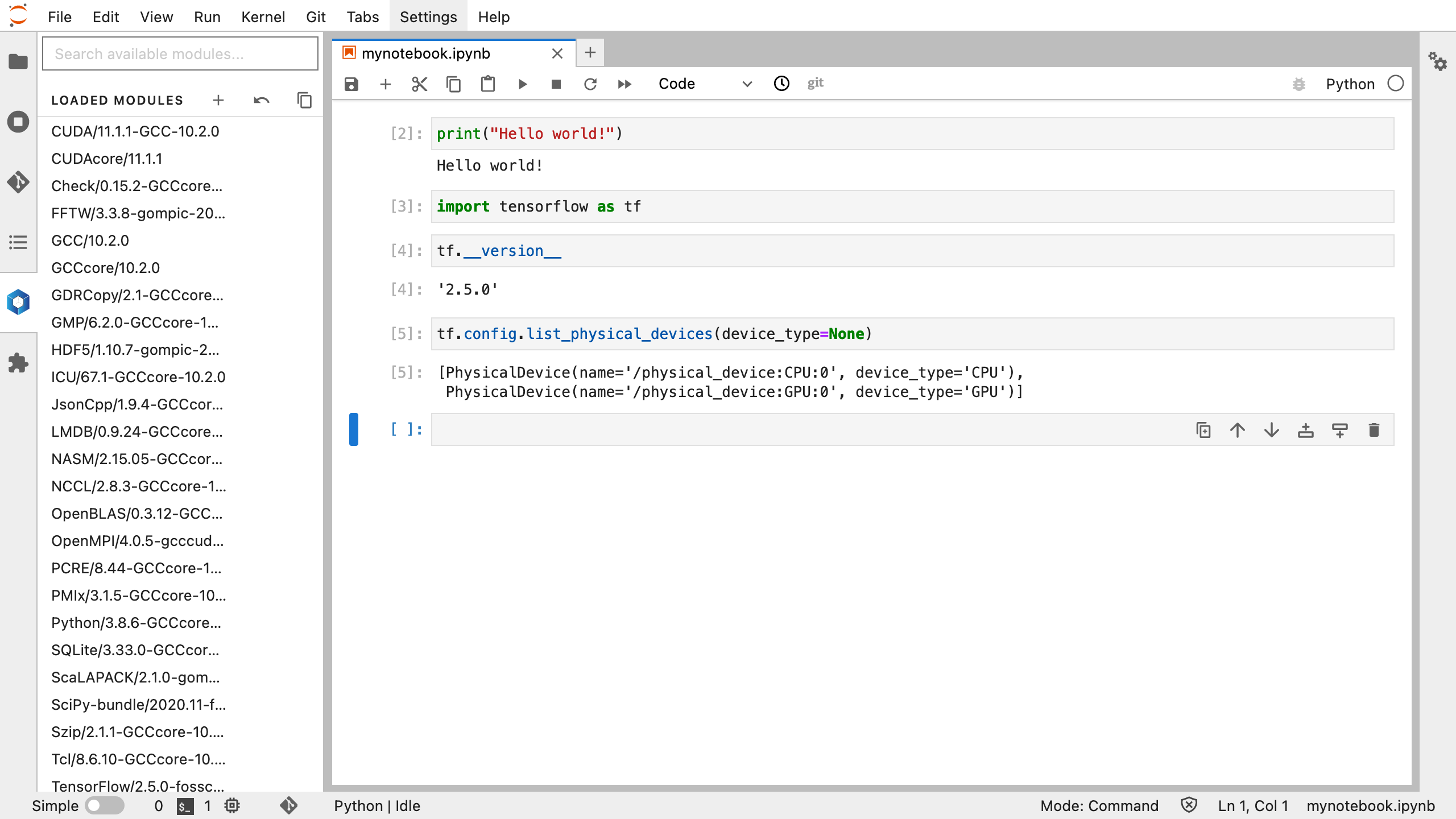

File Edit View Run Kernel Git Tabs Settings Help
Search available modules...
LOADED MODULES
CUDA/11.1.1-GCC-10.2.0
CUDAcore/11.1.1
Check/0.15.2-GCCcore...
FFTW/3.3.8-gompic-20...
FFmpeg/4.3.1-GCCcore...
FriBidi/1.0.10-GCCcore...
GCC/10.2.0
GCCcore/10.2.0
GDRCopy/2.1-GCCcore...
GMP/6.2.0-GCCcore-1...
LAME/3.100-GCCcore-...
LibTIFF/4.1.0-GCCcore-...
MPFR/4.1.0-GCCcore-1...
NASM/2.15.05-GCCcor...
NCCL/2.8.3-GCCcore-...
Ninja/1.10.1-GCCcore-1...
OpenBLAS/0.3.12-GCC...
OpenMPI/4.0.5-gcccud...
PMIx/3.1.5-GCCcore-1...
Pillow/8.0.1-GCCcore-1...
PyTorch/1.8.1-fosscuda...
PyYAML/5.3.1-GCCcor...
Python/3.8.6-GCCcore...
SQLite/3.33.0-GCCcor...
ScaLAPACK/2.1.0-gom...
mynotebook.ipynb
Code
git
Python
[1]: print("Hello world!")
Hello world!
[2]: import torch
[3]: torch.__version__
[3]: '1.8.1'
[ ]:
Restore collection
Select a collection to restore :
default
Cancel
Restore
• Restore environment to default
Simple
0
1
Python | Idle
Mode: Command
Ln 1, Col 1
mynotebook.ipynb

https://github.com/baskerville-hpc/baskerville-portal

Your turn

- Restore default environment and restart kernel
- Module load TensorFlow
- import tensorflow as tf
- Check the software version number with tf.__version__
- Query visible GPU devices with the command

```
tf.config.list_physical_devices(
    device_type=None
)
```


File
Edit
View
Run
Kernel
Git
Tabs
Settings
Help
Search available modules...
LOADED MODULES
CUDA/11.1.1-GCC-10.2.0
CUDAcore/11.1.1
Check/0.15.2-GCCcore...
FFTW/3.3.8-gompic-20...
GCC/10.2.0
GCCcore/10.2.0
GDRCopy/2.1-GCCcore...
GMP/6.2.0-GCCcore-1...
HDF5/1.10.7-gompic-2...
ICU/67.1-GCCcore-10.2.0
JsonCpp/1.9.4-GCCcor...
LMDB/0.9.24-GCCcore...
NASM/2.15.05-GCCcor...
NCCL/2.8.3-GCCcore-1...
OpenBLAS/0.3.12-GCC...
OpenMPI/4.0.5-gcccud...
PCRE/8.44-GCCcore-1...
PMIx/3.1.5-GCCcore-10...
Python/3.8.6-GCCcore...
SQLite/3.33.0-GCCcor...
ScaLAPACK/2.1.0-gom...
SciPy-bundle/2020.11-f...
Szip/2.1.1-GCCcore-10....
Tcl/8.6.10-GCCcore-10....
TensorFlow/2.5.0-fossc...
mynotebook.ipynb
Code
git
Python
[2]:
print("Hello world!")
Hello world!
[3]:
import tensorflow as tf
[4]:
tf.__version__
[4]:
'2.5.0'
[5]:
tf.config.list_physical_devices(device_type=None)
[5]:
[PhysicalDevice(name='/physical_device:CPU:0', device_type='CPU'),
PhysicalDevice(name='/physical_device:GPU:0', device_type='GPU')]
[ ]:
Simple
0
1
Python | Idle
Mode: Command
Ln 1, Col 1
mynotebook.ipynb

b) Conda Environments

- Conda is a package and environment manager for Python

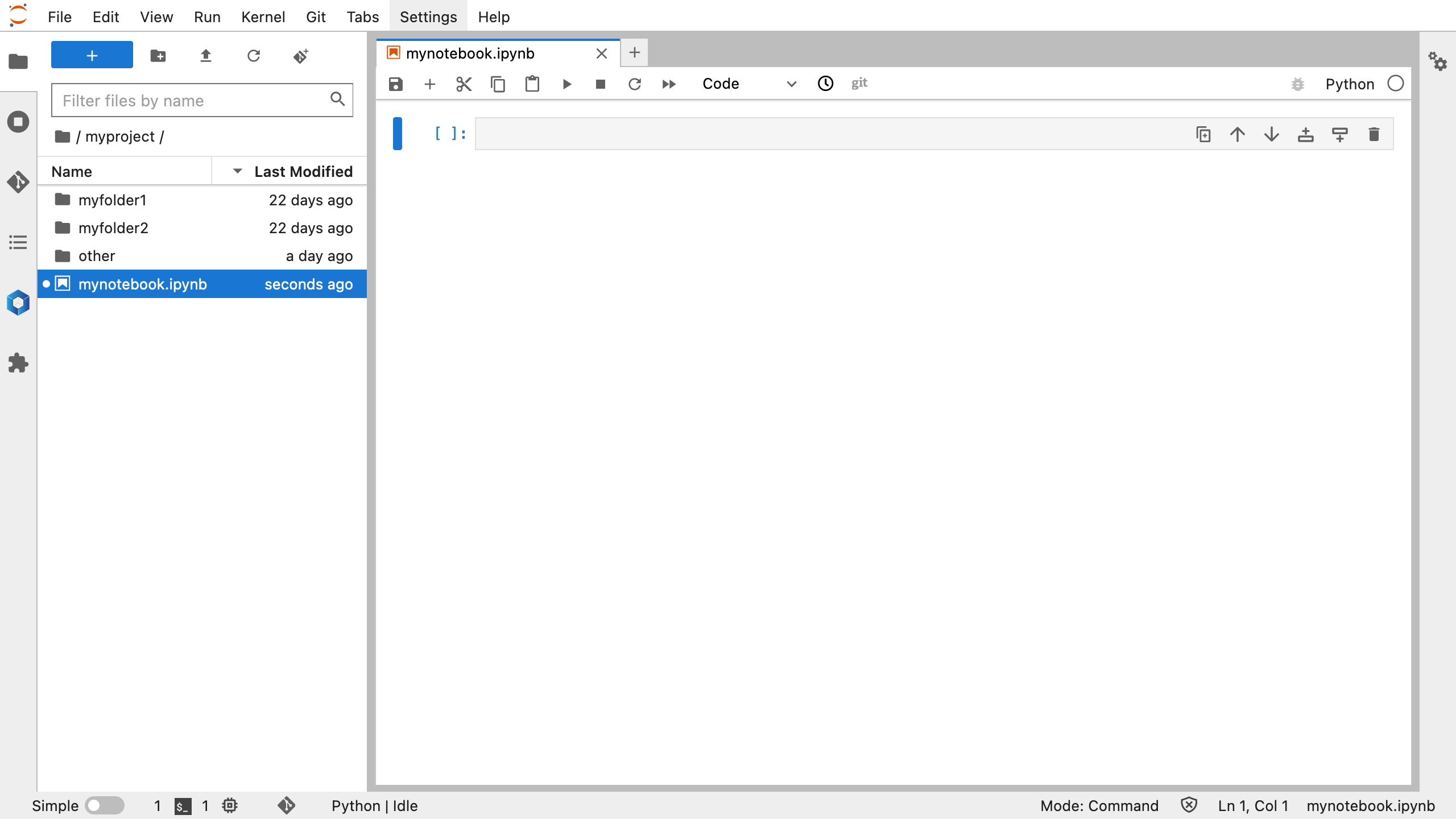
- Steps to create a Conda Environment for JupyterLab:

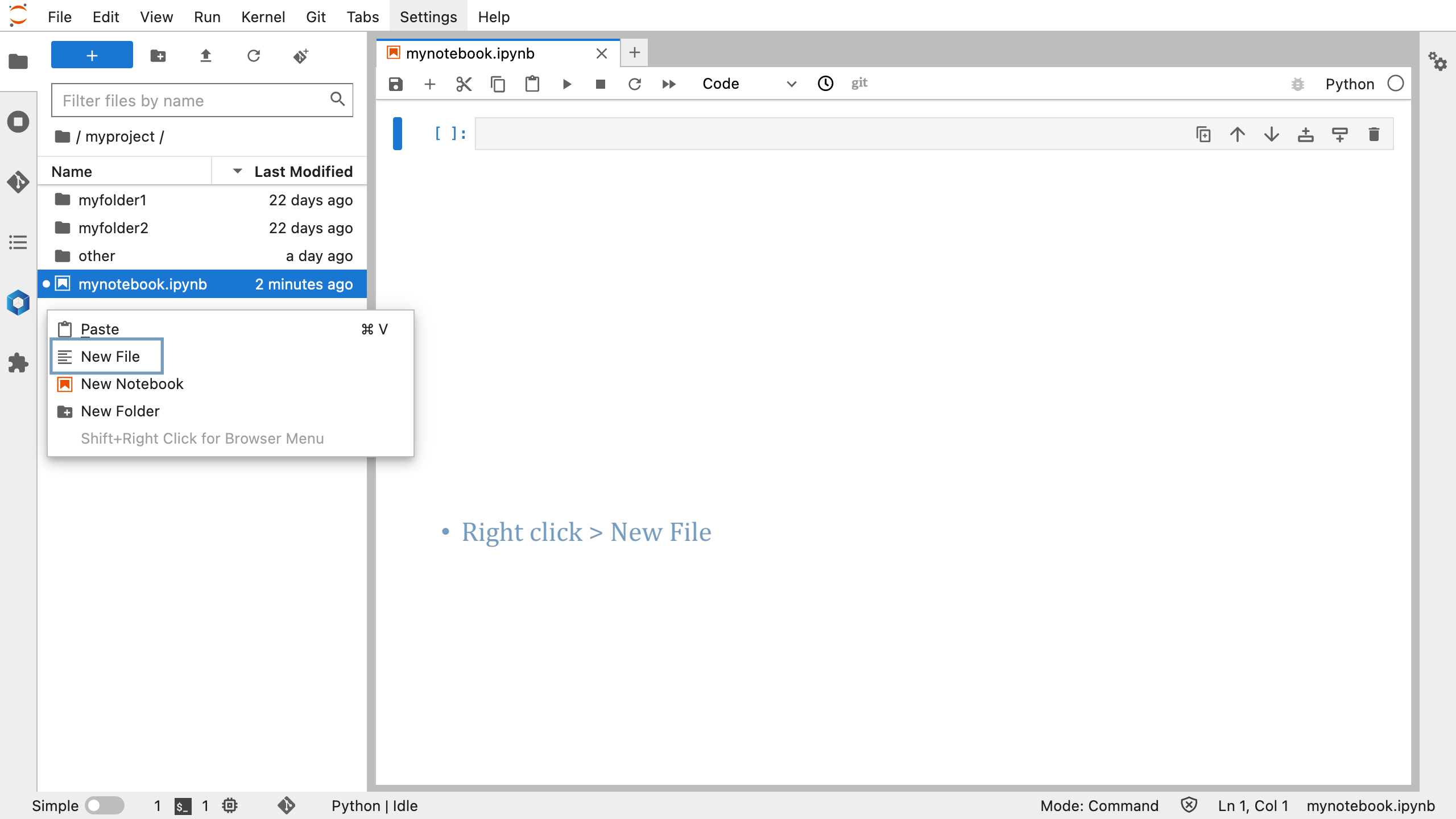
    i. Create a Conda environment in your **project folder** using a batch script in the Terminal
    ii. Relaunch the JupyterLab server to load the new Conda kernel
    iii. (Optional) Use the same JupyterLab session to modify the environment

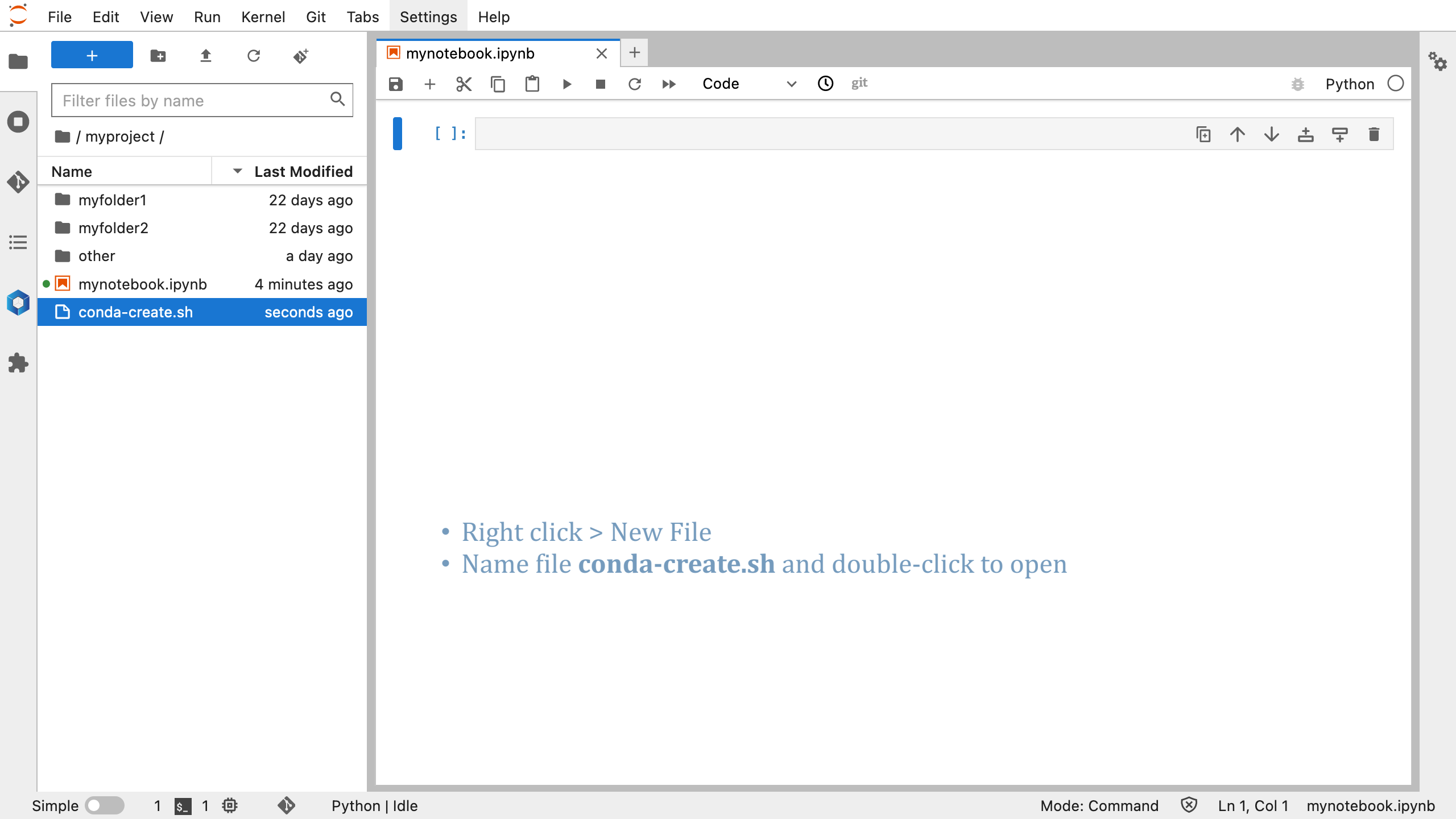
3. JupyterLab

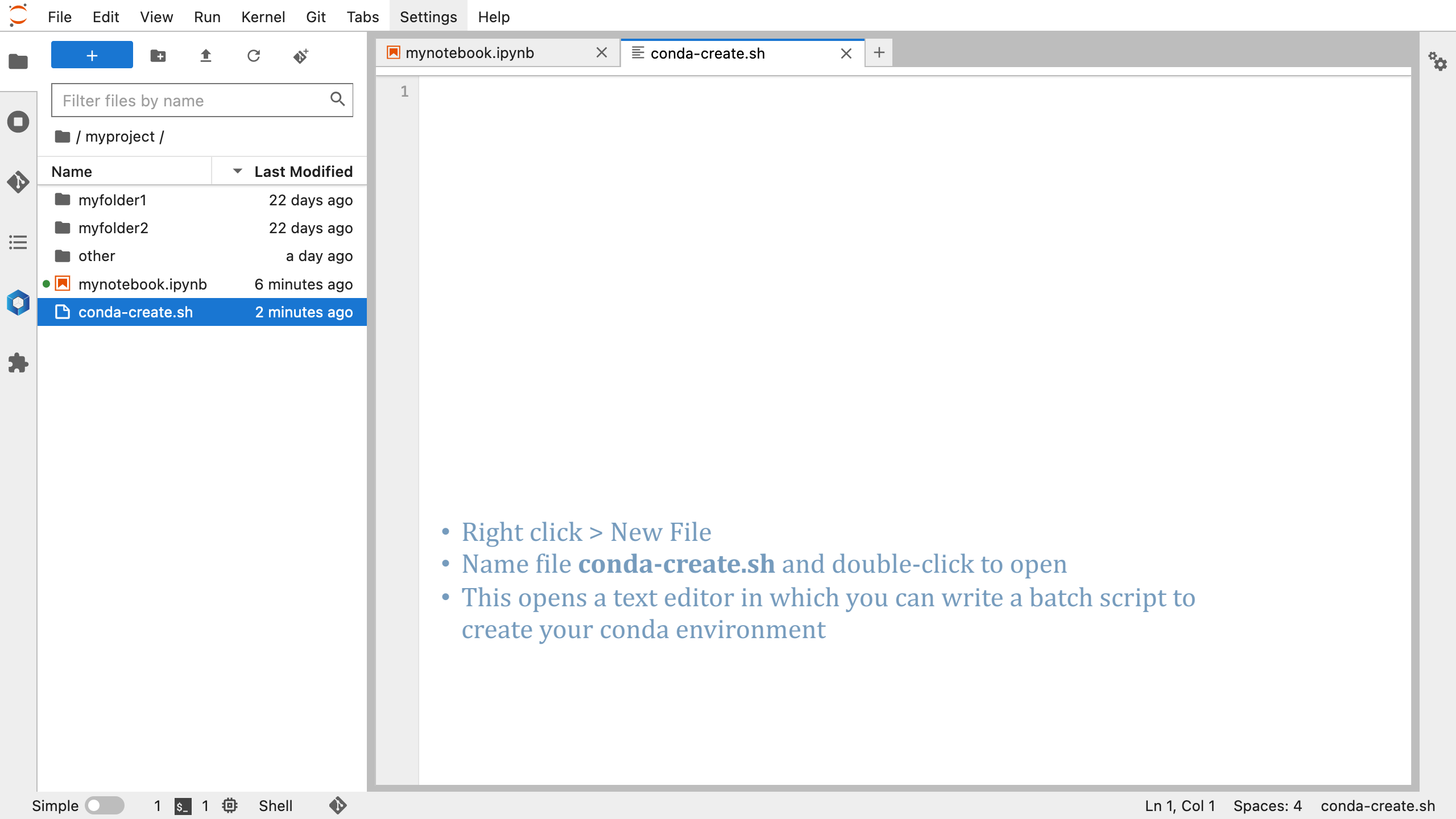
b) Conda Environments

(i) Create your Conda Environment


File
Edit
View
Run
Kernel
Git
Tabs
Settings
Help
Filter files by name
/ myproject /
Name
Last Modified
myfolder1
22 days ago
myfolder2
22 days ago
other
a day ago
mynotebook.ipynb
seconds ago
mynotebook.ipynb
Code
git
Python
[ ]:
Simple
1
1
Python | Idle
Mode: Command
Ln 1, Col 1
mynotebook.ipynb


File
Edit
View
Run
Kernel
Git
Tabs
Settings
Help
Filter files by name
/ myproject /
Name
Last Modified
myfolder1
22 days ago
myfolder2
22 days ago
other
a day ago
mynotebook.ipynb
2 minutes ago
Paste
⌘ V
New File
New Notebook
New Folder
Shift+Right Click for Browser Menu
mynotebook.ipynb
Code
git
Python
[ ]:
• Right click > New File
Simple
1
1
Python | Idle
Mode: Command
Ln 1, Col 1
mynotebook.ipynb


File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
myfolder1 22 days ago
myfolder2 22 days ago
other a day ago
mynotebook.ipynb 4 minutes ago
conda-create.sh seconds ago
mynotebook.ipynb
Code
git
Python
[ ]:
• Right click > New File
• Name file conda-create.sh and double-click to open
Simple
1
1
Python | Idle
Mode: Command
Ln 1, Col 1
mynotebook.ipynb


File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
myfolder1 22 days ago
myfolder2 22 days ago
other a day ago
mynotebook.ipynb 6 minutes ago
conda-create.sh 2 minutes ago
mynotebook.ipynb
conda-create.sh
1
• Right click > New File
• Name file conda-create.sh and double-click to open
• This opens a text editor in which you can write a batch script to create your conda environment
Simple
1
1
Shell
Ln 1, Col 1
Spaces: 4
conda-create.sh

File Edit View Run Kernel Git Tabs Settings Help

Filter files by name

/ myproject /

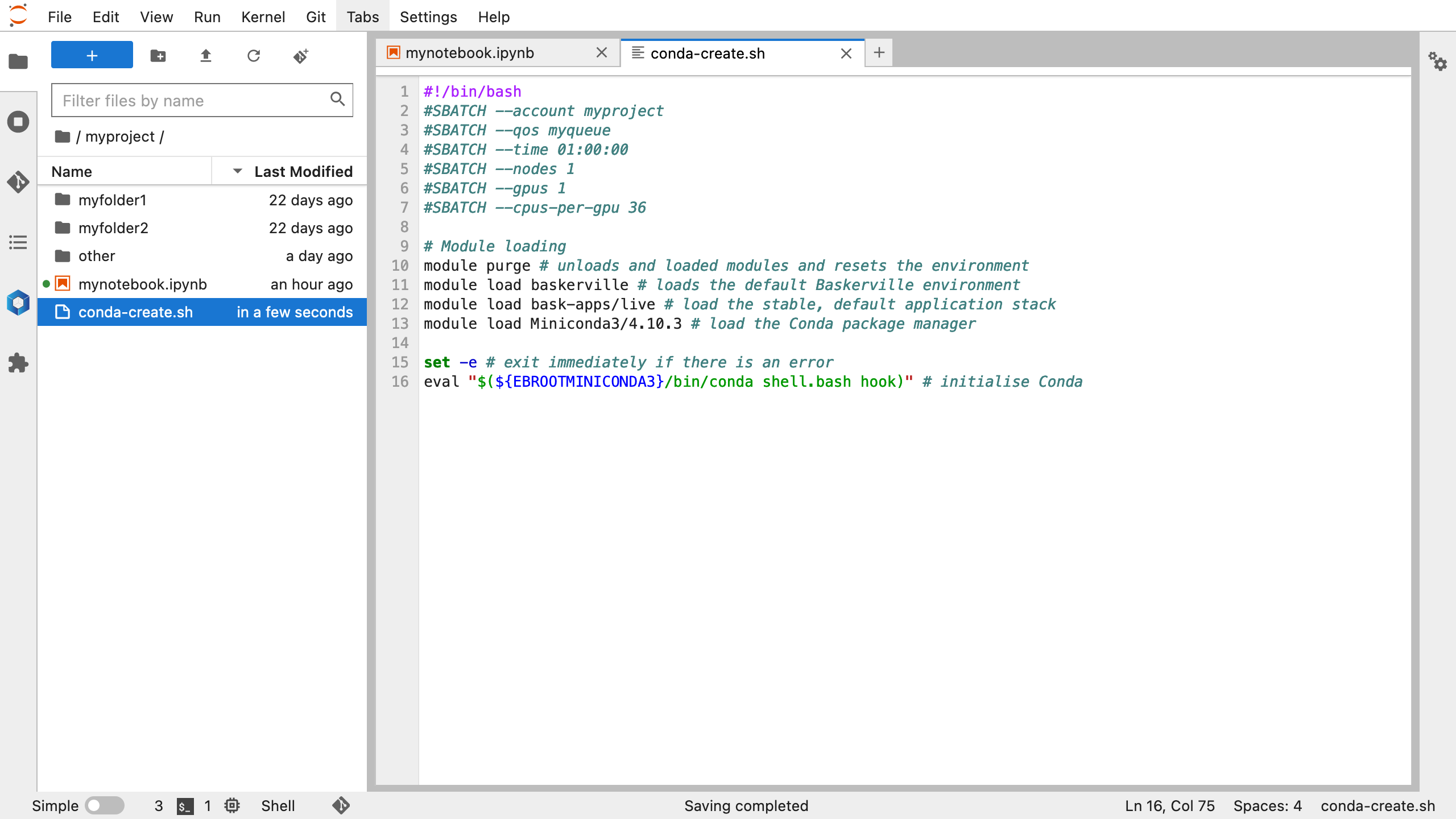
Name	Last Modified
myfolder1	22 days ago
myfolder2	22 days ago
other	a day ago
mynotebook.ipynb	11 minutes ago
conda-create.sh	seconds ago

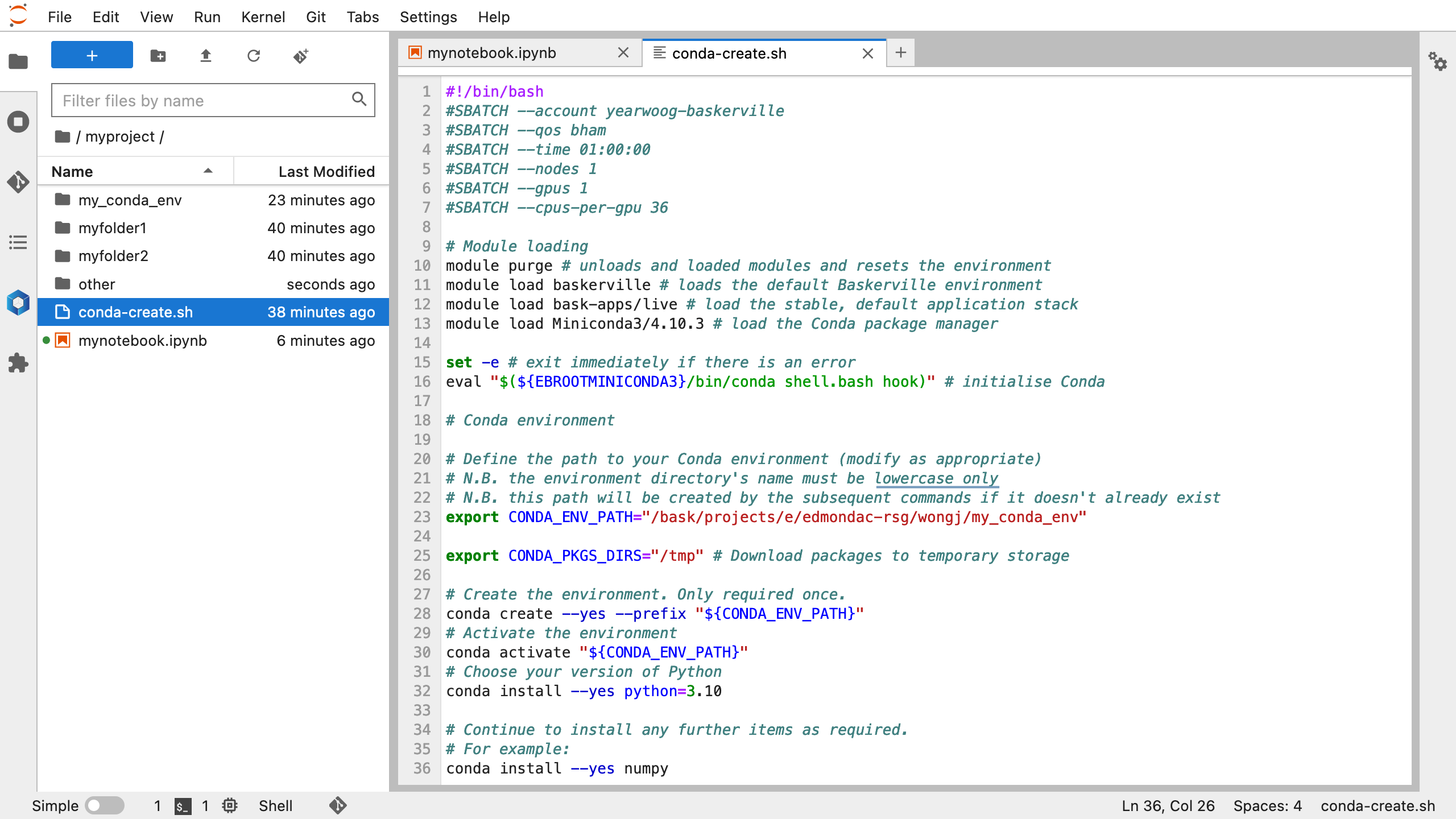
mynotebook.ipynb | conda-create.sh

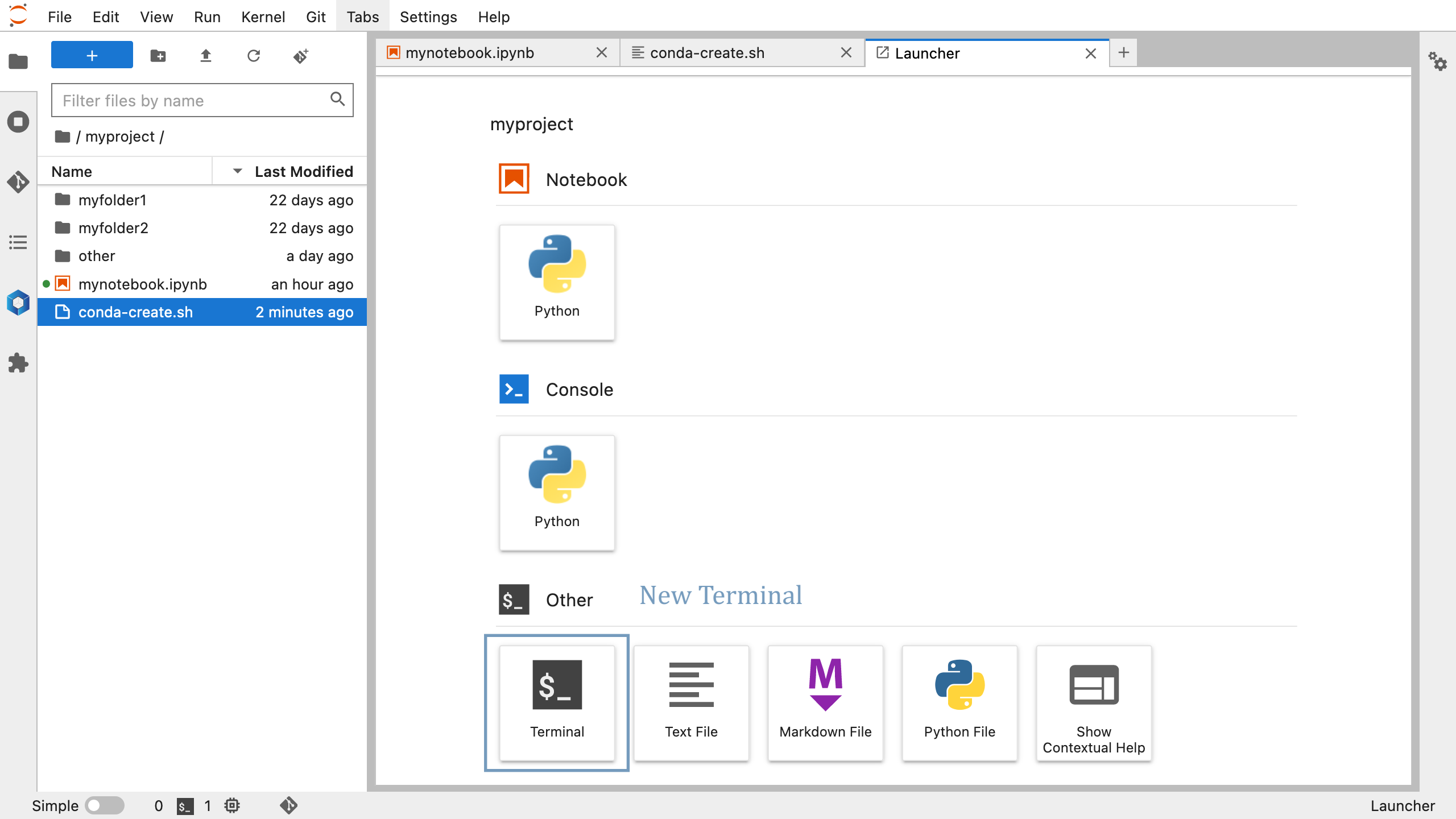
```
#!/bin/bash
#SBATCH --account myproject
#SBATCH --qos myqueue
#SBATCH --time 01:00:00
#SBATCH --nodes 1
#SBATCH --gpus 1
#SBATCH --cpus-per-gpu 36
```

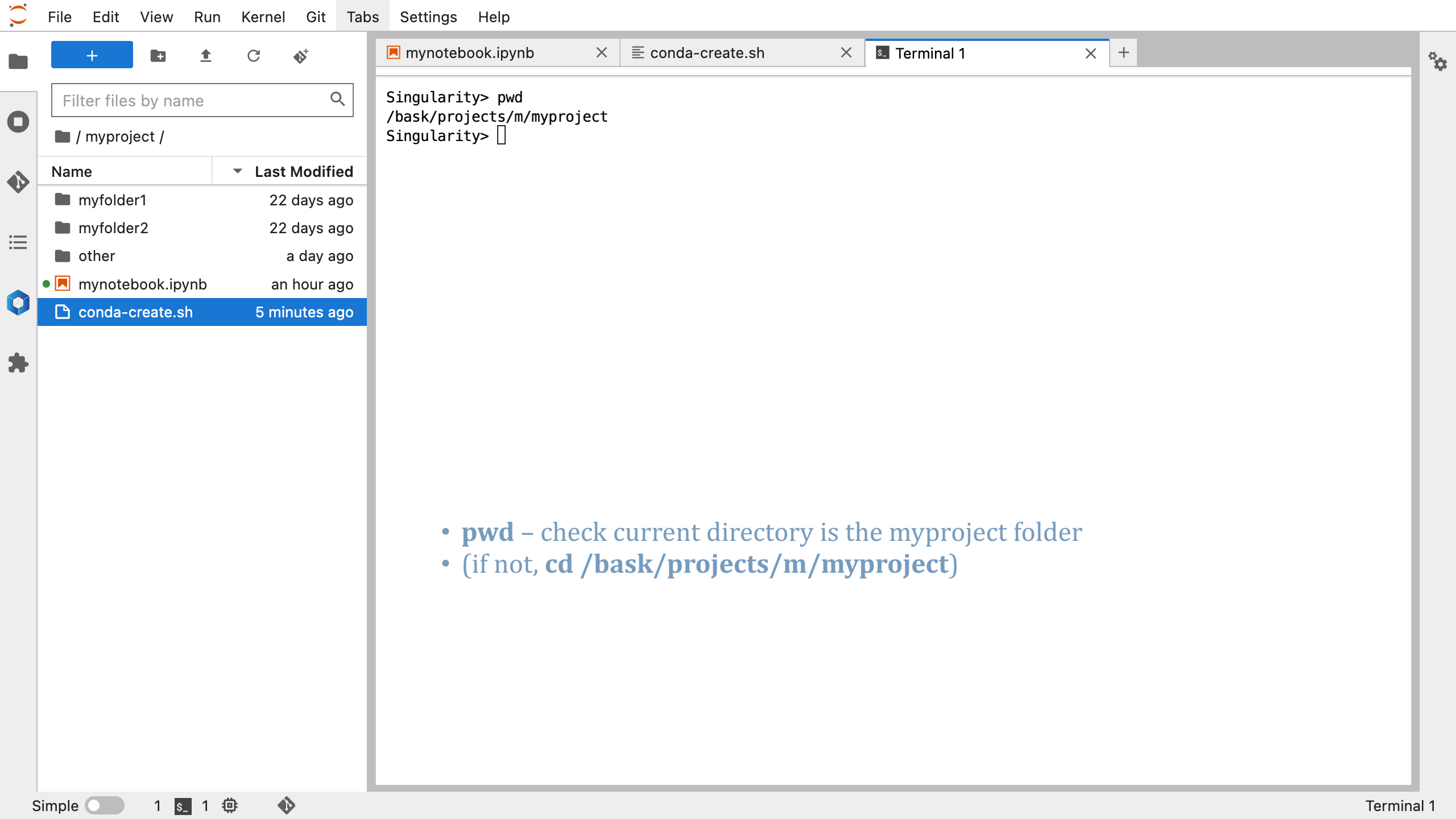
- **account** and **qos** details can be double checked with **my_baskerville** command in the Terminal
- request a modest amount of time for an increased chance of your job starting straight away
- 1 node has 4 GPUs and 144 CPU cores, therefore 144/4 = 36 cores and 4/4 = 1 GPU are the minimum resources available to build the environment (even if we requested less cores, this still takes 1 GPU out of service due to distribution of system architecture)

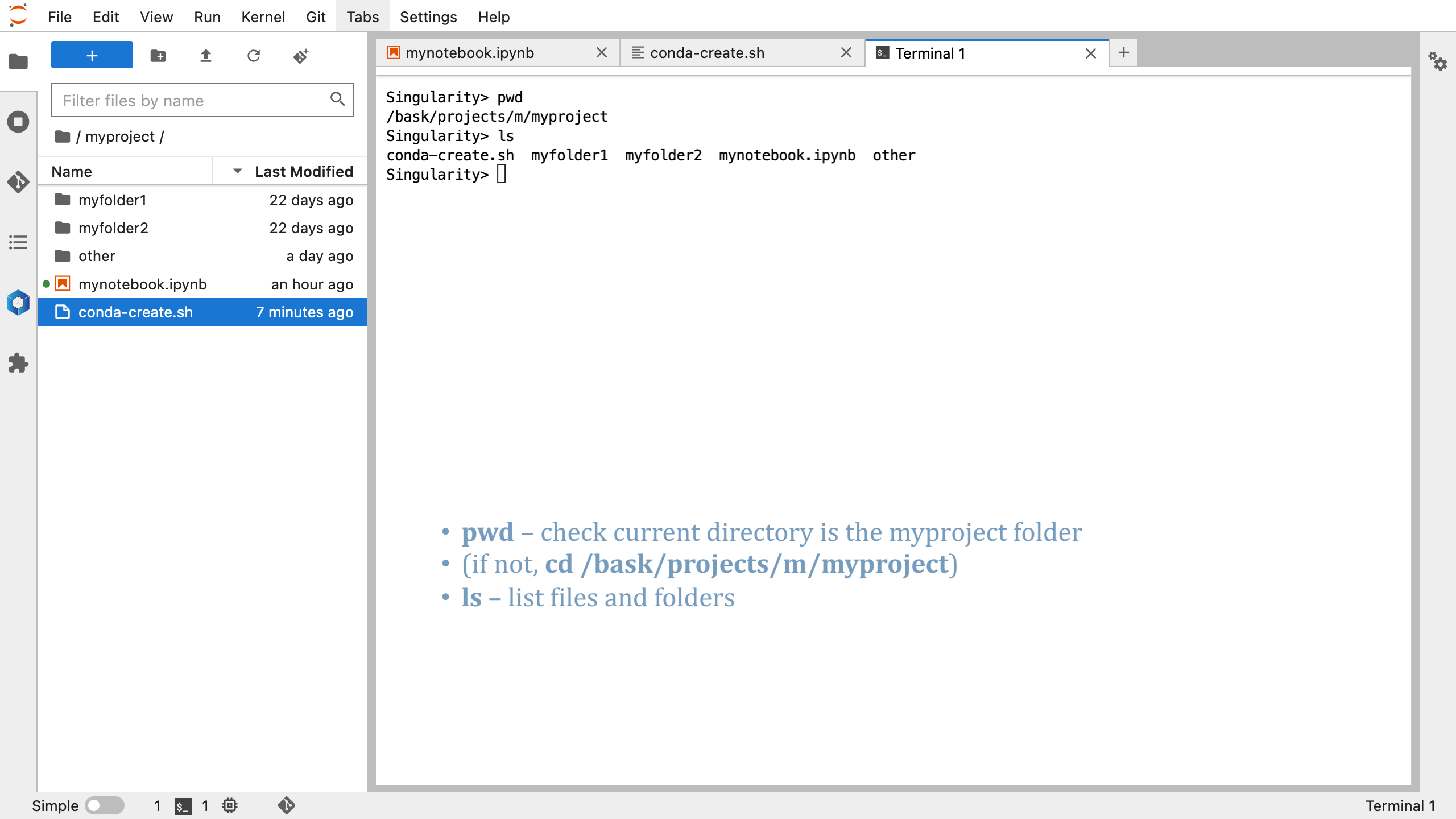
Simple 2 1 Shell Ln 7, Col 26 Spaces: 4 conda-create.sh

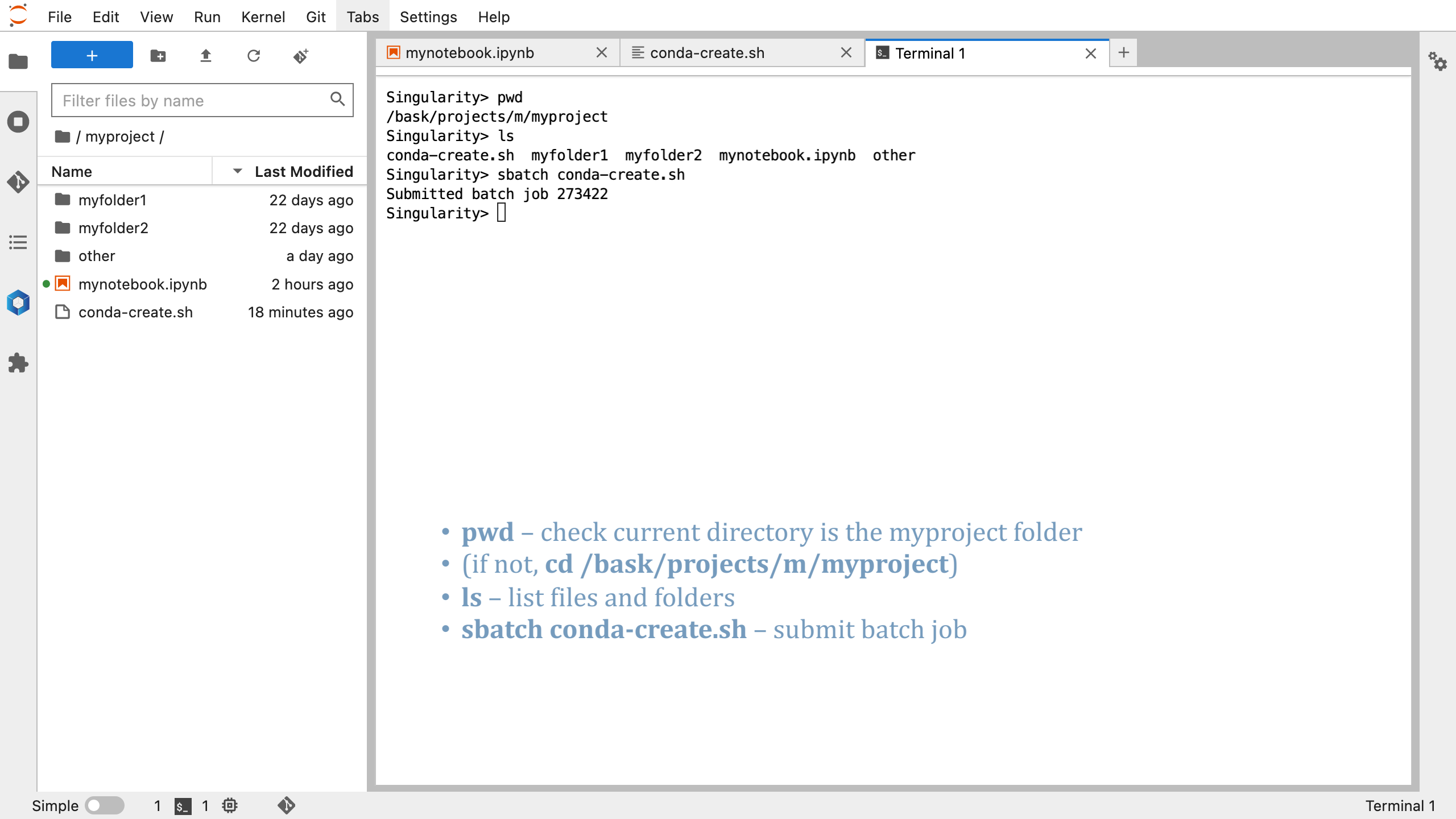

File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
myfolder1 22 days ago
myfolder2 22 days ago
other a day ago
mynotebook.ipynb an hour ago
conda-create.sh in a few seconds
mynotebook.ipynb
conda-create.sh
#!/bin/bash
#SBATCH --account myproject
#SBATCH --qos myqueue
#SBATCH --time 01:00:00
#SBATCH --nodes 1
#SBATCH --gpus 1
#SBATCH --cpus-per-gpu 36
Module loading
module purge # unloads and loaded modules and resets the environment
module load baskerville # loads the default Baskerville environment
module load bask-apps/live # load the stable, default application stack
module load Miniconda3/4.10.3 # load the Conda package manager
set -e # exit immediately if there is an error
eval "$(${EBROOTMINICONDA3}/bin/conda shell.bash hook)" # initialise Conda
Simple 3 1 Shell
Saving completed
Ln 16, Col 75 Spaces: 4 conda-create.sh

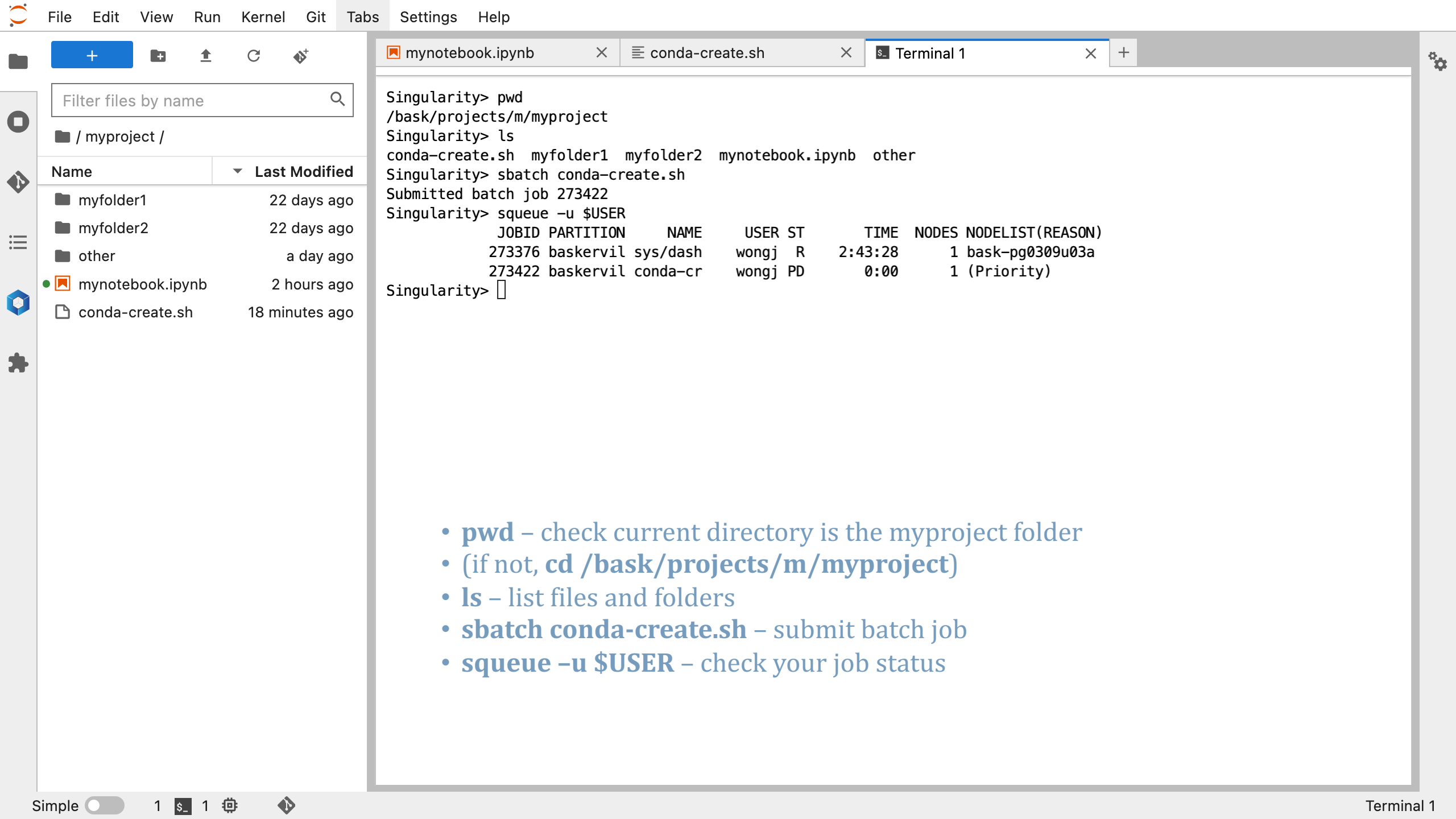

File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
my_conda_env 23 minutes ago
myfolder1 40 minutes ago
myfolder2 40 minutes ago
other seconds ago
conda-create.sh 38 minutes ago
mynotebook.ipynb 6 minutes ago
mynotebook.ipynb
conda-create.sh
#!/bin/bash
#SBATCH --account yearwoog-baskerville
#SBATCH --qos bham
#SBATCH --time 01:00:00
#SBATCH --nodes 1
#SBATCH --gpus 1
#SBATCH --cpus-per-gpu 36
Module loading
module purge # unloads and loaded modules and resets the environment
module load baskerville # loads the default Baskerville environment
module load bask-apps/live # load the stable, default application stack
module load Miniconda3/4.10.3 # load the Conda package manager
set -e # exit immediately if there is an error
eval "$(${EBROOTMINICONDA3}/bin/conda shell.bash hook)" # initialise Conda
Conda environment
Define the path to your Conda environment (modify as appropriate)
N.B. the environment directory's name must be lowercase only
N.B. this path will be created by the subsequent commands if it doesn't already exist
export CONDA_ENV_PATH="/bask/projects/e/edmondac-rsg/wongj/my_conda_env"
export CONDA_PKGS_DIRS="/tmp" # Download packages to temporary storage
Create the environment. Only required once.
conda create --yes --prefix "${CONDA_ENV_PATH}"
Activate the environment
conda activate "${CONDA_ENV_PATH}"
Choose your version of Python
conda install --yes python=3.10
Continue to install any further items as required.
For example:
conda install --yes numpy
Simple 1 1 Shell
Ln 36, Col 26 Spaces: 4 conda-create.sh


File
Edit
View
Run
Kernel
Git
Tabs
Settings
Help
Filter files by name
/ myproject /
Name
Last Modified
myfolder1
22 days ago
myfolder2
22 days ago
other
a day ago
mynotebook.ipynb
an hour ago
conda-create.sh
2 minutes ago
mynotebook.ipynb
conda-create.sh
Launcher
myproject
Notebook
Python
Console
Python
Other
New Terminal
Terminal
Text File
Markdown File
Python File
Show Contextual Help
Simple
0
1
Launcher


File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
myfolder1 22 days ago
myfolder2 22 days ago
other a day ago
mynotebook.ipynb an hour ago
conda-create.sh 5 minutes ago
mynotebook.ipynb
conda-create.sh
Terminal 1
Singularity> pwd
/bask/projects/m/myproject
Singularity>
• pwd – check current directory is the myproject folder
• (if not, cd /bask/projects/m/myproject)
Simple
1
1
Terminal 1


File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
myfolder1 22 days ago
myfolder2 22 days ago
other a day ago
mynotebook.ipynb an hour ago
conda-create.sh 7 minutes ago
mynotebook.ipynb
conda-create.sh
Terminal 1
Singularity> pwd
/bask/projects/m/myproject
Singularity> ls
conda-create.sh myfolder1 myfolder2 mynotebook.ipynb other
Singularity>
• pwd – check current directory is the myproject folder
• (if not, cd /bask/projects/m/myproject)
• ls – list files and folders
Simple
1
1
Terminal 1


File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
myfolder1 22 days ago
myfolder2 22 days ago
other a day ago
mynotebook.ipynb 2 hours ago
conda-create.sh 18 minutes ago
mynotebook.ipynb
conda-create.sh
Terminal 1
Singularity> pwd
/bask/projects/m/myproject
Singularity> ls
conda-create.sh myfolder1 myfolder2 mynotebook.ipynb other
Singularity> sbatch conda-create.sh
Submitted batch job 273422
Singularity>
• pwd – check current directory is the myproject folder
• (if not, cd /bask/projects/m/myproject)
• ls – list files and folders
• sbatch conda-create.sh – submit batch job
Simple
1
1
Terminal 1


File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
myfolder1 22 days ago
myfolder2 22 days ago
other a day ago
mynotebook.ipynb 2 hours ago
conda-create.sh 18 minutes ago
mynotebook.ipynb
conda-create.sh
Terminal 1
Singularity> pwd
/bask/projects/m/myproject
Singularity> ls
conda-create.sh myfolder1 myfolder2 mynotebook.ipynb other
Singularity> sbatch conda-create.sh
Submitted batch job 273422
Singularity> squeue -u $USER
JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)
273376 baskervil sys/dash wongj R 2:43:28 1 bask-pg0309u03a
273422 baskervil conda-cr wongj PD 0:00 1 (Priority)
Singularity>
• pwd – check current directory is the myproject folder
• (if not, cd /bask/projects/m/myproject)
• ls – list files and folders
• sbatch conda-create.sh – submit batch job
• squeue –u $USER – check your job status
Simple
1
1
Terminal 1

File Edit View Run Kernel Git Tabs Settings Help

Filter files by name

/ myproject /

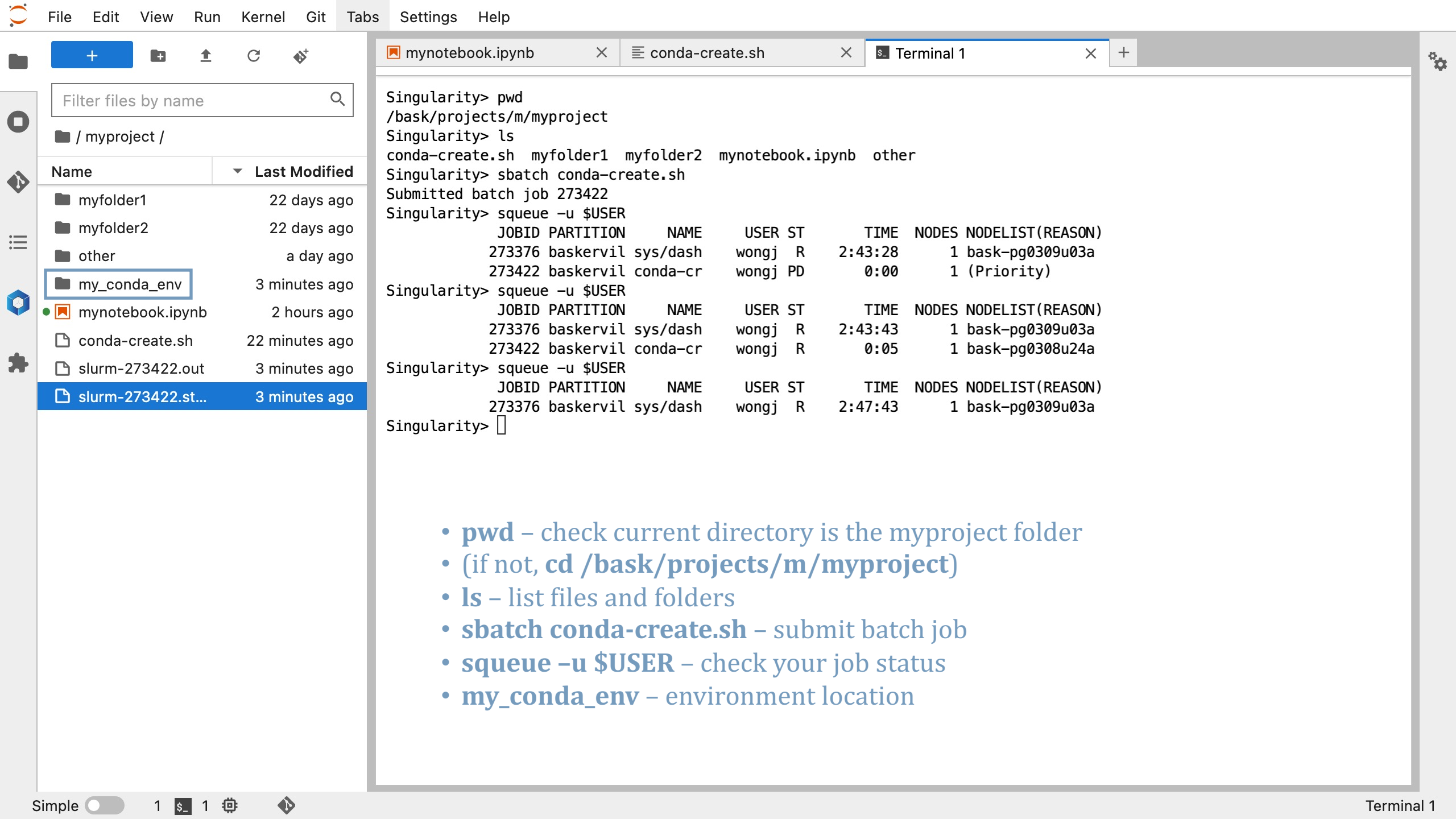
Name	Last Modified
myfolder1	22 days ago
myfolder2	22 days ago
other	a day ago
mynotebook.ipynb	2 hours ago
conda-create.sh	18 minutes ago
slurm-273422.st...	seconds ago

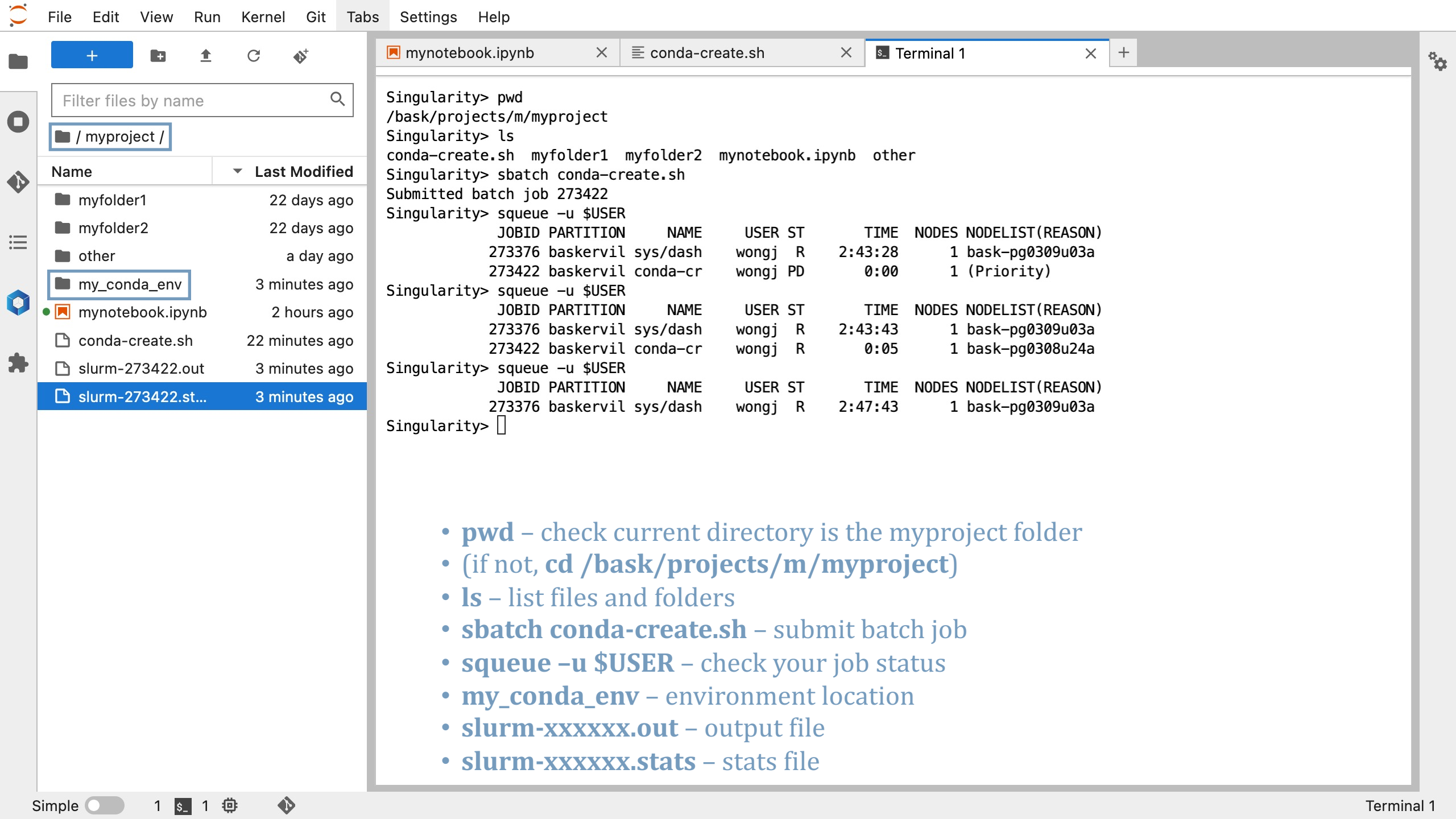
mynotebook.ipynb | conda-create.sh | Terminal 1

```
Singularity> pwd
/bask/projects/m/myproject
Singularity> ls
conda-create.sh  myfolder1  myfolder2  mynotebook.ipynb  other
Singularity> sbatch conda-create.sh
Submitted batch job 273422
Singularity> squeue -u $USER
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
            273376 baskervil sys/dash    wongj  R    2:43:28      1 bask-pg0309u03a
            273422 baskervil conda-cr    wongj PD       0:00      1 (Priority)
Singularity> squeue -u $USER
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
            273376 baskervil sys/dash    wongj  R    2:43:43      1 bask-pg0309u03a
            273422 baskervil conda-cr    wongj  R       0:05      1 bask-pg0308u24a
Singularity>
```

- **pwd** – check current directory is the myproject folder
- (if not, **cd /bask/projects/m/myproject**)
- **ls** – list files and folders
- **sbatch conda-create.sh** – submit batch job
- **squeue –u $USER** – check your job status

Simple 1 1 Terminal 1


File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
myfolder1 22 days ago
myfolder2 22 days ago
other a day ago
my_conda_env 3 minutes ago
mynotebook.ipynb 2 hours ago
conda-create.sh 22 minutes ago
slurm-273422.out 3 minutes ago
slurm-273422.st... 3 minutes ago
mynotebook.ipynb
conda-create.sh
Terminal 1
Singularity> pwd
/bask/projects/m/myproject
Singularity> ls
conda-create.sh myfolder1 myfolder2 mynotebook.ipynb other
Singularity> sbatch conda-create.sh
Submitted batch job 273422
Singularity> squeue -u $USER
JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)
273376 baskervil sys/dash wongj R 2:43:28 1 bask-pg0309u03a
273422 baskervil conda-cr wongj PD 0:00 1 (Priority)
Singularity> squeue -u $USER
JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)
273376 baskervil sys/dash wongj R 2:43:43 1 bask-pg0309u03a
273422 baskervil conda-cr wongj R 0:05 1 bask-pg0308u24a
Singularity> squeue -u $USER
JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)
273376 baskervil sys/dash wongj R 2:47:43 1 bask-pg0309u03a
Singularity>
• pwd – check current directory is the myproject folder
• (if not, cd /bask/projects/m/myproject)
• ls – list files and folders
• sbatch conda-create.sh – submit batch job
• squeue –u $USER – check your job status
• my_conda_env – environment location
Simple
1 1
Terminal 1


File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
myfolder1 22 days ago
myfolder2 22 days ago
other a day ago
my_conda_env 3 minutes ago
mynotebook.ipynb 2 hours ago
conda-create.sh 22 minutes ago
slurm-273422.out 3 minutes ago
slurm-273422.st... 3 minutes ago
mynotebook.ipynb
conda-create.sh
Terminal 1
Singularity> pwd
/bask/projects/m/myproject
Singularity> ls
conda-create.sh myfolder1 myfolder2 mynotebook.ipynb other
Singularity> sbatch conda-create.sh
Submitted batch job 273422
Singularity> squeue -u $USER
JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)
273376 baskervil sys/dash wongj R 2:43:28 1 bask-pg0309u03a
273422 baskervil conda-cr wongj PD 0:00 1 (Priority)
Singularity> squeue -u $USER
JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)
273376 baskervil sys/dash wongj R 2:43:43 1 bask-pg0309u03a
273422 baskervil conda-cr wongj R 0:05 1 bask-pg0308u24a
Singularity> squeue -u $USER
JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)
273376 baskervil sys/dash wongj R 2:47:43 1 bask-pg0309u03a
Singularity>
• pwd – check current directory is the myproject folder
• (if not, cd /bask/projects/m/myproject)
• ls – list files and folders
• sbatch conda-create.sh – submit batch job
• squeue –u $USER – check your job status
• my_conda_env – environment location
• slurm-xxxxxx.out – output file
• slurm-xxxxxx.stats – stats file
Simple
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Terminal 1

File Edit View Run Kernel Git Tabs Settings Help

New
New Launcher ⇧ ⌘ L

Open from Path...
Open from URL...

New View for
New Console for Activity

Close Tab ⌥ W
Shutdown Terminal ^ ⇧ Q
Close All Tabs

Save ⌘ S
Save As... ⇧ ⌘ S
Save All

Reload from Disk
Revert to Checkpoint
Rename...

Download

Save and Export Notebook As...

Save Current Workspace As...
Save Current Workspace

Print... ⌘ P

Log Out
Shut Down

Restart session

mynotebook.ipynb | conda-create.sh | Terminal 1

```
gularity> pwd
sk/projects/m/myproject
gularity> ls
da-create.sh  myfolder1  myfolder2  mynotebook.ipynb  other
gularity> sbatch conda-create.sh
mitted batch job 273422
gularity> squeue -u $USER
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
            273376 baskervil sys/dash    wongj  R    2:43:28      1 bask-pg0309u03a
            273422 baskervil conda-cr    wongj PD       0:00      1 (Priority)
gularity> squeue -u $USER
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
            273376 baskervil sys/dash    wongj  R    2:43:43      1 bask-pg0309u03a
            273422 baskervil conda-cr    wongj  R       0:05      1 bask-pg0308u24a
gularity> squeue -u $USER
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
            273376 baskervil sys/dash    wongj  R    2:47:43      1 bask-pg0309u03a
gularity>
```

- **pwd** – check current directory is the myproject folder
- (if not, **cd /bask/projects/m/myproject**)
- **ls** – list files and folders
- **sbatch conda-create.sh** – submit batch job
- **squeue –u $USER** – check your job status
- **my_conda_env** – environment location
- **slurm-xxxxxx.out** – output file
- **slurm-xxxxxx.stats** – stats file

Simple 1 1 Terminal 1

3. JupyterLab

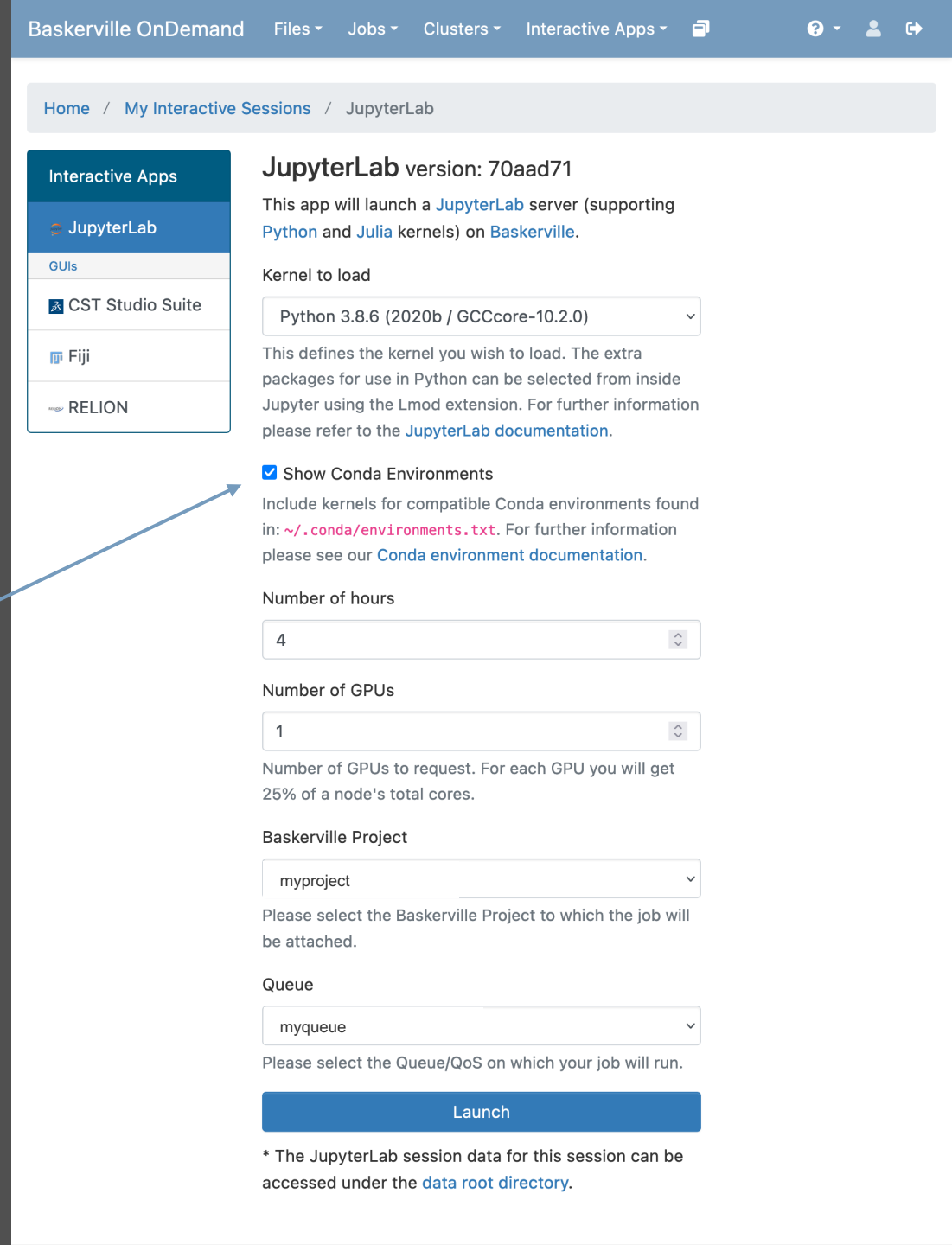
b) Conda Environments

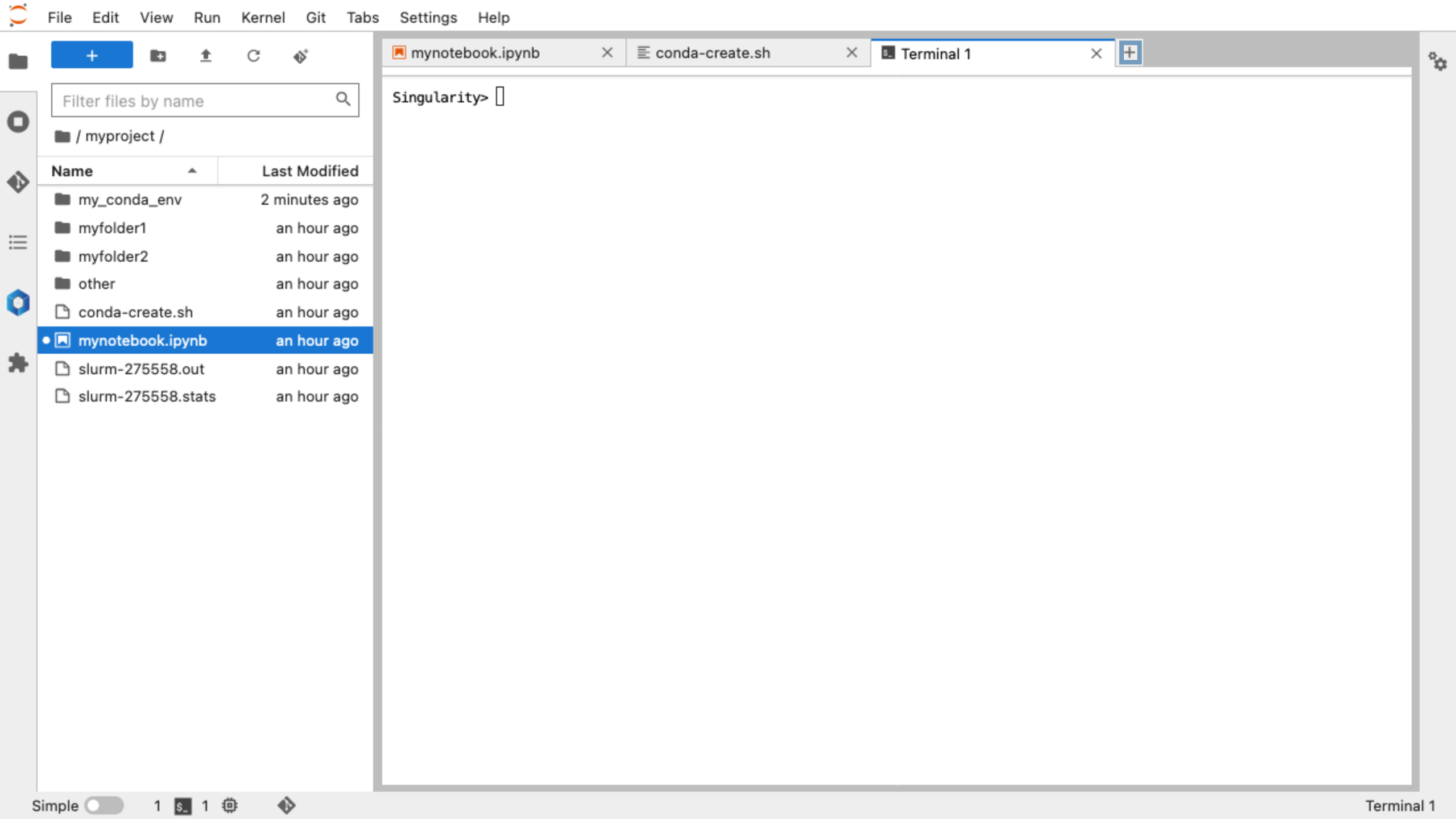
(ii) Relaunch JupterLab and load new kernel

Relaunch JupyterLab and load new kernel

This time, tick to enable

Show Conda Environments




File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
my_conda_env 2 minutes ago
myfolder1 an hour ago
myfolder2 an hour ago
other an hour ago
conda-create.sh an hour ago
mynotebook.ipynb an hour ago
slurm-275558.out an hour ago
slurm-275558.stats an hour ago
mynotebook.ipynb
conda-create.sh
Terminal 1
Singularity>
Simple
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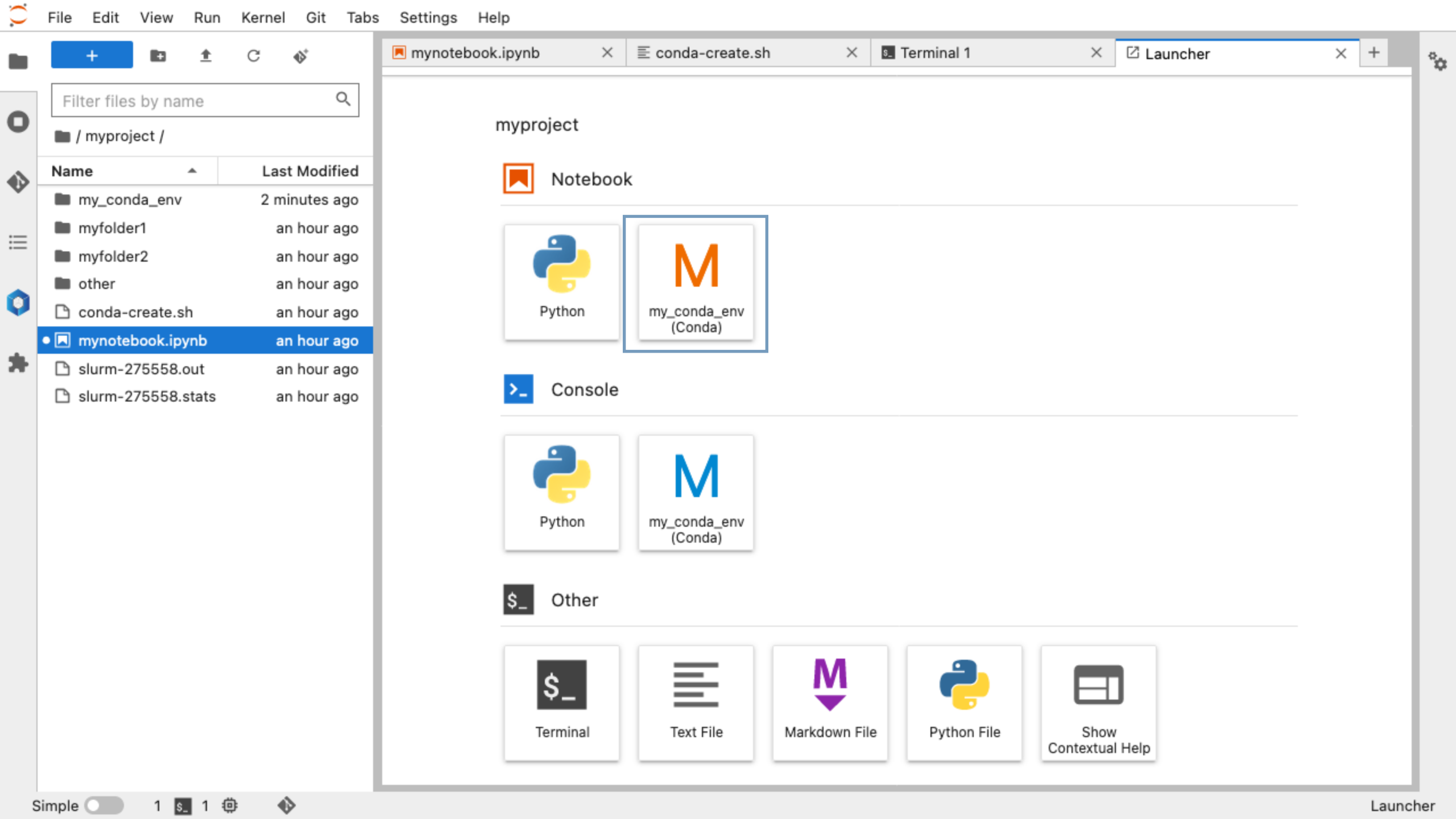
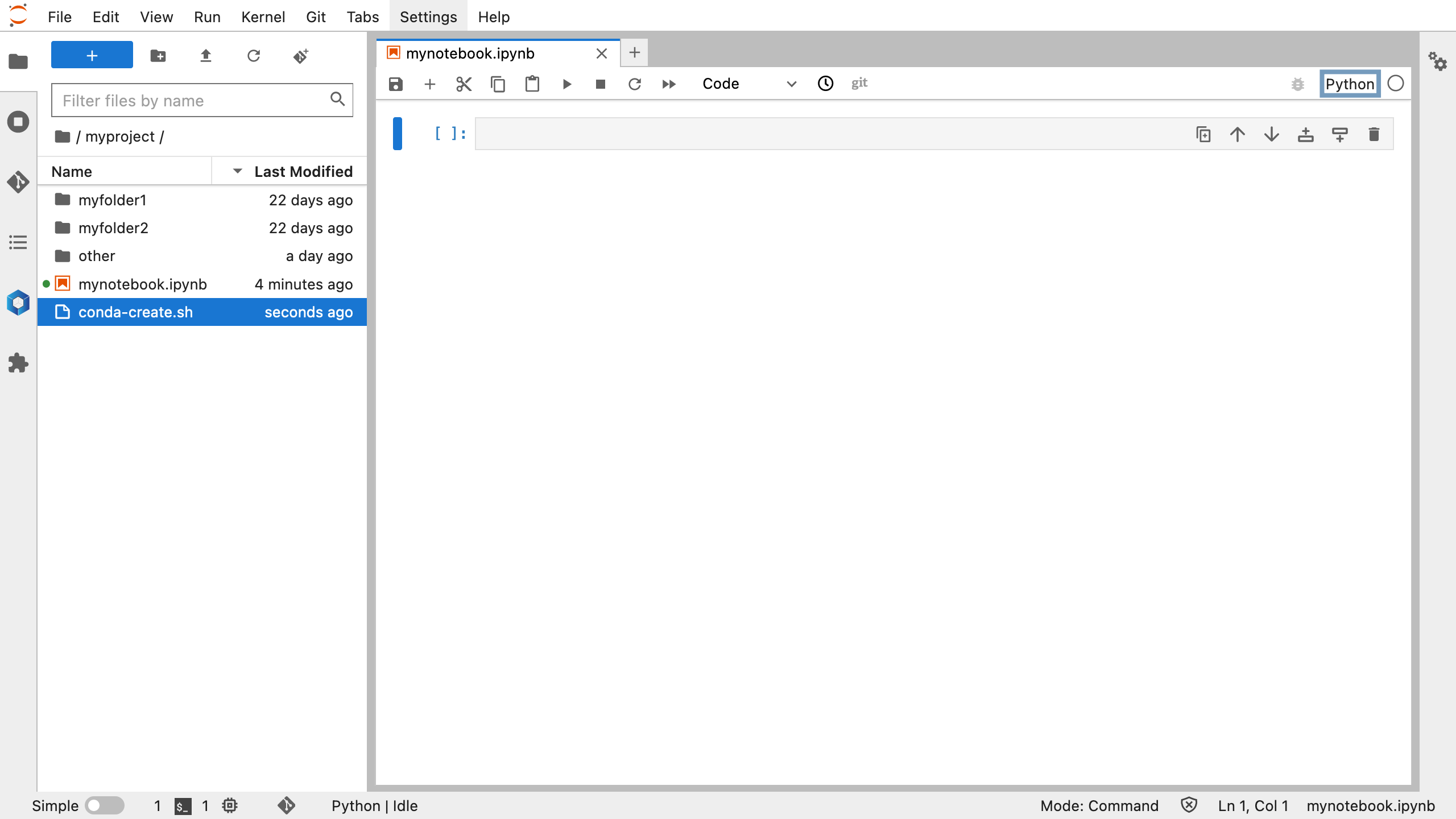
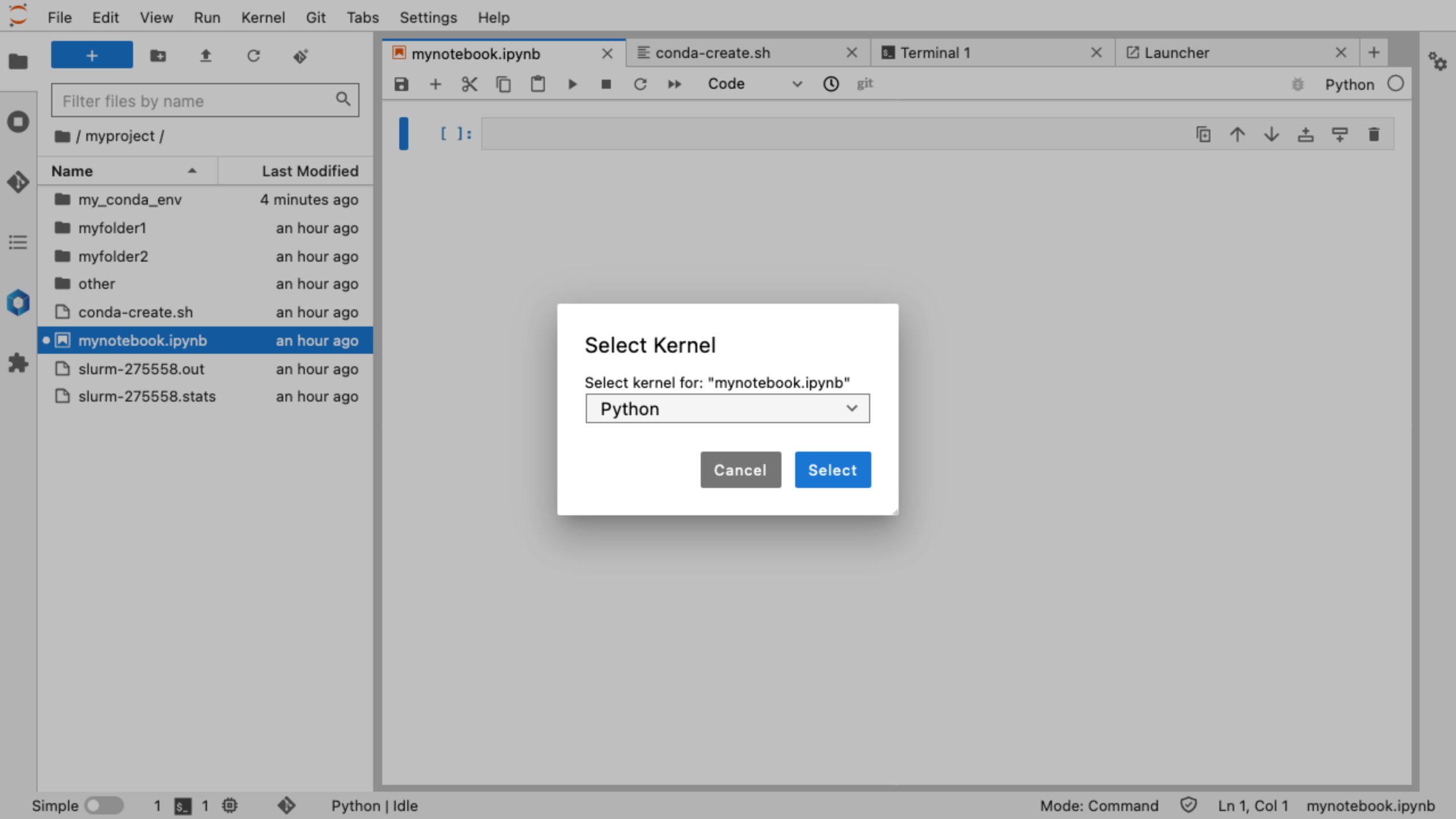
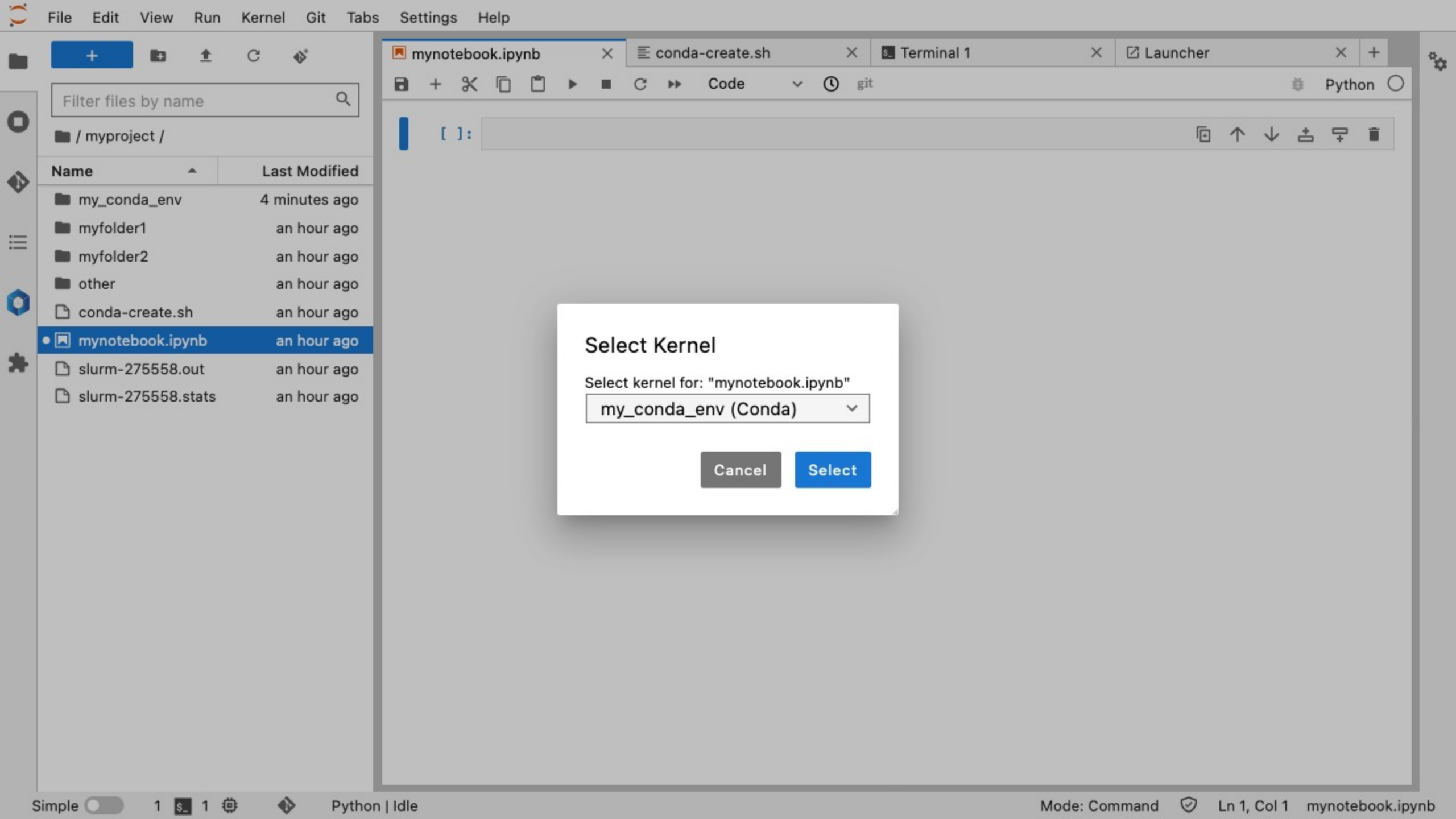
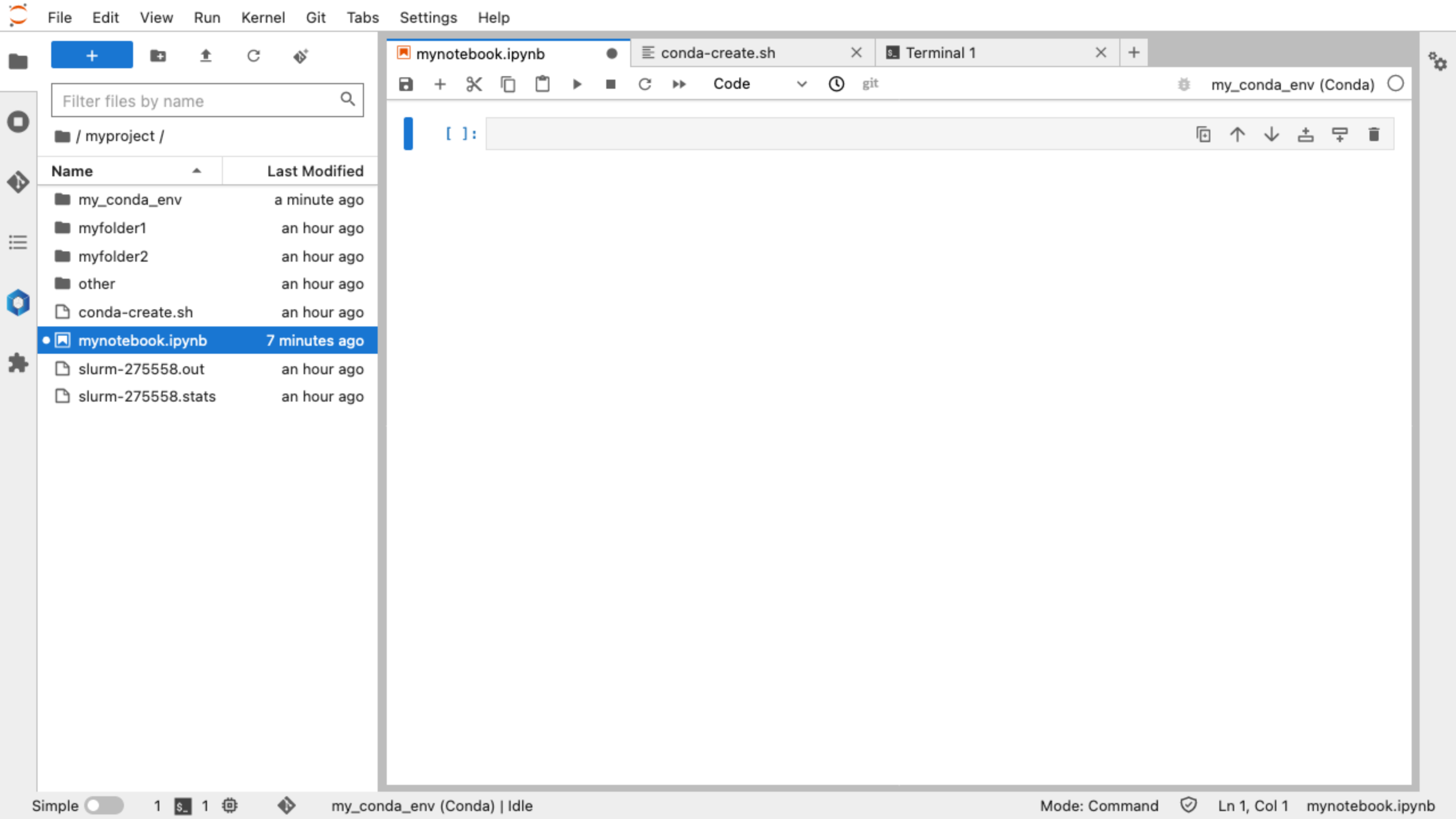
Terminal 1

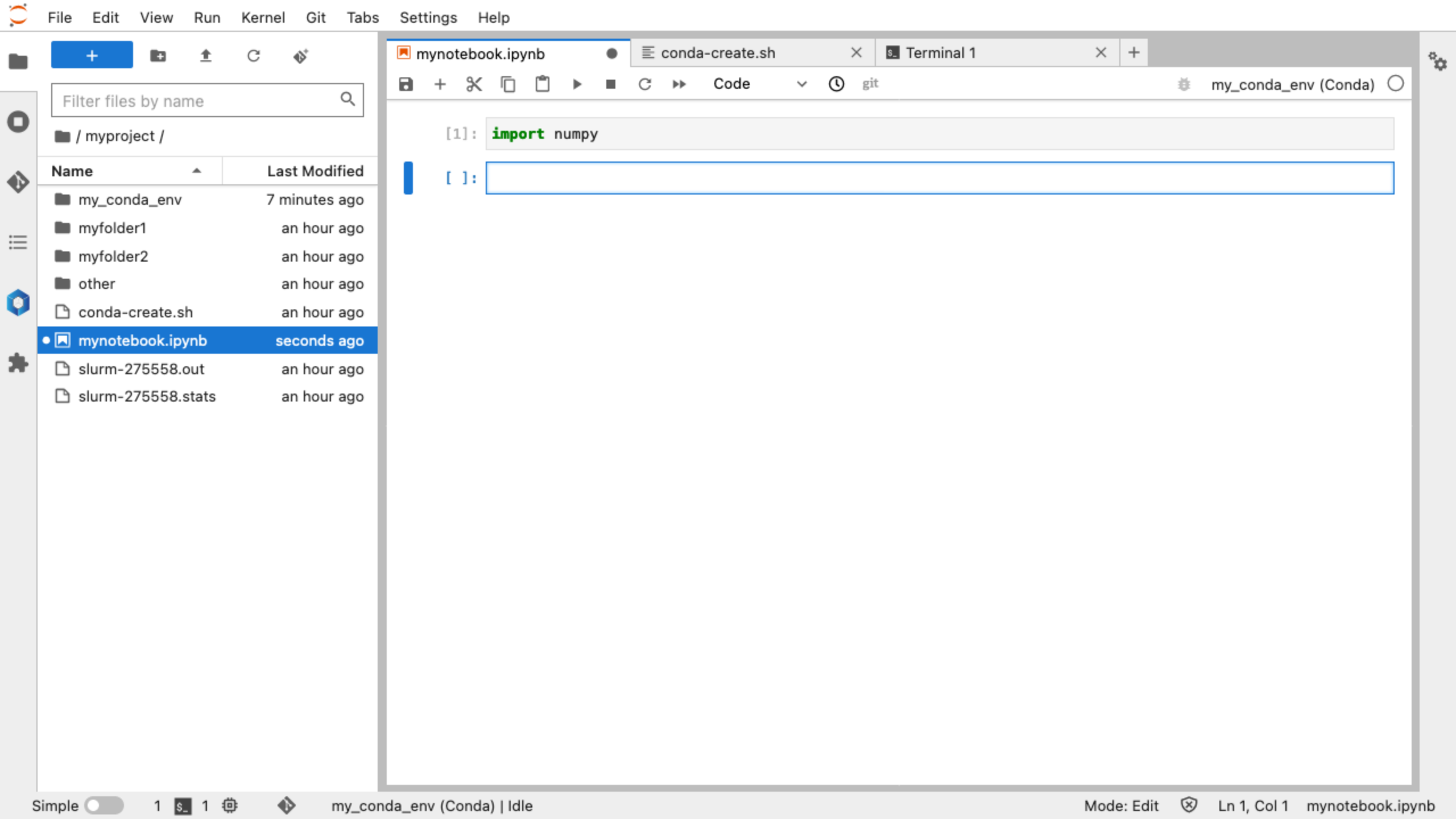

File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
my_conda_env 2 minutes ago
myfolder1 an hour ago
myfolder2 an hour ago
other an hour ago
conda-create.sh an hour ago
mynotebook.ipynb an hour ago
slurm-275558.out an hour ago
slurm-275558.stats an hour ago
mynotebook.ipynb
conda-create.sh
Terminal 1
Launcher
myproject
Notebook
Python
my_conda_env (Conda)
Console
Python
my_conda_env (Conda)
Other
Terminal
Text File
Markdown File
Python File
Show Contextual Help
Simple
1
1
Launcher

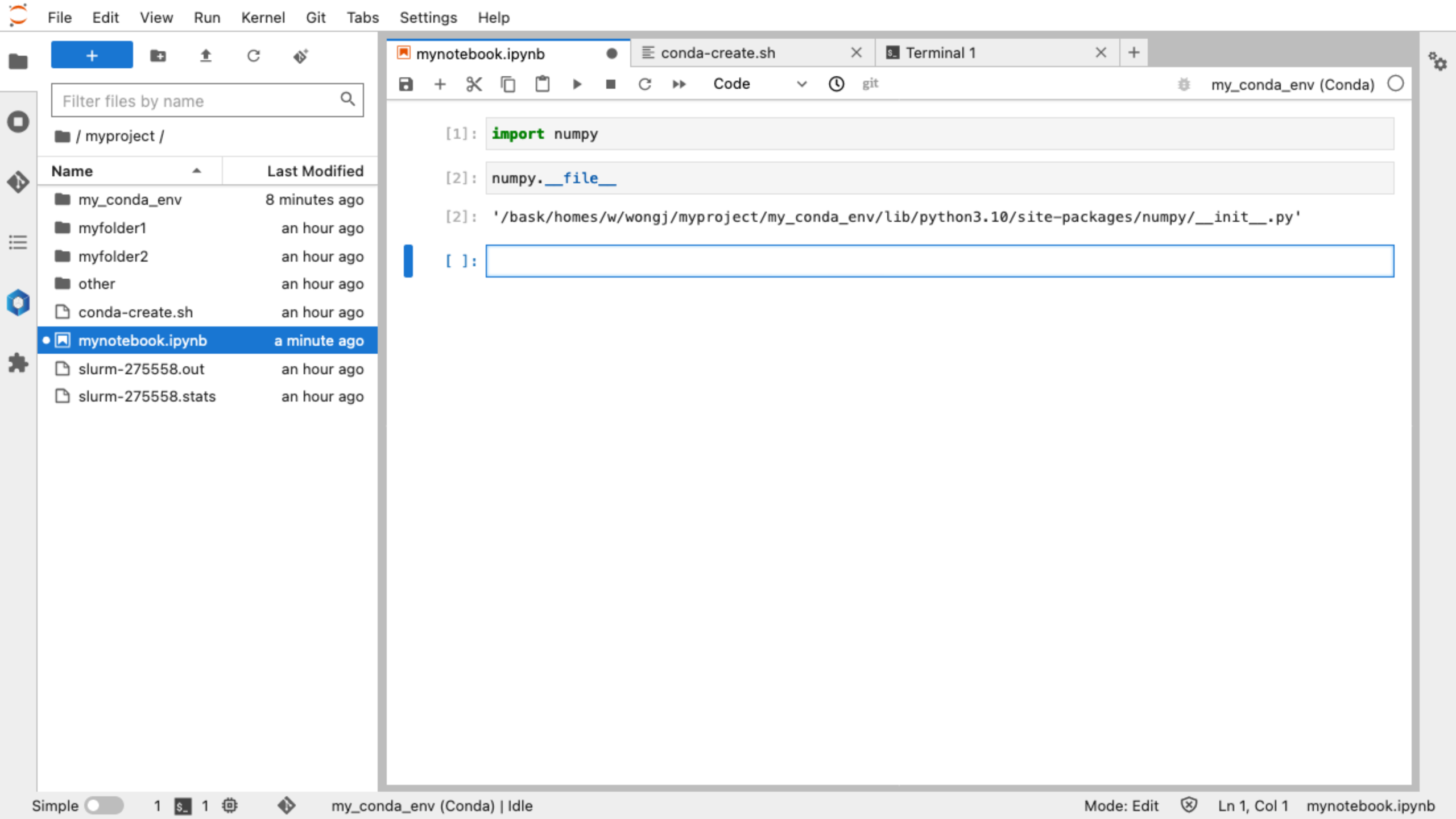

File
Edit
View
Run
Kernel
Git
Tabs
Settings
Help
Filter files by name
/ myproject /
Name
Last Modified
myfolder1
22 days ago
myfolder2
22 days ago
other
a day ago
mynotebook.ipynb
4 minutes ago
conda-create.sh
seconds ago
mynotebook.ipynb
Code
git
Python
[ ]:
Simple
1
1
Python | Idle
Mode: Command
Ln 1, Col 1
mynotebook.ipynb


File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
my_conda_env 4 minutes ago
myfolder1 an hour ago
myfolder2 an hour ago
other an hour ago
conda-create.sh an hour ago
mynotebook.ipynb an hour ago
slurm-275558.out an hour ago
slurm-275558.stats an hour ago
mynotebook.ipynb
conda-create.sh
Terminal 1
Launcher
Code
git
Python
[ ]:
Select Kernel
Select kernel for: "mynotebook.ipynb"
Python
Cancel
Select
Simple
1
1
Python | Idle
Mode: Command
Ln 1, Col 1
mynotebook.ipynb


File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
my_conda_env 4 minutes ago
myfolder1 an hour ago
myfolder2 an hour ago
other an hour ago
conda-create.sh an hour ago
mynotebook.ipynb an hour ago
slurm-275558.out an hour ago
slurm-275558.stats an hour ago
mynotebook.ipynb
conda-create.sh
Terminal 1
Launcher
Code
git
Python
[ ]:
Select Kernel
Select kernel for: "mynotebook.ipynb"
my_conda_env (Conda)
Cancel
Select
Simple
1
1
Python | Idle
Mode: Command
Ln 1, Col 1
mynotebook.ipynb


File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
my_conda_env a minute ago
myfolder1 an hour ago
myfolder2 an hour ago
other an hour ago
conda-create.sh an hour ago
mynotebook.ipynb 7 minutes ago
slurm-275558.out an hour ago
slurm-275558.stats an hour ago
mynotebook.ipynb
conda-create.sh
Terminal 1
Code
git
my_conda_env (Conda)
[ ]:
Simple
1
1
my_conda_env (Conda) | Idle
Mode: Command
Ln 1, Col 1
mynotebook.ipynb

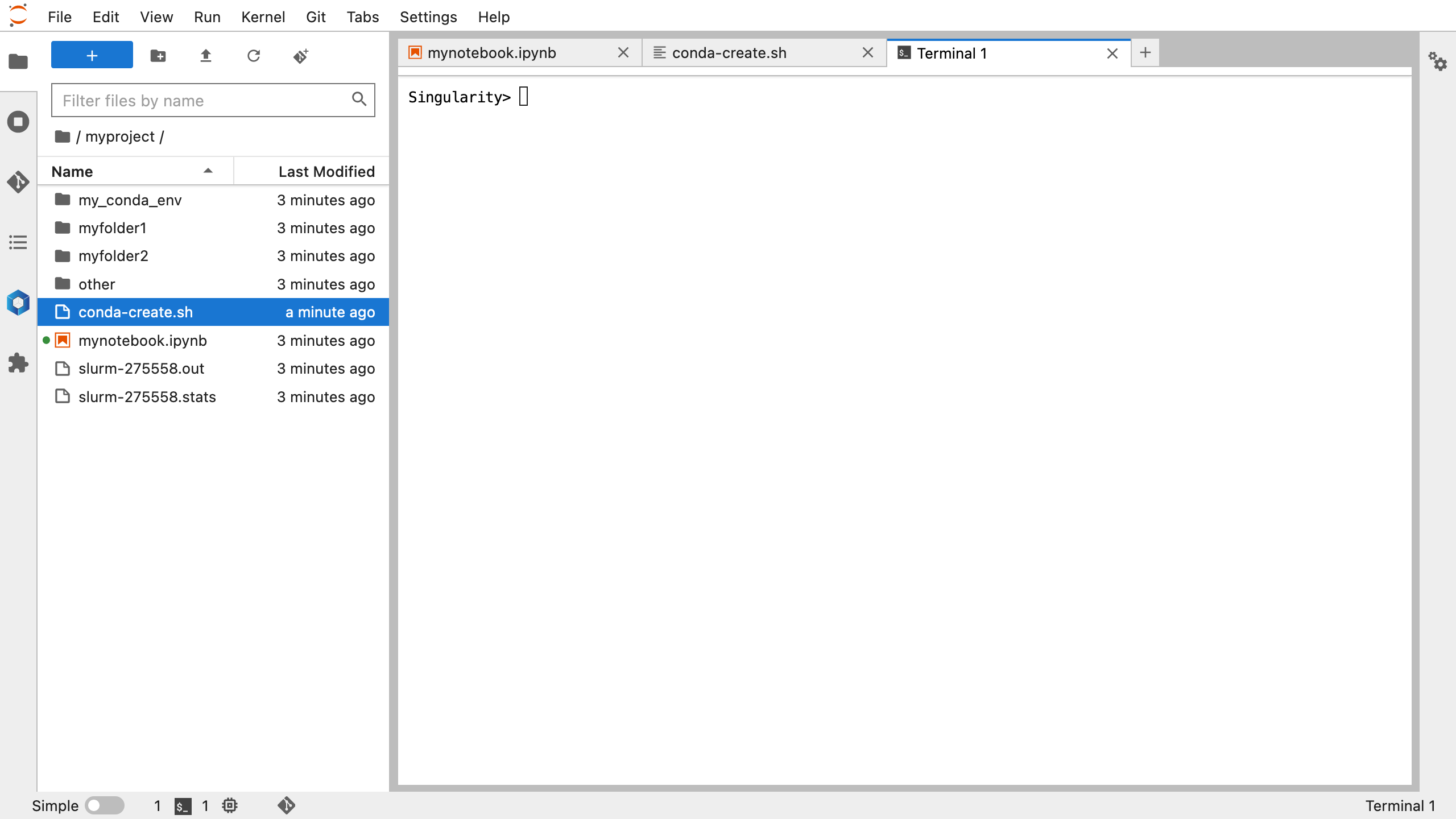

File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
my_conda_env 7 minutes ago
myfolder1 an hour ago
myfolder2 an hour ago
other an hour ago
conda-create.sh an hour ago
mynotebook.ipynb seconds ago
slurm-275558.out an hour ago
slurm-275558.stats an hour ago
mynotebook.ipynb
conda-create.sh
Terminal 1
Code
git
my_conda_env (Conda)
[1]: import numpy
[ ]:
Simple
1
1
my_conda_env (Conda) | Idle
Mode: Edit
Ln 1, Col 1
mynotebook.ipynb

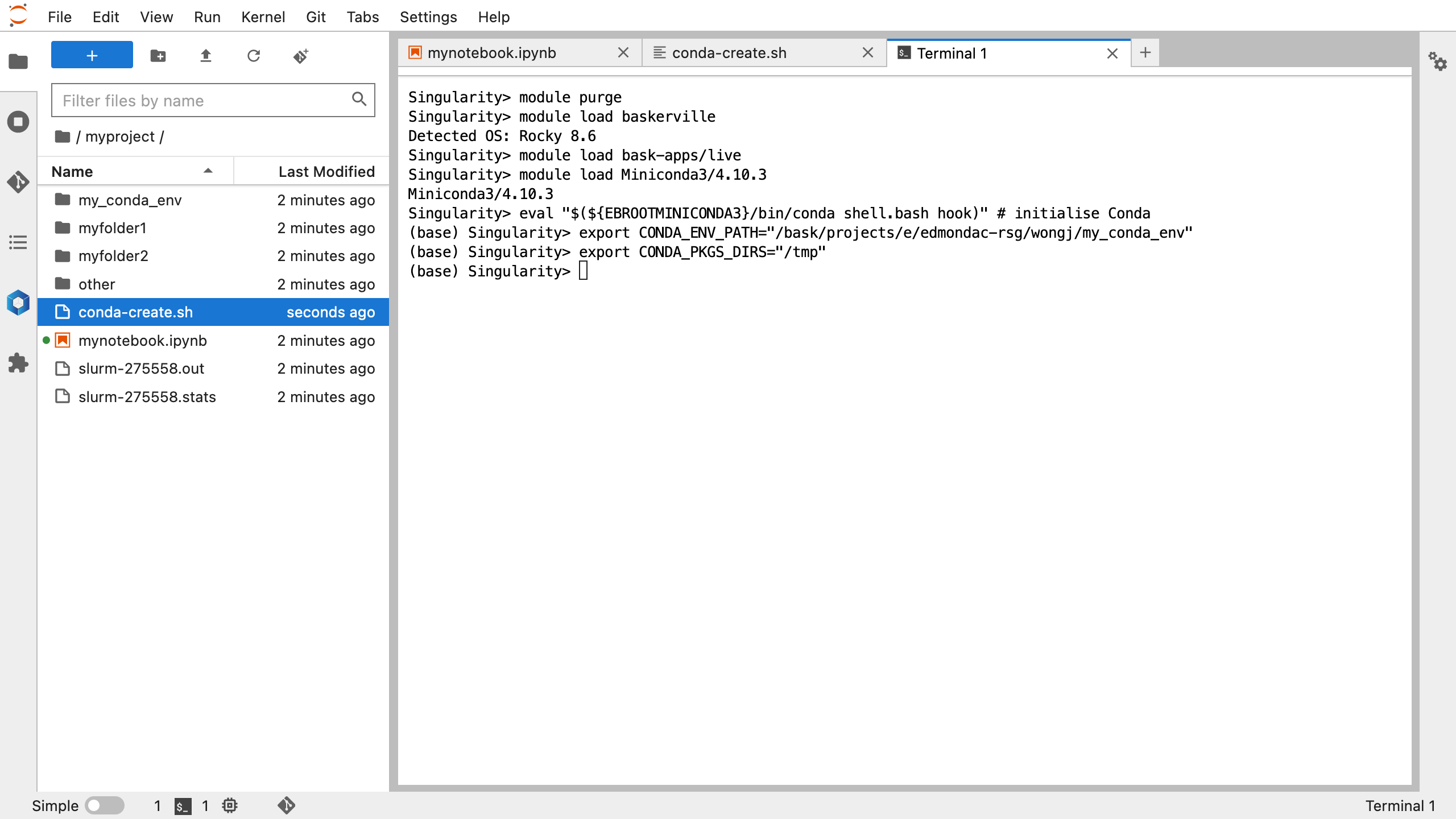

File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
my_conda_env 8 minutes ago
myfolder1 an hour ago
myfolder2 an hour ago
other an hour ago
conda-create.sh an hour ago
mynotebook.ipynb a minute ago
slurm-275558.out an hour ago
slurm-275558.stats an hour ago
mynotebook.ipynb
conda-create.sh
Terminal 1
Code
git
my_conda_env (Conda)
[1]: import numpy
[2]: numpy.__file__
[2]: '/bask/homes/w/wongj/myproject/my_conda_env/lib/python3.10/site-packages/numpy/__init__.py'
[ ]:
Simple
1
1
my_conda_env (Conda) | Idle
Mode: Edit
Ln 1, Col 1
mynotebook.ipynb

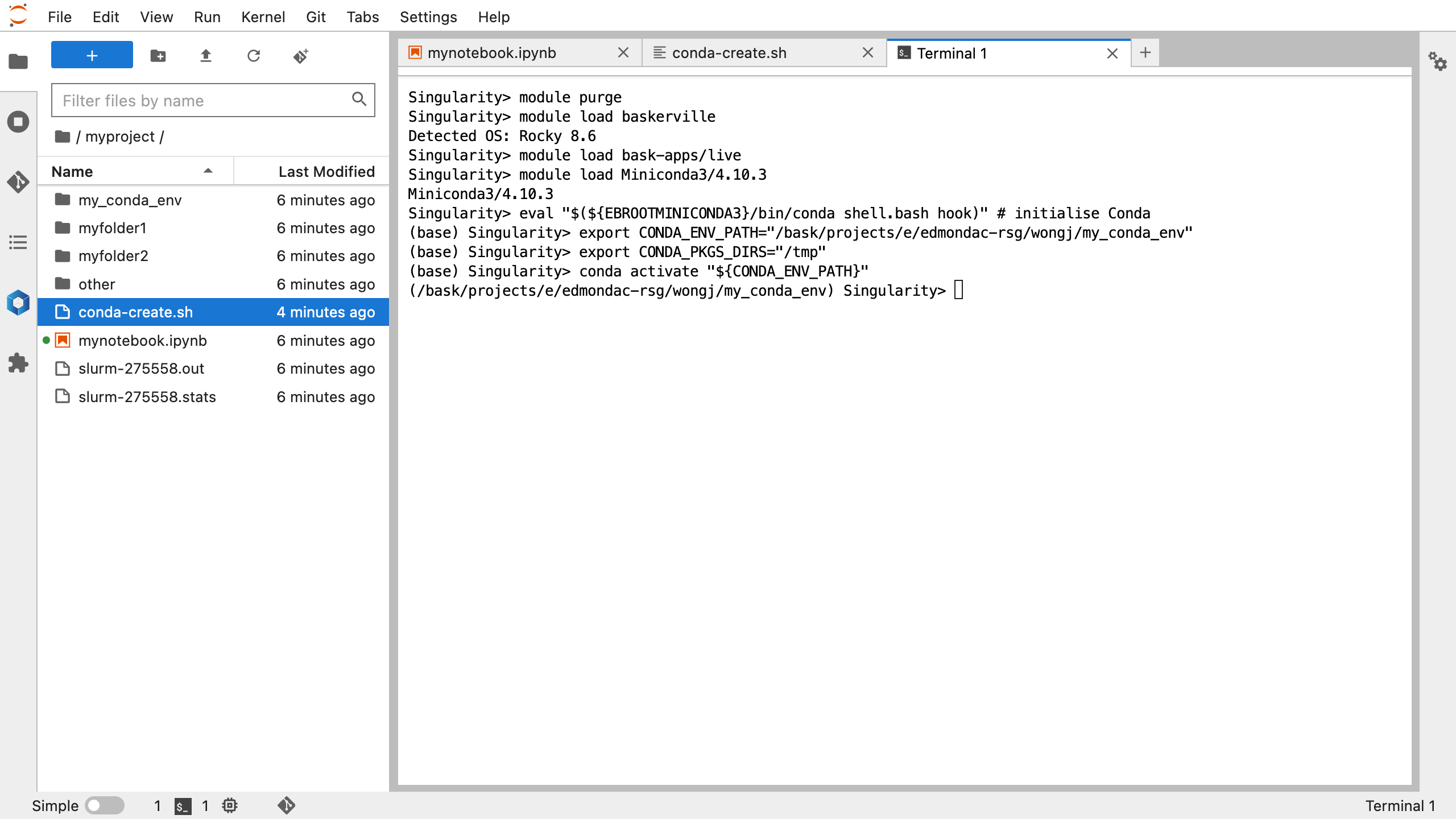
3. JupyterLab

b) Conda Environments

(iii) Modifying your environment


File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
my_conda_env 3 minutes ago
myfolder1 3 minutes ago
myfolder2 3 minutes ago
other 3 minutes ago
conda-create.sh a minute ago
mynotebook.ipynb 3 minutes ago
slurm-275558.out 3 minutes ago
slurm-275558.stats 3 minutes ago
mynotebook.ipynb
conda-create.sh
Terminal 1
Singularity>
Simple 1 1
Terminal 1


File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
my_conda_env 2 minutes ago
myfolder1 2 minutes ago
myfolder2 2 minutes ago
other 2 minutes ago
conda-create.sh seconds ago
mynotebook.ipynb 2 minutes ago
slurm-275558.out 2 minutes ago
slurm-275558.stats 2 minutes ago
mynotebook.ipynb
conda-create.sh
Terminal 1
Singularity> module purge
Singularity> module load baskerville
Detected OS: Rocky 8.6
Singularity> module load bask-apps/live
Singularity> module load Miniconda3/4.10.3
Miniconda3/4.10.3
Singularity> eval "$(${EBROOTMINICONDA3}/bin/conda shell.bash hook)" # initialise Conda
(base) Singularity> export CONDA_ENV_PATH="/bask/projects/e/edmondac-rsg/wongj/my_conda_env"
(base) Singularity> export CONDA_PKGS_DIRS="/tmp"
(base) Singularity>
Simple
1
1
Terminal 1


File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
my_conda_env 6 minutes ago
myfolder1 6 minutes ago
myfolder2 6 minutes ago
other 6 minutes ago
conda-create.sh 4 minutes ago
mynotebook.ipynb 6 minutes ago
slurm-275558.out 6 minutes ago
slurm-275558.stats 6 minutes ago
mynotebook.ipynb
conda-create.sh
Terminal 1
Singularity> module purge
Singularity> module load baskerville
Detected OS: Rocky 8.6
Singularity> module load bask-apps/live
Singularity> module load Miniconda3/4.10.3
Miniconda3/4.10.3
Singularity> eval "$(${EBROOTMINICONDA3}/bin/conda shell.bash hook)" # initialise Conda
(base) Singularity> export CONDA_ENV_PATH="/bask/projects/e/edmondac-rsg/wongj/my_conda_env"
(base) Singularity> export CONDA_PKGS_DIRS="/tmp"
(base) Singularity> conda activate "${CONDA_ENV_PATH}"
(/bask/projects/e/edmondac-rsg/wongj/my_conda_env) Singularity>
Simple
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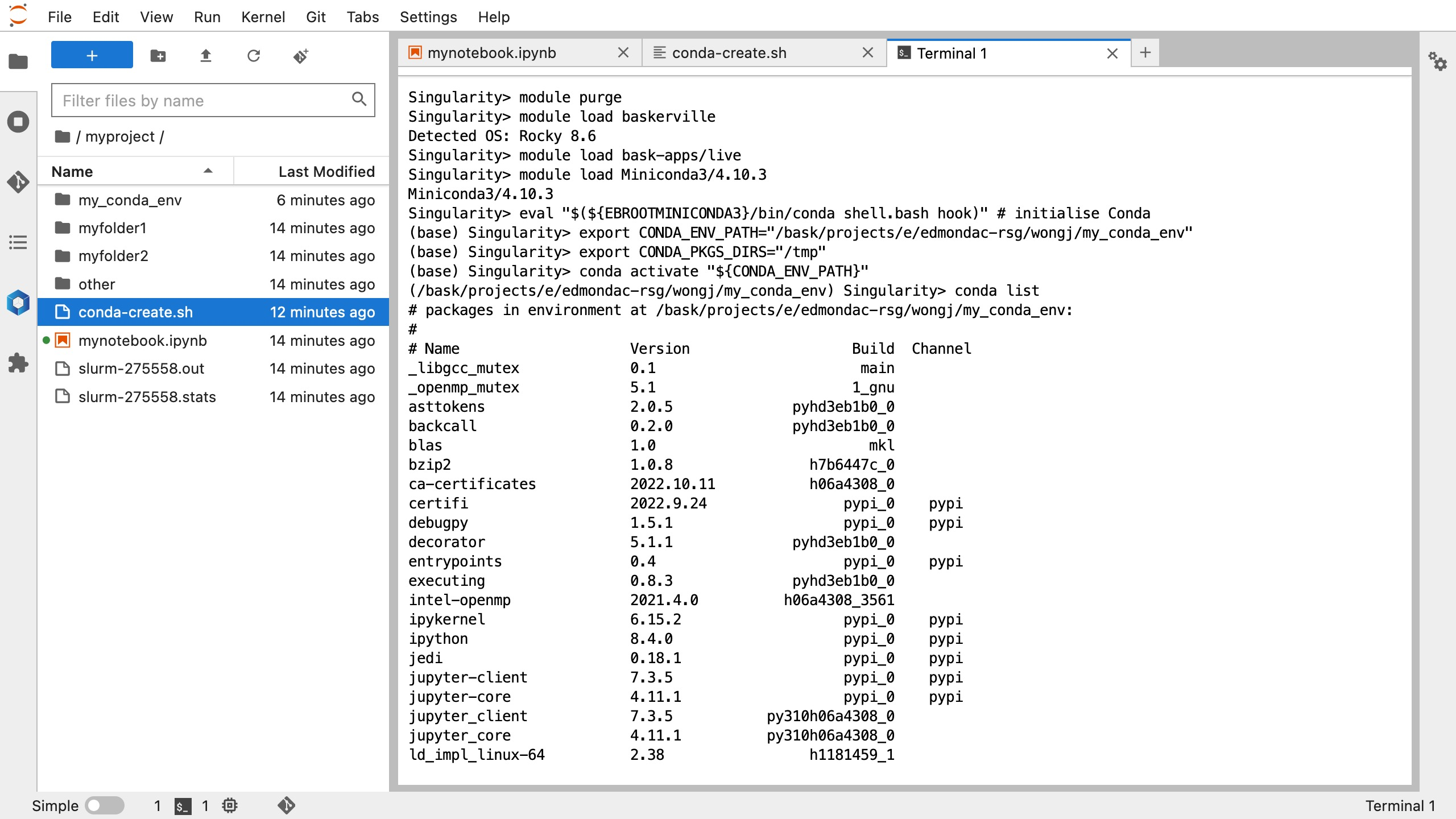
Terminal 1


File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
my_conda_env 6 minutes ago
myfolder1 14 minutes ago
myfolder2 14 minutes ago
other 14 minutes ago
conda-create.sh 12 minutes ago
mynotebook.ipynb 14 minutes ago
slurm-275558.out 14 minutes ago
slurm-275558.stats 14 minutes ago
mynotebook.ipynb
conda-create.sh
Terminal 1
Singularity> module purge
Singularity> module load baskerville
Detected OS: Rocky 8.6
Singularity> module load bask-apps/live
Singularity> module load Miniconda3/4.10.3
Miniconda3/4.10.3
Singularity> eval "$(${EBROOTMINICONDA3}/bin/conda shell.bash hook)" # initialise Conda
(base) Singularity> export CONDA_ENV_PATH="/bask/projects/e/edmondac-rsg/wongj/my_conda_env"
(base) Singularity> export CONDA_PKGS_DIRS="/tmp"
(base) Singularity> conda activate "${CONDA_ENV_PATH}"
(/bask/projects/e/edmondac-rsg/wongj/my_conda_env) Singularity> conda list
packages in environment at /bask/projects/e/edmondac-rsg/wongj/my_conda_env:
#
Name Version Build Channel
_libgcc_mutex 0.1 main
_openmp_mutex 5.1 1_gnu
asttokens 2.0.5 pyhd3eb1b0_0
backcall 0.2.0 pyhd3eb1b0_0
blas 1.0 mkl
bzip2 1.0.8 h7b6447c_0
ca-certificates 2022.10.11 h06a4308_0
certifi 2022.9.24 pypi_0 pypi
debugpy 1.5.1 pypi_0 pypi
decorator 5.1.1 pyhd3eb1b0_0
entrypoints 0.4 pypi_0 pypi
executing 0.8.3 pyhd3eb1b0_0
intel-openmp 2021.4.0 h06a4308_3561
ipykernel 6.15.2 pypi_0 pypi
ipython 8.4.0 pypi_0 pypi
jedi 0.18.1 pypi_0 pypi
jupyter-client 7.3.5 pypi_0 pypi
jupyter-core 4.11.1 pypi_0 pypi
jupyter_client 7.3.5 py310h06a4308_0
jupyter_core 4.11.1 py310h06a4308_0
ld_impl_linux-64 2.38 h1181459_1
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Terminal 1

File Edit View Run Kernel Git Tabs Settings Help

Filter files by name

/ myproject /

Name	Last Modified
my_conda_env	6 minutes ago
myfolder1	15 minutes ago
myfolder2	15 minutes ago
other	15 minutes ago
conda-create.sh	13 minutes ago
mynotebook.ipynb	15 minutes ago
slurm-275558.out	15 minutes ago
slurm-275558.stats	15 minutes ago

mynotebook.ipynb | conda-create.sh | Terminal 1

```
mkl_random                1.2.2           py310h00e6091_0
ncurses                   6.3                  h5eee18b_3
nest-asyncio              1.5.5                pypi_0    pypi
numpy                     1.23.3               pypi_0    pypi
numpy-base                1.23.3          py310h8e6c178_0
openssl                   1.1.1q               h7f8727e_0
packaging                 21.3               pyhd3eb1b0_0
parso                     0.8.3              pyhd3eb1b0_0
pexpect                   4.8.0              pyhd3eb1b0_3
pickleshare               0.7.5           pyhd3eb1b0_1003
pip                       22.2.2               pypi_0    pypi
prompt-toolkit            3.0.20             pyhd3eb1b0_0
psutil                    5.9.0                pypi_0    pypi
ptyprocess                0.7.0              pyhd3eb1b0_2
pure_eval                 0.2.2              pyhd3eb1b0_0
pygments                  2.11.2             pyhd3eb1b0_0
pyparsing                 3.0.9                pypi_0    pypi
python                    3.10.6               haa1d7c7_1
python-dateutil           2.8.2              pyhd3eb1b0_0
pyzmq                     23.2.0               pypi_0    pypi
readline                  8.2                  h5eee18b_0
setuptools                65.5.0               pypi_0    pypi
six                       1.16.0             pyhd3eb1b0_1
sqlite                    3.39.3               h5082296_0
stack_data                0.2.0              pyhd3eb1b0_0
tk                        8.6.12               h1ccaba5_0
tornado                   6.2                  pypi_0    pypi
traitlets                 5.1.1              pyhd3eb1b0_0
tzdata                    2022f                h04d1e81_0
wcwidth                   0.2.5              pyhd3eb1b0_0
wheel                     0.37.1             pyhd3eb1b0_0
xz                        5.2.6                h5eee18b_0
zeromq                    4.3.4                h2531618_0
zlib                      1.2.13               h5eee18b_0
(/bask/projects/e/edmondac-rsg/wongj/my_conda_env) Singularity>
```

Simple 1 1 Terminal 1

File Edit View Run Kernel Git Tabs Settings Help

Filter files by name

/ myproject /

Name	Last Modified
my_conda_env	7 minutes ago
myfolder1	16 minutes ago
myfolder2	16 minutes ago
other	16 minutes ago
conda-create.sh	14 minutes ago
mynotebook.ipynb	16 minutes ago
slurm-275558.out	16 minutes ago
slurm-275558.stats	16 minutes ago

mynotebook.ipynb | conda-create.sh | Terminal 1

```
mkl_random                1.2.2           py310h00e6091_0
ncurses                   6.3                  h5eee18b_3
nest-asyncio              1.5.5                   pypi_0    pypi
numpy                     1.23.3                  pypi_0    pypi
numpy-base                1.23.3          py310h8e6c178_0
openssl                   1.1.1q               h7f8727e_0
packaging                 21.3               pyhd3eb1b0_0
parso                     0.8.3              pyhd3eb1b0_0
pexpect                   4.8.0              pyhd3eb1b0_3
pickleshare               0.7.5           pyhd3eb1b0_1003
pip                       22.2.2                  pypi_0    pypi
prompt-toolkit            3.0.20             pyhd3eb1b0_0
psutil                    5.9.0                   pypi_0    pypi
ptyprocess                0.7.0              pyhd3eb1b0_2
pure_eval                 0.2.2              pyhd3eb1b0_0
pygments                  2.11.2             pyhd3eb1b0_0
pyparsing                 3.0.9                   pypi_0    pypi
python                    3.10.6               haa1d7c7_1
python-dateutil           2.8.2              pyhd3eb1b0_0
pyzmq                     23.2.0                  pypi_0    pypi
readline                  8.2                  h5eee18b_0
setuptools                65.5.0                  pypi_0    pypi
six                       1.16.0             pyhd3eb1b0_1
sqlite                    3.39.3               h5082296_0
stack_data                0.2.0              pyhd3eb1b0_0
tk                        8.6.12               h1ccaba5_0
tornado                   6.2                     pypi_0    pypi
traitlets                 5.1.1              pyhd3eb1b0_0
tzdata                    2022f                h04d1e81_0
wcwidth                   0.2.5              pyhd3eb1b0_0
wheel                     0.37.1             pyhd3eb1b0_0
xz                        5.2.6                h5eee18b_0
zeromq                    4.3.4                h2531618_0
zlib                      1.2.13               h5eee18b_0
(/bask/projects/e/edmondac-rsg/wongj/my_conda_env) Singularity> conda install pandas --yes
```

Simple 1 1 Terminal 1

File Edit View Run Kernel Git Tabs Settings Help

Filter files by name

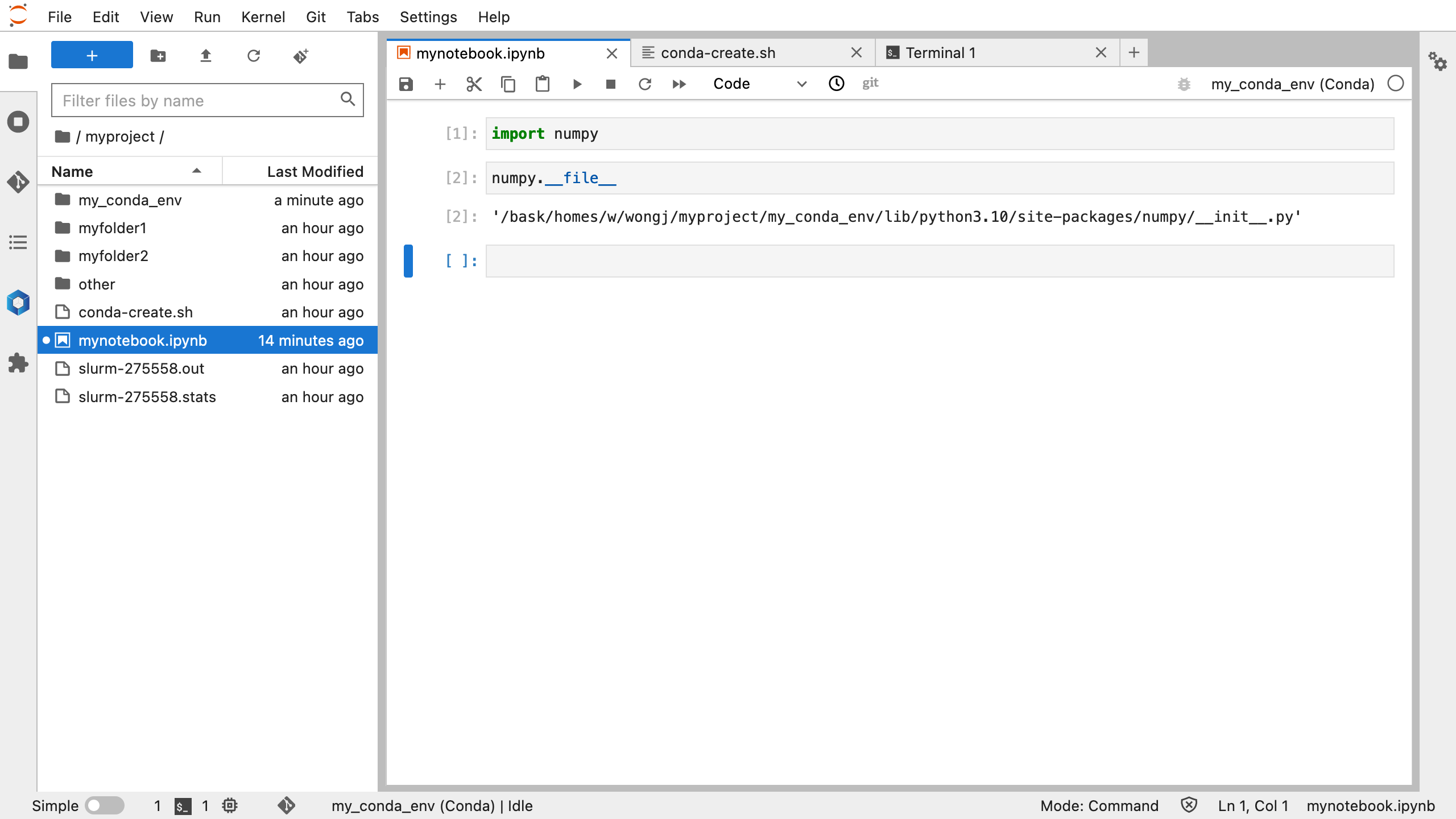
/ myproject /

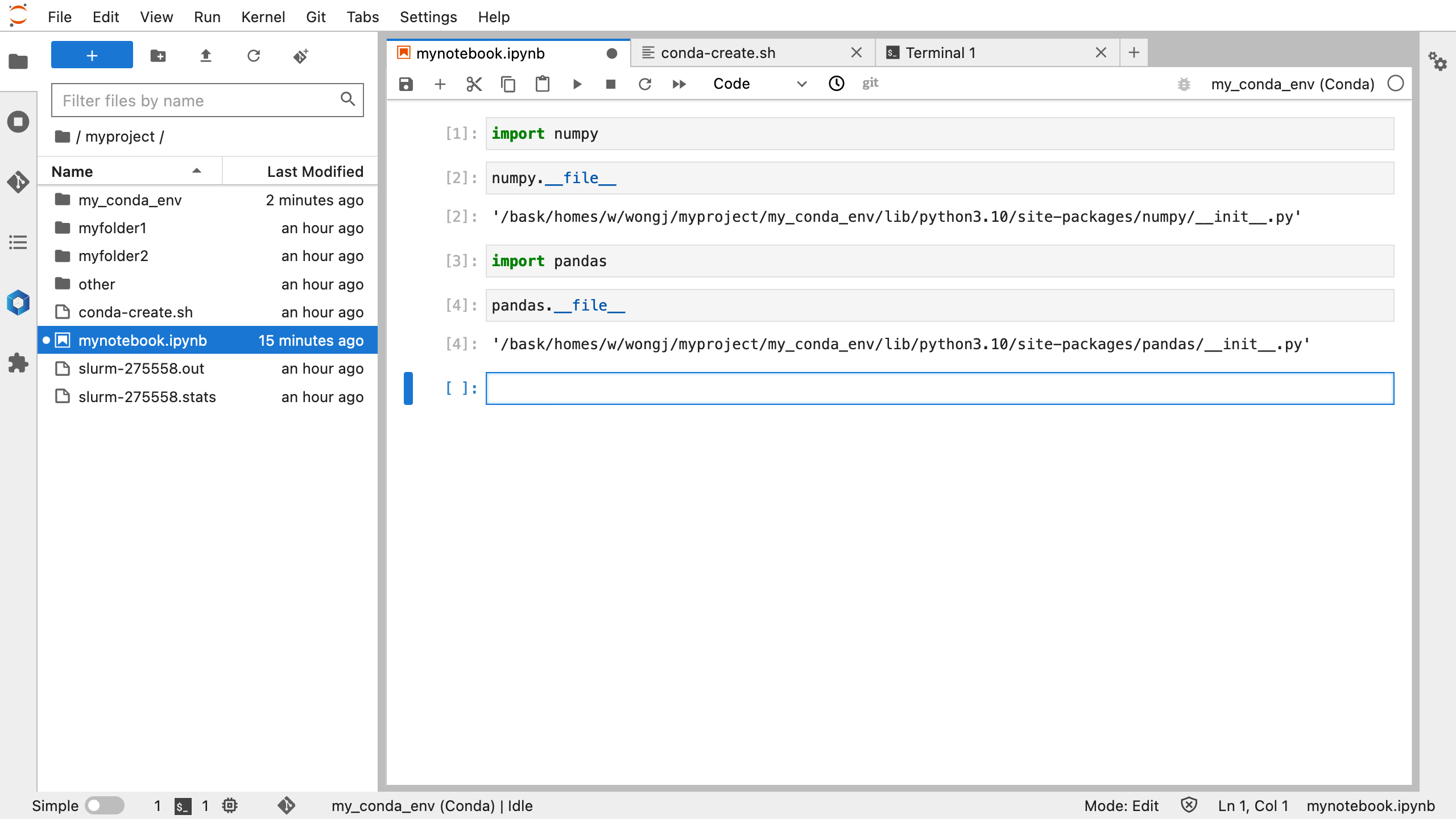
Name	Last Modified
my_conda_env	seconds ago
myfolder1	17 minutes ago
myfolder2	17 minutes ago
other	17 minutes ago
conda-create.sh	15 minutes ago
mynotebook.ipynb	17 minutes ago
slurm-275558.out	17 minutes ago
slurm-275558.stats	17 minutes ago

mynotebook.ipynb | conda-create.sh | Terminal 1

```
  environment location: /bask/projects/e/edmondac-rsg/wongj/my_conda_env

  added / updated specs:
    - pandas


The following packages will be downloaded:

    package                    |            build
    ---------------------------|-----------------
    bottleneck-1.3.5           |  py310ha9d4c09_0         274 KB
    numexpr-2.8.3              |  py310hcea2de6_0         321 KB
    pandas-1.4.4               |  py310h6a678d5_0        25.5 MB
    pytz-2022.1                |  py310h06a4308_0         196 KB
    ------------------------------------------------------------
                                           Total:        26.3 MB

The following NEW packages will be INSTALLED:

  bottleneck         pkgs/main/linux-64::bottleneck-1.3.5-py310ha9d4c09_0
  numexpr            pkgs/main/linux-64::numexpr-2.8.3-py310hcea2de6_0
  pandas             pkgs/main/linux-64::pandas-1.4.4-py310h6a678d5_0
  pytz               pkgs/main/linux-64::pytz-2022.1-py310h06a4308_0



Downloading and Extracting Packages
bottleneck-1.3.5     | 274 KB    | ############################################################################ | 100%
numexpr-2.8.3        | 321 KB    | ############################################################################ | 100%
pandas-1.4.4         | 25.5 MB   | ############################################################################ | 100%
pytz-2022.1          | 196 KB    | ############################################################################ | 100%
Preparing transaction: done
Verifying transaction: done
Executing transaction: done
(/bask/projects/e/edmondac-rsg/wongj/my_conda_env) Singularity>
```

Simple 1 1 Terminal 1


File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
my_conda_env a minute ago
myfolder1 an hour ago
myfolder2 an hour ago
other an hour ago
conda-create.sh an hour ago
mynotebook.ipynb 14 minutes ago
slurm-275558.out an hour ago
slurm-275558.stats an hour ago
mynotebook.ipynb
conda-create.sh
Terminal 1
Code
git
my_conda_env (Conda)
[1]: import numpy
[2]: numpy.__file__
[2]: '/bask/homes/w/wongj/myproject/my_conda_env/lib/python3.10/site-packages/numpy/__init__.py'
[ ]:
Simple
1
1
my_conda_env (Conda) | Idle
Mode: Command
Ln 1, Col 1
mynotebook.ipynb

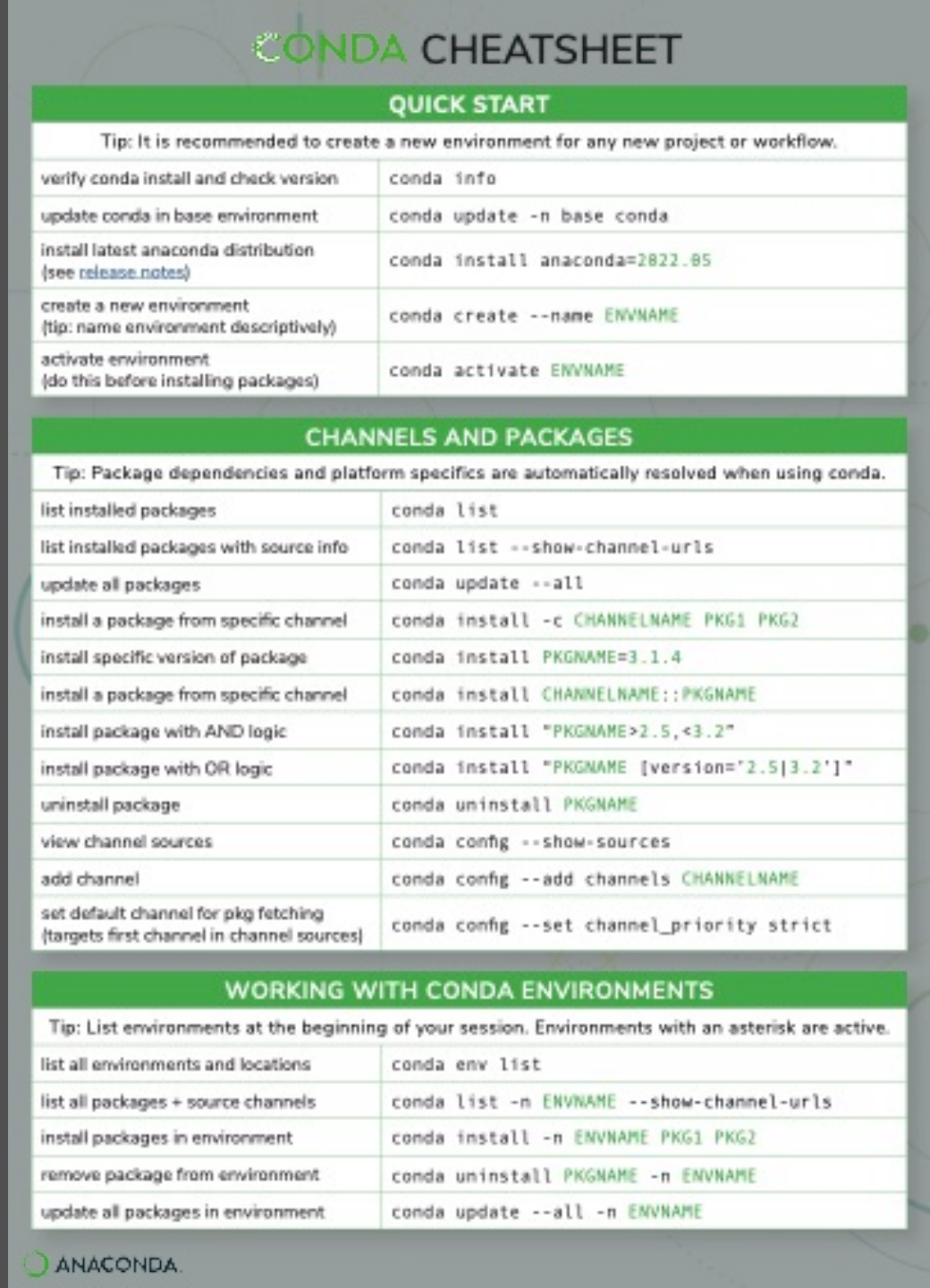

File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
/ myproject /
Name
Last Modified
my_conda_env 2 minutes ago
myfolder1 an hour ago
myfolder2 an hour ago
other an hour ago
conda-create.sh an hour ago
mynotebook.ipynb 15 minutes ago
slurm-275558.out an hour ago
slurm-275558.stats an hour ago
mynotebook.ipynb
conda-create.sh
Terminal 1
Code
git
my_conda_env (Conda)
[1]: import numpy
[2]: numpy.__file__
[2]: '/bask/homes/w/wongj/myproject/my_conda_env/lib/python3.10/site-packages/numpy/__init__.py'
[3]: import pandas
[4]: pandas.__file__
[4]: '/bask/homes/w/wongj/myproject/my_conda_env/lib/python3.10/site-packages/pandas/__init__.py'
[ ]:
Simple
1
1
my_conda_env (Conda) | Idle
Mode: Edit
Ln 1, Col 1
mynotebook.ipynb

More Conda commands

Consult the Cheat Sheet

https://docs.conda.io/projects/conda/en/latest/user-guide/cheatsheet.html

https://github.com/baskerville-hpc/baskerville-portal



CONDA CHEATSHEET

QUICK START

Tip: It is recommended to create a new environment for any new project or workflow.

verify conda install and check version	`conda info`
update conda in base environment	`conda update -n base conda`
install latest anaconda distribution (see release notes)	`conda install anaconda=2022.05`
create a new environment (tip: name environment descriptively)	`conda create --name ENVNAME`
activate environment (do this before installing packages)	`conda activate ENVNAME`

CHANNELS AND PACKAGES

Tip: Package dependencies and platform specifics are automatically resolved when using conda.

list installed packages	`conda list`
list installed packages with source info	`conda list --show-channel-urls`
update all packages	`conda update --all`
install a package from specific channel	`conda install -c CHANNELNAME PKG1 PKG2`
install specific version of package	`conda install PKGNAME=3.1.4`
install a package from specific channel	`conda install CHANNELNAME::PKGNAME`
install package with AND logic	`conda install "PKGNAME>2.5,<3.2"`
install package with OR logic	`conda install "PKGNAME [version='2.5|3.2']"`
uninstall package	`conda uninstall PKGNAME`
view channel sources	`conda config --show-sources`
add channel	`conda config --add channels CHANNELNAME`
set default channel for pkg fetching (targets first channel in channel sources)	`conda config --set channel_priority strict`

WORKING WITH CONDA ENVIRONMENTS

Tip: List environments at the beginning of your session. Environments with an asterisk are active.

list all environments and locations	`conda env list`
list all packages + source channels	`conda list -n ENVNAME --show-channel-urls`
install packages in environment	`conda install -n ENVNAME PKG1 PKG2`
remove package from environment	`conda uninstall PKGNAME -n ENVNAME`
update all packages in environment	`conda update --all -n ENVNAME`

ANACONDA.

Tips

- Do **not** mix Module Loading and Conda Environments
  - This can result in version conflicts and incompatible software
- Module loading is preferred where possible
  - These system-wide applications are built and optimised specifically for Baskerville, resulting in better performance and compatability
  - Not easily customisable if the module you want does not exist, although we are happy to install more module applications at your request
- Conda Environments are customisable, but can be large
  - When modifying your Conda environment, add the **conda install** commands into your shell script for reproducibility (helpful for troubleshooting)
  - Run **conda env remove --prefix <$CONDA_ENV_PATH>** to delete an environment
  - Run **conda clean --all** to clear your Conda cache in your home folder
- Remember to shutdown your JupyterLab notebook when you are done
- Consult **https://docs.baskerville.ac.uk/portal/portal/** for more advice

https://github.com/baskerville-hpc/baskerville-portal

Final Task – PyTorch Conda Environment

- Create another Conda environment using a shell script
- **conda install --yes pytorch torchvision pytorch-cuda=11.6 -c pytorch -c nvidia**
- Launch a JupyterLab server
  - **import torch**
  - Check **torch.__path__**
  - Check **torch.__version__**
  - Query visible GPU devices with the commands from **pytorch-gpu.py**

```
import torch

use_cuda = torch.cuda.is_available()

if use_cuda:
    print('__CUDNN VERSION:', torch.backends.cudnn.version())
    print('__Number CUDA Devices:',
torch.cuda.device_count())
    print('__CUDA Device
Name:',torch.cuda.get_device_name(0))
    print('__CUDA Device Total Memory
[GB]:',torch.cuda.get_device_properties(0).total_memory/1e9)
```

pytorch-gpu.py

Congratulations!

Useful links:

- **https://docs.baskerville.ac.uk/**
- **https://admin.baskerville.ac.uk/**
- **https://apps.baskerville.ac.uk/**
- **https://portal.baskerville.ac.uk/**
- **https://github.com/baskerville-hpc/baskerville-portal**

Email:

- **baskerville-tier2-support@contacts.bham.ac.uk**