DKRZ
DEUTSCHES
KLIMARECHENZENTRUM

Introduction to

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(DKRZ)

ML Workshop March 5, 2024

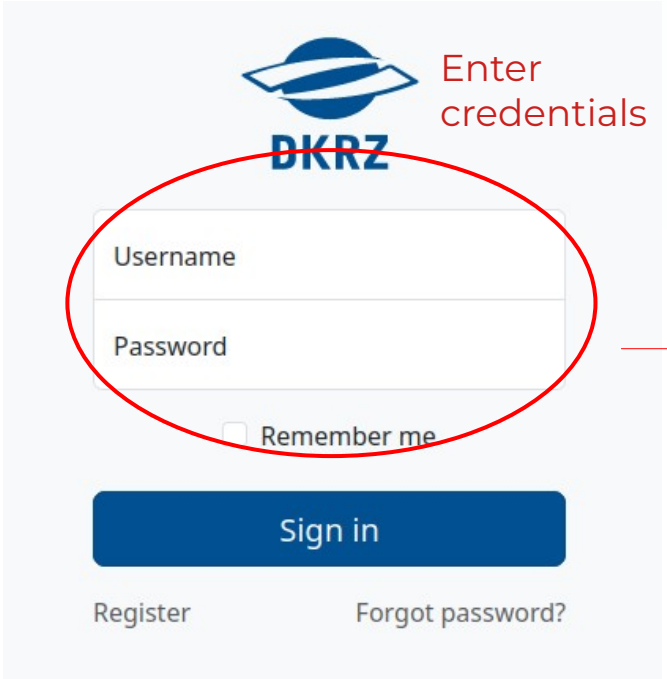
Overview

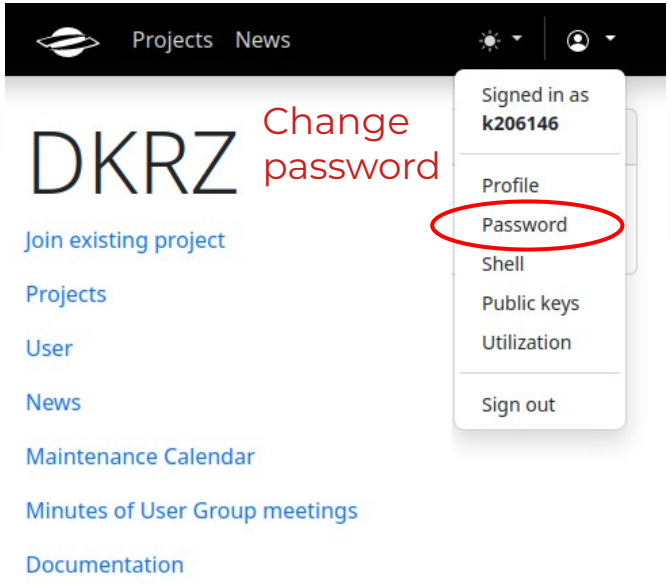
- **Setup** of the Hands-on
- What is **PyTorch**?
- Hands-on: basics of PyTorch
- Hands-on: code example

Setup the **PyTorch** hands-on

Setup - Step 1

Go to https://luv.dkrz.de

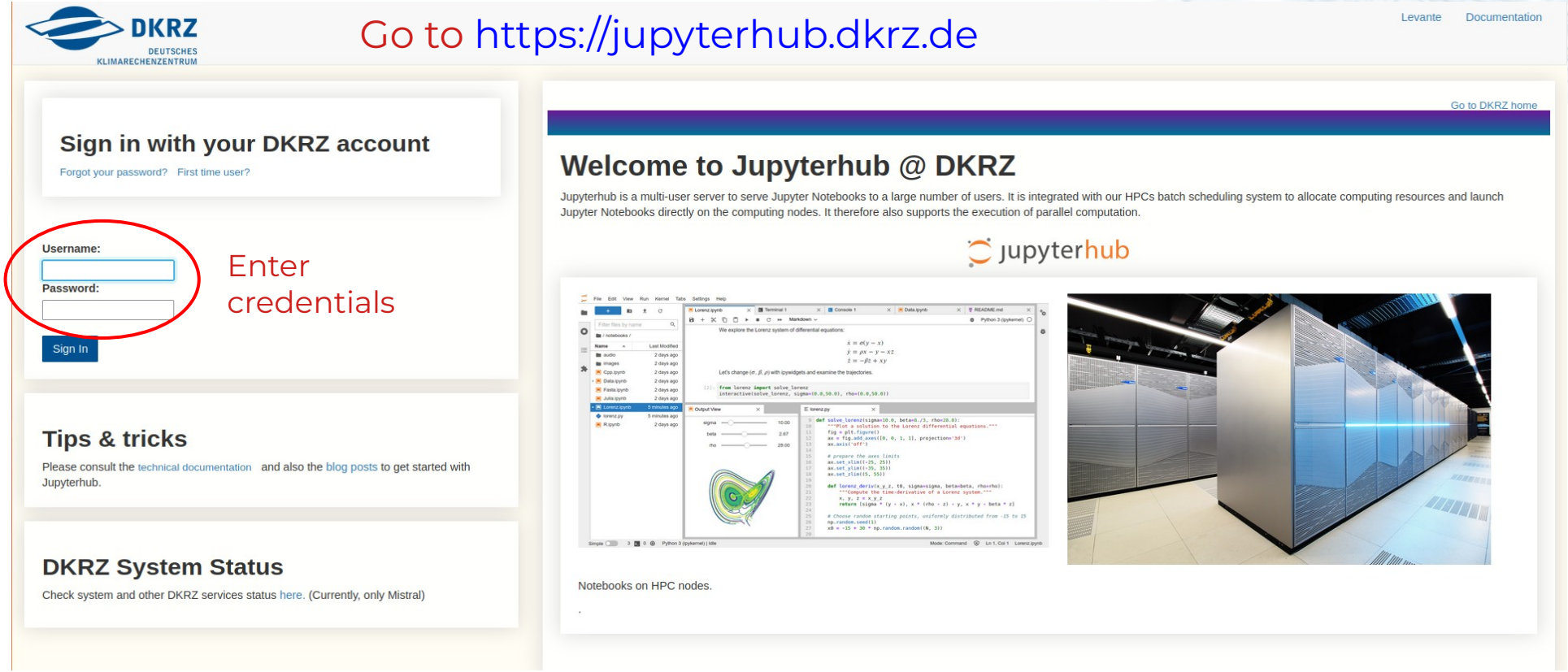




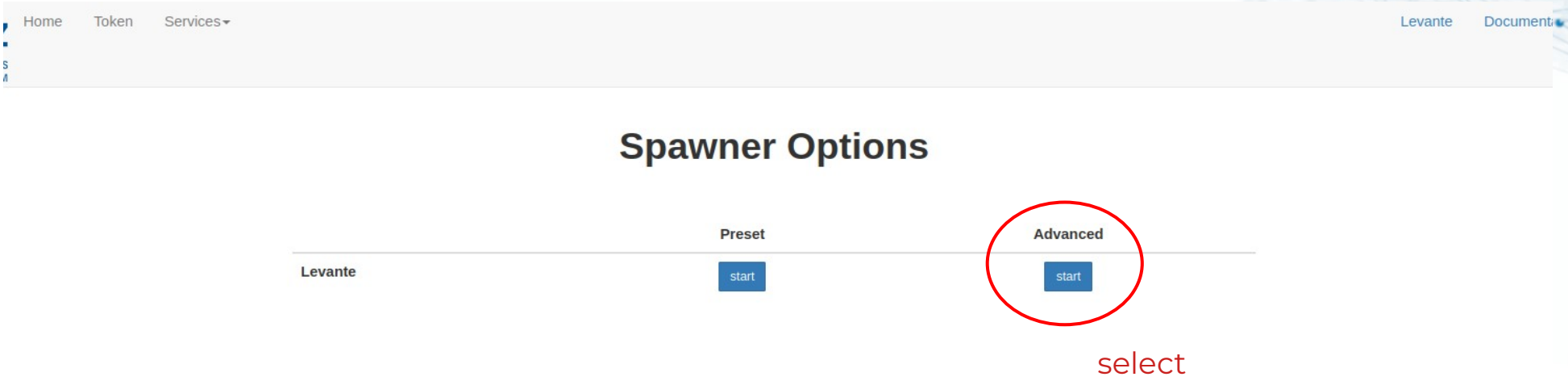
Last name	First name	Username
Behncke	Jacqueline	k206090
Bouarar	Idir	k206091
Custódio	Danilo	k206092
Fauer	Felix	k206093
Filipa	Viegas	k206094
Gieße	Céline	k206095
Gorges	Ksenia	k206096
Grawe	David	k206097
Halder	Suman	k206098
Hauke	Clara	k206099
Hossain	Akil	k206100
Kowalczyk	Lorena	k206101
Krüger	Julian	k206102
Linke	Olivia	k206103
Lucio	Etor	k206104
Mchedlishvili	Alexander	k206105
Nnamchi	Hyacinth	k206106
Olonscheck	Dirk	k206107
Pasternack	Alexander	k206108
Pohlmann	Holger	k206109
Sanchez	Antonio	k206110
Savita	Abhishek	k206111
Vogt	Judith	k206112
Wang	Xiaoxue	k206113
Weinkaemmerer	Jan	k206114
Winkler	Marius	k206115
Zhu	Xiuhua	k206116

Setup - Step 2

Go to https://jupyterhub.dkrz.de

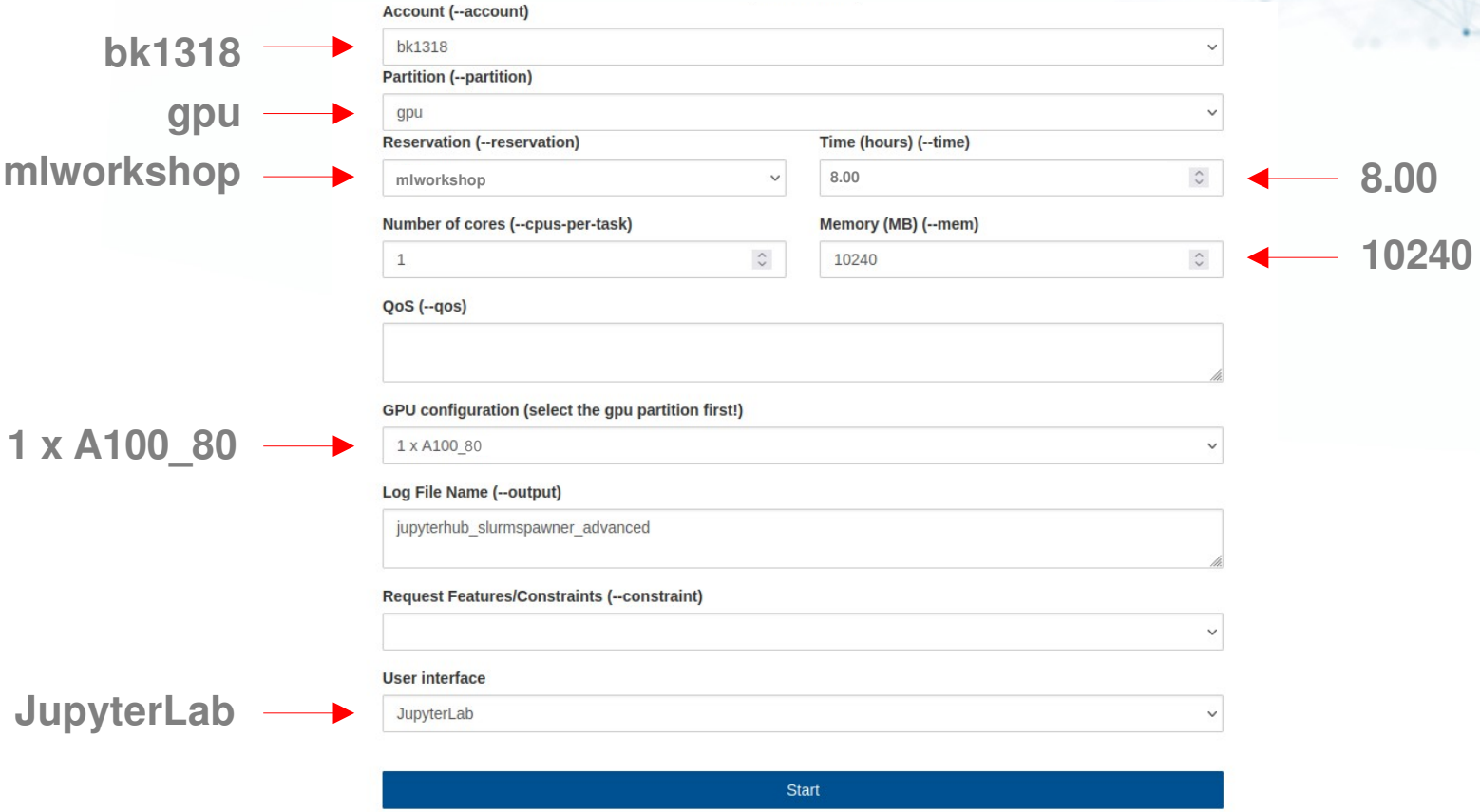


Setup - Step 3

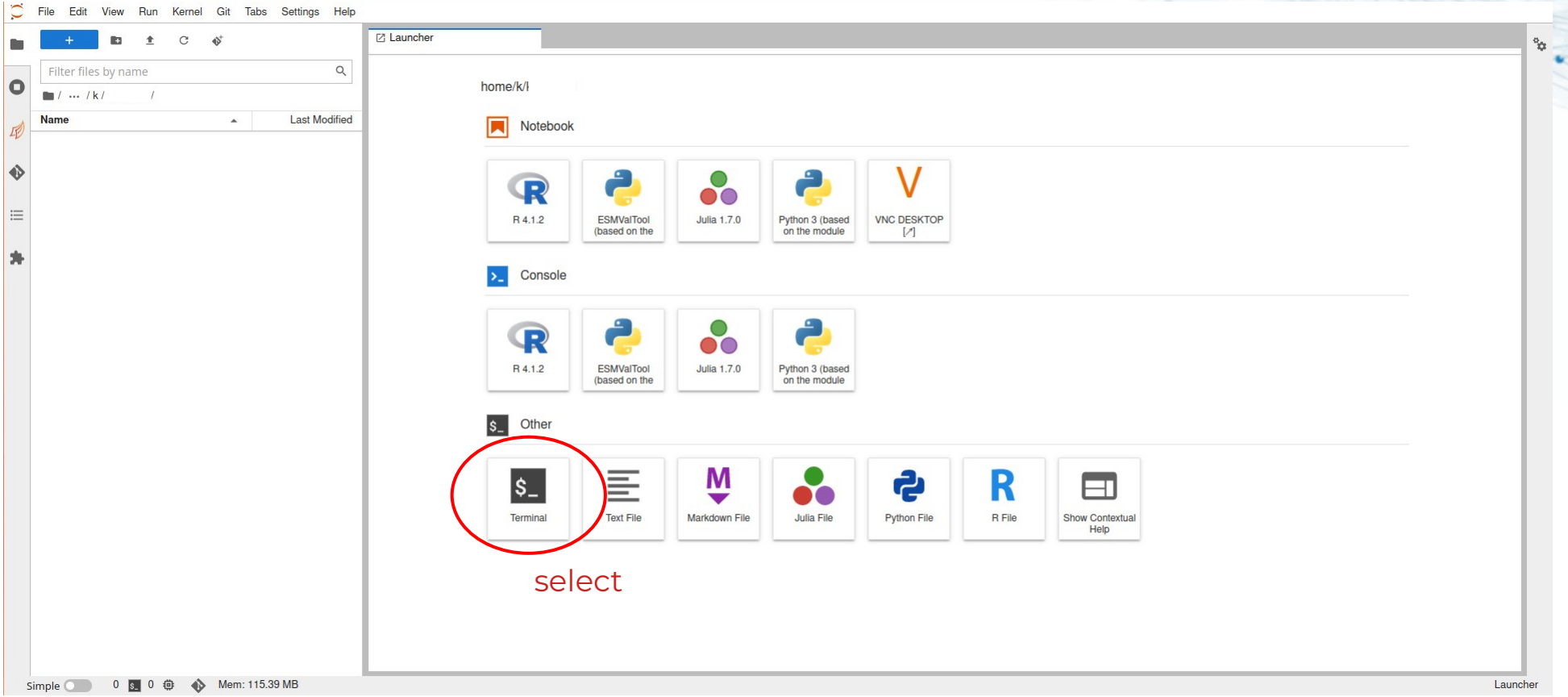


select

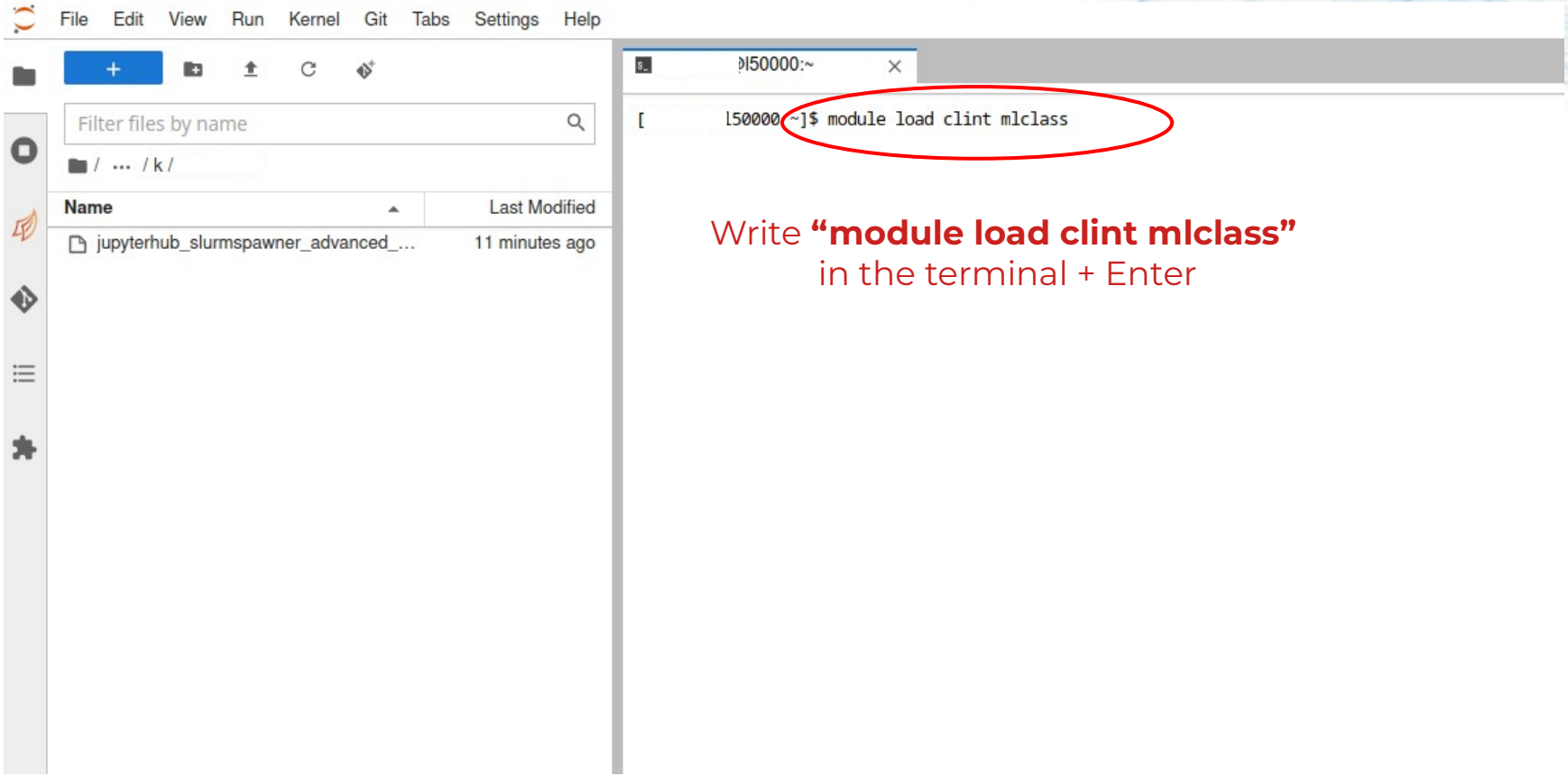
Setup - Step 4


bk1318
gpu
mlworkshop
1 x A100_80
JupyterLab
Account (--account)
bk1318
Partition (--partition)
gpu
Reservation (--reservation)
mlworkshop
Time (hours) (--time)
8.00
8.00
Number of cores (--cpus-per-task)
1
Memory (MB) (--mem)
10240
10240
QoS (--qos)
GPU configuration (select the gpu partition first!)
1 x A100_80
Log File Name (--output)
jupyterhub_slurmspawner_advanced
Request Features/Constraints (--constraint)
User interface
JupyterLab
Start

Setup - Step 5

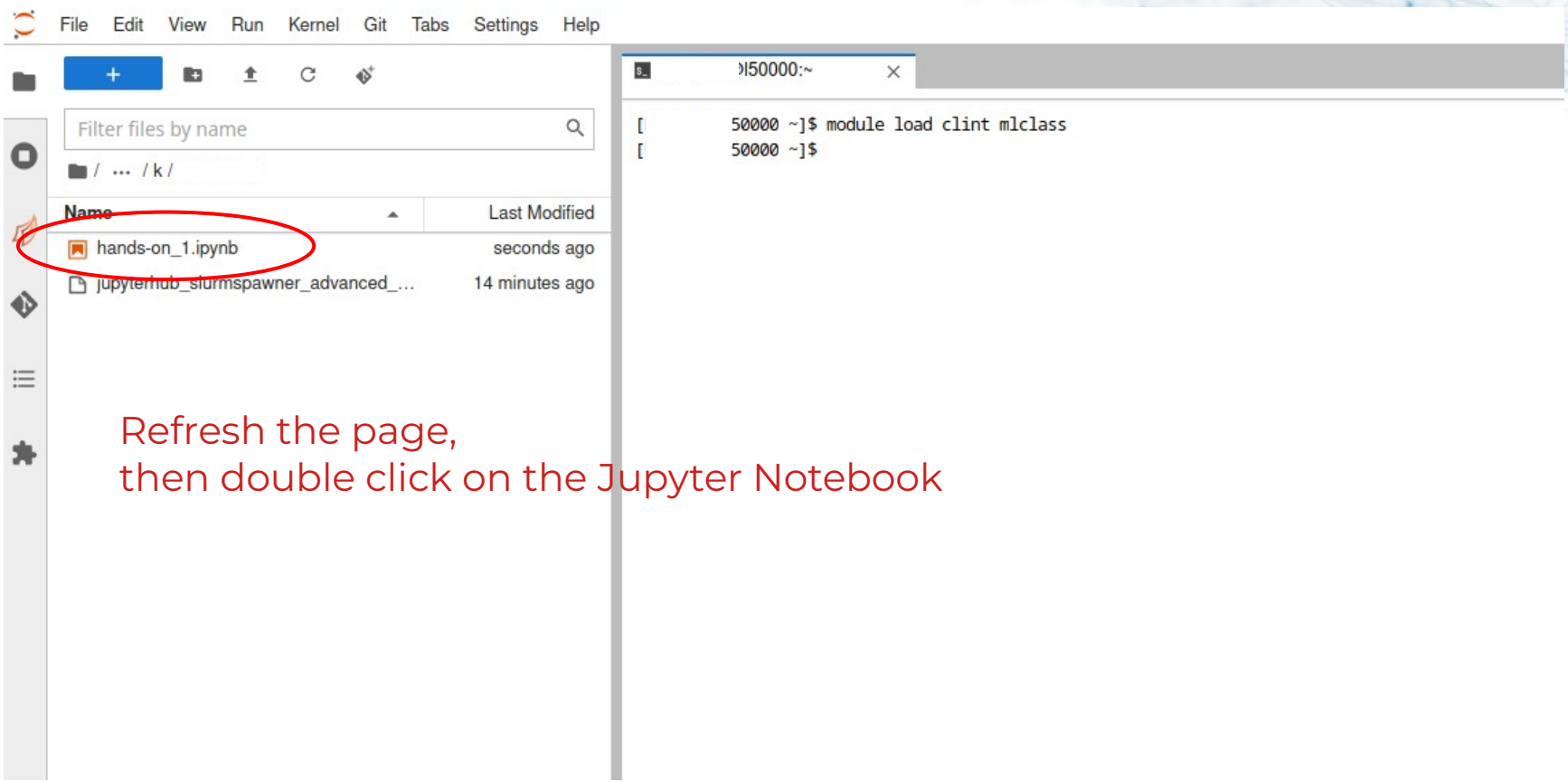

File Edit View Run Kernel Git Tabs Settings Help
Filter files by name
Name
Last Modified
Launcher
home/k/l
Notebook
R 4.1.2
ESMValTool (based on the
Julia 1.7.0
Python 3 (based on the module
VNC DESKTOP
Console
R 4.1.2
ESMValTool (based on the
Julia 1.7.0
Python 3 (based on the module
Other
Terminal
Text File
Markdown File
Julia File
Python File
R File
Show Contextual Help
select
Simple
Mem: 115.39 MB
Launcher

Setup - Step 6



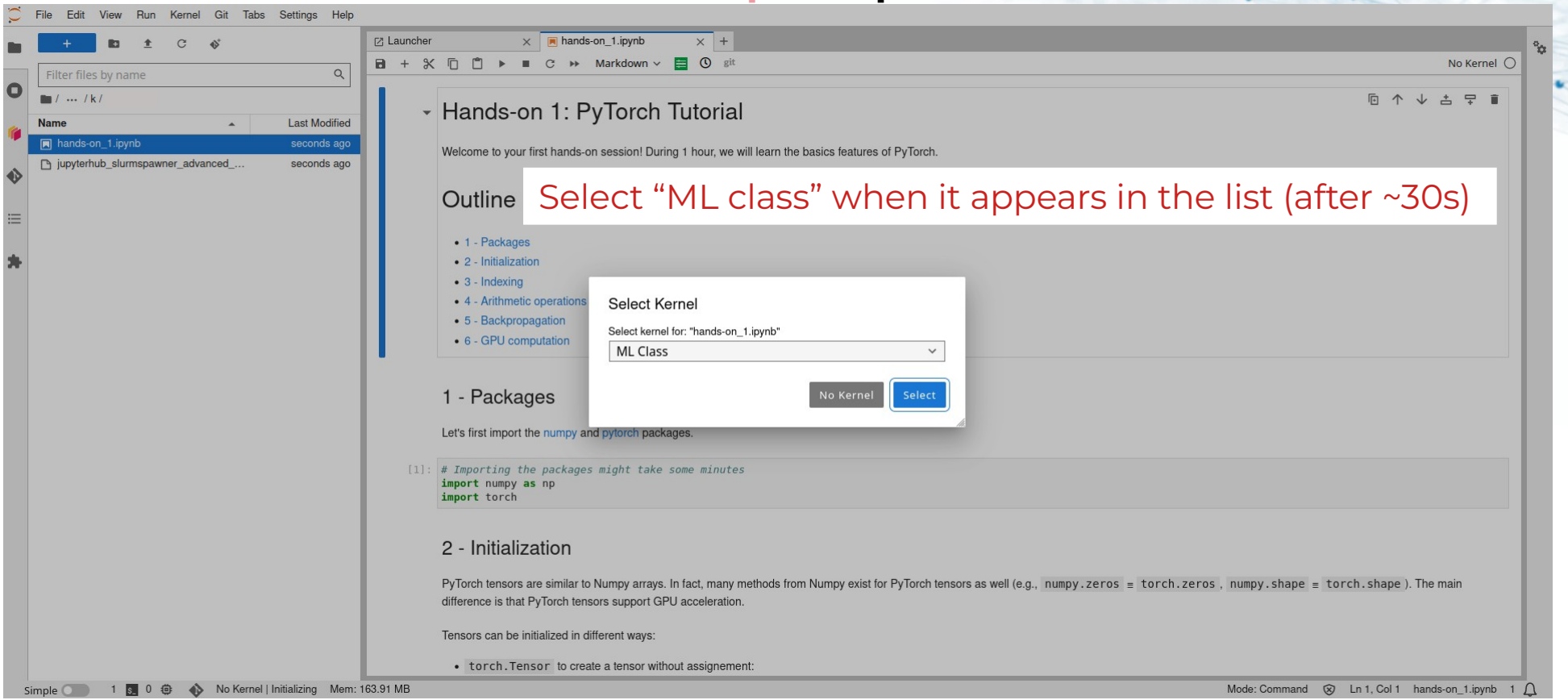
Write **“module load clint mlclass”**
in the terminal + Enter

Setup - Step 7



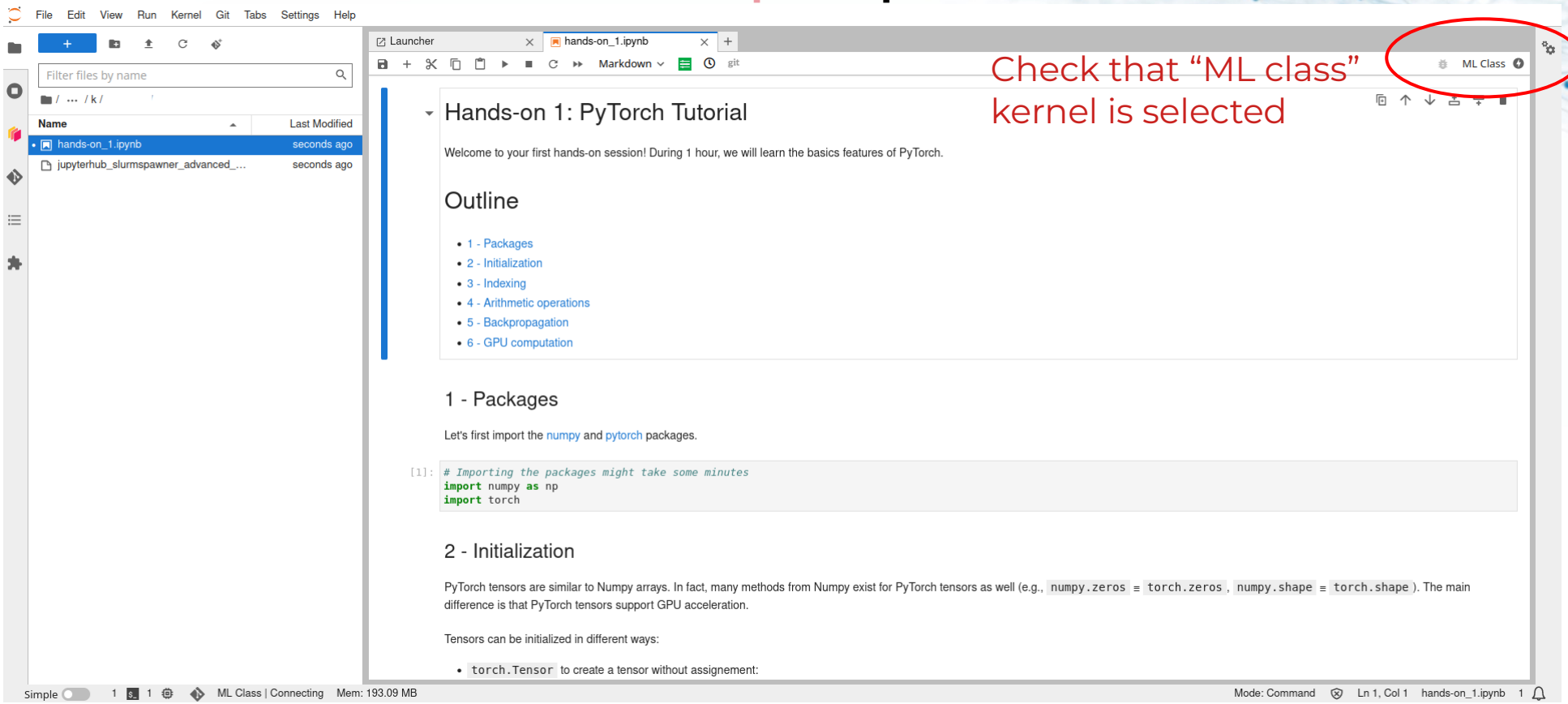
Refresh the page,
then double click on the Jupyter Notebook

Setup - Step 8


File Edit View Run Kernel Git Tabs Settings Help
Launcher
hands-on_1.ipynb
Filter files by name
Name
Last Modified
hands-on_1.ipynb
seconds ago
jupyterhub_slurmspawner_advanced_...
seconds ago
Markdown
No Kernel
Hands-on 1: PyTorch Tutorial
Welcome to your first hands-on session! During 1 hour, we will learn the basics features of PyTorch.
Outline
Select “ML class” when it appears in the list (after ~30s)
1 - Packages
2 - Initialization
3 - Indexing
4 - Arithmetic operations
5 - Backpropagation
6 - GPU computation
Select Kernel
Select kernel for: "hands-on_1.ipynb"
ML Class
No Kernel
Select
1 - Packages
Let's first import the numpy and pytorch packages.
[1]:
# Importing the packages might take some minutes
import numpy as np
import torch
2 - Initialization
PyTorch tensors are similar to Numpy arrays. In fact, many methods from Numpy exist for PyTorch tensors as well (e.g., numpy.zeros = torch.zeros , numpy.shape = torch.shape). The main difference is that PyTorch tensors support GPU acceleration.
Tensors can be initialized in different ways:
torch.Tensor to create a tensor without assignement:
Simple
No Kernel | Initializing
Mem: 163.91 MB
Mode: Command
Ln 1, Col 1
hands-on_1.ipynb

Setup the **PyTorch** hands-on

Setup - Step 9



Setup the **PyTorch** hands-on

Setup - Step 10