

Getting Started with **Jupyter Hub**

Étienne Plésiat

(DKRZ)

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Getting started with Jupyter Hub

Setup - Step 1



DKRZ
DEUTSCHES
KLIMARECHENZENTRUM

Go to <https://jupyterhub.dkrz.de>

Levante Documentation

Go to DKRZ home

Sign in with your DKRZ account

[Forgot your password?](#) [First time user?](#)

Username:

Password:

Sign In

Enter
credentials

Tips & tricks

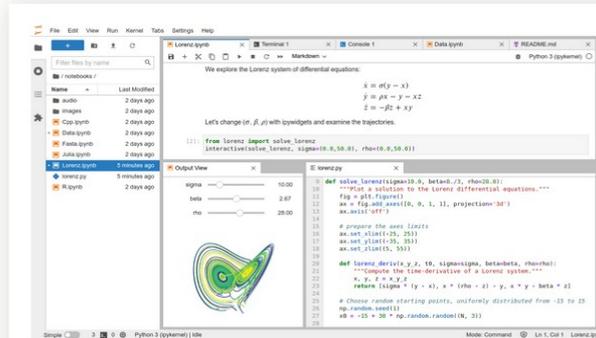
Please consult the [technical documentation](#) and also the [blog posts](#) to get started with Jupyterhub.

DKRZ System Status

Check system and other DKRZ services status [here](#). (Currently, only Mistral)

Welcome to Jupyterhub @ DKRZ

Jupyterhub is a multi-user server to serve Jupyter Notebooks to a large number of users. It is integrated with our HPCs batch scheduling system to allocate computing resources and launch Jupyter Notebooks directly on the computing nodes. It therefore also supports the execution of parallel computation.



Notebooks on HPC nodes.



Getting started with Jupyter Hub

Setup - Step 2

Spawner Options



Getting started with Jupyter Hub

Setup - Step 3

bk1444 → Account (--account) bk1444

gpu → Partition (--partition) gpu

deeplearning → Reservation (--reservation) deeplearning

Time (hours) (--time) 4.00 ← **8.00**

Number of cores (--cpus-per-task) 1

Memory (MB) (--mem) 10240 ← **10240**

QoS (--qos)

1 x A100_80 → GPU configuration (select the gpu partition first!) 1 x A100_80

Log File Name (--output) jupyterhub_slurmspawnner_advanced

Request Features/Constraints (--constraint)

JupyterLab → User interface JupyterLab

Start

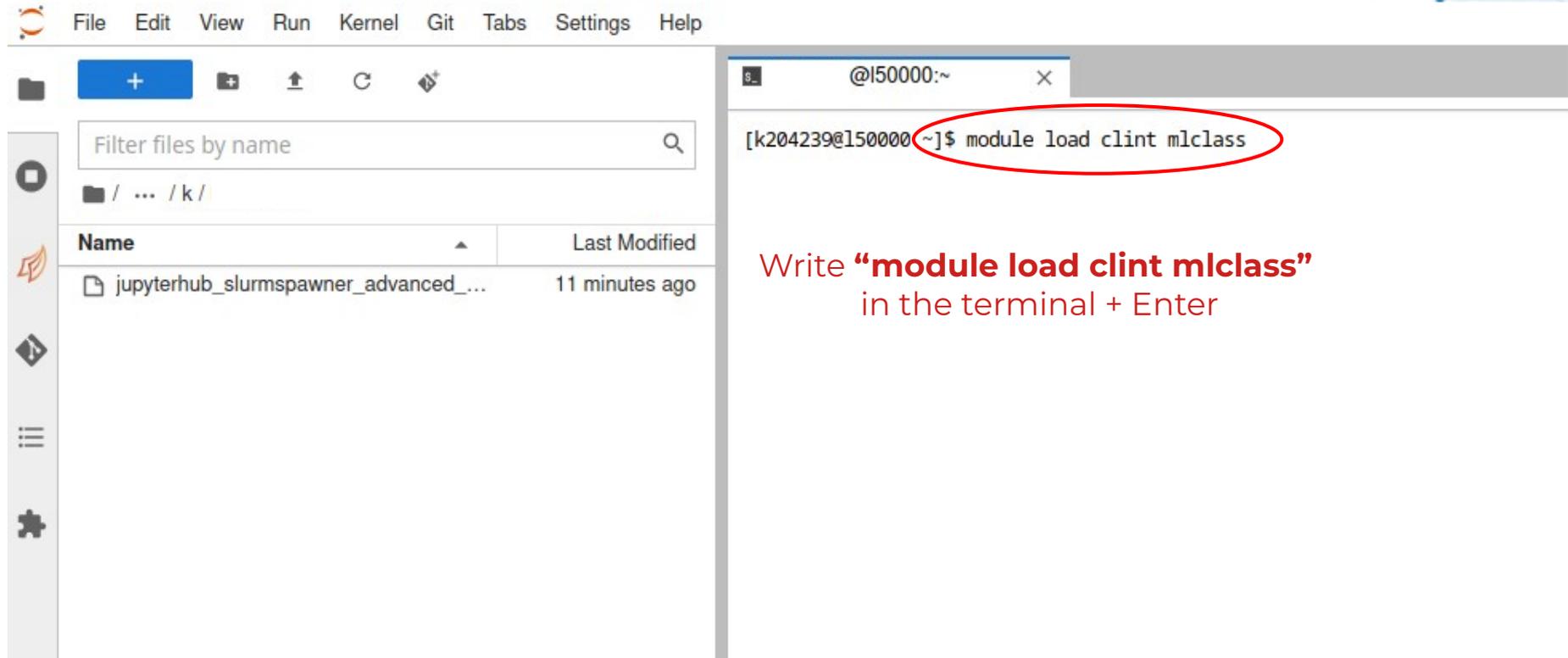
Getting started with Jupyter Hub

Setup - Step 4

The screenshot displays the Jupyter Hub Launcher interface. The top navigation bar includes 'File', 'Edit', 'View', 'Run', 'Kernel', 'Git', 'Tabs', 'Settings', and 'Help'. Below this is a search bar for 'Filter files by name' and a file browser showing the path 'home/k/l'. The main area is divided into three sections: 'Notebook', 'Console', and 'Other'. The 'Notebook' section contains icons for R 4.1.2, ESMValTool (based on the), Julia 1.7.0, Python 3 (based on the module), and VNC DESKTOP [1]. The 'Console' section contains icons for R 4.1.2, ESMValTool (based on the), Julia 1.7.0, and Python 3 (based on the module). The 'Other' section contains icons for Terminal, Text File, Markdown File, Julia File, Python File, R File, and Show Contextual Help. The 'Terminal' icon, which features a black square with a white '\$ _' symbol, is circled in red. Below the 'Terminal' icon, the word 'select' is written in red. The bottom status bar shows 'Simple' mode, memory usage of 115.39 MB, and the word 'Launcher' in the bottom right corner.

Getting started with Jupyter Hub

Setup - Step 5



The screenshot displays the Jupyter Hub web interface. On the left is a file browser with a search bar and a table of files. On the right is a terminal window. The terminal prompt is `[k204239@l50000 ~]$`, and the command `module load clint mlclass` has been entered. The command text is circled in red. Below the terminal, red text provides instructions.

Name	Last Modified
jupyterhub_slurmspawnner_advanced_...	11 minutes ago

```
[k204239@l50000 ~]$ module load clint mlclass
```

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

Getting started with Jupyter Hub

Setup - Step 6

The screenshot shows the Jupyter Hub interface. On the left, a file browser sidebar displays the directory structure. The current path is `/intro_pytorch/`. A file named `hands-on_1.ipynb` is highlighted in blue and circled in red. A red arrow points from the text "Go to the directory called 'intro_pytorch'" to the path in the sidebar. Below the sidebar, red text says "Open (double-click) 'hands-on_1.ipynb'". The main area shows a "Launcher" tab with a "Notebook" icon. Below this, there are several environment cards. The first row includes "1 Python 3 (based on the module python3/2023.0 1)", "0 Python 3 (based on the module python3/unstable)", "AI Weather", and "Bash". The second row shows four more Python environment cards.

File browser sidebar:

- Filter files by name
- Path: `/intro_pytorch/`
- File: `hands-on_1.ipynb` (22 hours ago)

Main area:

- Launcher
- Notebook
- Environment cards: 1 Python 3, 0 Python 3, AI Weather, Bash, and four more Python 3 cards.

Getting started with Jupyter Hub

Setup - Step 7

The screenshot shows the Jupyter Hub interface. The top menu includes File, Edit, View, Run, Kernel, Git, Tabs, Settings, and Help. The main area displays a file browser with a search bar and a list of files: hands-on_1.ipynb (22 hours), hands-on_2.ipynb (20 hours), and utils.py (22 hours). A 'Select Kernel' dialog box is open, showing the selected kernel for 'hands-on_1.ipynb'. The dialog lists several options, with 'ML Class' highlighted at the bottom.

Select Kernel

Select kernel for: "hands-on_1.ipynb"

- 1 Python 3 (based on the module python3/2023.01) ▾
- 0 Python 3 (based on the module python3/unstable)
- AI Weather
- Bash
- ESMValTool (based on the latest module esmvaltool)
- Julia 1.7.0
- ML (based on the latest module pytorch)
- ML Class**

Getting started with Jupyter Hub

Setup - Step 8

Check that "ML class" kernel is selected

The screenshot shows the Jupyter Hub interface. On the left is a file browser with a search bar and a table of files. The file 'hands-on_1.ipynb' is selected. The main area shows a Jupyter notebook titled 'hands-on_1.ipynb' with a kernel dropdown menu set to 'ML Class', which is circled in red. The notebook content includes a title 'Hands-on 1: PyTorch Tutorial', a welcome message, and an outline of topics.

Name	Modified
hands-on_1.ipynb	22 hours ago

Kernel: ML Class

Hands-on 1: PyTorch Tutorial

Welcome to your first hands-on session! During 1 hour, we will learn the basics features of PyTorch.

Outline

- 1 - Packages
- 2 - Initialization
- 3 - Indexing
- 4 - Arithmetic operations

Getting started with Jupyter Hub

Setup - Step 9

File Edit View Run Kernel Git Tabs Settings Help

Filter files by name

/ ... / / intro_pytorch /

Name	Modified
hands-on_1.ipynb	1 minute ago

Launcher hands-on_1.ipynb

Run the first cell to import the packages (it takes ~30-60s)

1 - Packages

Let's first import the `numpy` and `pytorch` packages.

```
[*]: # Importing the packages might take some minutes
import numpy as np
import torch

# Even though PyTorch supports parallelism, we will be using only one
torch.set_num_threads(1)
```

2 - Initialization