

Getting Started with **Jupyter Hub**

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DL Workshop for Climate Scientists

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Getting started with Jupyter Hub

Setup - Step 1



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.

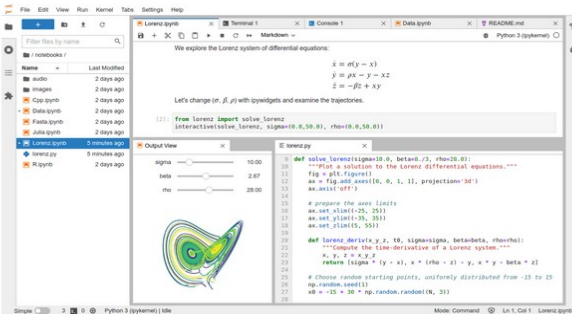
DKRZ System Status

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.





```
File Edit View Run Kernel Help
Lorenz.ipynb Terminal 1 Console 1 Data.ipynb README.md Python 3 (ipykernel)
We explore the Lorenz system of differential equations:
x' = sigma*(y - x)
y' = rho*x - y - x*z
z' = x*y + beta - z
Let's change (sigma, rho, beta) with widgets and examine the trajectories.
In [2]: from IPython import InteractiveShell
InteractiveShell.run_cell('sigma=10, rho=28, beta=8')
Out[2]:
sigma: 10.00
rho: 28.00
beta: 8.00
def solve_lorenz(sigma, rho, beta):
    """Solve the Lorenz system of differential equations"""
    fig = plt.figure()
    ax = fig.add_subplot(1, 1, projection='3d')
    ax.set_xlabel('x')
    ax.set_ylabel('y')
    ax.set_zlabel('z')
    # prepare the axes limits
    ax.set_xlim(-20, 20)
    ax.set_ylim(-20, 20)
    ax.set_zlim(-20, 20)
    def lorenz_deriv(x, y, z, t):
        """Compute the time derivative of a Lorenz system"""
        x, y, z = x, y, z
        return (sigma*(y - x), rho*x - y - x*z, x*y + beta - z)
    # choose random starting points, uniformly distributed from -10 to 10
    x0 = -10 + 20 * np.random.random(N, 1)
    y0 = -10 + 20 * np.random.random(N, 1)
    z0 = -10 + 20 * np.random.random(N, 1)
```



Notebooks on HPC nodes.

Getting started with Jupyter Hub

Setup - Step 2

Spawner Options

Levante

	Preset	Advanced
	start	start

select

Getting started with Jupyter Hub

Setup - Step 3

bk1444 → Account (--account) bk1444

gpu → Partition (--partition) gpu

dlws → Reservation (--reservation) dlws

Time (hours) (--time) 8.00 ← **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. On the left is a sidebar with a file browser and a search bar. The main area is titled 'Launcher' and shows the current directory as 'home/k/l'. It is divided into three sections: 'Notebook', 'Console', and 'Other'. The 'Other' section contains several icons, with the 'Terminal' icon (a black square with a white '\$_') circled in red. Below the red circle, the word 'select' is written in red. The status bar at the bottom shows 'Simple' mode, 0 files, 0 kernels, and a memory usage of 115.39 MB.

File Edit View Run Kernel Git Tabs Settings Help

Filter files by name

home/k/l

Launcher

Notebook

R 4.1.2 ESMValTool (based on the Julia 1.7.0 Python 3 (based on the module VNC DESKTOP [1]

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

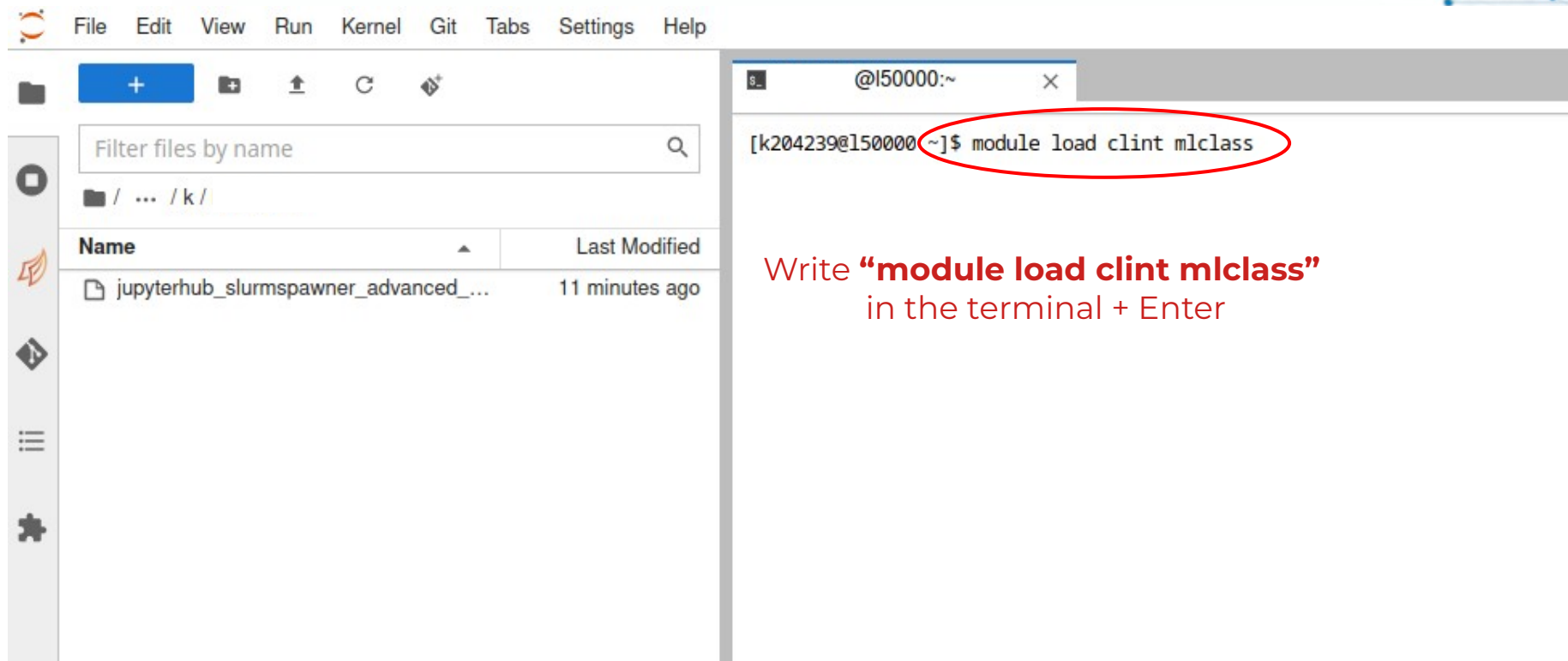
select

Simple 0 0 0 Mem: 115.39 MB

Launcher

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 labeled 'Filter files by name' and a table of files. The table has columns 'Name' and 'Last Modified'. One file is listed: 'jupyterhub_slurmspawnner_advanced_...' with a modification time of '11 minutes ago'. On the right is a terminal window titled '@l50000:~'. The terminal shows the command `[k204239@l50000 ~]$ module load clint mlclass`, where the command is circled in red. To the right of the terminal, red text reads: 'Write **“module load clint mlclass”** in the terminal + Enter'.

Name	Last Modified
jupyterhub_slurmspawnner_advanced_...	11 minutes ago

Getting started with Jupyter Hub

Setup - Step 6

The screenshot shows the Jupyter Hub interface. On the left is a sidebar with icons for file management, search, and settings. The main area is divided into two panes. The left pane shows a file browser with a search bar and a list of files. The right pane shows the main workspace with a 'Launcher' tab and a grid of notebook templates.

File browser details:

Name	Modified
hands-on_1.ipynb	22 hours ago

Main workspace details:

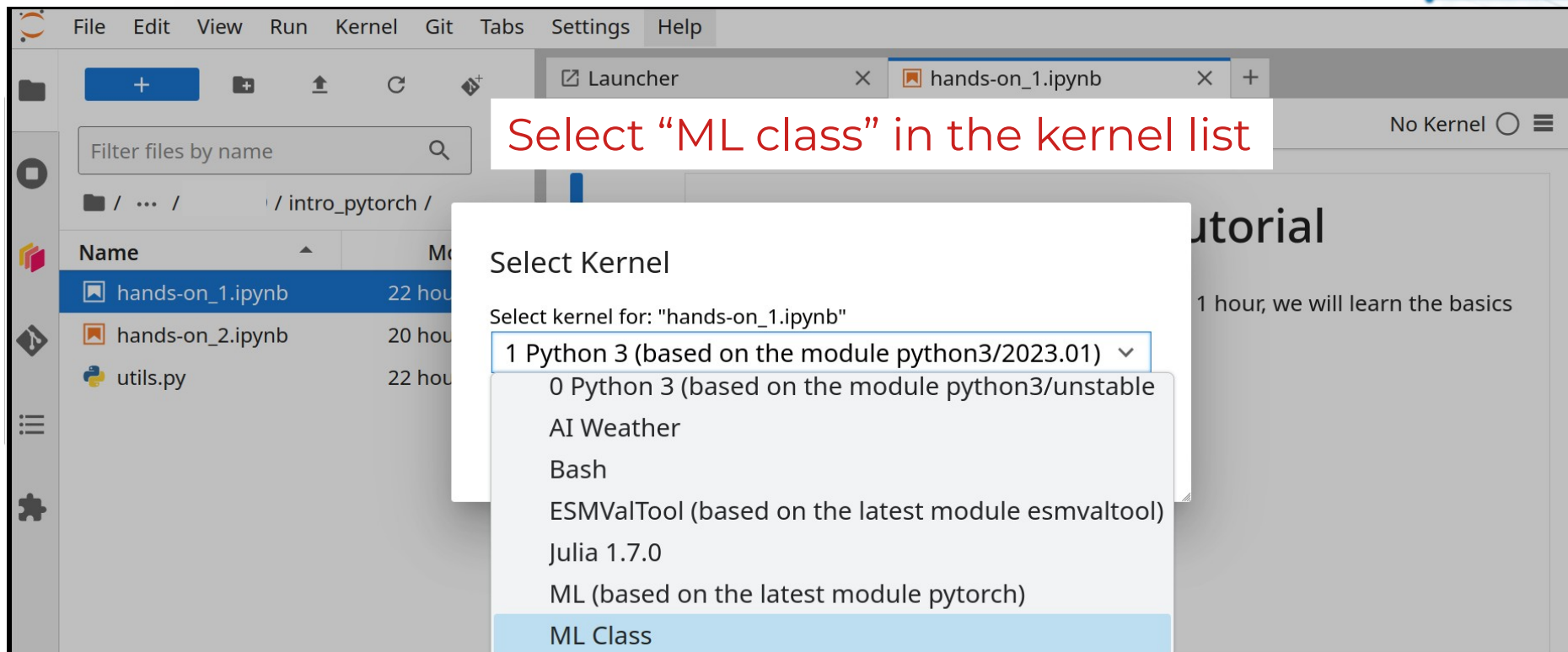
- Launcher tab
- Notebook icon
- Grid of notebook templates:
 - 1 Python 3 (based on the module python3/2023.0 1)
 - 0 Python 3 (based on the module python3/unstable)
 - AI Weather
 - Bash

Annotations:

- Red arrow pointing to the file browser path: `/ intro_pytorch /`
- Red circle around the file `hands-on_1.ipynb`
- Red text: "Go to the directory called 'intro_pytorch'" (with arrow to path)
- Red text: "Open (double-click) 'hands-on_1.ipynb'" (with circle around file)

Getting started with Jupyter Hub

Setup - Step 7



The screenshot shows the Jupyter Hub web interface. At the top, there's a menu bar with 'File', 'Edit', 'View', 'Run', 'Kernel', 'Git', 'Tabs', 'Settings', and 'Help'. Below the menu, there's a toolbar with icons for adding, uploading, and refreshing. The main area shows a file browser with a search bar 'Filter files by name'. A list of files is displayed: '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 a list of available kernels. The text 'Select "ML class" in the kernel list' is overlaid on the dialog. The background shows a notebook titled 'Tutorial' with the text '1 hour, we will learn the basics'.

Select "ML class" in the kernel list

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 displays the Jupyter Hub web interface. On the left, a sidebar shows a file browser for the 'intro_pytorch' directory, containing a file named 'hands-on_1.ipynb' modified 22 hours ago. The main area shows the 'Launcher' tab for 'hands-on_1.ipynb'. In the top right of the launcher, the 'ML Class' kernel is selected, indicated by a red circle around the radio button. The notebook content includes a title 'Hands-on 1: PyTorch Tutorial', a welcome message, and an outline with four items: 1 - Packages, 2 - Initialization, 3 - Indexing, and 4 - Arithmetic operations.

File Edit View Run Kernel Git Tabs Settings Help

Filter files by name

/ ... / intro_pytorch /

Name	Modified
• hands-on_1.ipynb	22 hours ago

Launcher hands-on_1.ipynb

Markdown

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

The screenshot displays the Jupyter Hub interface. On the left, a file browser shows a directory structure with 'hands-on_1.ipynb' selected. The main area shows a notebook with two cells:

- 1 - Packages**: A code cell containing the following code:

```
[*]: # 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)
```

A red annotation is present: **Run the first cell to import the packages (it takes ~30-60s)**
- 2 - Initialization**: A code cell that is currently empty.