

#### 0 0 0 0 0 JUPYTERHUB-01 0 0 0 0 0 FIRST STEPS ON THE JUPYTERHUB PYTHON & MATLAB SERVER 0 0 0 0 0 0 0 Bill Incal BR Excision In the migrat . 🖌 matlah se 📕 matlab.test.ip last more 0 0 0 Simeon Beinlich beinlich@fhi.mpg.de PP&B Computer Support Group Fritz-Haber-Institut der Max-Planck-Gesellschaft

FRITZ-HABER-INSTITUT | SIMEON BEINLICH

SCIENTIFIC COMPUTING INFRASTRUCTURE AT FHI

BERLIN, GERMANY | 26<sup>TH</sup> MARCH 2025

# REGISTRATION

In order to use the jupyterhub server, please register here: https://root.compute.fhi.mpg.de.

#### Enter your:

- Full name
- FHI email address
- Choose a user/project name (ideally the FHI username)
- Use case

#### Specify whether you need a virtual desktop session as well!

Shortly after you will receive a confirmation email with your login credentials.





#### FHI Compute Manager

Welcome to the FHI Compute Manager!

**Create User / Project** Account

#### Your Full Name

Fhi User

Your E-Mail

fhiusername@fhi.mpg.de

#### Your username / projectname

fhiusername

Use-case

Access Jupyterhub and a virtual desktop session for python postprocessing.

Create Account

# REGISTRATION | LOGIN CREDENTIALS

Shortly after you will receive a confirmation email with your login credentials.

Dear User,

You can now log in to the compute servers, e.g. jupyterhub-01, analysis-01, gpu-01, storage-01, etc. instances with your new compute credentials:

- username: yourusername
- initial password: yourpassword

Please keep this information safe, and change your initial password!



Dear User frosch,

You can now log in to the compute servers, e.g. jupyterhub-01, analysis-01, gpu-01, storage-01, etc. instances with your new compute credentials: - username: frosch

- initial password: qgbqetqtb

Please change your password immediately as described here: - Changing your password: <u>https://gitlab.fhi.mpg.de/fhi-hpc/jupyterhub-</u> compute/-/wikis/Access

# CHANGING YOUR PASSWORD

#### Visit: root.compute.fhi.mpg.de.

Click on Change Password.

#### Enter your

- **username**: *yourusername*
- initial password: yourpassword

#### Set a

• new password

Please use at least 8 characters containing letters, numbers, and symbols.



#### **FHI Compute Manager**

Welcome to the FHI Compute Manager!





yourfhiusername

........

Old Password:

New Password

**Confirm New Password** 

.....

Change Password

BERLIN, GERMANY | 26<sup>TH</sup> MARCH 2025





# CHANGING YOUR PASSWORD

#### Visit: root.compute.fhi.mpg.de.

Click on Change Password.

#### Enter your

- username: yourusername
- initial password: yourpassword

#### Set a

• new password

Please use at least 8 characters containing letters, numbers, and symbols.

After changing your password, you will be asked, whether you also **want to restart all your VNC sessions to inherit the password**. Continue with this, **if you plan on using a desktop session**!

### FHI Compute Manager

Welcome to the FHI Compute Manager!





yourfhiusername

Old Password:

New Password

**Confirm New Password** 

•••••

Change Password





# LOGIN IN TO JUPYTERHUB

Open a browser (we recommend Chrome) and visit:

jupyterhub-01.compute.fhi.mpg.de

Enter your:

- **username**: *myusername*
- password: new password

Click Sign In

#### 🔵 jupyter<mark>hub</mark>

Sightin		
Username:		
myusername		
Password:		
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	Sign in	



# LOGIN IN TO JUPYTERHUB

Open a browser (we recommend Chrome) and visit:

jupyterhub-01.compute.fhi.mpg.de

Enter your:

- **username**: *myusername*
- password: new password

Click Sign In

After your session has started up, you will arrive at a fresh session.





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### JUPYTERHUB START PAGE

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FILE BROWSER

Browse and manage your files and folders.

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### FILE BROWSER

Browse and manage your files and folders.

#### STORAGE SPACES

On First arrival you are in your Jupyterhub home directory /.

home: /home/yourusername
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 Best starting point for new users

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On First arrival you are in your Jupyterhub home directory /.

home: /home/yourusername
 shome directory of the Jupyterhub Server
 Best starting point for new users

#### OTHER STORAGE SPACES

These are linked to the folders in your home directory!

- data: /mnt/data/yourusername Access from any compute server This is the place for your data!
- local: /mnt/local/yourusername
   Fast reading / writing of files
   If you have many tiny files / a lot of random IO
- ext: /mnt/ext/yourusername:
  - Storage extension >100TB Only on request!





### FILE BROWSER

Browse and manage your files and folders.

### RUNNING SESSIONS

Please shut them down, if you don't need them!

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FILE BROWSER

Browse and manage your files and folders.

### RUNNING SESSIONS

Please shut them down, if you don't need them!

### PS: HUB CONTROL PANEL

Your session will keep running in the background if you log out or if you close your browser!

If you are done using Jupyterhub, shut your entire session down in the hub control panel!





Go to File > Hub Control Panel



### FILE BROWSER

Browse and manage your files and folders.

### RUNNING SESSIONS

Please shut them down, if you don't need them!

### OUTLINE

For using Markdown headings in notebooks!

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#### FILE BROWSER

Browse and manage your files and folders.

#### RUNNING SESSIONS

Please shut them down, if you don't need them!

### OUTLINE

For using Markdown headings in notebooks!

#### JUPYTERHUB EXTENSIONS Please do not modify them for now!

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Create new notebooks, scripts or launch consoles and terminals.



Click the | + | button or create a new tab.

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SCIENTIFIC COMPUTING INFRASTRUCTURE AT FHI



Create new notebooks, scripts or launch consoles and terminals.

### NOTEBOOKS

Mix of script, interactive session and documentation.

• Matlab or Python (choose your environment)

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Create new notebooks, scripts or launch consoles and terminals.

### NOTEBOOKS

Mix of script, interactive session and documentation.

• Matlab or Python (choose your environment)

### CONSOLES

A purely *interactive session* (temporary).

• Matlab or Python (choose your environment)

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Create new notebooks, scripts or launch consoles and terminals.

### NOTEBOOKS

Mix of script, interactive session and documentation.

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### CONSOLES

A purely *interactive session* (temporary).

• Matlab or Python (choose your environment)

### TERMINAL

A normal terminal shell.

- Manage your Python environments
- Run Shell / Python scripts or any other commands.

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Create new notebooks, scripts or launch consoles and terminals.

### NOTEBOOKS

Mix of script, interactive session and documentation.

• Matlab or Python (choose your environment)

### CONSOLES

A purely *interactive session* (temporary).

• Matlab or Python (choose your environment)

### TERMINAL

A normal terminal shell.

- Manage your Python environments
- Run Shell / Python scripts or any other commands.

### SCRIPTS

Create modules or standalone scripts.

• Import them or run them in a terminal.

☑ Launcher

Notebook

jody-druce-env-

2

Open MATLAB

[7]

jody-druce-env

2

py-3.13

Pvthon 3

(ipykernel)

my-env

Python 3

(ipykernel)

my-env

\$\_ Other

Console

MATLAB Kerne

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MATLAB Kernel

jody-druce-env-

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py-3.13

jody-druce-env-

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# JUPYTERHUB - FULL MATLAB SESSION

You can as well run entire, full MATLAB sessions on Jupyterhub!

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# JUPYTERHUB - H5WEB FOR EXPLORING HDF5 FILES

#### The integrated **H5web** viewer is a convenient alternative to HDFview for exploring *HDF5* and *Nexus* Files.



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# JUPYTERHUB - DOWNLOAD / UPLOAD FILES

#### For now, just download and upload files via Jupyterhub. Later you can use the Storage System for more complex transfers!



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# JUPYTERHUB - TRAINING MATERIAL

#### You can find Training Material in ~/data/shared/Training:

#### • Python-Introduction:

A collection of Resources, from basics to simple Pandas CSV processing.

#### • Archive-Introduction:

Interacting with the FHI Archive System - With Plain Python or Via GUI-style Widgets

#### • DASK-Introduction:

A simple Framework to Parallelize your Analysis. Starting with trivially parallelizable file processing

#### • HDF5-Introduction:

Accessing HDF5 Files with python and HDF5web - a first look.

#### • Matlab-Introduction:

*Very simple plotting example using a matlab notebook (or the Matlab Jupyterlab App).* 

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	Archive-Introduction	5 days ago
*	DASK Introduction	3 days ago
	Example Data	3 days ago
	HDF5 Introduction	3 days ago
	Matlab Introduction	3 days ago
	Python Introduction	3 days ago

# FURTHER TOPICS & LINKS



#### MORE TRAINING MATERIAL

Visit root.compute.fhi.mpg.de/training

### PPB WIKI | HPC

General Information.

### FHI GITLAB | HPC DOCUMENTATION

Jupyterhub Wiki | Virtual Desktop Wiki | Storage Wiki

Questions, issues, needing help? Please mail: beinlich@fhi.mpg.de or call: +49 30 8431 5270