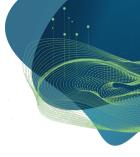


JupyterHub Training

Mariela Sanchez, Adnan Haidar, Elias Werner

Dresden, 27th of October 2022



GEFÖRDERT VOM



Bundesministerium für Bildung und Forschung

SACHSEN Diese Maßnahme wird gefördert durch die Bundesregierung aufgrund eines Beschlusses des Deutschen Bundestages. Diese Maßnahme wird mitfinanziert durch Steuermittel auf der Grundlage des von den Abgeordneten des Sächsischen Landtags beschlossenen Haushaltes.



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https://scads.ai/



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flows

Mariela Sanchez, Research Associate, ZIH

Adnan Haidar,

ficial Intelligence

Elias Werner,

Data Science for synthetic data evaluation

Data Science, Robotics Tactile Sense using Arti-

performance analysis of data science work-

Research Associate, ScaDS.Al

Research Associate, ScaDS.Al





1 Introduction – Agenda

1 Introduction

2 Jupyter overview

- 3 Access and Basics of the ZIH HPC system
- 4 Data Management via Jupyter
- 5 Collaborative Research and Teaching with Jupyter on HPC
- 6 Hands On session: Prepare a Jupyter "environment" for collaborative working
- 7 Conclusion, Q&A and Supplementary



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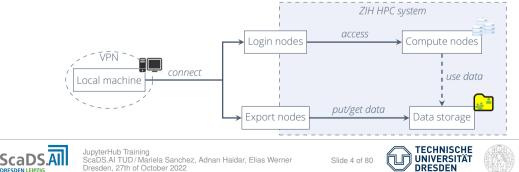




1 Recap: What is an HPC machine?

- Cluster of many single nodes (single "computers") for pooling their resources (computation and memory)
- Job scheduler *Slurm* manages resource/hardware allocation
- Software environment can be set up easily via a module system
- Collaborative working spirit, shared machine
- HPC project required for interaction

Technical workflow:



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1 HPC system - Taurus

- Name: HPC-Cluster Taurus
- **Model**: The second high-performance computing/memory complex (HRSK-II)
- Facility: Center for Information Services and High Performance Computing (ZIH)
- Details:
 - More than 60,000 cores,
 - ▶ 720 GPUs,
 - Flexible storage hierarchy with about 16 PB total capacity,
 - Linux, shared login nodes, filesystems, batchsystem Slurm,
 - Perfect platform for highly scalable, data-intensive and compute-intensive applications.





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1 JupyterHub - a Good Mean for Interacting with HPC

- Jupyter useful for data analysis
- Jupyter as an interface to an HPC system for many users
- Users access to complex computing infrastructures from the JupyterHub
- Jupyter provides remote access to Jupyter Notebooks





Taken from: geohackweek.github.io/Introductory/05-Jupyter-tutorial/

A GROUP OF PEOPLE.



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Asking the audience:

- 1) What is your main discipline of work?
 - A. Humanities and Social Sciences
 - B. Natural Sciences
 - C. Life Sciences
 - D. Engineering Sciences

2) Which programming language you use mostly in Jupyter?

- A. Python
- **B**. R
- C. Julia
- D. Others
- 3) What is the OS you use to initialize and use Jupyter?
- 4) What are your main reasons for joining this training event?



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1 Structure of the Presentation

- Jupyter
 - Features
 - Usability
 - Functionalities
- HPC basics
 - Access
 - Data management
 - Software management
- Collaborative working with HPC and Jupyter notebook
 - Shared system principles
 - Workflow
 - Useful features
- Hands-on session



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1 Intention of the Presentation

- Making things understandable esp. for **frequent JH users** including teachers and researchers.
- Complete workflow examples are shown, here: based on Python code (can be used as blueprint for other software/tools).
- From the user's perspective: What are the most important things to work with JH on HPC?

🧪 Note

We do not want to show everything that is possible. We want to show, what is needed to get started

🧪 Note

We do **not** want to show *the* complete architecture and advanced properties of Jupyter. We want you to comprehend how Jupyter works and HPC principles behind JH tool with concrete examples

💧 Hint

Please ask and interrupt our presentation immediately if something is not clear! Use your mic or the chat.



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2 Jupyter overview – Agenda

1 Introduction

2 Jupyter overview

- 3 Access and Basics of the ZIH HPC system
- 4 Data Management via Jupyter
- 5 Collaborative Research and Teaching with Jupyter on HPC
- 6 Hands On session: Prepare a Jupyter "environment" for collaborative working
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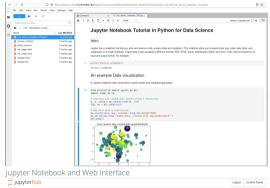


Jupyter Notebook documents:

- Dynamic notebook documents include:
 - Plots
 - Images
 - Video
 - Equations
 - Narrative text

•••

- Notebook web application enables to:
 - Run and edit code
 - Build hierarchical documents
 - Computations results as PDF, HTML, etc



× /	
Files Running Clusters	
Select items to perform actions on them.	Upload New • D
0 • BAMT	Name Last Modified File size
D	seconds ago
D general log	7 months apo 2.6 GB

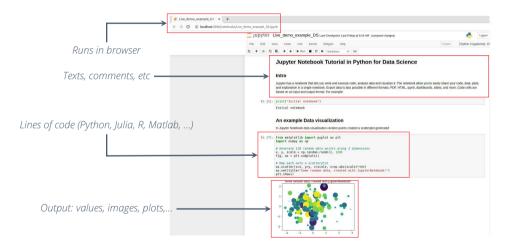


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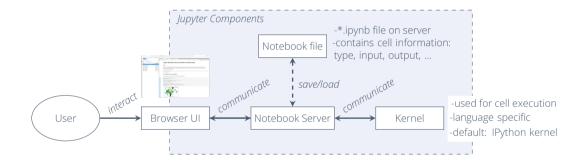


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structure according to: jupyter.readthedocs.io/.../content-architecture



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Jupyter Kernels:

- IPython: basic Python kernel with features for interactive computing
- IRKernel: basic R kernel
- IJulia: basic Julia kernel
- MATLAB Kernel: Basic kernel for Matlab language
- ITorch: IPython kernel with visualizations of images
- IPykernel: another Python kernel

🧪 Note

Jupyter supports over 100 programming languages. For more details: https://github.com/jupyter/jupyter/wiki/Jupyter-kernels



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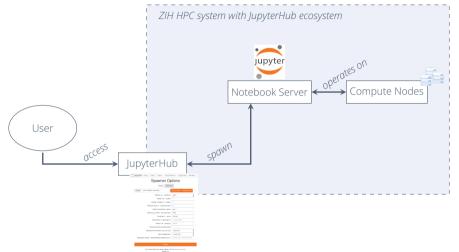


jupyter

Jupyter kernels



iulia

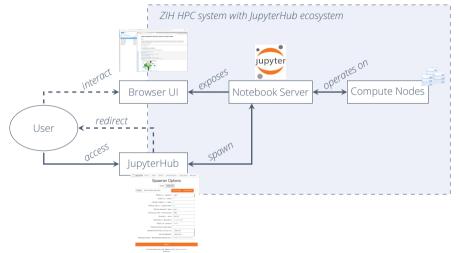


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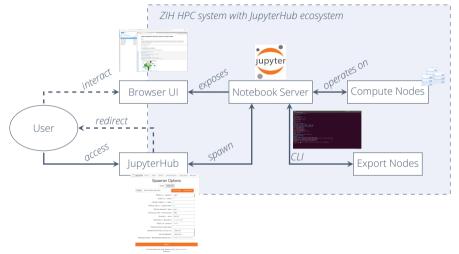


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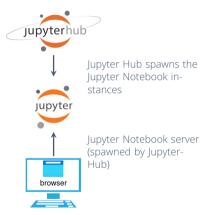
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One single node of Jupyter:

- Each user a whole new instance of Jupyter software
- The instance has all necessary features to interact with the HPC:
 - Web browser
 - Jupyter Notebook
 - Kernel
 - others: Jupyter lab, etcetera

🖍 Note

Jupyter Hub has many interesting properties to explore for intermediate and basic users.



Adapted from: opencredo.com/blogs/writing-a-custom-jupyterhub-spawner/



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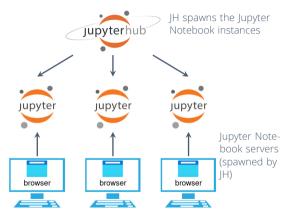
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The ecosystem of JH under HPC:

- A multi-user Hub with multiple instances of single-users
- Set up in HPC system
- Built for multiple user log in
- The instances are single Jupyter structures
- A interactive interaction with HPC in every instance



Adapted from:

opencredo.com/blogs/writing-a-custom-jupyterhub-spawner/



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2 Jupyter Scenario: Research

Paulina is a researcher, she has some of her experiments ready



She wants to share them with other researchers

Adapted from: Beg, Marijan, et al. "Using Jupyter for reproducible scientific workflows."



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2 Jupyter Scenario: Research She describes her experiments as a Jupyter Notebook Paulina is a researcher. she has some of her 2 experiments ready ·(*) 1 Ď¥° Her Jupyter Notebook She wants to share is a mix of code. them with other visualizations. researchers annotations, among others

Adapted from: Beg, Marijan, et al. "Using Jupyter for reproducible scientific workflows."



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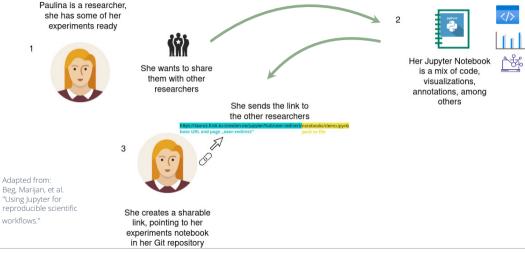
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2 Jupyter Scenario: Research

She describes her experiments as a Jupyter Notebook





1

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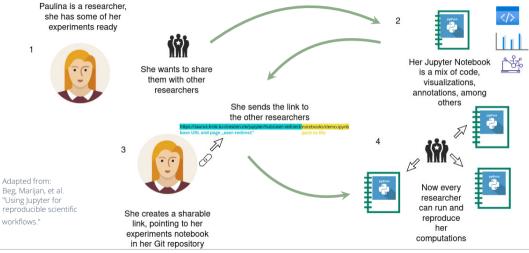
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2 Jupyter Scenario: Research

She describes her experiments as a Jupyter Notebook





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2 Jupyter Scenario: Teaching

John is a University Professor



He wants to provide the lecture in Jupyter notebooks with a consistent software environment for all the students

Adapted from: Beg, Marijan, et al. "Using Jupyter for reproducible scientific workflows."

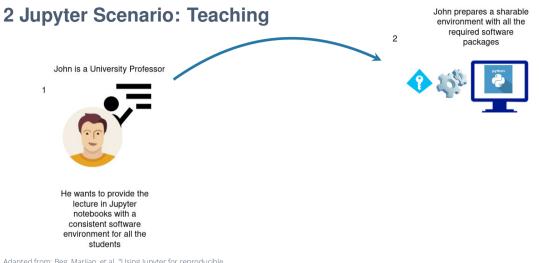


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Adapted from: Beg, Marijan, et al. "Using Jupyter for reproducible scientific workflows."

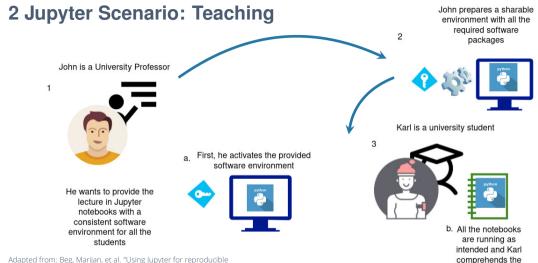


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Adapted from: Beg, Marijan, et al. "Using Jupyter for reproducible scientific workflows."

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lecture

3 Access and Basics of the ZIH HPC system – Agenda

- 1 Introduction
- 2 Jupyter overview
- 3 Access and Basics of the ZIH HPC system Organizational, Access and Permissions, Software management
- 4 Data Management via Jupyter
- 5 Collaborative Research and Teaching with Jupyter on HPC
- 6 Hands On session: Prepare a Jupyter "environment" for collaborative working
- 7 Conclusion, Q&A and Supplementary



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3 JupyterHub Project on the ZIH System

Working on the JupyterHub system requires an HPC project. An HPC project on the ZIH system includes:

- project directory and login with existing or without existing ZIH Login
- project members (at least project leader and project administrator)
- resource quotas for compute time (CPU/GPU hours) and storage

Ele	ctronic HPC Project Application Form for ZIH
CONTENT -	
	Application lists
	is page: lications for the current call, which are not finalized yet. Inalized applications for the current call.
During the application process data is s	splayed for the actions allowed for that record. aved automatically by changing a panel or clicking on the "SAVE"-Button. d like to edit or create a new application by clicking on the new button. The following actions are available
	tion and create a new one with that data.
delete: Delete the application record. delete: Load an active application from	a province excelor and add the data
files: Show a list of files uploaded for	
O New Project Application: Create a ne	
print: Display a summary of a finalize	d application as PDF for printing.
E-mail address of principal investigator (Pf):	E-mail address of person to contact (PC):
matthias.kraeusslein@tu-dresden.de	none -
🕼 change PI/PC (re-login required)	



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3 JupyterHub Project on the ZIH System

There are different possibilities to work with HPC:

- create a new project
 - fill the application form: https://hpcprojekte.zih.tu-dresden.de/
 - find additional information in the wiki:
 - https://doc.zih.../application/project_request_form/
- Join an existing project, new researchers in an existing project, teaching purposes

💧 Hint

Kindly mention the HPC resource usage in the acknowledgment section of all publications https://doc.zih.tu-dresden.de/application/acknowledgement/



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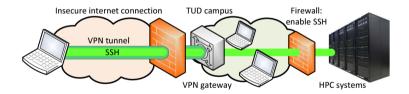




3 VPN to Access Services

To access ZIH services:

- from within the TU Dresden campus via secure shell (ssh).
- install VPN tool at your local machine.
 - OPENVPN client (recommended variant).
 - Cisco AnyConnect Secure Mobility Client





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3 Accessing the JupyterHub

Different ways to access the ZIH system:

JupyterHub

- browser based approach
- most easiest way for beginners



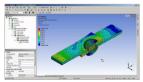
SSH connection

- "classical" approach
- command line interface (CLI) knowledge is necessary



desktop visualization

- esp. in case of using GUI-based software
- e.g. Ansys, Vampir,...



💧 Hint

For getting in touch with the system and also development purposes the approach with JuypterHub is recommended.



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3 Accessing the JupyterHub

To access JupyterHub to use:

- use the browser link (https://taurus.hrsk.tu-dresden.de/jupyter)
- 2. Start session by clicking Start my server button Allocation of resources via the GUI Spawner Option
 - Simple Option
 - Advanced Option

Utilization Bar

• Number of GPUs/CPUs available per node

More information in the https://doc.zih..../access/jupyterhub

Spawner Options





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wiki





3 Simple Option Resources

Spawner Options

Very important!

If you have finished your work please explicitely stop your server.



Simple form offers most important settings to start quickly:

- Intel Hashwell or IBM Power9
- Numbers of CPUs cores and threads
- GPUs

Architecture	IBM Power9	Intel Haswell
CPUs per node	2 x IBM Power9 (22 cores@2.80 GHz)	2x Intel Xeon 2680v3 (12 cores@2.50GHz
Memory per node	256GB RAM DDR4 2666MHz	64GB RAM 128 GB SSD
GPUs per node	6x NVIDIA VOLTA V100	4x NVIDIA Tesla K80



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3 Accessing the JupyterHub Advanced Option

Accessing the JupyterHub Advanced Option:

- Preset Option
 - Save own configurations as additional presets
 - Those are saved in browser or lost
 - Use import/export features to save as text
 - You can delete preset

	Curr	ent Utiliza	atio	n		
Slurm Interac GPU (GPU (e presets Default Partitions tive Partition NVIDIA Tesia K60) NVIDIA Ampece A100) SMP System HPE Superdome Flex NC		256	cores on ron gpus on alp cores on julia	ha	
1	Sir	mple Advanc	ed.			
Preset	GPU (NVIDIA Ampere A100)			✓ Save prese	t Delete preset	
	Partition (-ppartition): Nodeist (w. wnodeist): Nodes (-4,nodes): Number of tasks (-rtasks): CPUs per tasks (-ccpus-per-task): Generic resources (gres): Memory per CPU (mem-per-cpu):	<pre>diples no specific no 1 1 6 gpu:1 10312</pre>	odes	default haswell interactive gpu2 hpdff ml dev romeo alpha julia		~
	Runtime (-t,time):	8:00:00				
	Reservation (reservation): Project (-A,account): Preload modules (module load):	no reservatio default	n			
	Standard environment (package list):	hiera_gccco	re-10.2	2.0_python-3.8.6		×
	Launch application:	JupyterLab				×
	Workspace scope (NotebookApp.notebook_dir=):	default (your	home	directory)		

Spawr



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3 JupyterHub Advanced Option

Customise available resources via advanced form:

- Every parameters of advanced form can be set.
- Partitions, Nodes, Number of tasks.
- CPU, GPUs, Memory and Run-Time.
- Project, Modules.
- Standard environment, Workspace.

💧 Hint

The resource parameters refer to the Slurm parameters of the srun, salloc and sbatch commands when using an ssh connection to the HPC system.

Partition (-p,partition):	alpha-interactive
Nodelist (-w,nodelist):	no specific nodes
Nodes (-N,nodes):	1
Number of tasks (-n,tasks):	1
CPUs per task (-c,cpus-per-task):	6
Generic resources (gres):	gpu:1
Memory per CPU (mem-per-cpu):	10312
Runtime (-t,time):	8:00:00
Reservation (reservation):	no reservation
Project (-A,account):	default
Preload modules (module load):	none
Standard environment (package list):	hiera_gcccore-10.2.0_python-3.8.6
Launch application:	JupyterLab
Workspace scope (NotebookApp.notebook dir=):	default (your home directory)



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3 Software Management by Loading Modules

A module system:

- is a user interface that provides utilities for the dynamic modification of a user's environment (e.g. \$PATH variable)
- enables to smoothly switch between different versions of installed software packages and libraries
- in Jupyter, modules are available via Preload modules parameter

💧 Hint

More information about module management: https://doc.zih..../software/modules/



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3 Software Management - Preload Modules

- The Preload modules parameter for loading modules when spawning the JupyterHub server
- Preloaded modules will be available during the whole session
- After spawning, loading modules in the Jupyter terminal is not possible Only preloaded modules will be available in the Jupyter notebook files.

	Simple	Advanced			
Preset			 Save preset 	Delete preset	
Partition (-p,partition)	default				~
Nodelist (-w,nodelist)	no specific node	15			
Nodes (-N,nodes)	1				
Number of tasks (-n,tasks)	1				
CPUs per task (-c,cpus-per-task)	1				
Generic resources (gres)	no generic reso	urces			
Memory per CPU (mem-per-cpu)	1000				
Runtime (-t,time)	8:00:00				
Reservation (reservation)	no reservation				
Protect (A,account)	default				
Preload modules (module load)	× PyTorch/1.6.0- × TensotFlow/2.2		-Python-3.7.4 19b-Python-3.7.4		
Steedard environment (package list)					v
Launch application	JupyterLab				v
Workspace scope (~ NotebookApp.notebook_dir=)		me directory)			



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3 Module Commands - Example

A **module** usage is quite straight forward and the following table lists the basic commands.

```
Example
1
   # Show all module options
   marie@local$ module help
 2
   # List active modules in the user environment
 Δ
   marie@local$ module list
 5
   # Remove modules from the user environment
 8
   marie@local$ module purge
 9
   # Load module "modname" in the user environment
   marie@local$ module load <modname>
   # Remove module "modname" from the user environment
14 marie@local$ module unload <modname>
```



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3 Standard Environments in JupyterHub

Standard environment through advanced option open a list with all included python-packages:



💧 Hint

This list shows all packages of the currently selected conda environment. This depends on your settings for partition (CPU architecture) and standard environment. The default Python kernel uses conda environments.

List of available standard environments, namely: https://doc.zih.../access/jupyterhub/standard-environments



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3 Terminal, Tensorboard, WebVNC, RStudio

- JupyterHub launcher supports additional tools:
 - ▶ Terminal: access the compute node via CLI
 - WebVNC: spawn a graphical user interface on the compute node
 - Tensorboard: access the Tensorboard functionality
 - RStudio: connect to RStudio suite on the compute node
- Tools and features are updated regularly depending on the needs of the users
- Availability of features depending on the *standard environment*





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3 CLI in JupyterHub



The terminal in the JupyterHub enables to:

- interact with ZIH system via CLI
- manage software and data with CLI commands

LSTM_PCA_FixedForceLevel_IX	Terminal 2	×
Module Python/3.8.6, GCCcore/10. (python-env-python3.8.6-20210715 Usage: ws_find [options] [worksp	-1421) ws_find	inloa
<pre>(python-env-python3.8.6-20210715 python: error while loading shar (python-env-python3.8.6-20210715 2_RandForcePCA.1pynb ANN_1_FixedForceLevel_UR5.ipynb CNN EX1.ipynb datax.hdf5 datay.hdf5 DIR Features_1FixedForce_tabels.ipynb GRU_fFixedForce-tabels.ipynb (python-env-python3.8.6-20210715</pre>	ed libraries: libpython3. -1421) ls GRU_FixedForce-MA.py GRUFixedForce-MA.py GRU_LOMEMI.ipynb jupyter-session-29401068 jupyter-session-29401068 jupyter-session-29401067 kfold.ipynb K Fold Task A-Multi clas Location_DNN.ipynb	8.so y .log .log '.log



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3 CLI Commands under the Hood: Jupyter Magic

The IPython Jupyter kernel supports Jupyter magic commands that:

- add additional functionality to Jupyter notebooks
- provide CLI functionality by the %%bash and ! magic commands

💧 Hi	int							
See ipyt	the Jupyter hon.readthedocs.io//	documentation magics.html	to	learn	more	about	magic	commands:
E E	xample							
[3]:	<pre>%bash cd /beegfs/ws/1/s4122485-jh_ mkdir test_magic ls -l</pre>		[5]: 1	d /heenfs/ws	/1/s4122485-il			
	total 42757 drwxr-xr-x 4 s4122485 p_scads 2 Oct 17 15:21 JPEGIm -Twr-r-r- 1 s4122485 p_scads 789 Oct 17 13:22 LICENSI -Twr-r-r 1 s4122485 p_scade 4370936 Oct 17 13:22 LICENSI		to				t 17 15:21 JPEGIma t 17 13:22 LICENSE	



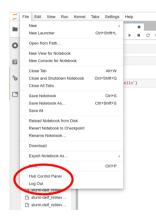
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3 JupyterHub Stop a Session





👠 Warning

Work finished do not forget to logout and stop your server! Otherwise, the resources will not be available to others and account for your **CPU quota**!



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4 Data Management via Jupyter – Agenda

1 Introduction

2 Jupyter overview

- 3 Access and Basics of the ZIH HPC system
- 4 Data Management via Jupyter Data Management via Jupyter
- 5 Collaborative Research and Teaching with Jupyter on HPC
- 6 Hands On session: Prepare a Jupyter "environment" for collaborative working
- 7 Conclusion, Q&A and Supplementary



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4 Data Management on HPC System

- many systems to store data that differ in capacity, bandwidth, IOPS rate etc
- organization of these storage systems in **files systems**
- many file systems, users, data require mechanisms for data management (duration, size, permission)
- the concept of work-spaces is used on the ZIH system for data management

🗄 Hint

for this presentation: a file system refers to a "place" to store data and a **workspace** refers to the "access" to that place



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4 Filesystem Storage Overview

- Each filesystems serves as respective capacity, performance, duration, lifetime.
- User creates a workspace with defined expiration date.
- A workspace can be extended multiple times, depending on the filesystem.

scope	filesystem	speed	size	duration
local	/tmp	+++		
Global temporary	/beegfs	++		
Global temporary	/ssd	+	-	
Global temporary	/scratch	-	+	+
Global permanent	/projects /home		++	++
archiving	/warm_archive		+++	+++

note 🖍

 $/\mathrm{projects}$ and $/\mathrm{home}$ are permanent filesystems without expiration date



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4 Workspace management in JupyterHub

To manage workspaces in Jupyter, use dedicated ws commands via:

- the CLI from the JupyterHub
- Jupyter magic commands within a notebook cell to execute bash scripts

Description	Command
Find available workspace filesystems	$ws_findlist$
Allocate workspace	ws_allocate
List your workspaces and get information (duration, path,)	ws_list
Extend workspace	ws_extend
Delete workspaces	ws_release

🕈 Note

Find additional commands in the docs: https://doc.zih..../data/lifecycle/workspaces/



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4 Workspace - Example

A workspace is a directory, with an associated expiration date, created on behalf of a user in a certain filesystem.

```
Example
1
   # Show available file systems for using workspaces
   marie@compute$ ws find -1
 2
 4
   # List all allocated workspaces
   marie@compute$ ws list
 5
   # Allocate a workspace "test-workspace" in filesystem "scratch"
 8
   marie@compute$ ws allocate -F scratch test-workspace
 9
   # Extend lifetime of a workspace called "test-workspace"
   marie@compute$ ws allocate -F scratch test-workspace 10
12
   # Delete workspace
14 marie@compute$ ws_release test-workspace
```



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4 Accessing Data: Linking Workspaces

- It might be valuable to links workspaces within a certain directory, e.g., your home directory.
- The command "ws_register" DIR to create link of workspace within the Home DIR directory
- via the Workspace scope parameter, set a workspace as the default directory for the notebook data

🛕 Warning

The **workspace scope** parameter is only for setting a specific working directory as default through the spawn menu. It is not related to the workspace principles on the system.

Spawner Options



Spawn



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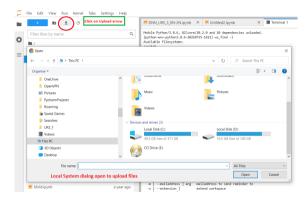
Very important





4 Data transfer to the JupyterHub

With JupyterHub GUI, data can be uploaded, downloaded with into workspace or home directory.





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4 Data transfer to the ZIH System, Windows 🎘

With an WinScp software, data can be uploaded, downloaded with a GUI to workspace or home directory for windows

Local Mark I	iles Commands	Senion Optio	ns Remote Help						
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acha26304	tauserport/vsk	au-dresden.de	X 🚇 New Session						
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4 Data Transfer on HPC System

There are two methods for exchanging data on HPC:

- scp, rsync, and sftp
- Datamover, to move data faster inside the ZIH
- for datamover you have to use commands prefixed with dt: dtcp, dtwget, dtmv, dtrm, dtrsync, dttar, dtls

More information in the wiki: https://doc.zih..../access/data/transfer/

Example: Access From Linux using scp





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4 Data Transfer on HPC System

Command examples prefixed with dt for transfer files from one filesystem to another filesystem

듣 Example

```
1 # dtcp for copying data from one filesystem to another filesystem
2 marie@login$ dtcp -r <fs_origin>/results <fs_destination>/.
3
4 # dtmv for moving data from one filesystem to another filesystem
5 marie@login$ dtmv <fs_origin>/ws/results <fs_destination>/ws/ws-archive/.
6
7 # dttar for archive data "results.gz" from one filesystem to another filesystem
8 marie@login$ dttar -czf <fs_destination>/results.tgz <fs_origin>/ws/results
```



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5 Collaborative Research and Teaching with Jupyter on HPC – Agenda

1 Introduction

2 Jupyter overview

3 Access and Basics of the ZIH HPC system

4 Data Management via Jupyter

5 Collaborative Research and Teaching with Jupyter on HPC

6 Hands On session: Prepare a Jupyter "environment" for collaborative working

7 Conclusion, Q&A and Supplementary



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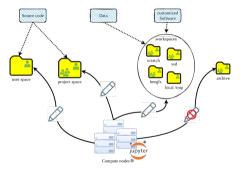


5 Collaborative Principles on HPC

- consider access/permission restrictions on the cluster
- level 1: permissions of files/directories need to be configured (esp. data and customized software environments)
- level 2: read/write connection between parts of the cluster (login nodes, compute nodes, storage)

Distinguish between: data, software environment, source code:

- data: in workspaces with group access
- software environment:
 - module system
 - ▶ in workspaces with group access
- source code:
 - user space or directory in project space
 - collaborative management via external version control, e.g. Git





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5 Accessing Data and Sharing Software: Permissions Management on ZIH system

On the ZIH system, we use Linux permissions:

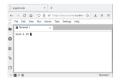
- distinguish **r**ead, **w**rite and e**x**ecute permissions
- assignable to user/owner, group (HPC project), other, all
- works on directory level and file level

Reading permissions with ls -l command:

💧 Hint

The chown and chgrp command change the owner and group of the directory/file

Example 1 # Check permissions of directory 2 marie@compute\$ ls -1 /scratch/ws/1/Marie-ml-ws/ 3 # Output 4 -rwxr-xr-- 1 marie marie_group 10 11. Nov 11:11 textfile.txt 5 drwx------ 1 marie marie_group 4096 11. Nov 11:12 marie_dir



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5 Accessing Data and Sharing Software: Permissions Management on ZIH system

Permission management is done by the 'chmod' command via CLI. Syntax:

chmod [ugoa]*([-+=]([rwxXst]*|[ugo]))+|[-+=][0-7]+ myfile

- ugoa = user/owner, group, other, all
- -+= = remove(-), add(+), set(=) permissions
- rwx = read, write, execute
- for more information: man chmod

📃 Example

- 1 # Give read and execute access to the group of the file
- 2 marie@compute\$ chmod g+rx /scratch/ws/1/Marie-ml-ws/marie_dir -R
- 3 # Check permissions of directory

```
4 marie@compute$ ls -l /scratch/ws/1/Marie-ml-ws/
```

- 5 # Output
- 6 drwxr-x--- 1 marie marie_group 4096 11. Nov 11:12 marie_dir





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5 Customized Software Environments with Python

- Python virtual environments create isolated working environments
- You can install packages, without interfere with other environments
- Multiple environments can be installed on one system simultaneously
- conda or virtualenv are state-of-the-art systems to create virtual environments

🛕 Warning

 $\tt conda$ virtual environments may infer with the module system on HPC. Therefore we recommend using <code>virtualenv</code> and <code>pip</code> instead of <code>conda</code>

More information in the wiki: https://doc.zih..../software/python_virtual_environments



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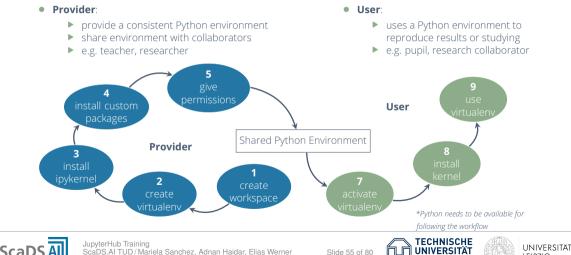


5 Shared Python Environment and Jupyter Kernels

We assume two roles for collaboration:

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5 Shared Python Environment: Example - Provider

```
Example
   # Create a virtual environment in the workspace
   marie@compute$ virtualenv --system-site-packages jh venv
 2
 3
   # Activate the environment
 4
   marie@compute$ source jh venv/bin/activate
   # Install the ipykernel package to use the environment in JupyterHub
    (jh_venv) marie@compute$ pip install ipykernel
 9
   # Install additional packages
    (jh venv) marie@compute$ pip install [...]
   # Set permissions of the workspace to share environment with collaborators
14 marie@compute$ chmod g+rx /scratch/ws/1/jh ws/ -R
```



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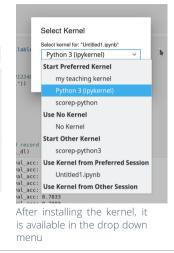


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5 Shared Python Environment: Example - User

📃 Example



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5 Persistence of Environments

- Goal: long-term storage and distribution of a Python software environment
- Conda and pip provide mechanisms to persist environments via a file
- Permanently store files in Git repository, e.g. repository for lecture series
- Restore environments by creating new environments based on the file

듣 Example

pip:

- 1 # Store packages of "env_pre" in "req.txt" and restore in fresh environment "env_post"
- 2 (env_pre) marie@compute\$ pip freeze > req.txt
- 3 (env_post) marie@compute\$ pip install -r req.txt







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5 Share a Spawn Link

- JupyterHub allows to share spawn options, e.g. Slurm parameters or work directory, via a link
- Every parameter of advanced form can be set as parameter
- If a parameter is not set, the default value will be loaded
- Setting the parameters in the form also sets the parameters in your browsers URL line:
- 💧 🚭 https://taurus.hrsk.**tu-dresden.de**/jupyter/hub/spawn#/~(partition~'romeo ☆

	Simp	le Advar	nced		
Preset	~	Save pres	set	Delete preset	
	Partition (-p, -	-partition):	roi	meo	~
	Nodelist (-w,	nodelist):	no	specific nodes	
	Nodes (-N	,nodes):	1		
1	Number of tasks (-	n,tasks):	1		
CPUs	per task (-c,cpus	-per-task):	4		
	Generic resource	es (gres):	no	generic resource	s
Memo	ry per CPU (men	n-per-cpu):	250	00	

📃 Example

https://taurus.hrsk.tu-dresden.de/jupyter/hub/spawn#/~(partition~'romeo~cpuspertask~'4~mempercpu~'2500) base URL and page "spawn" encoded spawn parameters



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5 Git Pull Feature

- Clone a public git repository into users work directory via nbgitpuller extension
- Distribute notebooks, data and other material to students or colleagues
- Use nbgitpuller link generator

📃 Example

https://taurus.hrsk.tu-dresden.de/jupyter/hub/user-redirect/...

base URL and page "user-redirect"

...git-pull?repo=https://github.com/jdwittenauer/ipython-notebooks&urlpath=/tree/ipython-notebooks/notebooks/language/Intro.ipynb

call to nbgitpuller extension with "repo" and "urlpath" parameter

- clone repository *ipython-notebooks* into work directory
- open *Intro.ipynb* notebook



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5 Git Pull Feature: NBGitpuller Link Generator

			Jupyter	Hub Launch fi	om Canvas	Binder
https://taurus.hrsk.tu-	dresden.de/jupyter/hub/user-redirect/git-pull?repo=https%3A%2F	%2Fgithub.o	com%2Felwe	r%2FJH_HPC	_demo&url	path=lab
JupyterHub URL	https://taurus.hrsk.tu-dresden.de/jupyter/					~
Git Repository URL	https://github.com/elwer/JH_HPC_demo	✓	branch	master		~
			Use main inst	ead of master for ne	w GitHub repo:	sitories
File to open	handson_diving_meets_ai.ipynb					~
	This file or directory from within the repo will open when user clicks the link.					
Application to Open	O Classic Jupyter Notebook					
	○ RetroLab					
	JupyterLab					
	O RStudio					
	O Shiny					
	O Custom URL					
	Relative URL to redirect user to					



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5 Git Pull Feature: Private Repository

- Git pull feature also possible for private repositories, e.g. repository in GitLab Chemnitz
- Access tokens provide access to your repository for the "outer world"
- Permissions and expiration of tokens definable by yourself

Workflow:

- 1. Create access token in repository settings
- Adapt link to repository for Git HTTPS cloning: https://<username>:<access-token>@<repository-url>
- 3. Use nbgitpuller link generator

🖍 Note

GitLab Chemnitz creates a "Bot user" when creating an access token. Use this user for the link generation. The username is created as follows: project_project_id_bot. You can find the project_id in your repository settings. More information: gitlab.hrz.tu-chemnitz.de/.../project_access_tokens



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5 Git Pull Feature: Private Repository - Example(1)

🦊 🗮 Menu			
M My Project		④ Your new access token has been created.	×
	0	Project Access Tokens Generate project access tokens acoped to this project for your applications that need access to the Gittab APJ. You can also use project access tokens with Git to authenticate over HTTP(S). Learn more.	Your new project access token _tkCKDYGBMfCxeo9DUlg Make sure you save it - you won't be able to access it again. Add a project access token Enter the name of your application, and we'll return a unique project access token. Token name For example, the application using the token or the purpose of the token. Do not give sensitive information for the name of the token, as it will be visible to all project members.
Le Analytics			Expiration date

🛕 Warning

The token is only visible at creation time. On the page you can find multiple options for configuring a specific token (access role, scopes, expiration date) as well as revoking access for existing tokens.



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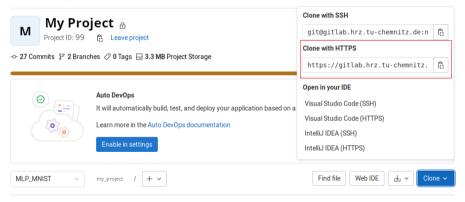
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5 Git Pull Feature: Private Repository - Example(2)

Scads-Al > My Project





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5 Git Pull Feature: Private Repository - Example(3)

Workflow Example:

- get access token
- get git repository link
- get project id Bot username: project_99_bot

🔶 🗏 Menu					
M My Project		Scads-Al → My Project → General Set	ings		
Project information		-			
Repository		Q Search page			
D Issues	0				
13 Merge requests	0	Naming, topics, avatar			
🕼 CI/CD		Update your project name, topics, desc	ription, and avatar.		
D Security & Compliance		Project name	Projec	ct ID	
Deployments		My Project	99	j.	
🖰 Packages & Registries		Topics			
Infrastructure		Search for topic			
👜 Monitor					
La Analytics		Project description (optional)			
X Snippets					
Settings					
General		Repository size limit (MB)			
Integrations					

- now: create link for Git HTTPS cloning https://project_99_bot:_tkagshd63Sd@gitlab.hrz.tu-chemnitz.de/scads-ai/my_project.git
- use the link in the nbgitpuller link generator



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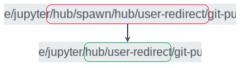


5 Combine Parameter Sharing and Git Pull

- You can also combine the *parameter sharing* and the *git pull* feature via a single link
- Concatenation of links can be done manually or:
 - 1. create the parameter sharing link
 - insert the link as JupyterHub URL in the nbgitpuller link generator and add git pull functionality

👠 Warning

When **combining** the link via the nbgitpuller link generator, the link might be defective and needs to be fixed.



듣 Example

https://taurus.hrsk.tu-dresden.de/jupyter/hub/user-redirect/...

base URL and page "user-redirect"

...git-pull?repo=https://github.com/jdwittenauer/ipython-notebooks&urlpath=/tree/ipython-notebooks/notebooks/language/intro.ipynb...

call to nbgitpuller extension with "repo" and "urlpath" parameter

...#/~(partition~'romeo~cpuspertask~'4~mempercpu~'2500)

encoded spawn parameters



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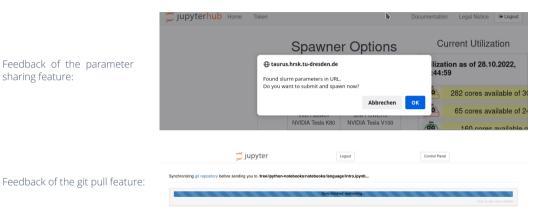
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5 JupyterHub Link Feedback

Feedback of the parameter sharing feature:





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5 Short URLs

💧 Hint

Short URL services shorten your links and may provide further functionality, e.g.

- expiration date
- maximum number of accesses

We recommend to use the TUD Short link service for that purposes: https://tud.link/create/

UNIVERSITAT DRESDEN	Short URL Service
Create Short-URL +	How to use?
Target URL: C_demo%2Fhandson_diving_meets_al.ipynb&branch=master	Shorten
Your short URL: https://tud.link/ud4i Link copied.	
Short-URL Settings	
+ enable password protection	
+ limit validity period + define maximum access count	
+ create a deactivation link + hide the referrer	
+ create a QR code	
in Deutsch anzeigen A	ccessibility Privacy Contact



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6 Hands On session: Prepare a Jupyter "environment" for collaborative working – Agenda

1 Introduction

2 Jupyter overview

- 3 Access and Basics of the ZIH HPC system
- 4 Data Management via Jupyter
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- 6 Hands On session: Prepare a Jupyter "environment" for collaborative working
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6 HandsOn: Diving meets AI

Dataset: NOAA Puget Sound Nearshore Fish 2017-2018

- 77.739 images from underwater video
- 30.384 images with fish and crustaceans, annotated as *animal*
- remaining images annotated as *empty*
- more information about the dataset: lila.science/.../noaa-puget-sound-nearshore-fish

📐 Warning

Please use your personal ZIH login credentials we sent you for the following tasks! Use the reservation p_scads_jupyterhub_773 for the --reservation parameter to reduce scheduling time.





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6 Setting

💧 Hint

We distinguish between *source code, data* and *software*. In this example, we already prepared the source code in a git repository.

- A Jupyter notebook with the source code is available in a Git repository: https://github.com/elwer/JH_HPC_demo
- The NOAA fish dataset is available in the workspace: /beegfs/ws/1/s4122485-jh_ws/NOAA
- Aim: Share your experiences with the dataset with your colleagues
- The example consists of two parts:
 - 1. Prepare and share your setup (data and software)
 - 2. Test the setup



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6 Part 1a: Prepare the workspace and the data

Concrete tasks (data part):

- 1. Open the browser and spawn a Jupyter server:
 - Advanced option (see slide 30)
 - Partition: alpha
 - Runtime: 2hours
 - Reservation: p_scads_jupyterhub_773
- 2. Open a terminal after spawning (see slide 37)
- 3. Create a workspace teaching_ws on beegfs file system (see slide 44)
 - create a directory data for the data in teaching_ws
 - create a directory sw for the software in teaching_ws
 - note down/remember the workspace directory (it is required later)
- 4. Copy the data from /beegfs/ws/1/s4122485-jh_ws/NOAA to [...]/teaching_ws/data either via the datamover nodes (see slide 49) or simple cp command



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Provider

6 Part 1b: Prepare the software

Concrete tasks:

- 1. Load the Python module: module load modenv/scs5 Python/3.9.5
- 2. Create a Python virtual environment in [...]/teaching_ws/sw and activate it (see slide 56)
- 3. Install the ipykernel package (see slide 56)
- 4. Install additional packages (see slide 56):
 - pip3 install torch torchvision torchaudio --extra-index-url https://download.pytorch.org/whl/cu113
 - pip install tqdm matplotlib
- Give the group read and execute permissions to [...]/teaching_ws and all subdirectories (see slide 53)
- 6. Log out from your session and stop it(see slide 39)

🛕 Warning

Important: This example is only for demonstration purposes. When interacting with the HPC, always prefer pre-installed Modules instead of installing the software on your own.



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6 Part 1c: Prepare for sharing

Concrete tasks:

- Via the spawner advanced interface: Create a link for sharing the resources (see slide 59):
 - partition: alpha
 - nodes: 1
 - CPUs: 6
 - GPUs: 1
 - memory per CPU: 2500M
 - runtime: 2hours
 - reservation: p_scads_jupyterhub_773
 - preload modules: Python/3.9.5
 - standard environment: production
 - workspace_scope: your workspace directory
- Insert the link in the nbgitpuller website as JupyterHub URL (see slide 60/61)
- Add the Git Repository URL and the File to open to combine both links (see slide 61/62)
- Shorten the link (see slide 64) and communicate the link to the group via the chat



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6 Part 2: Test the setup



Concrete task:

- 1. Use some link from the chat to start a JupyterHub (not your own)
- 2. Activate and install the virtual environment from the workspace of your group members either via CLI or Jupyter magic (see slide 38)
- 3. Select the installed Kernel
- 4. Execute the Jupyter notebook and explore the data set

🛕 Warning

This part will only work, if the person that created your link, carefully followed all the steps in part 1.



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6 Basic CLI Commands

Command	Description
ls	list files and/or directories
cd <path_destination></path_destination>	change directory
mkdir <directory_name></directory_name>	create a new directory
pwd	Show full path of the current directory
cp <path_source> <path_destination></path_destination></path_source>	copy a file
cp -r <path_source> <path_destination></path_destination></path_source>	copy a directory
mv <path_source> <path_destination></path_destination></path_source>	move a file or directory
rm <path_source></path_source>	delete a file or directory
wget	get datasets from the web (using HTTP, HTTPS, FTP and FTPS)



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6 Troubleshooting

- Problems when spawning:
 - delete cookies
 - delete access tokens
 - ▶ check whether your spawner is still running via squeue --me command in CLI (ssh connection)
- General:
- check the jupyter-session-XXXXXXX.log file in your HOME directory
- it gives a lot of insights of your notebook servers behaviour (e.g. if module (pre-)load was successful)
- Pika Job Monitoring tool shows you utilization statistics of your notebook server
- ssh connection to the node with the notebook server software (get name of the node via squeue --me), then ssh taurusi_nodeID, lets you investigate your computing node(s) further

💧 Hint

Having a look in the compendium is always useful: doc.zih.tu-dresden.de



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7 Conclusion, Q&A and Supplementary – Agenda

- 1 Introduction
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7 Conclusions

- The Jupyter universe is big (extensions, plugins, use cases, people)
- JupyterHub offers an easy access to HPC resources
- HPC is a complex task JupyterHub abstracts some of the complexity
- Versatile features for collaborative working
- We proposed one approach but typically there is not only one solution



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7 Conclusions

- In case of questions start at the official docs for the ZIH system: https://doc.zih.tu-dresden.de/
- Software ecosystems are changing dynamically, esp. in ML: with HPC systems it is hard to react immediately
- Contact us with your own ideas, experiences and wishes!

🖍 Note

logins (scads0xx) will work for further 10 days

- if your are interested afterwards please apply for your own HPC project
- for starting purposes we recommend a "Schnupperprojekt" without a detailed project description

ScaDS.AI

Thank you

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