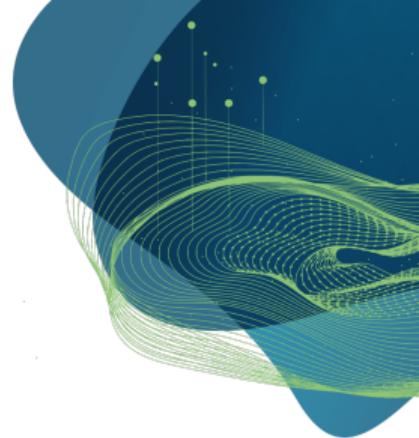




DRESDEN LEIPZIG

CENTER FOR SCALABLE DATA ANALYTICS AND  
ARTIFICIAL INTELLIGENCE



## Introduction to High Performance Computing

Physics of Life - Bio Image Analysis Training School

Neringa Jurenaite, Apurv D. Kulkarni, Taras Lazariv

Dresden, 29 August 2023

GEFÖRDERT VOM



Bundesministerium  
für Bildung  
und Forschung

SACHSEN



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# Instructors



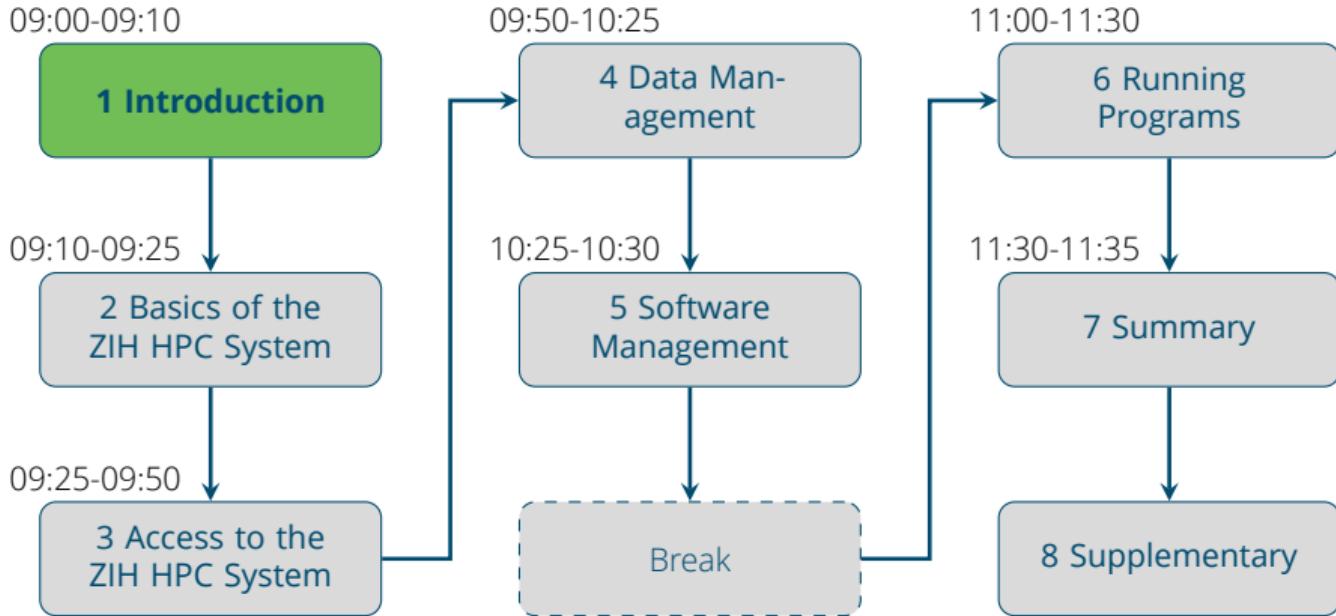
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Statistics, Machine Learning, Deep Learning



# Intention of this Training

- Making things understandable esp. for new users without a background in computer science
- Complete workflow examples are shown which are based on Python (can be used as a blueprint for other software/tools)
- From the user's perspective: What are the most important things to work with ML on an HPC cluster?

## Note

- We do **not** want to show everything possible. We want to show what is needed to get started.
- We do **not** want to show the perfect HPC-ML workflow. We want you to comprehend ML principles with an HPC machine starting with concrete examples.

## Hint

Please interrupt and ask immediately if something is not clear.

# What is an HPC machine?

## Terminology

- **Compute or login Node:** An individual computer, part of an HPC cluster
- **CPU, Core:** Central Processing Unit. A modern CPU is composed of numerous cores
- **Cluster:** A group of machines interconnected in a way that work together as a single system

### Note

**HPC cluster** is a relatively tightly coupled collection of compute nodes, the interconnect typically allows for high bandwidth, low latency communication. Access to the cluster is provided through a login node. A resource manager and scheduler provide the logic to schedule jobs efficiently on the cluster.



# Why do we use HPC?

## ❓ Question

What are the things that we look for, while performing our task on a computer? What are the issues that we come across?  
Computation? Memory? or both?

- **High speed:** Massive calculations in a relative short time
- **Reduced cost:** Faster answers mean less money; Affordable cloud-based HPC
- **Scalability**
- **Innovation:** Science, technology, business, and academia
- More information on HPC:  
[https://hpc-wiki.info/hpc/HPC\\_Wiki](https://hpc-wiki.info/hpc/HPC_Wiki)

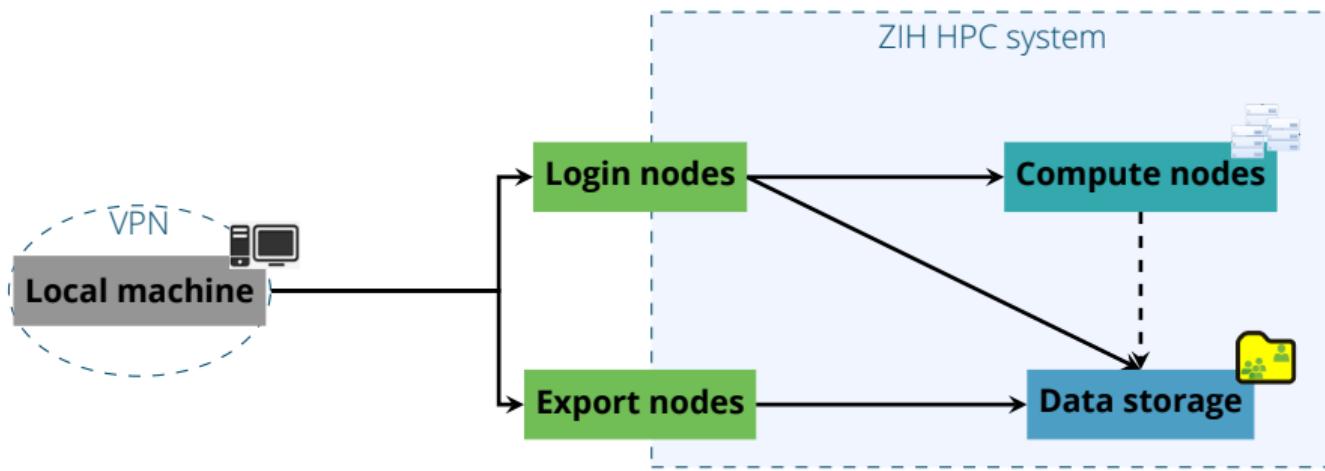


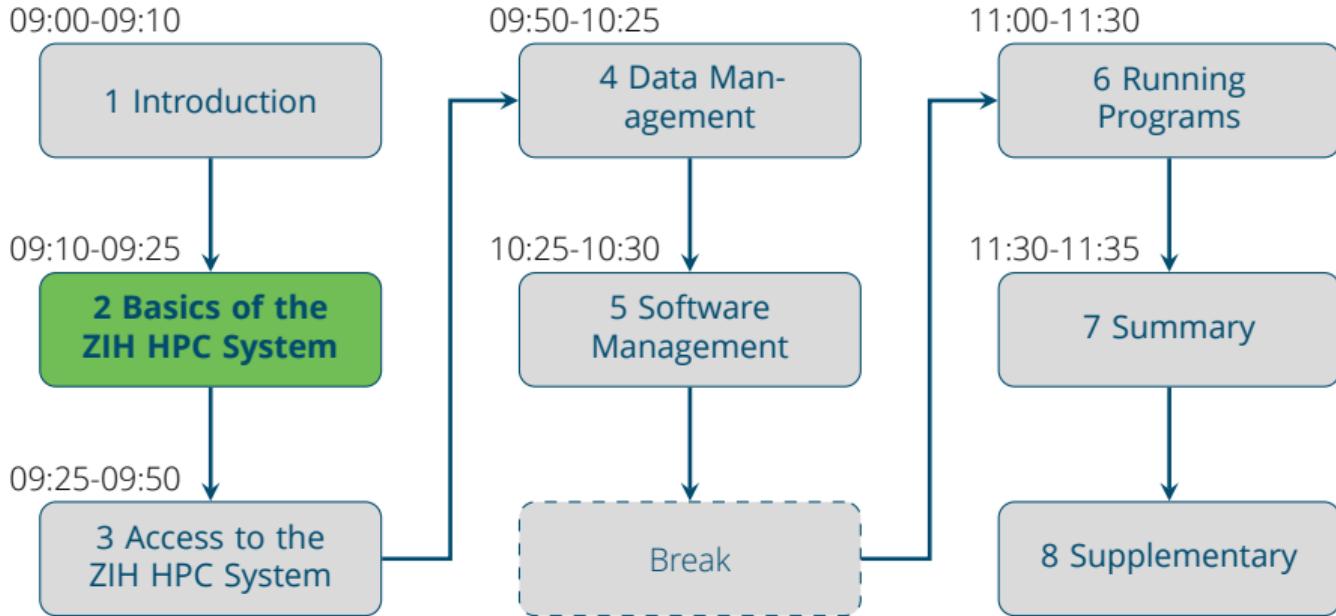
# HPC system - Taurus

- **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,
  - ▶ GPU partition with 128 dual GPU. All nodes have local SSD.
  - ▶ 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.



# The ZIH System





# Typical Workflow

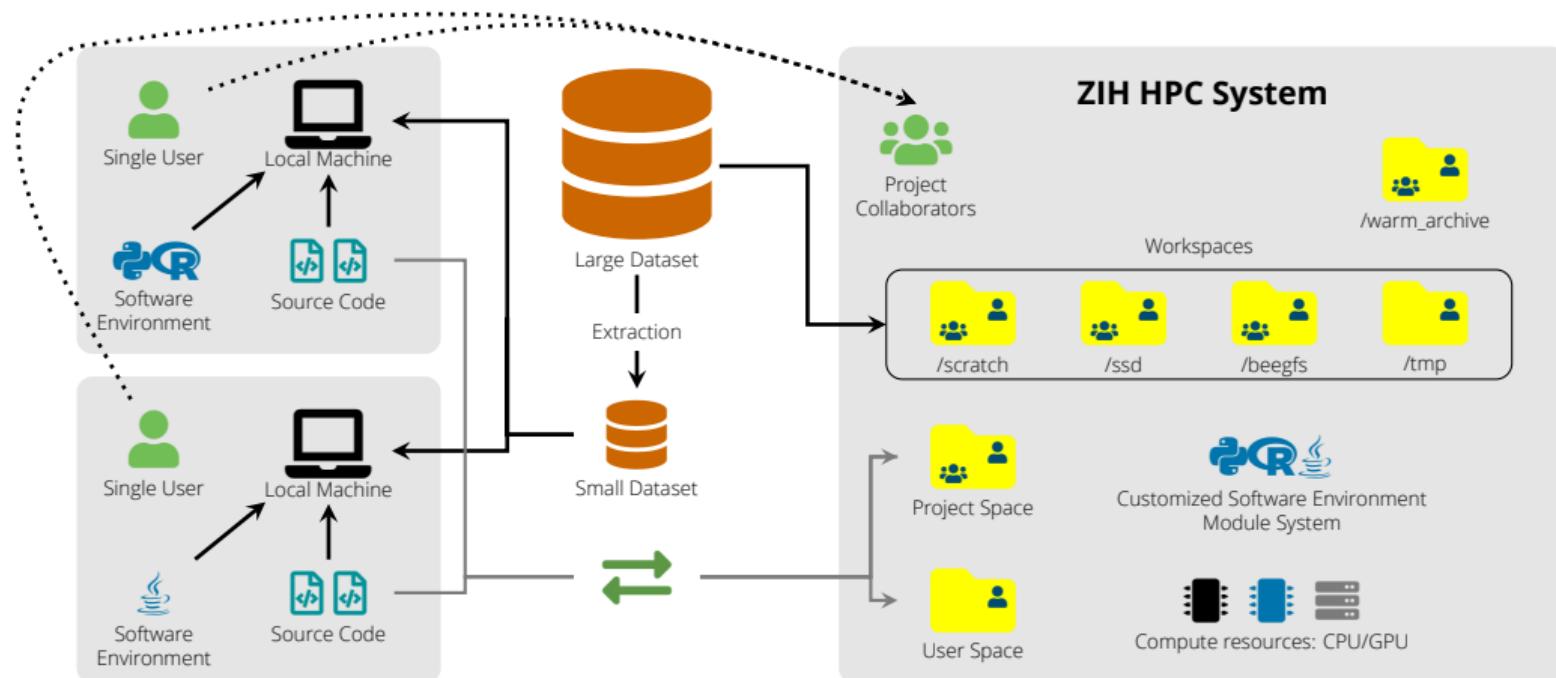
Recommended workflow to achieve a productive command line (CLI) based pipeline (some steps are optional)

1. Local machine: development of a pipeline as prototype (maybe with virtual environments like virtualenv or conda), usage of IDE or within jupyter notebook
2. Local machine: fully working CLI-based pipeline for small model/data
3. HPC machine: switch to a compute cluster with need for larger resources
4. HPC machine: use graphical front-end as jupyter notebook for testing purposes (software, hardware, algorithms)
5. HPC machine: fully working CLI-based pipeline with full data

## 💡 Hint

See the official docs for the ZIH system: <https://doc.zih.tu-dresden.de/>.

# Switching from Local Machines to HPC Systems

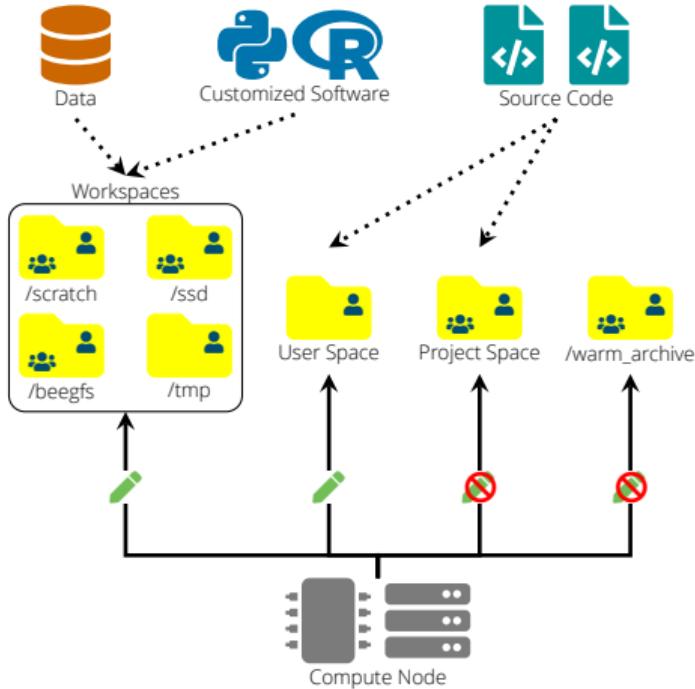


# Collaborative Working

- We can achieve a collaborative working environment at two different levels based on the access/permission restrictions on the cluster:
  - Consideration 1: setting permissions to **different users** in your project (esp. important for data and customized software environments)
  - Consideration 2: Defined access possibilities based on **which node** you are on (login or compute) and on **which storage filesystem** you are trying to access (e.g. beegfs vs archive)
- It is important to distinguish usage of data, software environment, source code.

## Hint

- Data:** in workspaces with group access
- Software environment:** module system or workspaces with group access
- Source code:** user space or user specific directory in the project space



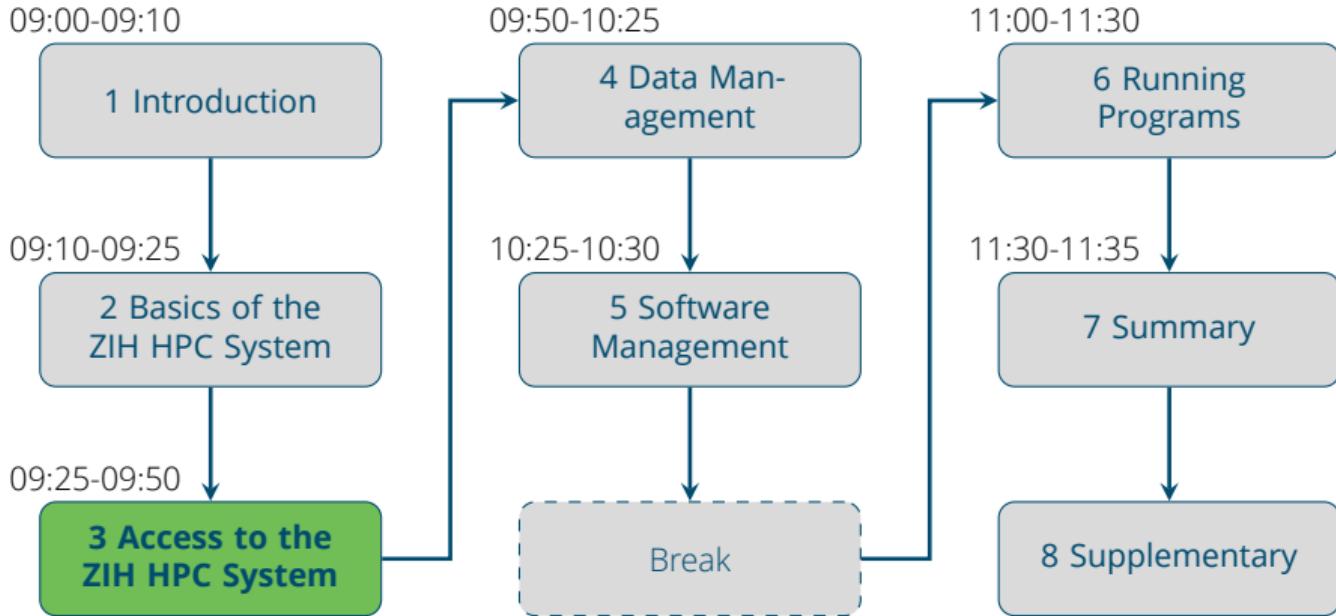
# HPC project application

The ZIH system is structured by HPC projects. A HPC project on the ZIH system includes:

- project directory
- project group (linux group)
- project members (at least project leader and project administrator)
- resource quotas for compute time (CPU/GPU hours) and storage

There are different possibilities to work with the ZIH HPC:

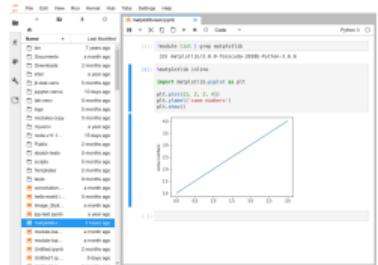
- create a new project
  - ▶ fill in the application form: <https://hpcprojekte.zih.tu-dresden.de/>
  - ▶ find additional information on the wiki: 
- join an existing project: e.g. new researchers in an existing project, teaching purposes



# Access the ZIH HPC System

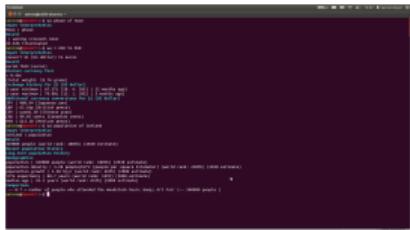
## JupyterHub

- browser based approach
- easiest way for beginners



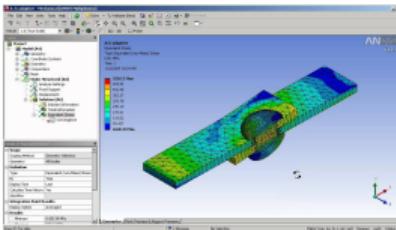
## SSH connection (CLI)

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



## Desktop visualization

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



## Note

- When working from **outside of the university network**, the ZIH HPC system can be accessed **only via Virtual Private Network (VPN)**
- Please use **provided** login information for this training

## Hint

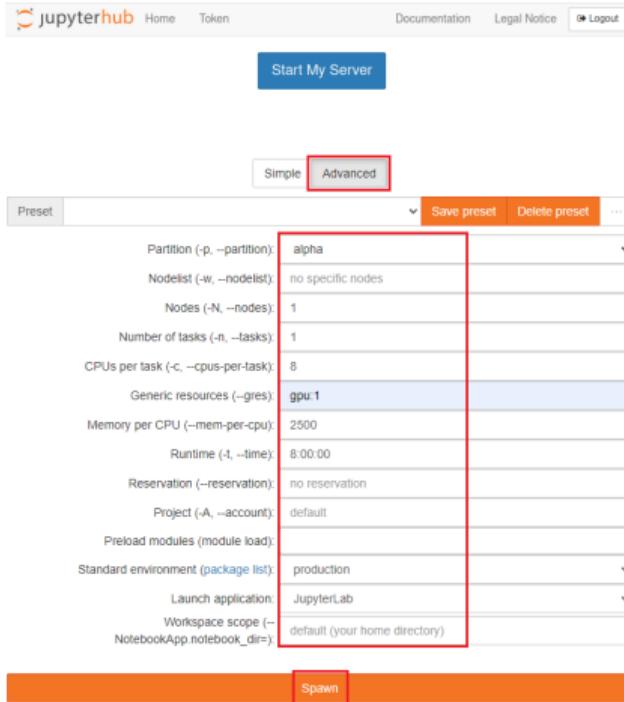
More info on VPN: [↗](#)

# Access via JupyterHub

1. Connect to TU Dresden network via VPN, if you are accessing outside university network
2. Go to following JupyterHub link using any browser:  
<https://taurus.hrsk.tu-dresden.de/jupyter>
3. Login using ZIH-ID and password
4. Click on "Start My Server". This doesn't start any job.
5. Allocate resources via the spawner interface, and click on "Spawn" to start job

## Hint

More information in the wiki: [!\[\]\(397cc4c04b5e7ea225dbaa029a5dee1f\_img.jpg\)](#)



The screenshot shows the JupyterHub interface with the following configuration:

- Simple** tab is selected.
- Advanced** tab is visible above the configuration fields.
- Preset** dropdown is set to "alpha".
- Partition (-p, --partition)**: alpha
- Nodelist (-w, --nodelist)**: no specific nodes
- Nodes (-N, --nodes)**: 1
- Number of tasks (-n, --tasks)**: 1
- CPUs per task (-c, --cpus-per-task)**: 8
- Generic resources (-gres)**: gpu:1
- Memory per CPU (-mem-per-cpu)**: 2500
- Runtime (-t, --time)**: 8:00:00
- Reservation (-reservation)**: no reservation
- Project (-A, --account)**: default
- Preload modules (module load)**: (empty)
- Standard environment (package list)**: production
- Launch application**: JupyterLab
- Workspace scope (-NotebookApp.notebook\_dir=)**: default (your home directory)

A red box highlights the "alpha" preset in the dropdown and the "gpu:1" entry in the generic resources field.

**Spawn** button is at the bottom right.

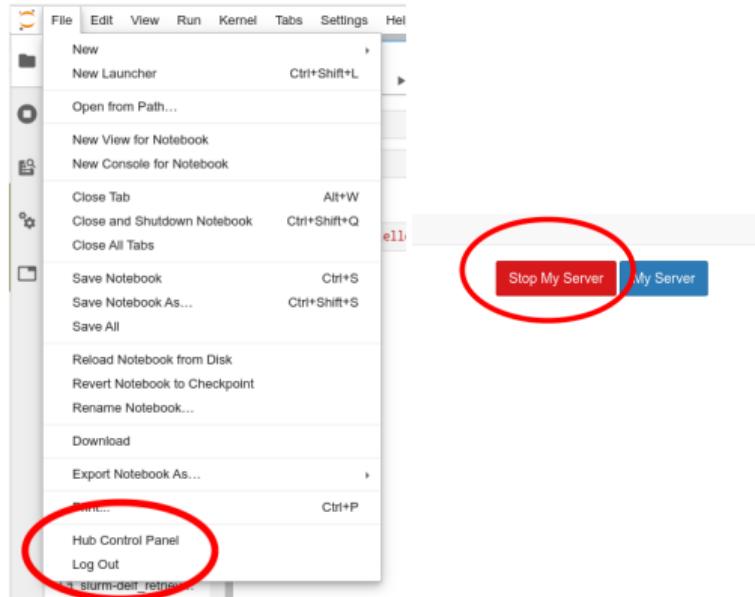
# Access via JupyterHub

- When using JupyterHub do not forget to **logout** and then **stop your server!** Otherwise, the resources will not be available to others and will be included in your CPU quota!

## Hint

In case of any issues while accessing/launching JupyterNotebook, it is recommended to:

- clear browser cookies and cache, and/or
- use incognito/private browser mode



# Access via SSH connection (CLI)

ZIH systems can be accessed via CLI using SSH connection.

1. Connect to TU Dresden network via VPN, if you are accessing outside university network
2. Launch terminal
3. Connect to ZIH HPC login-nodes via `ssh` using ZIH-ID, login-node address (`taurus.hrsk.tu-dresden.de`) and ZIH account password
4. Allocate resources via `srun` or `sbatch`



Hint

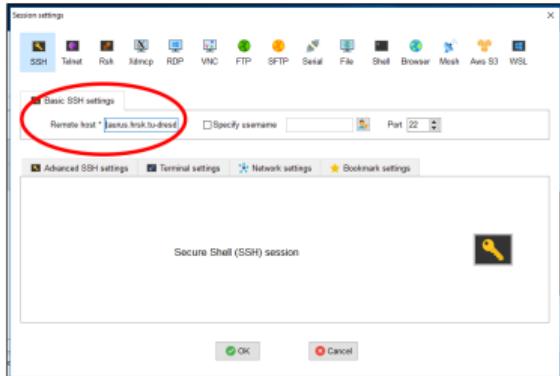
More info at: [🔗](#)

## Example

```
1 # Connect to the cluster via SSH
2 marie@local$ ssh marie@taurus.hrsk.tu-dresden.de
3
4 # Allocate resources via srun (for an interactive session)
5 marie@login$ srun --partition=alpha --gres=gpu:1 --cpus-per-task=8 --mem=8000 --time=6:00:00
   --account=p_scads_trainings --reservation=p_scads_trainings_1149 --pty bash
6
7 # Now you can use the resources
8 marie@compute$ [...]
```

# Access via SSH connection (CLI) (contd.)

- Accessing the ZIH system from a **Windows system**  is done via SSH client
- We recommend using **MobaXterm** (download free version at <https://mobaxterm.mobatek.net/download.html>)

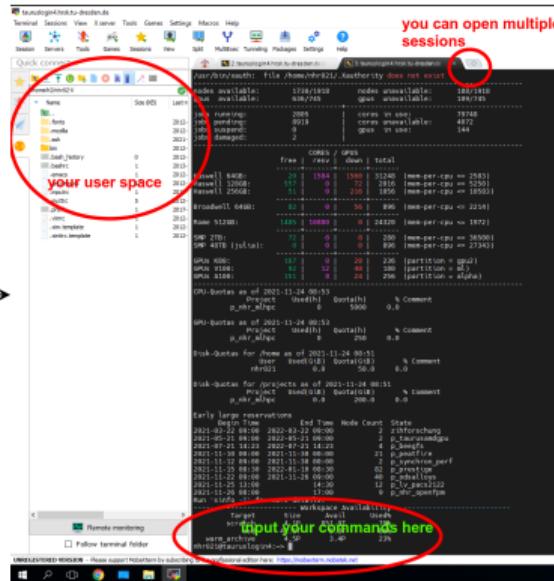


Remote host: **taurus.hrsk.tu-dresden.de**  
username:<ZIH-ID>

 Hint

More info at: 

successful login →



# Try it Yourself

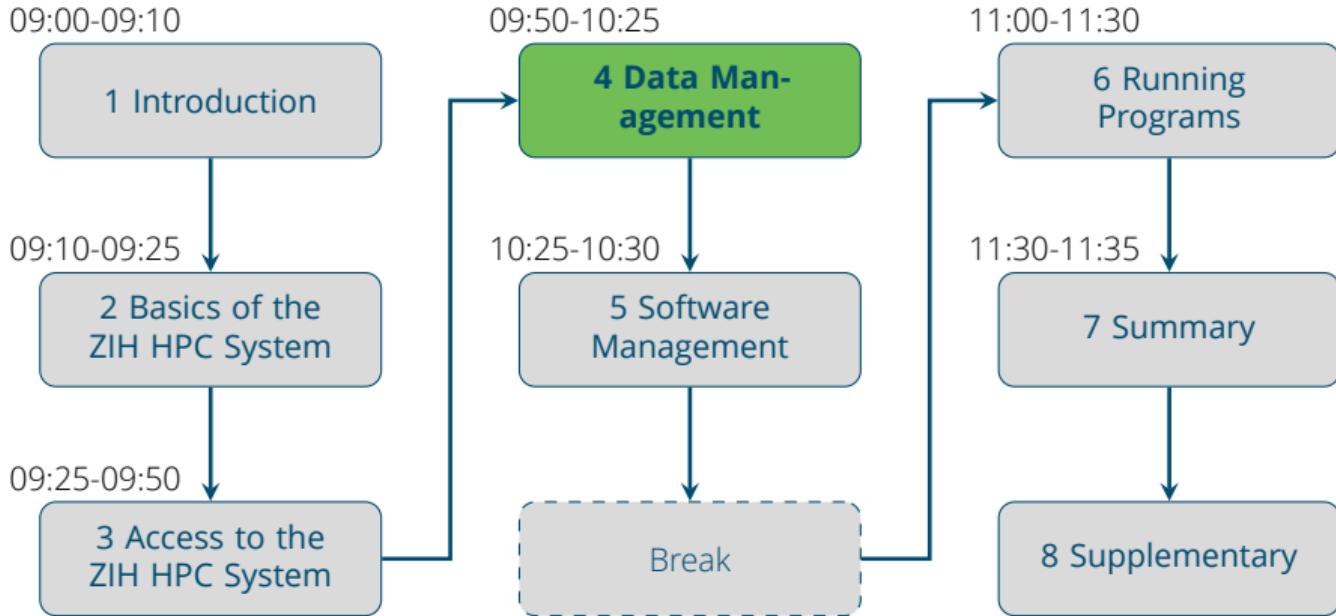
- Accessing HPC via MobaXterm, JupyterHub
- Use basic CLI Commands
- Use nano open, modify and save a text file

Once you are logged in try doing following commands in CLI:

- copy/insert from/to with CLI: **Ctrl +Shift +c** or **Ctrl +Shift +v**
- copy/insert from/to in MobaXterm: just select/Shift+insert or right-click-mouse
- use arrow up and down for command history
- use Tab-completion
- nano is command line text editor for Linux



More info about basic CLI commands can be found at 51



# Filesystems

- There are different areas for storing your data on the ZIH HPC system, called **filesystems**
- The filesystems have different properties (available space, time limit, size, permission rights). Therefore, choose the one that fits your project best.
- You need to create a workspace for your data on one of these filesystems.

## Note

For this presentation: a filesystem refers to a "space/place" to store data and a workspace refers to the "access" you created to that filesystem

- Overview of filesystems

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

## Note

There are also other archives available via datamover nodes.

# Workspaces

- On the ZIH system, data has a **limited lifetime** depending on the filesystem
- User creates a workspace on filesystems with defined **expiration date**
- Data is **deleted** automatically after expiration.



**Note**  
`/projects` and `/home` are permanent filesystems **without expiration** date

Some commands to manage workspaces on the ZIH system:

Command	Description
<code>ws_find --list</code>	Find available workspace filesystems
<code>ws_allocate -F &lt;filesystem&gt; &lt;name_of_your_ws&gt; &lt;duration_of_your_ws&gt;</code>	Allocate workspace
<code>ws_list</code>	List your workspaces and get information
<code>ws_extend -F &lt;filesystem&gt; &lt;name_of_your_ws&gt; &lt;duration&gt;</code>	Extend workspace



**Hint**  
More info at: [↗](#)

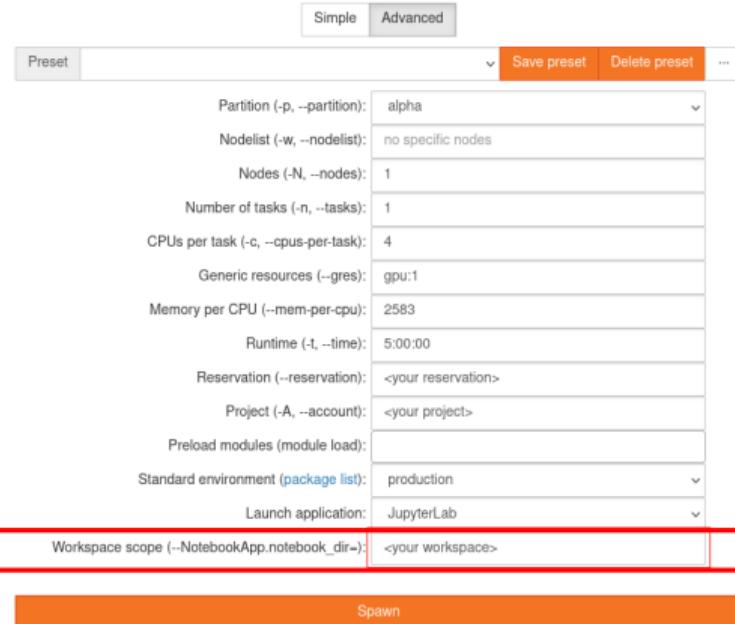
# Workspaces

## Example

```
1 #Check the available filesystems
2 marie@login$ ws_find --list
3
4 #Create a beegfs workspace and retrieve workspace path
5 marie@login$ ws_allocate -F beegfs myworkspace 10
6
7 #Check workspace information (e.g. duration, path,...)
8 marie@login$ ws_list
9
10 #Create a directory for the data in the workspace
11 marie@login$ mkdir /beegfs/ws/1/marie-myworkspace/src
12
13 #Create a directory for the model in the workspace
14 marie@login$ mkdir /beegfs/ws/1/marie-myworkspace/output
```

# Workspace: JupyterHub

- On JupyterHub, the working directory can be set in the spawner options
- Set **Workspace scope** parameter to the full path of required workspace
- Specified workspace will be set as the default directory for the notebook execution



The screenshot shows a configuration interface for a JupyterHub spawner. At the top, there are tabs for "Simple" and "Advanced". Below that is a "Preset" dropdown with "alpha" selected, and buttons for "Save preset" and "Delete preset".  
  
The configuration fields include:

- Partition (-p, --partition): alpha
- Nodelist (-w, --nodelist): no specific nodes
- Nodes (-N, --nodes): 1
- Number of tasks (-n, --tasks): 1
- CPUUs per task (-c, --cpus-per-task): 4
- Generic resources (--gres): gpu:1
- Memory per CPU (--mem-per-cpu): 2583
- Runtime (-t, --time): 5:00:00
- Reservation (--reservation): <your reservation>
- Project (-A, --account): <your project>
- Preload modules (module load):
- Standard environment (package list): production
- Launch application: JupyterLab

  
A red box highlights the "Workspace scope (--NotebookApp.notebook\_dir=)" field, which contains "<your workspace>".  
  
At the bottom is a large orange "Spawn" button.

# Access Permissions

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

```
1 chmod [class] [operator] [mode] myobject  
2 chmod [ugoa] [-+=] [rwx] myobject
```

where:

- class = [ugoa] = **u**ser/owner, **g**roup, **o**ther, **a**ll three classes
- operator = [-+=] = remove(-), add(+), set(=) the specified modes for the specified classes
- mode = [rwx] = **r**ead, **w**rite, **e**xecute



**Hint**

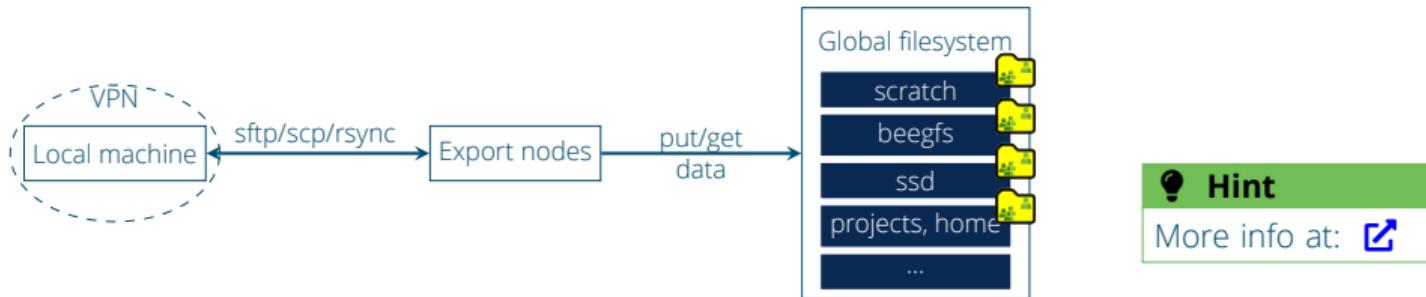
More info at: [? and ↗](#) or [man chmod](#)

## Example

```
1 # check permissions of myobject i.e. the workspace  
2 marie@login$ ls -l /beegfs/ws/1/marie-myworkspace/  
3  
4 # give "read, write and execute" access to the group that owns myobject  
5 # -R means recursively i.e. on all files and directories at myobject  
6 marie@login$ chmod g+rwx -R /beegfs/ws/1/marie-myworkspace/
```

# Datatransfer: Local Machine and ZIH System

- Connection with local machine in VPN to export nodes via `scp`, `sftp`, `rsync`
- Transfer data to your target directory via export node



## Example

```
1 marie@local$ scp myscript.py marie@taurusexport.hrsk.tu-dresden.de:/home/marie/
2 marie@local$ rsync -avz myscript.sbatchr marie@taurusexport.hrsk.tu-dresden.de:/home/marie/
3 marie@local$ rsync -avz requirements.txt
                         marie@taurusexport.hrsk.tu-dresden.de:/beegfs/ws/1/marie-myworkspace/
```

# Datatransfer: External sources

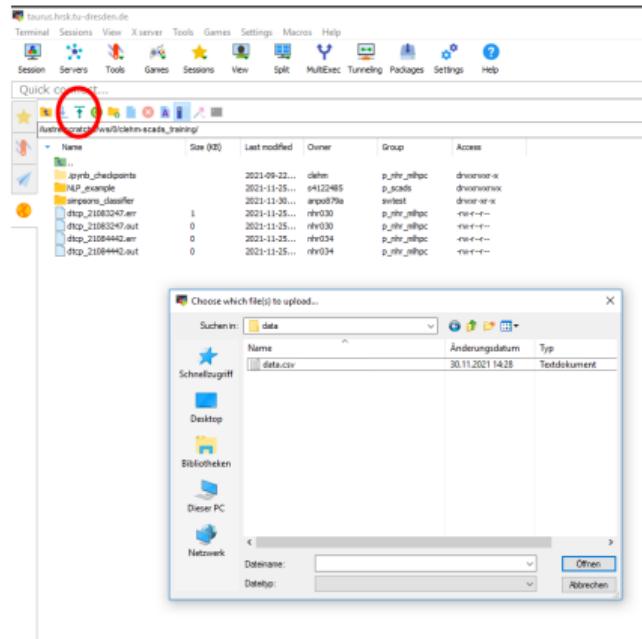
- Any file from external sources can also be downloaded on ZIH HPC system directly using commands like `wget`.

## Example

```
1 #Use wget command to get dataset from the web
2 marie@compute$ wget --directory-prefix=/beegfs/ws/1/marie-myworkspace
   https://cloudstore.zih.tu-dresden.de/index.php/s/bm9HMTRGbN9ibrn/download/myfile.txt
3
4 #Check the content of the file with the nano editor
5 marie@compute$ nano /beegfs/ws/1/marie-myworkspace/myfile.txt
```

# Datatransfer: Windows

With an SSH client (such as MobaXterm), data can be copied with a GUI



# Datatransfer: Large vs Small Data

- Runtime of applications on login nodes is **limited** to 10min
- Data transfer that takes longer than that, will be **canceled**
- Therefore, it is recommended to use **export nodes** for large data transfer (might take longer)

## Note

For very small data (up to 100MB), you can also use the login nodes (i.e. a single script file)

# Datatransfer: Within the ZIH system

- Special data transfer nodes for moving large data between different filesystems
- Commands for data handling and transfer are prefixed with `dt`

► `dtcp`, `dtls`, `dtrmv`, `dtrm`, `dtrsync`, `dttar`

► `dtqueue --me` to check the status of the data transfer

► These commands create a **Slurm job** with dedicated resources to conduct the data handling/transfer.

## Hint

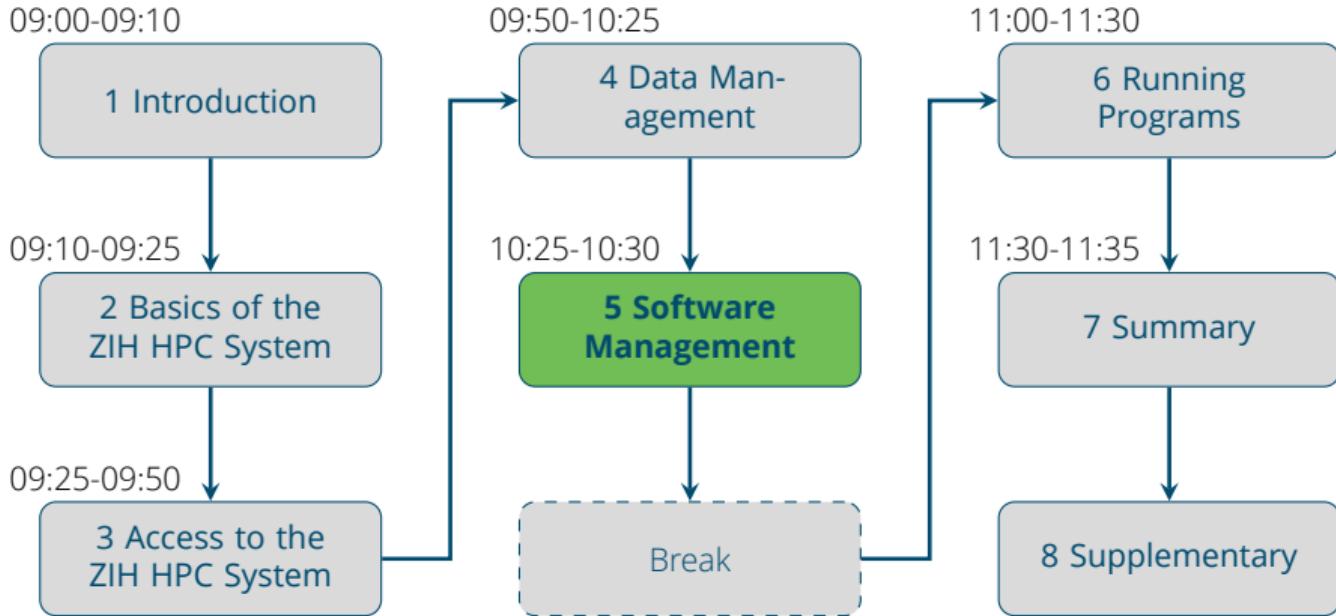
More info at: [🔗](#)

## Example

```
1 # Copy the training data into beegfs workspace directory
2 marie@login$ cp myscript.py /beegfs/ws/1/marie-myworkspace/src/
```

## Example

```
1 # Copy the training data into beegfs workspace directory
2 marie@login$ dtcp myscript.sbatch /beegfs/ws/1/marie-myworkspace/src/
3
4 # Check copy job status
5 marie@login$ dtqueue --me
```

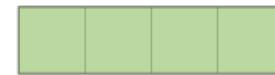
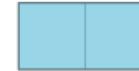
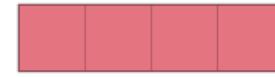


# Module System

- On the ZIH system, software is organized in modules.
- A **module** is a user interface, that:
  - ▶ allows you to easily switch between different versions of software
  - ▶ dynamically sets up user's environment (PATH, etc.) and loads dependencies
- ZIH HPC system use **EasyBuild** framework to build and install scientific frameworks.



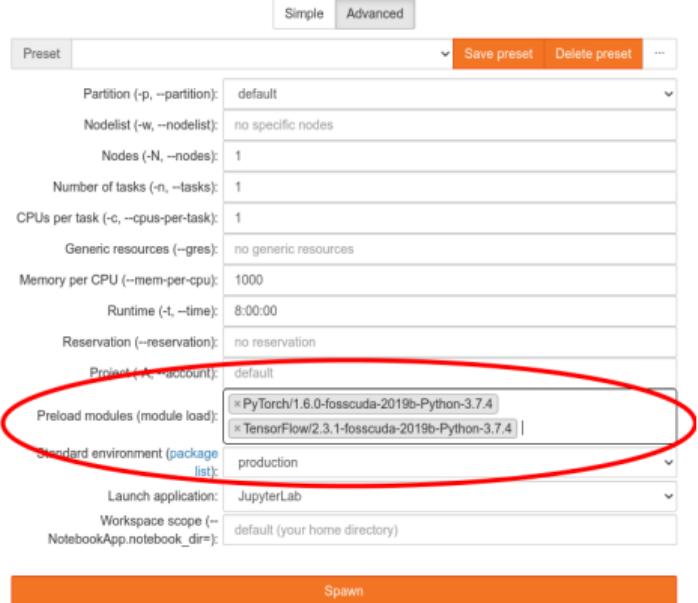
Hint  
More info at: [link](#) and [link](#)



**EasyBuild**.io  
building software with ease

# Module Management: JupyterHub

**Preload** modules before spawning a notebook



Simple Advanced

Preset:   ...

Partition (-p, --partition): default

Nodelist (-w, --nodelist): no specific nodes

Nodes (-N, --nodes): 1

Number of tasks (-n, --tasks): 1

CPUs per task (-c, --cpus-per-task): 1

Generic resources (-gres): no generic resources

Memory per CPU (-mem-per-cpu): 1000

Runtime (-t, --time): 8:00:00

Reservation (-reservation): no reservation

Project (-A, --account): default

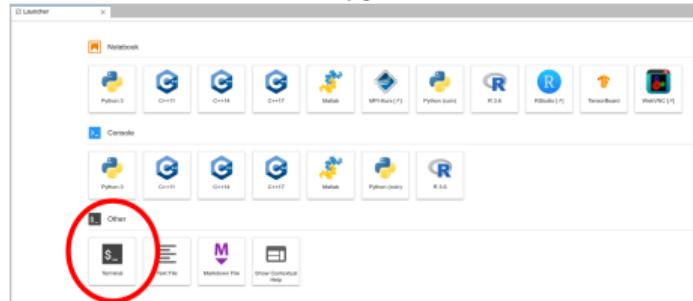
Preload modules (module load):

Standard environment (package list): production

Launch application: JupyterLab

Workspace scope (-NotebookApp.notebook\_dir): default (your home directory)

After spawning (without preloading modules), loading modules in the JupyterHub terminal **doesn't** make them available inside Jupyter Notebook



# Module Management: CLI

After allocating resources, setting up your software can be done using following module commands:

Command	Description
<code>module avail/spider &lt;your software&gt;</code>	Find required software
<code>module show &lt;module name&gt;</code>	Show additional module information
<code>module load &lt;module name&gt;</code>	Load module
<code>module list</code>	List all loaded modules
<code>module rm &lt;module name&gt;</code>	Unload module
<code>module purge</code>	Unload all module
<code>module save</code>	Save modules for next login

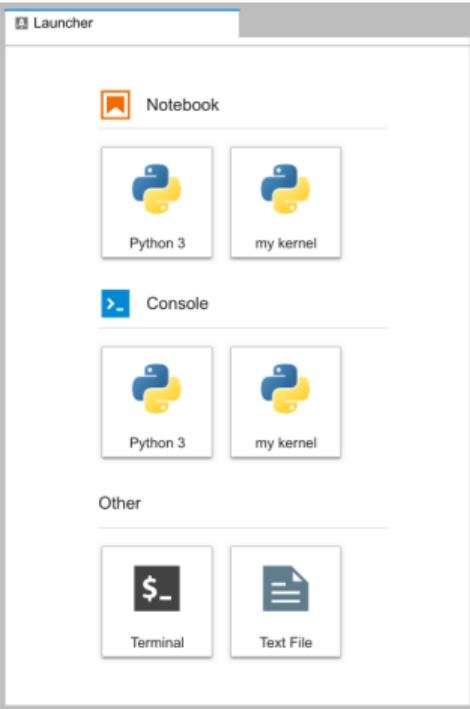
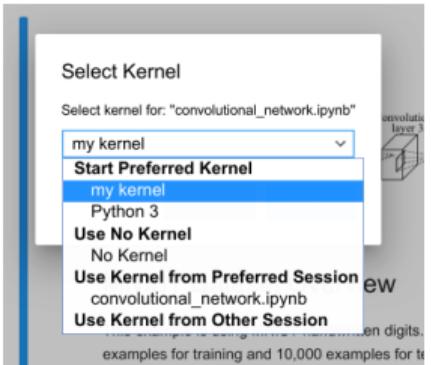
## Example

```
1 marie@compute$ module load modenv/hiera GCC/10.2.0 CUDA/11.1.1 OpenMPI/4.0.5 PyTorch/1.9.0
   tqdm/4.56.2 matplotlib/3.3.3
2
3 marie@compute$ module list
```

# Custom Jupyter Kernel

Allows you to install your own preferred Python packages and use them in your notebooks.

- You can switch kernels of existing notebooks in the menu
- Your kernels are listed on the launcher page



## Hint

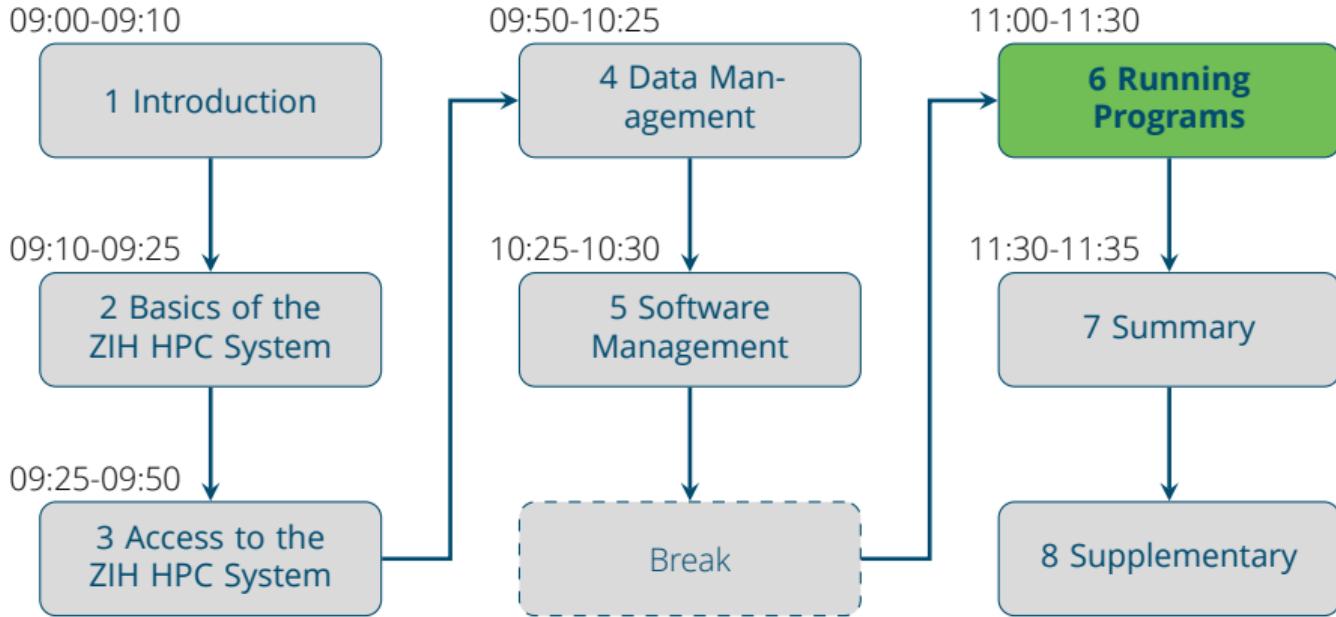
To create and use your own kernel, see here: [↗](#) and [↗](#)

# Python Virtual Environment + Kernel

- Virtual environments are isolated run-time environments and allow users to install additional Python packages
- For managing virtual environments on the ZIH HPC system, `virtualenv` is preferred to be used, which is a part of the Python modules

## Example

```
1 # Load default Python
2 marie@compute$ module load Python
3
4 # Install virtual environment
5 marie@compute$ virtualenv --system-site-packages /path/to/desired/location/my-env
6
7 # Activate the virtual environment
8 marie@compute$ source /path/to/desired/location/my-env/bin/activate
9
10 # User can now install additional packages using pip command
11 (env) marie@compute$ pip install -r requirements.txt
12
13 # register and name your kernel
14 (env) marie@compute$ pip install ipykernel
15 (env) marie@compute$ python -m ipykernel install --user --name my-env --display-name="my kernel"
```



# Workload Management System

- User-defined calculations, programs etc. are **not run directly** and **interactively** on an HPC system (as commonly on a personal workstation or laptop)
- Running some program on an HPC machine means running it within a **temporary resource allocation**
- The definition of a program and a resource allocation is a **job**

## Note

Most crucial issue esp. for HPC beginners: You need to specify in advance compute, memory, and time resources according to your program's needs. We will refer to this later.

- On the ZIH system: job scheduling and workload management with **slurm**
  - ▶ **Manages** jobs and provides an **interface** for the users to submit their jobs
  - ▶ **Evaluates** resource requirements and **priorities**, **distributes** jobs to suitable compute nodes -> "job queue"



More details about job schedulers can be found at: [https://hpc-wiki.info/hpc/Scheduling\\_Basics](https://hpc-wiki.info/hpc/Scheduling_Basics)

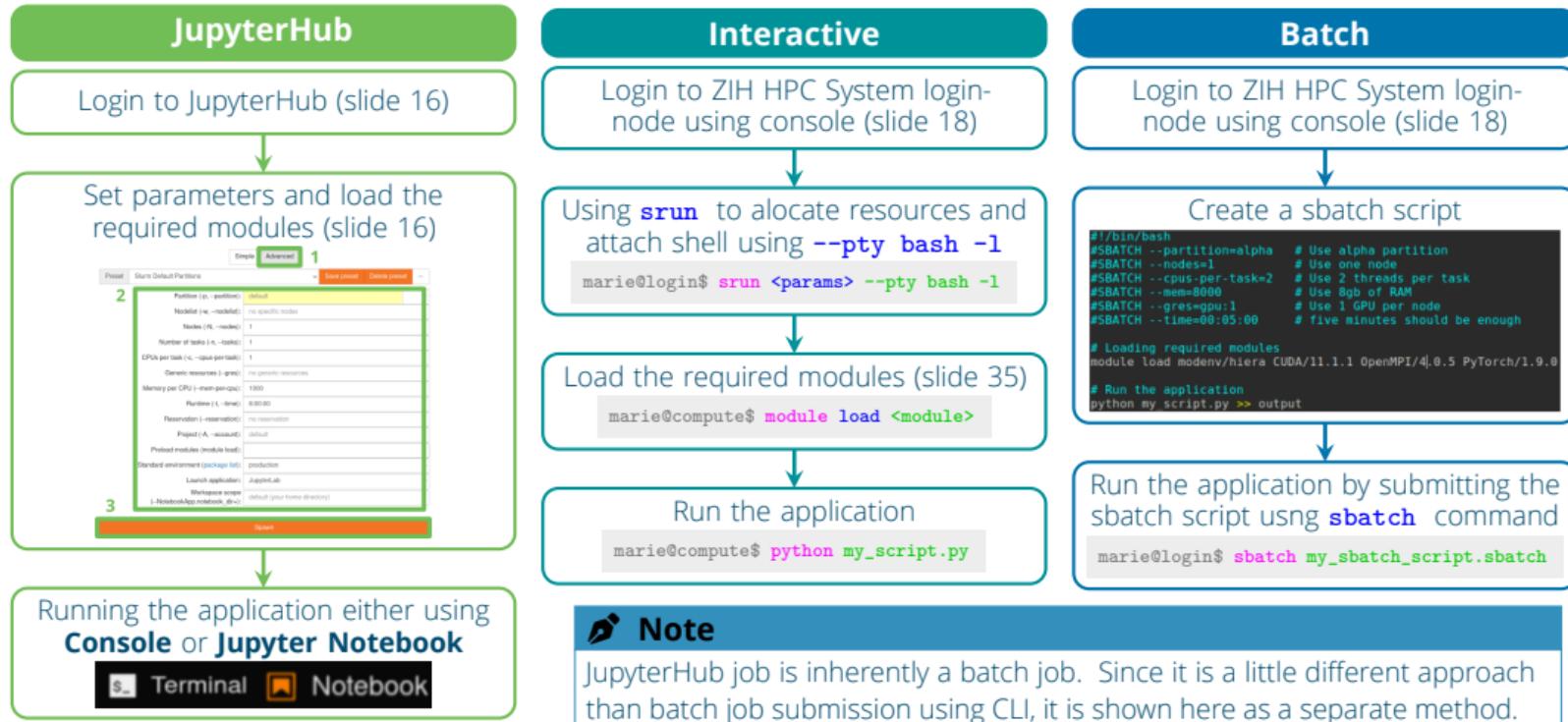
# Job Scheduler Basics: Slurm

- Some basic commands used to manage Slurm jobs

Type	Command	Description
Job submission	<code>srun &lt;params&gt; &lt;command-to-run&gt;</code>	Allocate resources and execute an application (interactive)
	<code>sbatch &lt;params&gt; &lt;command-to-run&gt;</code>	Run a command, script etc. with dedicated hardware resources (non-interactive)
Job management	<code>scancel &lt;jobid&gt;</code>	Cancel job
	<code>squeue --me</code>	List own jobs in queue and retrieve jobid
	<code>whypending &lt;jobid&gt;</code>	Get info why a job has not started yet
	<code>sinfo &lt;params&gt;</code>	View information about nodes and partitions

- Hardware limits can be found at: [🔗](#)
- More slurm parameters can be found at: [🔗](#)
- Additional commands in the docs can be found at: [🔗](#)

# Job Scheduler Basics: Running Jobs



# Slurm Parameters: Example

- Source code is stored in <workspace-full-path>/myscript.py
- alpha partition: `--partition=alpha`
- one node (no distributed application): `--nodes=1`
- two CPUs for preprocessing: `--cpus-per-task=2`
- 8GB memory for the data: `--mem=8000`
- one GPU : `--gres=gpu:1`
- run the job for 1 hr: `--time=01:00:00`
- account: `--account=p_scads_trainings` (only for this login)
- reservation: `--reservation=p_scads_trainings_1149` (only for today)

## Hint

- Typically, the most crucial parameters are `--gres` , `--cpus-per-task` , `--mem` , `--time` .
- Choosing the right parameters needs application-specific knowledge and experience.
- For more insights on resources use the performance monitoring tool PIKA (see slide 53).

# Slurm Parameters: JupyterHub

- Many slurm parameters are usable directly in the JupyterHub GUI (“Advanced” mode)
- Access overview is provided on slide 16.
- Note the choice of Standard environment and workspace option.
- Once the the JupyterHub is spawned, open **your-script.ipynb** notebook execute the code in it.

**Spawner Options**

Very important!  
If you have finished your work please explicitly stop your server.

DCV problem (SOLVED)  
Now that we have also rebooted the JupyterHub server, everything is working as usual again.

Simple Advanced

Preset Save preset Delete preset

Partition (-p, --partition):	haswell
Nodelist (-w, --nodelist):	no specific nodes
Nodes (-N, --nodes):	1
Number of tasks (-n, --tasks):	1
CPUs per task (-c, --cpus-per-task):	1
Generic resources (-gres):	no generic resources
Memory per CPU (-mem-per-cpu):	2583
Runtime (-t, --time):	8:00:00
Reservation (-r, --reservation):	no reservation
Project (-A, --account):	default
Preload modules (-m, --load):	
Standard environment (package list):	production
Launch application:	JupyterLab
Workspace scope (-NotebookApp.notebook_dir):	default (your home direc

Spawn

# Slurm Parameters: Interactive Job

## Example

```
1 # Allocate resources via slurm and run a bash interactively (--pty)
2 marie@login$ srun --nodes=1 --partition=compute --gres=gpu:1 --cpus-per-task=2 --mem=8000 --time=
   01:00:00 --account=p_scads_trainings --reservation=p_scads_trainings_1149 --pty bash -l
3
4 # Now, within our temporary resource allocation, we run our interactive job
5 # [..do what you want and use the resources...]
6
7 marie@compute$ module load modenv/hiera GCC/10.2.0 CUDA/11.1.1 OpenMPI/4.0.5 PyTorch/1.10.0
   tqdm/4.56.2
8
9 marie@compute$ cd /beegfs/ws/1/marie-myworkspace/src
10
11 marie@compute$ python myscript.py
```

# Slurm Parameters: Batch Job

Create the a batch script (`myscript.sbatch`) with the any editor:

## Example

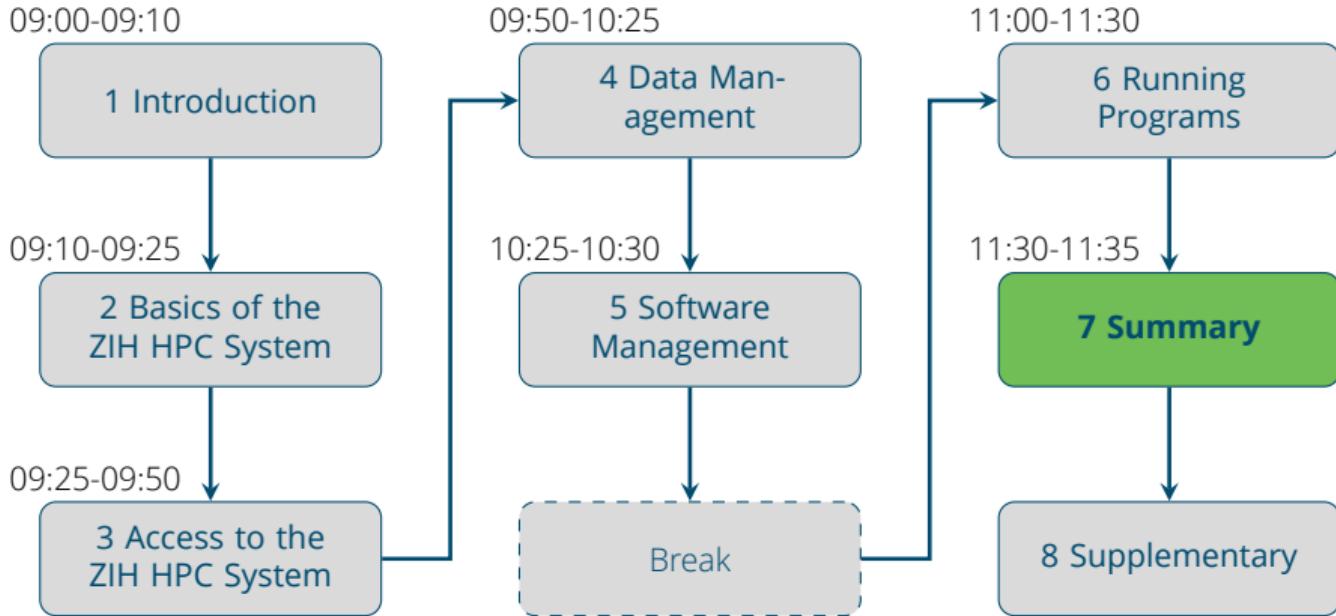
```
1 #!/bin/bash
2 #SBATCH --job-name=example
3 #SBATCH --nodes=1          # Number of nodes
4 #SBATCH --ntasks=1         # Run on a single CPU
5 #SBATCH --cpus-per-task=2  # use 2 threads per task
6 #SBATCH --gres=gpu:1       # 1 GPU per node
7 #SBATCH --time=0-00:05:00   # d-hh:mm:ss
8 #SBATCH --partition=alpha   # use alpha partition
9 #SBATCH --mem=2GB          # Memory per node
10 #SBATCH --output=%j.out     # Standard output and error log
11 #SBATCH --reservation=p_scads_trainings_1149
12 #SBATCH --account=p_scads_trainings
13
14 # From here code is executed line by line
15
16 module load modenv/hiera GCC/10.2.0 CUDA/11.1.1 OpenMPI/4.0.5 PyTorch/1.10.0 tqdm/4.56.2
17 cd /beegfs/ws/1/marie-myworkspace/src
18 python myscript.py
```

# Slurm Parameters: Batch Job

Run batch job files using command: `sbatch <jobfile>`

## Example

```
1 # run sbatch job file via sbatch command and retrieve the job id
2 marie@login$ sbatch myscript.sbatch
3 Submitted batch job 20815837
4 #show status of submitted job
5 marie@login$ squeue --me
```



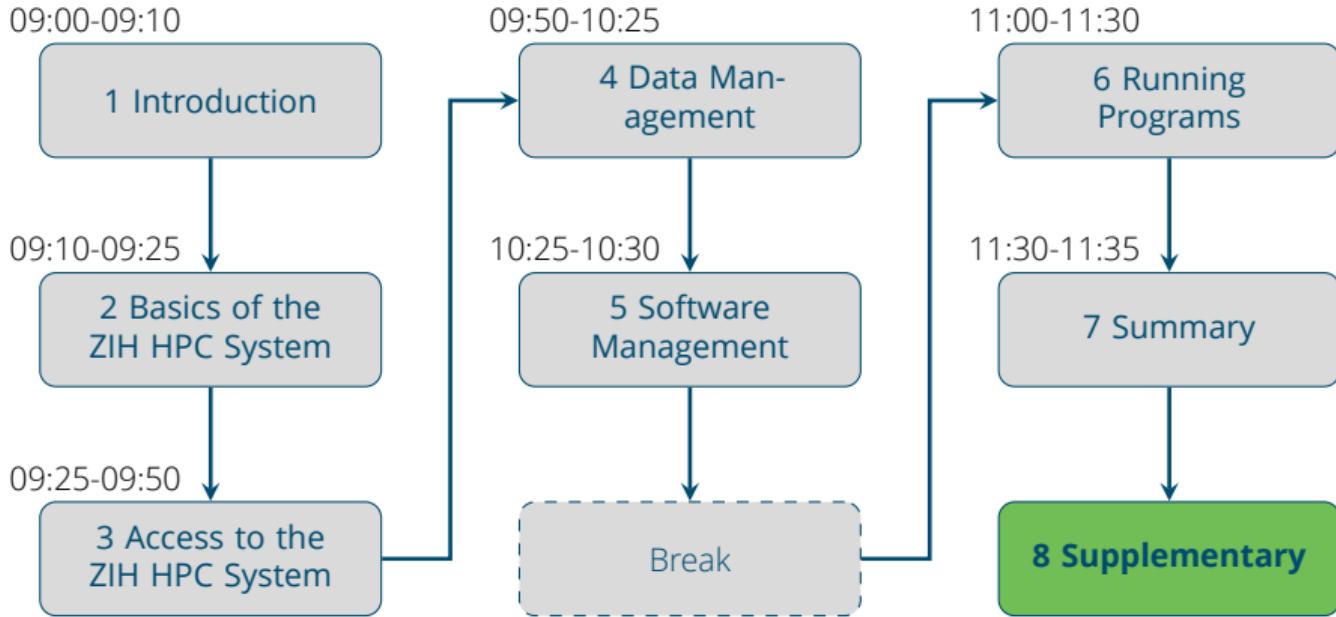
# 7 Summary

- There are three ways to work on HPC: JupyterHub, interactive, non-interactive.
- Do not use too much resources, **make resources free after you are done.**
- For more details read <https://doc.zih.tu-dresden.de/>
- Contact us with your own ideas, experiences and wishes!
- For getting support, esp. on ML, contact our ScaDS.AI service center <https://scads.ai/>.
- Logins (scads0xx) will work next 9 days, afterwards please apply for your own HPC project



Enjoy HPC!

Contact us on:  
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apurv.kulkarni@tu-dresden.de



# Basics: General terms

- **Secure shell (SSH)**: is a cryptographic network protocol
- **Integrated development environment (IDE)**: software application with comprehensive facilities for software development
- **Command-line interface (CLI)**: processes commands to a computer in the form of lines of text
- **Terminal, Bash, shell**: often used as synonym for CLI (esp. on Linux systems)



```

#PBS -l walltime=00:00:00
#PBS -l nodes=1:ppn=1
#PBS -l mem=8GB
#PBS -l scratch=10GB
#PBS -l vmem=8GB
#PBS -l gpus=1
#PBS -l walltime=00:05:00

#PBS -N myjob
#PBS -o myjob.out
#PBS -e myjob.err

cd /path/to/working/directory

# Run your job here
./myjob

```

Detailed description: A terminal window showing a PBS (Portable Batch System) script. The script defines resource requirements (nodes, memory, scratch space, GPUs, walltime), names the job, specifies output and error files, and changes to a working directory before running a command.

```

#!/bin/bash
#SBATCH --partition=alpha          # use alpha partition
#SBATCH --nodes=1                  # use one node
#SBATCH --ntasks=1                 # use one task per node
#SBATCH --mem=8000                # use 8GB of RAM
#SBATCH --gres=gpu:1              # use 1 GPU per node
#SBATCH --time=00:05:00            # five minutes should be enough

#A few lines of code are executed here
module load modernera GCC/10.2.0 CUDA/11.1.1 OpenMPI/4.0.5 PyTorch/1.9.0 tpm4/5.6.2
cd /scratch/username/job_id
python predict_text.py "the sun shone in the sky." >> fairytale

```

Detailed description: A terminal window showing a bash script being run. It includes a shebang line, module loading, a working directory change, and a python command with redirection.

# Basic CLI Commands

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

# Performance Analysis - Overview

- Performance analysis: basis for optimizing parallel programs on HPC w.r.t. run-time and efficiency
- challenging task for complex applications
- analysis of an application: collecting relevant information at runtime
- different approaches to collect info:
  - ▶ easiest way: simple monitoring of CPU/GPU processes and e.g. RAM (simple tools on OS level).
  - ▶ advanced possibilities: using advanced tools level for tracing and profiling (e.g. analysis with Score-P)
- user-friendly starting point: simple monitoring using PIKA for answering questions as:
  - ▶ Are supposedly parallelized parts of the program actually executed in parallel?
  - ▶ Is the GPU actually used?

# Performance Analysis – Job Monitoring with PIKA

- Simple approach for overview and to check used resources for a job: PIKA (hardware performance monitoring stack)
- monitoring during and after runtime: access PIKA web interface at [https://selfservice.zih.tu-dresden.de/l/index.php/hpcportal/jobmonitoring/z../jobs\\_and\\_resources](https://selfservice.zih.tu-dresden.de/l/index.php/hpcportal/jobmonitoring/z../jobs_and_resources)

The screenshot shows the HPC-Portal homepage. At the top, there's a navigation bar with the TECHNISCHE UNIVERSITÄT DRESDEN logo and links like 'Startseite', 'ZIH', 'Self Service Portal', and 'HPC-Portal'. Below this is a sidebar titled 'SELF SERVICE PORTAL' with various menu items such as 'Startseite', 'Abmeldung von Web-Anwendungen (Shibboleth-Logout)', 'Universitätswohnen', 'Zugangsvoraussetzung', 'Coupon einlösen', 'Mein Profil', 'Passwortverwaltung', 'Zertifikats-Management', and 'Login Antrag'. The main content area has a title 'HPC-PORTAL' and a search bar with tabs for 'Live', 'Job', 'Footprint', and 'Search'. The 'Live' tab is circled in red. Below the search bar, it says 'Total jobs: 1' and shows a table with columns for 'Name' and 'Project'. The table contains one row with 'bash' and 'p\_scads'. At the bottom, it says 'Stand 29.10.2021 12:53'.

The screenshot shows a date range selector with a calendar view from '29/10/2021 19:08' to '29/10/2021 18:48'. Below the calendar is a dropdown menu with options: 'Last hour', 'Last day', 'Last week', 'Last month', 'Last year', 'Last record', and 'All records'. The 'Last hour' option is currently selected.

Choose between "Live" (for running jobs) and "Jobs" (finished jobs with filtering by date/time if needed)

## Hint

More info about PIKA at: [↗](#)

# Available Resources on ZIH System

## General partitions:

- **romeo**: 192 nodes, 128 cores, 512GB RAM, 200GB /tmp
- **haswell**: 1456 nodes, 24 cores, 64/128/256GB RAM, 128GB /tmp
- **julia**: 1 node, 896 cores, 47TB RAM

## Machine Learning:

- **alpha**: 32 nodes, 48 cores, 1TB RAM, 3.5TB /tmp, 8x Nvidia A100-SXM4
- **ml**: 32 nodes, 44 cores IBM Power9, 256GB RAM, 6x Nvidia Volta V100

### 💡 Hint

There are some more partitions available. More info at: [!\[\]\(0d02338139225ba9482f9993590abfbe\_img.jpg\)](#)

# Workflow: Using git

Git is a version-control system, commonly used for managing source code and coordinating the work of multiple contributors on a software project.

Please consider the following basics while using git on the ZIH system:

- git is available on all cluster nodes
- can be used on HPC in the same way as in the shell of your local machine, e. g. `git clone`, `git add`, `git commit`, `git push` etc.
- every project collaborator is working on his own copy and changes are pushed to the remote repository
- no binary files are contained in the repo (this keeps the storage requirement low)
- cloned repo copies are located in user space



Using the same repo copy for different users will cause permission and access issues - DON'T DO THAT.

# Workflow: Using your favorite IDE

Instead of using the personal favorite IDE<sup>1</sup> (e.g. Eclipse, Code::Blocks, PyCharm, VisualStudio etc.) on an HPC system editors as vi or vim are available.

- Without establishing any SSH session, directories from the ZIH system can be mounted into the filesystem of the local machine with SSHFS:

## Example

```
1 marie@local$ sshfs <loginname>@taurus.hrsk.tu-dresden.de:</path/of/your/workspace/on/zihsystem/>
   </path/on/your/localmachine/> -o nonempty
```

- after calling SSHFS files are accessible from local file browsers and can be opened with your locally installed IDE

## Hint

For running source code on the ZIH system just open a CLI in an interactive session and execute the code there. Do not forget to save in your IDE and therewith writing changes to the ZIH filesystem.

<sup>1</sup>Integrated Development Environment