



INTERACTIVE HPC WITH JUPYTERLAB

Training Course – Welcome Day 2

2024-04-22..23 | JENS HENRIK GÖBBERT
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WELCOME

- Hello !
- Live document for this class
 - https://gitlab.jsc.fz-juelich.de/hedgedoc/3y3ppo_2Rq2ieO59LrBotg#
- Class repository
 - <https://gitlab.jsc.fz-juelich.de/jupyter4jsc/training-2024.04-jupyter4hpc>



Project training2412



Project title	Interactive High-Performance Computing with JupyterLab
Type	Computeproject
Principal Investigator	Jens Henrik Göbbert
Project Admin	Dr. Herwig Zilken
Project Mentor	Jens Henrik Göbbert
Start date	01.04.2024
End date	31.05.2024
Resource class	Training
Address	Forschungszentrum Jülich GmbH Wilhelm-Johnen-Straße 52428 Jülich Germany
Group name	training2412

As [PI](#) or [PA](#) of the project you are obliged to follow data protection regulations, in particular to maintain confidentiality. That means not to communicate or make data accessible to other persons without authorization by the data provider (even after the end of the project).

Active Budgets

Budget training2412 ?

JUSUF_CPU	Training fixed budget ⓘ	01.04.24–31.05.24
Total	<div><div></div></div> 64/30,000 core-h	
JUSUF_GPUS	Training fixed budget ⓘ	01.04.24–31.05.24
Total	<div><div></div></div> 0/30,000 core-h	

[Show extended statistics for PI/PAs](#)[Show extended statistics as SC Support](#)[Show extended statistics as Mentor](#)

The [jutil](#) tool on the systems can provide extended information about a budget.

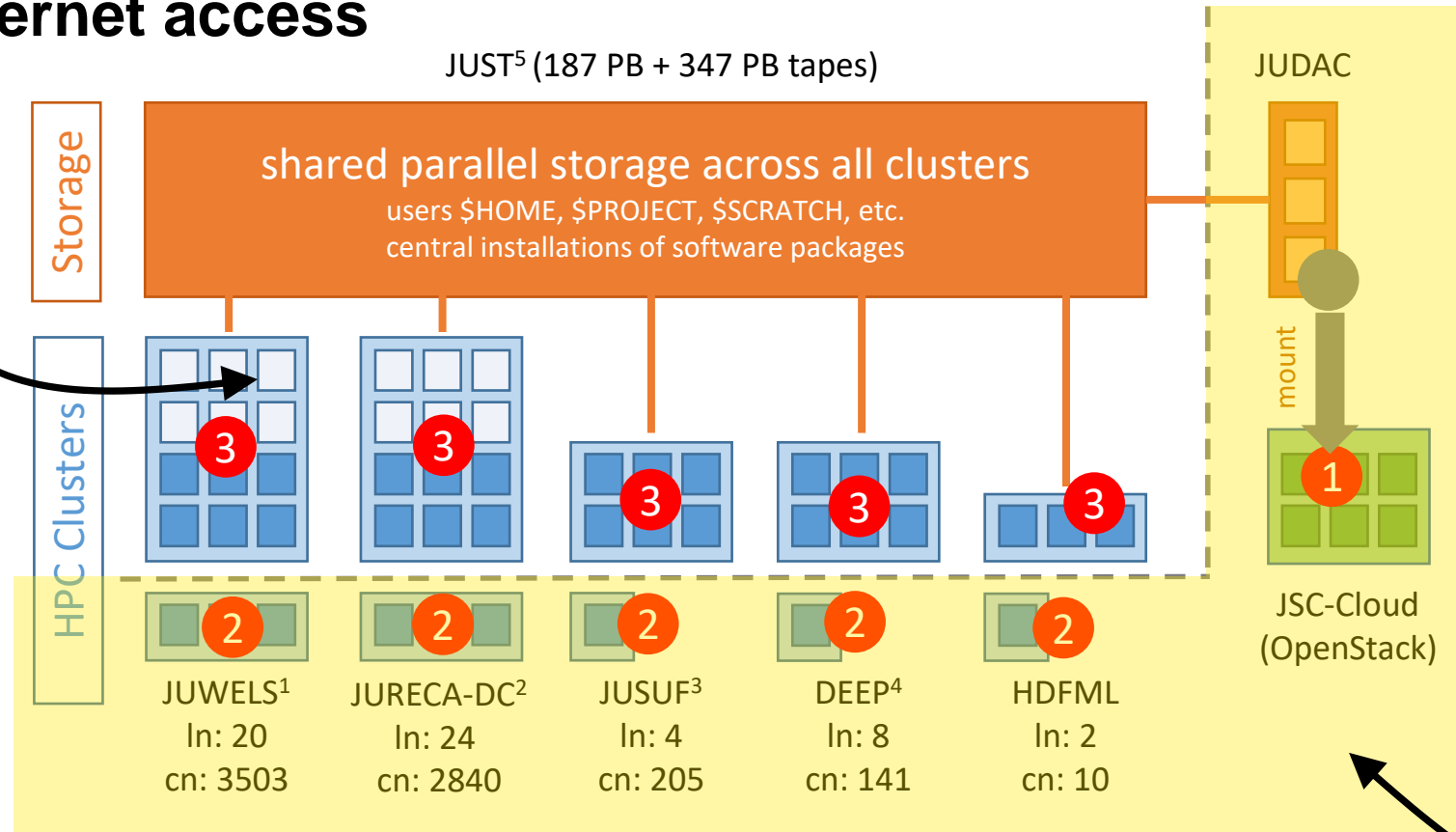
Storage Quota

Storage on just

scratch	<div><div></div></div> 0.00/90.00 TiB	<div><div></div></div> 1k/4,000k Inodes	08.04.24–31.05.24
project	<div><div></div></div> 0.00/14.90 TiB	<div><div></div></div> 27k/3,000k Inodes	08.04.24–31.05.24

JUPYTERLAB EVERYWHERE

NO internet access



no. login nodes = In
no. compute nodes = cn

[1] <https://apps.fz-juelich.de/jsc/hps/juwels/configuration.html>

[2] <https://apps.fz-juelich.de/jsc/hps/jureca/configuration.html>

[3] <https://apps.fz-juelich.de/jsc/hps/jusuf/configuration.html>

[4] https://www.fz-juelich.de/en/ias/jsc/systems/prototype-systems/deep_system

[5] <https://apps.fz-juelich.de/jsc/hps/just/configuration.html>

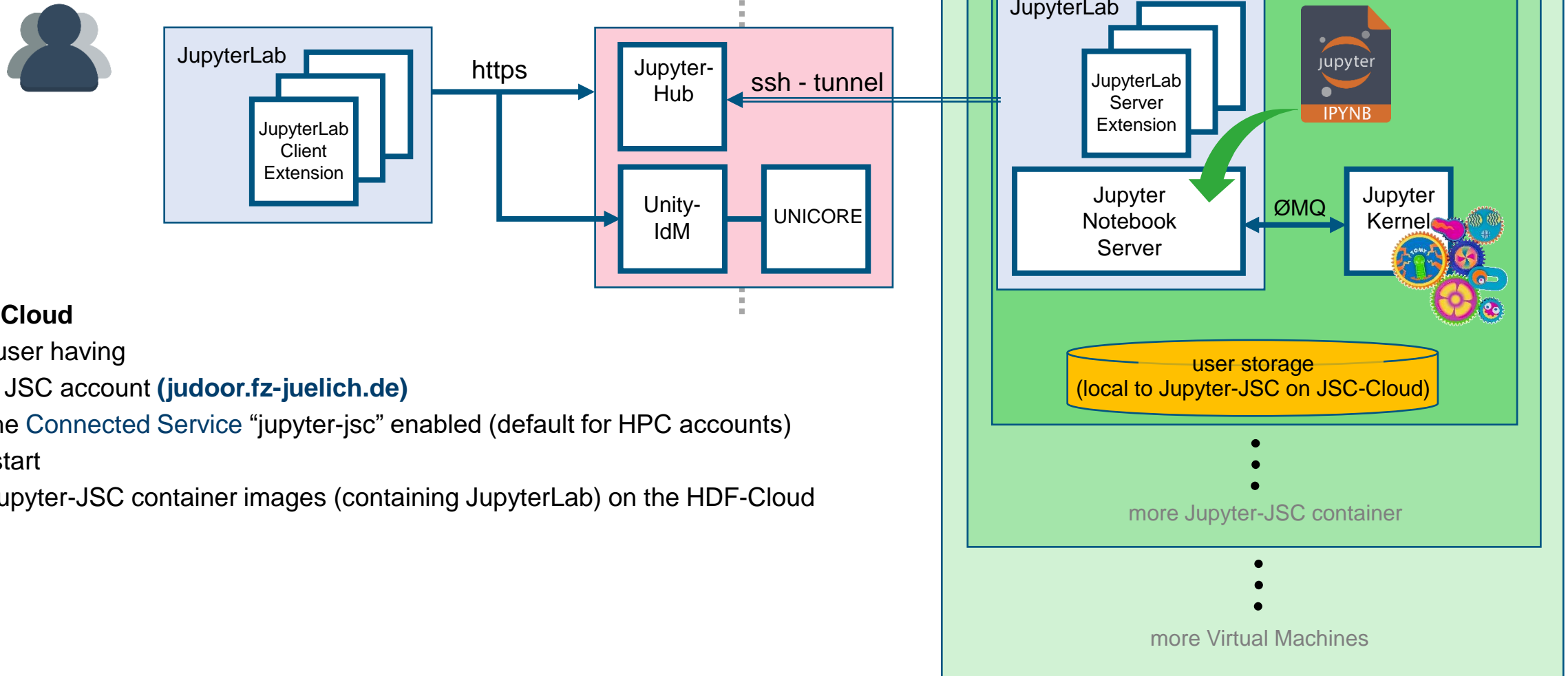
JupyterLab everywhere

- 1 JupyterLab on cloud
- 2 JupyterLab on login nodes
- 3 JupyterLab on compute nodes

internet access

JUPYTER-JSC WEBSERVICE

System: JSC-Cloud



JSC-Cloud

Any user having

- a JSC account (judoor.fz-juelich.de)
 - the [Connected Service](#) “jupyter-jsc” enabled (default for HPC accounts)
- can start
- Jupyter-JSC container images (containing JupyterLab) on the HDF-Cloud

JUPYTER-JSC WEBSERVICE

Start your JupyterLab

JÜLICH SUPERCOMPUTING CENTRE | JupyterLab JSC Status Documentation More Links

Your server is starting up...
You will be redirected automatically when it's ready for you.

Lab Info (click to expand)

2024-04-23 08:01:06:568: Sending request to Outpost service to start your service.
2024-04-23 08:01:06:645: Outpost communication successful.

Name	Configuration	Status	Actions
NEW JUPYTERLAB			
+			
✓ jusef_login_3.6	System JUSUF Partition LoginNode Project ccs4vs		Start
✓ jusef_3.6	System JUSUF Partition LoginNode Project ccs4vs		Start

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

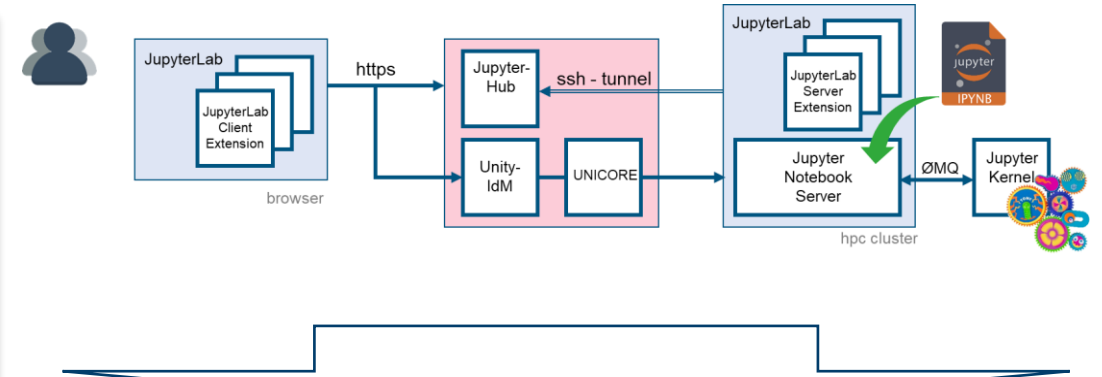
Jupyter-JSC
Supercomputing in Your Browser
Jupyter-JSC starts and provides access to your Jupyter Notebook servers running on JSC compute resources. These can be JUWELS, JURECA, JUSUF, HDFML or DEEP's login or compute nodes or even the HDF cloud - depending on the computing resources available to you.

Please use your JSC account to log in or register if you have not already done so. It's also possible to log in via Helmholtz AAI.

Log in Register

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HELMHOLTZ RESEARCH FOR GRAND CHALLENGES



GPU DASHBOARDS

- GPU Utilization
- GPU Memory
- GPU Resources
- PCIe Throughput
- WLink Throughput
- WLink Timeline
- Matching Resources

```
1 import math
2 import numpy as np
3 from numba import cuda
4 import numba.cuda.jit as jit
5 import sys
6
7 @jit(nopython=True)
8 def main():
9     # Run the simulation.
10     # 4 = 6.2 * 3.5, / size * 3
11     # 3 = 6.2 * 3.5, / size * 3
12     # 4 = 6.2 * 3.5, / size * 3
13     for i in range(1000000):
14         # ...
```

GPU Memory 332.48 MB

Variables

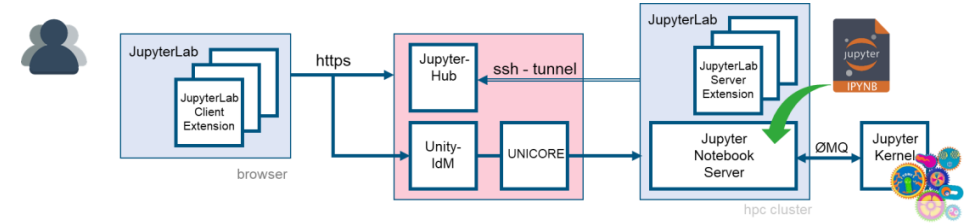
- math: module
- np: module
- cuda: module
- jit: module
- numba.cuda.compiler.Dispatcher
- size: 400
- iterations: 100
- my_numpy_array

Breakpoints

- hmp/jupyterlab_30146/402220956.py 4

JUPYTER-JSC WEBSERVICE

JupyterLab Configuration



Jupyter-JSC – Configuration

Available

- use
- sys
- CUR

Basic

Name	Configuration	Status	Actions
NEW JUPYTERLAB			
Lab Config	Name	jusuf_3.6	
Resources	Version	JupyterLab - 3.6	
Kernels and Extensions	System	JUSUF	
	Account	goebbert1	
	Project	training2412	
	Partition	batch	
	Reservation	None	
		None	
		jupyterlab-workshop-1	
▼ jusuf_3.6	System JUSUF	Partition LoginNode	Project training2412
		running	Logs
		Open	Stop

(this includes the decision for LoginNode and ComputeNode)

Extra options

- Partition == compute Resources
- Kernel and Extensions non-default JupyterKernel, Extensions, Proxies

Login Nodes
LoginNode
LoginNodeBooster
LoginNodeVis
Compute Nodes
batch
devel
develgpu
gpu
mem192

