



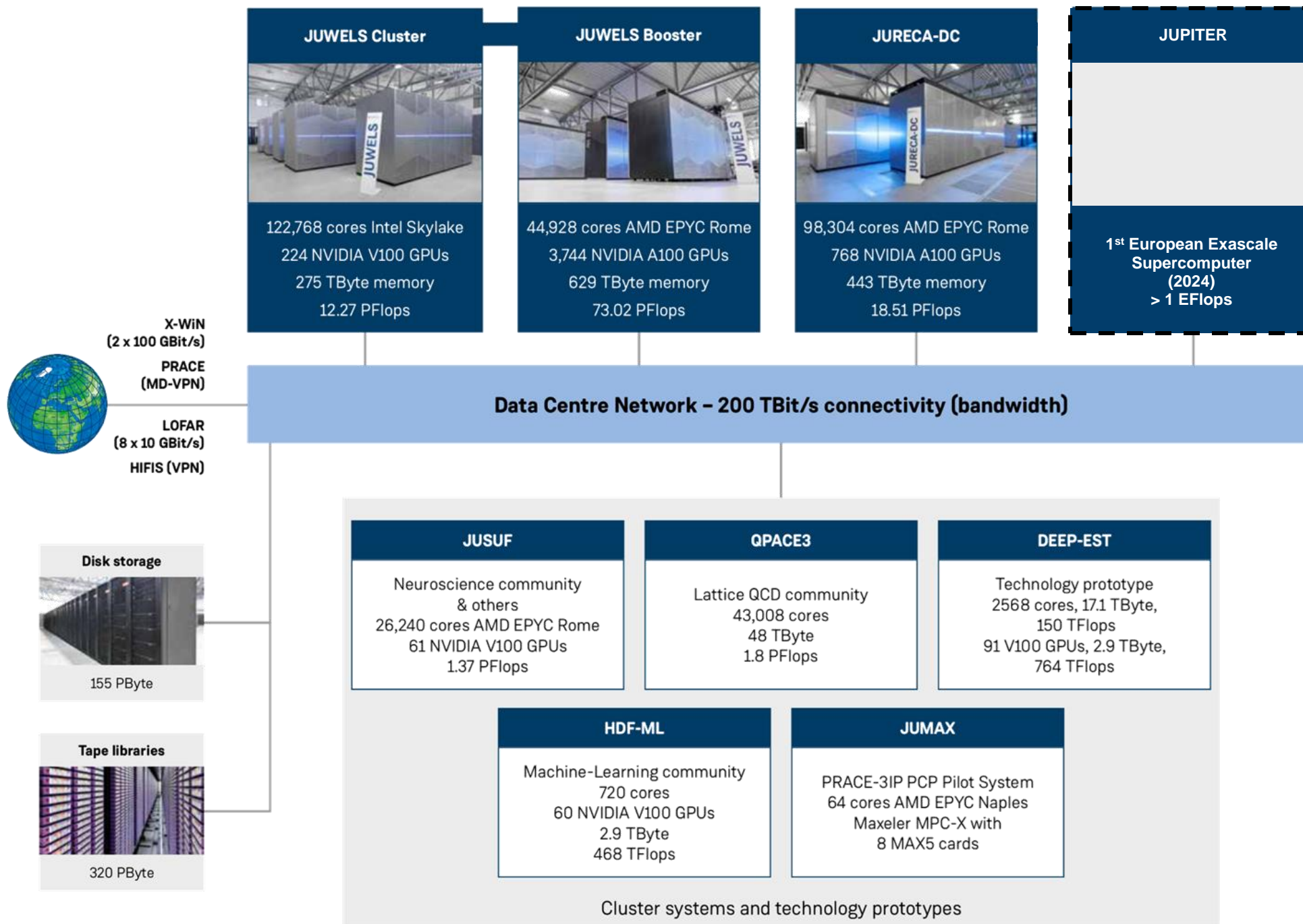
MATLAB FOR HPC AT JSC

On-boarding to the workshop

2023-11-06 | JENS HENRIK GÖBBERT (J.GOEBBERT@FZ-JUELICH.DE)

ON-BOARDING

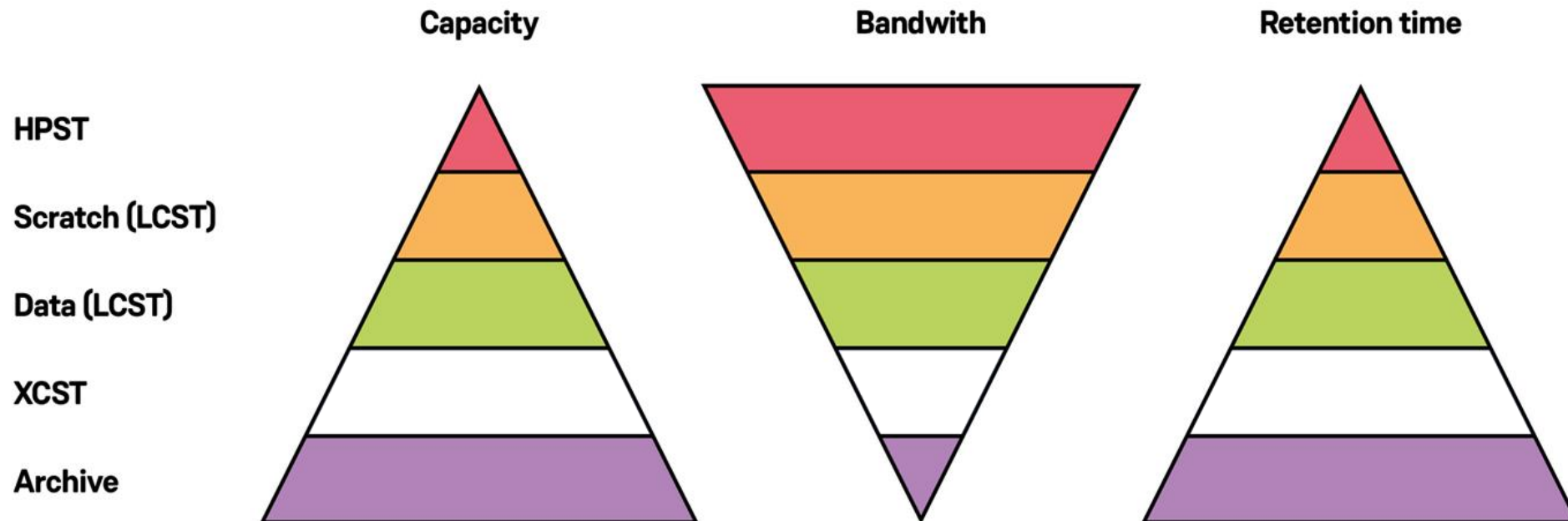
- Hello !
- Live document
 - <https://gitlab.jsc.fz-juelich.de/hedgedoc/krClbkrfRre-UaOX5V090g#>
- Slack channel
 - https://join.slack.com/t/matlabforhpc/shared_invite/zt-26e2ubbis-xHYoxSj0nsp6cKcOwjvNIA
- Access policy for MATLAB licenses at JSC
 - <https://www.fz-juelich.de/en/ias/jsc/services/user-support/software-tools/matlab>





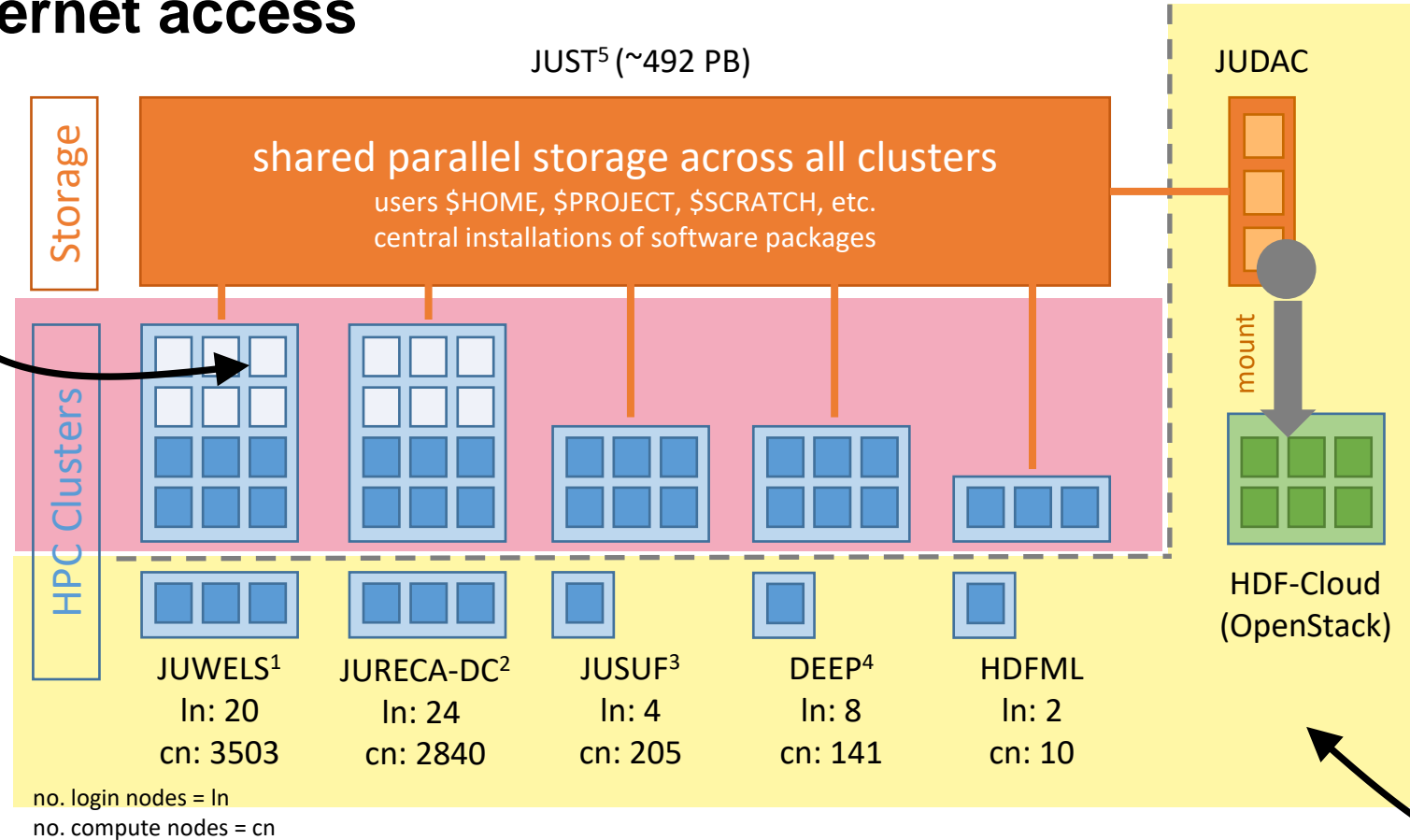
JUST (Juelich Storage cluster)

- One central storage infrastructure for HPC
- Total gross capacity
 - NVMe disks: ~2 PB
 - Spinning disks: ~180 PB
 - Tape: ~310 PB
- Software:
 - IBM Spectrum Scale
 - IBM Spectrum Protect
 - DDN Infinite Memory Engine
- **Project partners: DDN, IBM, Lenovo, ProCom**



SUMMARY – COMPUTE RESOURCES @ JSC

NO internet access



[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/cluster/configuration.html>

[4] https://www.fz-juelich.de/ias/jsc/EN/Expertise/Supercomputers/DEEP-EST/_node.html

[5] https://www.fz-juelich.de/ias/jsc/EN/Expertise/Datamanagement/OnlineStorage/JUST/Configuration/Configuration_node.html

ACCESS TO COMPUTE RESOURCES

1. REGISTER & LOGIN

PRE-ACCESS TODOS

1) Register & Login

- ✓ <https://judoor.fz-juelich.de>

2) Join the project „training2339“

- ✓ Wait to get joined by the project PI

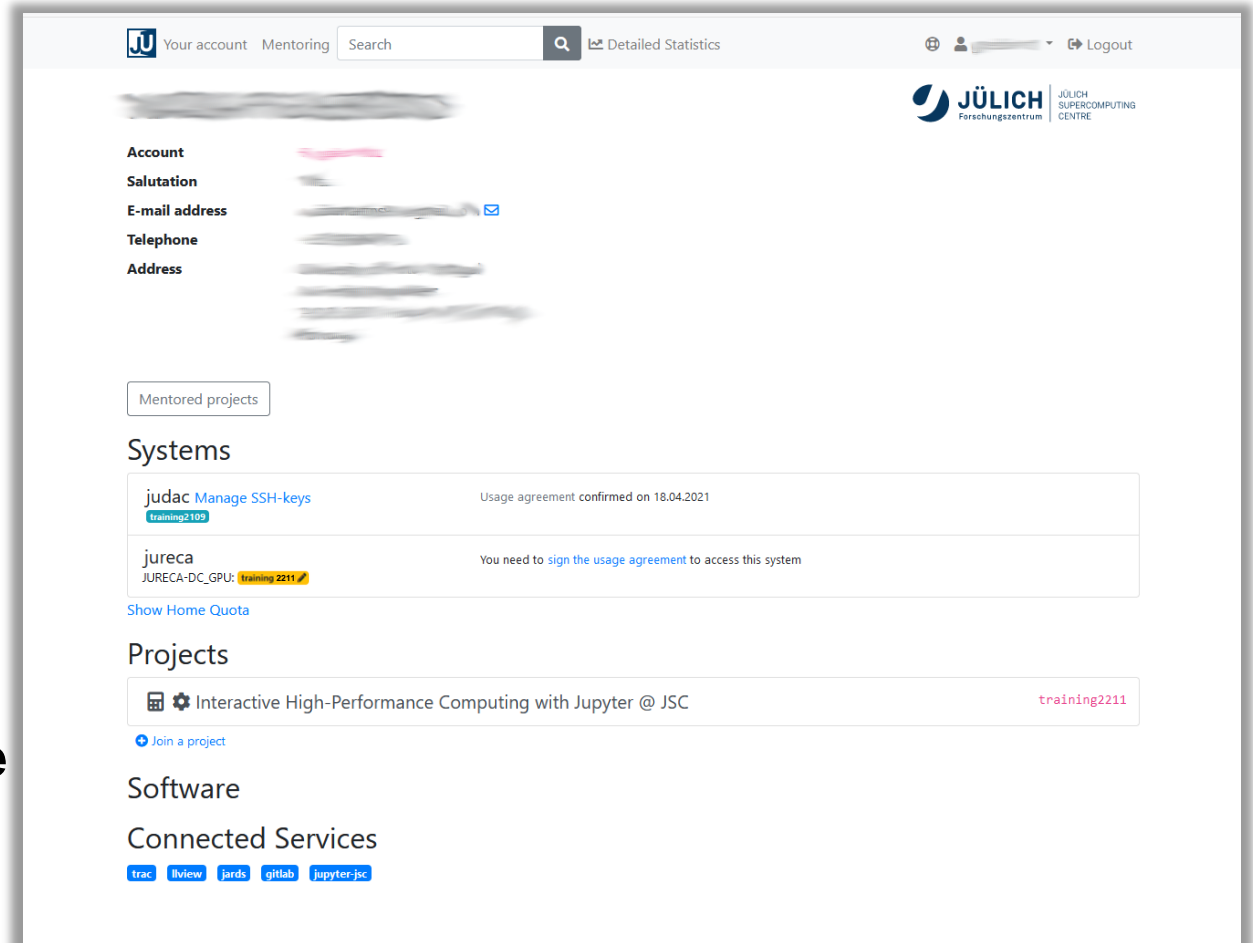
3) Sign usage agreement

- ✓ Wait for creation of HPC accounts

4) Request access to restricted software

- ✓ MATLAB

Waiting for access approval



For more details, please visit
<https://gitlab.jsc.fz-juelich.de/hedgedoc/krClbkrfRre-UaOX5V090g#Pre-Workshop-Todos>

PRE-ACCESS TODOS

1) I

2) v

3) s

4) l

<https://judoor.fz-juelich.de>



For more details

<https://gitlab.jsc.fz-juelich.de/hedgedoc/krClbkrfRre-UaOX5V090g#Pre-Workshop-Todos>

**ACCESS
TO COMPUTE RESOURCES**
2. JOIN THE PROJECT

PRE-ACCESS TODOS

1) Register & Login

- ✓ <https://judoor.fz-juelich.de>

2) Join the project „training2339“

- ✓ Wait to get joined by the project PI

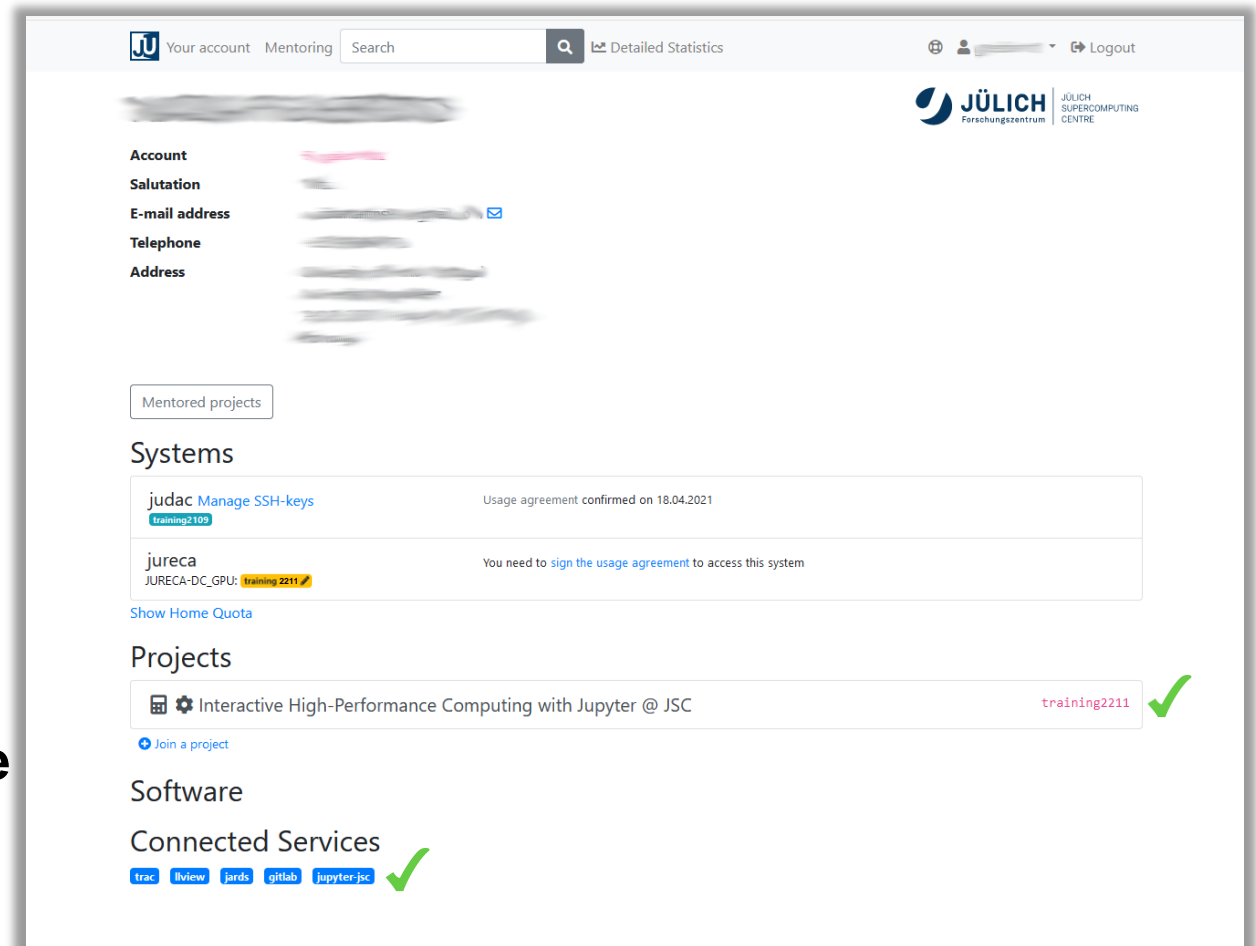
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PRE-ACCESS TODOS

1) I

2) J

3) S

4) I

<https://judoor.fz-juelich.de>

Project id =

„training2339“

For more de

<https://gitlab.jsc.fz-juelich.de/hedgedoc/krClbkrfRre-UaOX5V090g#Pre-Workshop-Todos>

PRE-ACCESS TODOS

1) Register & Login

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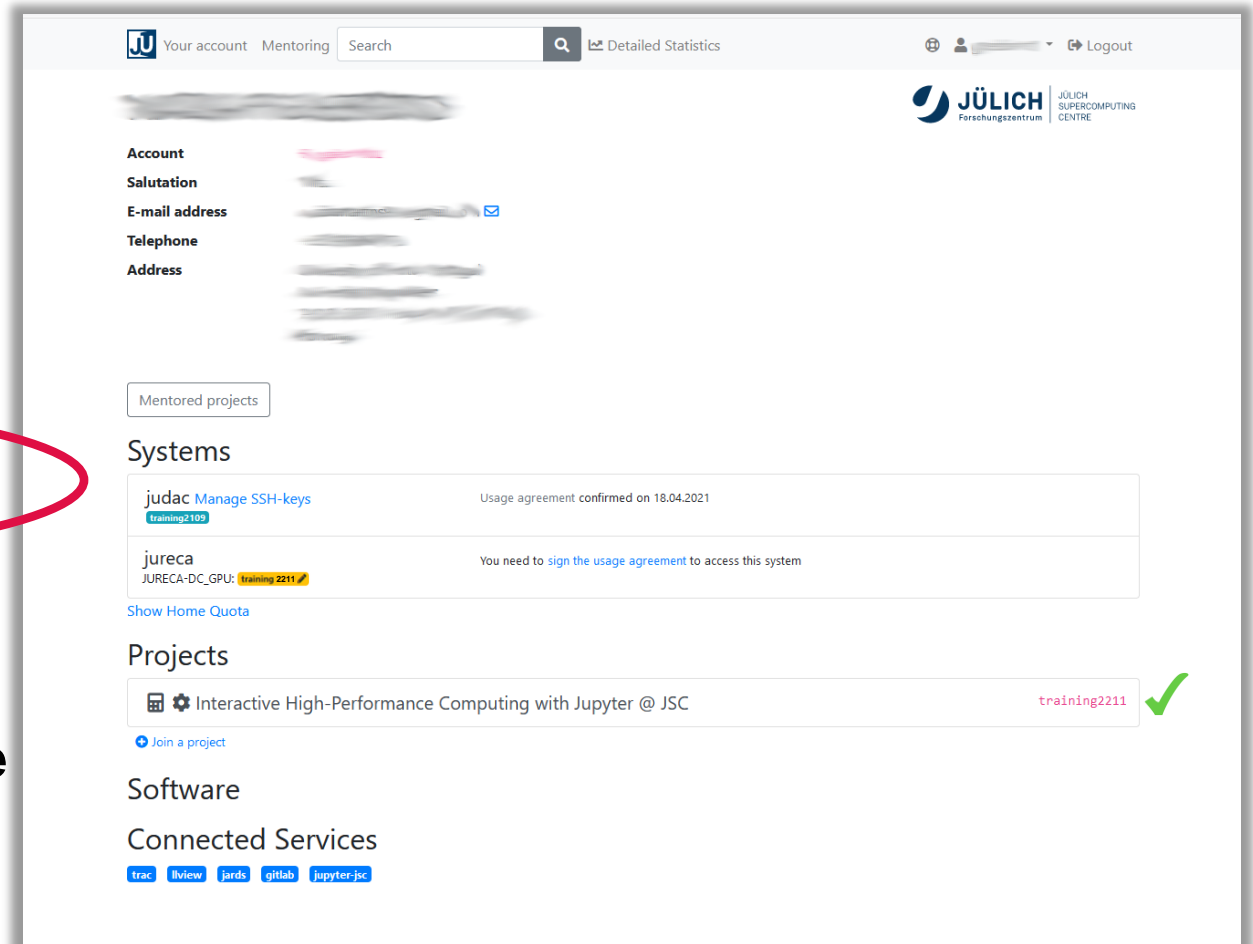
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Waiting for access approval



For more details, please visit
<https://gitlab.jsc.fz-juelich.de/hedgedoc/krClbkrfRre-UaOX5V090g#Pre-Workshop-Todos>

**ACCESS
TO COMPUTE RESOURCES
3. SIGN USAGE AGREEMENT**

PRE-ACCESS TODOS

1) Register & Login

- ✓ <https://judoor.fz-juelich.de>

2) Join the project „training2339“

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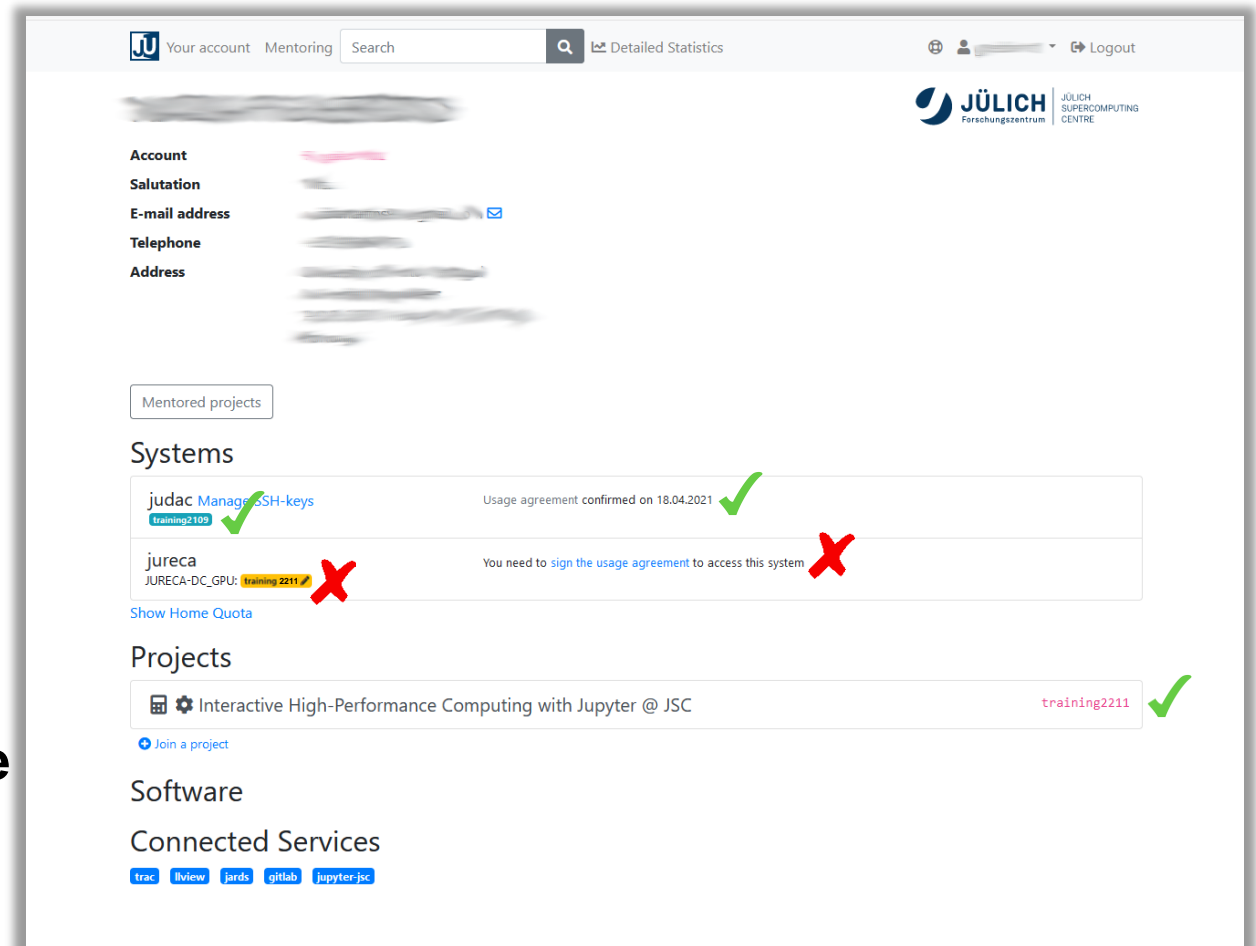
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For more details, please visit
https://gitlab.jsc.fz-juelich.de/hedgedoc/S46PXGluSiuMv1Vgw_UU_Q?view#Getting-Access

PRE-ACCESS TODOS

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<https://judoor.fz-juelich.de>

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For more details see
https://gitlab.jsc.fz-juelich.de/hedgedoc/S46PXGluSiuMv1Vgw_UU_Q?view#Getting-Access

PRE-ACCESS TODOS

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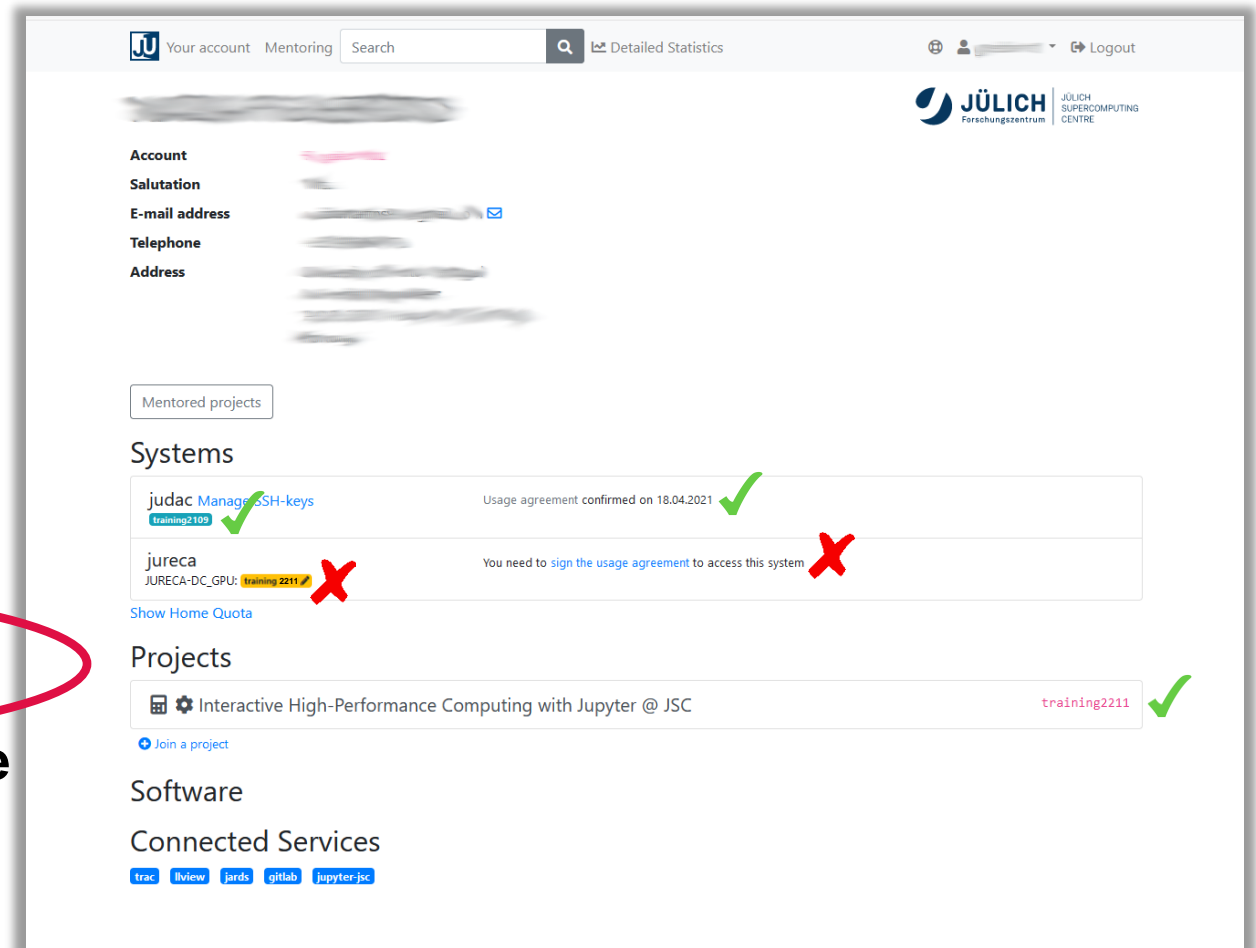
3) Sign usage agreement

- ✓ Wait for creation of HPC accounts

4) Request access to restricted software

- ✓ MATLAB

Waiting for access approval



For more details, please visit
https://gitlab.jsc.fz-juelich.de/hedgedoc/S46PXGluSiuMv1Vgw_UU_Q?view#Getting-Access

**ACCESS
TO COMPUTE RESOURCES**

4. REQUEST ACCESS TO RESTRICTED SOFTWARE

PRE-ACCESS TODOS

1) Register & Login

- ✓ <https://judoor.fz-juelich.de>

2) Join the project „training2339“

- ✓ Wait to get joined by the project PI

3) Sign usage agreement

- ✓ Wait for creation of HPC accounts

4) Request access to restricted software

- ✓ MATLAB

Waiting for access approval

The screenshot displays the 'Your account' page for 'Peter Supercomputing' at the Jülich Supercomputing Centre. The account details include the username 'supercomputing1', email 'peter.supercomputing@gmx.de', telephone '+49 2461 61 12345678', and address 'Juelich Supercomputing Centre Forschungszentrum Juelich GmbH, Wilhelm-Johnen-Str., 52425 Juelich, Germany'. The 'Systems' section lists 'judac' and 'juwels' with their respective usage agreements. The 'Projects' section shows 'MATLAB for HPC' and a 'Join a project' button. The 'Software' section has a yellow box highlighting the 'Request access to restricted software' button, with a yellow arrow pointing to it. The 'Connected Services' section lists 'trac', 'jards', 'gitlab', 'liview', and 'jupyter-js'. The footer contains links for 'Legal Notice', 'Privacy Policy', 'Forschungszentrum Jülich, JSC', 'Contact Support', and 'JuDoor Requests'.

For more details, please visit

https://gitlab.jsc.fz-juelich.de/hedgedoc/S46PXGluSiuMv1Vgw_UU_Q?view#Getting-Access

PRE-ACCESS TO DOCS

1) Reg



2) Join




3) Sign



4) Req




Wa

 Your account

supercomputing1 Logout

[Back to supercomputing1](#)

 JÜLICH SUPERCOMPUTING CENTRE

Software Access

Parts of the software at the supercomputers is only available via licenses or agreed service level agreements. Here you can get access to such software.

Access to licensed software

Select software for which you have a license. Deselect Software you don't want to use anymore.

- ☐ Dalton 2.0
- ☐ NAMD
- ☐ MOLPRO
- ☐ ADF_(2009.1b)
- ☐ AMBER
- ☐ CPMD
- ☐ UltraScan
- ☒ MATLAB


☒ I have been granted access to the HPC resources for the purpose of performing noncommercial academic research or teaching

[Send request](#)

Access to other restricted software


Container Runtime Engine


container


 JÜLICH Forschungszentrum

supercomputing1 Logout

[Back to supercomputing1](#)







training2339

Contact Support
JuDoor Requests

For more details, please visit
https://gitlab.jsc.fz-juelich.de/hedgedoc/S46PXGluSiuMv1Vgw_UU_Q?view#Getting-Access

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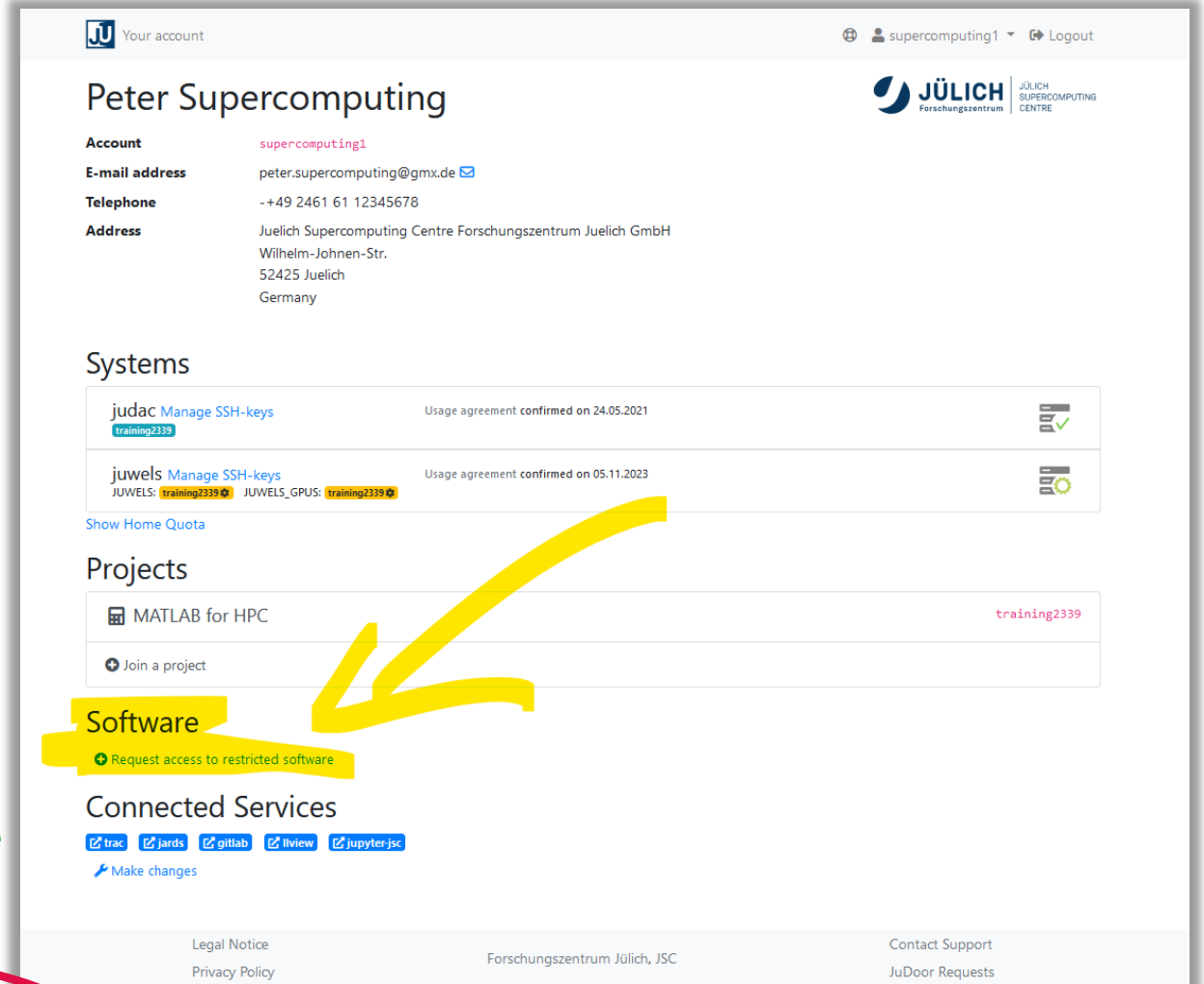
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For more details, please visit
https://gitlab.jsc.fz-juelich.de/hedgedoc/S46PXGluSiuMv1Vgw_UU_Q?view#Getting-Access

**ACCESS
TO COMPUTE RESOURCES
5. RESTER TO JUPYTER-JSC**

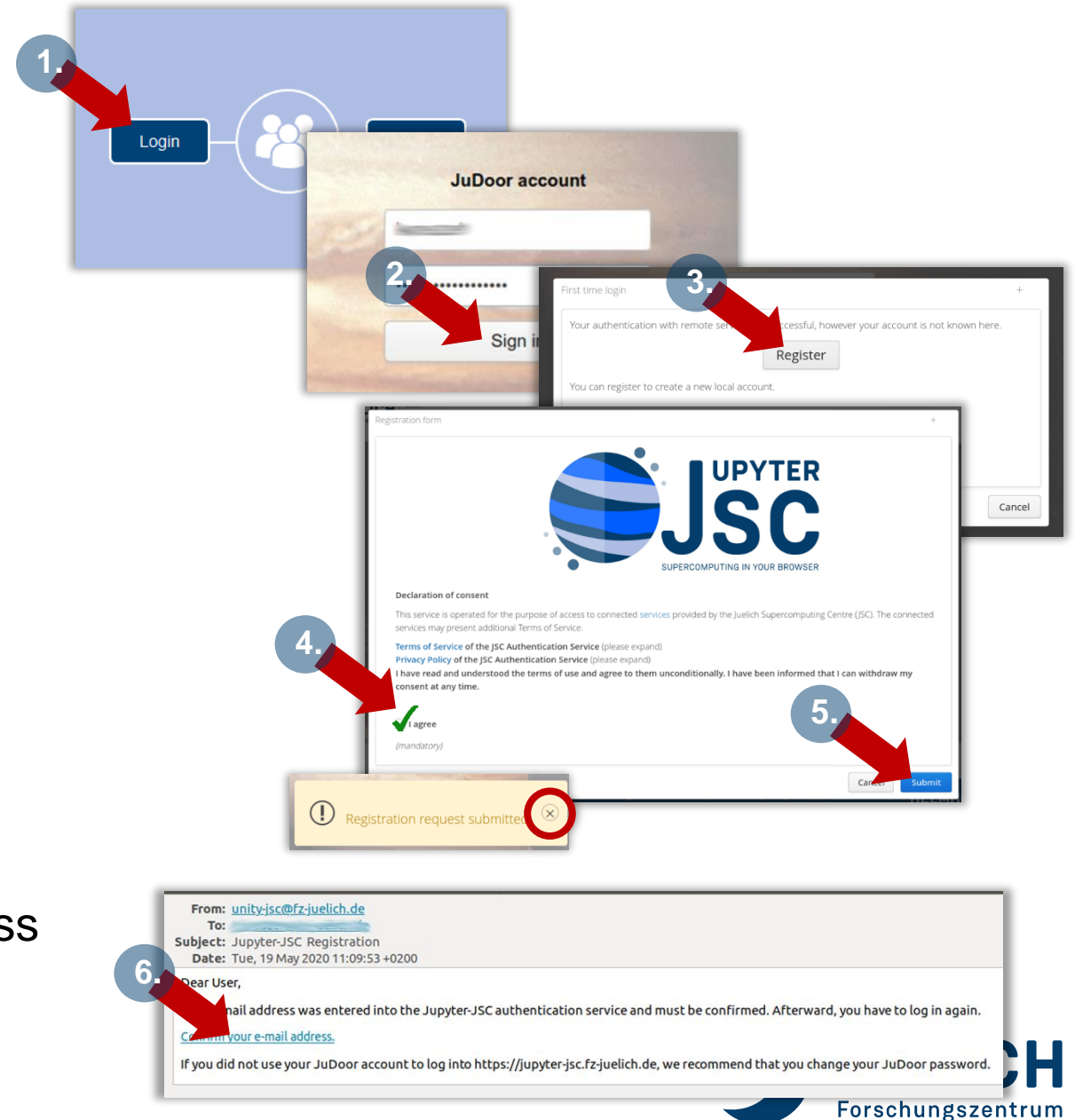
JUPYTER-JSC WEBSERVICE

First time login

=> <https://jupyter-jsc.fz-juelich.de>

Jupyter-JSC first time login

1. Login at <https://jupyter-jsc.fz-juelich.de>
2. Sign in with your JSC account
3. Register to Jupyter-JSC
4. Accept usage agreement
5. Submit the registration
6. Wait for email and confirm your email address



JUPYTER-JSC WEBSERVICE

First time

=> <https://jupyter-jsc.fz-juelich.de>

Jupyter

1. L

2. S

3. R

4. A

5. S

6. V

First check on
<https://judoor.fz-juelich.de>
if you are ready for Jupyter-JSC.

RECORDED WITH
SCREENCASTOMATIC

[Confirm your e-mail address.](#)

If you did not use your JuDoor account to log into <https://jupyter-jsc.fz-juelich.de>, we recommend that you change your JuDoor password.

**ACCESS
TO COMPUTE RESOURCES
5. START WEB-UI**

JUPYTER-JSC WEBSERVICE

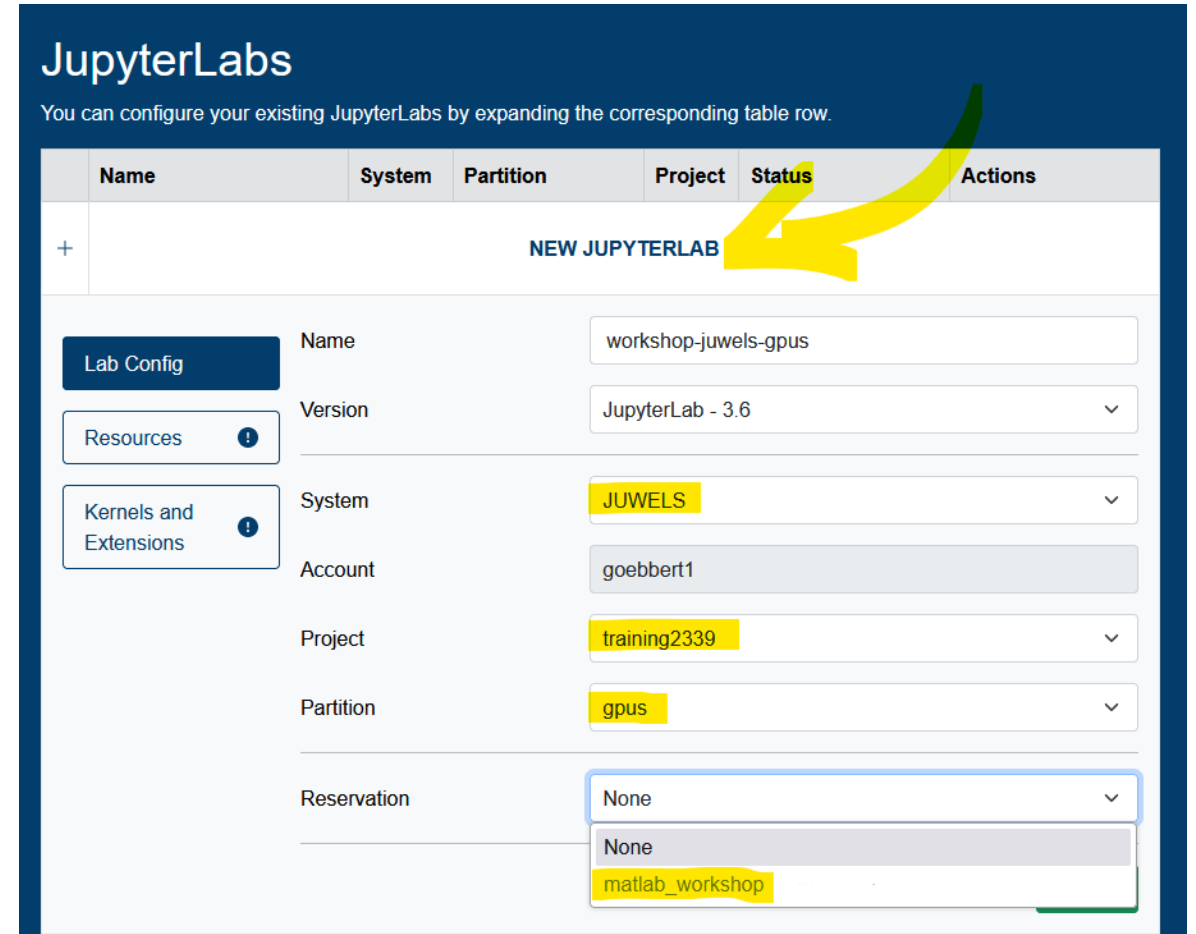
JupyterLab Configuration

Lab Config

- Version:
any name, e.g. "workshop-juwels"
- System:
JUWELS
- Account:
fixed
- Project:
training2339
- Partition:
gpu

Extra options

- Reservation
matlab_workshop



JupyterLabs

You can configure your existing JupyterLabs by expanding the corresponding table row.

Name	System	Partition	Project	Status	Actions
NEW JUPYTERLAB					

Lab Config

Resources ⓘ

Kernels and Extensions ⓘ

Name

workshop-juwels-gpus

Version

JupyterLab - 3.6

System

JUWELS

Account

goebbert1

Project

training2339

Partition

gpu

Reservation

None

None

matlab_workshop

JUPYTER-JSC WEBSERVICE

JupyterLab Configuration

Resources

- Nodes:
1
- GPUs:
4
- Runtime (minutes):
240

JupyterLabs

You can configure your existing JupyterLabs by expanding the corresponding table row.

Name	System	Partition	Project	Status	Actions
+ NEW JUPYTERLAB					
<div>Lab Config</div> <div>Resources</div> <div>Kernels and Extensions</div>		<div>Nodes [1,46] 1</div> <div>GPUs [1,4] 4</div> <div>Runtime (minutes) [10,1440] 240</div> <div>▶ Start</div>			

JUPYTER-JSC WEBSERVICE

Start your JupyterLab

The image shows three overlapping screenshots of the Jupyter-JSC web service interface. The top screenshot displays a 'Your server is starting up...' message with a table of server status. The middle screenshot shows the 'JupyterLabs' section with a '+ New' button and a table of existing labs. The bottom screenshot is the main landing page with a 'Supercomputing in Your Browser' banner and a list of available compute resources.

Name	System	Partition	Project	Status	Actions
juwels_cluster	JUWELS	devel	ccsys	76%	Cancel

Name	System	Partition	Project	Status	Actions
hdfcloud_3.3	HDF-Cloud	N/A	N/A		Start
juwelsbooster_login	JUWELS	LoginNodeBooster	ccstdf		Start
juwels_cluster	JUWELS	devel	ccsys	30%	Open Cancel

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.

Login Register

© Forschungszentrum Jülich Impressum Privacy Policy Support Terms of Service

HELMHOLTZ
RESEARCH FOR GRAND CHALLENGES

Your server is starting up...

You will be redirected automatically when it's ready for you.

Lab Info (click to expand)

95%

spawning...

Cancel

2023_11_05 23:07:36.365: Sending request to backend service to start your service.	+
2023_11_05 23:07:44.858: Backend communication successful.	+
2023_11_05 23:07:52.017: Your slurm job is currently in status PENDING.	+
2023_11_05 23:08:38.318: Setup ssh port-forwarding.	+
2023_11_05 23:08:38.794: Disk quota checked.	+
2023_11_05 23:08:38.960: Load default modules ...	+
2023_11_05 23:08:55.672: Load default modules done	+
2023_11_05 23:08:56.030: Add system specific configuration.	+
2023_11_05 23:08:59.732: Start JupyterLab	+

JUPYTER LAB WEBSERVICE

Start your

The screenshot displays the JupyterLab web interface. At the top, a menu bar includes 'File', 'Edit', 'View', 'Run', 'Kernel', 'Git', 'Tabs', 'Settings', and 'Help'. A status bar on the right shows 'Control Panel', 'CPU: 0%', 'Mem: 393 / 191580 MB', and a 'Launcher' tab. On the left, a sidebar contains 'FAVORITES' (with a '+' button circled in yellow), 'FILE BROWSER', and a list of files/directories. The main area is titled 'p/home/jusers/goebbert1' and shows a grid of application icons under the 'Notebook' section. A yellow arrow points from the 'FAVORITES' '+' button to the 'Open MATLAB' icon, which is also circled in yellow. Below the 'Notebook' section is a 'Console' section with another grid of icons. At the bottom, an 'Other' section (circled in yellow) contains icons for 'Terminal', 'LaTeX File', 'Text File', 'TypeScript File (Playground)', 'Markdown File', 'Julia File', and 'Python File'. The bottom status bar shows 'Simple', 'Mem: 360.07 / 191579.64 MB', and 'English (United States) Launcher'.