MATLAB FOR HPC AT JSC

On-boarding to the workshop

2023-11-06 I 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

https://jupyter.org

JUWELS Cluster

122,768 cores Intel Skylake
224 NVIDIA V100 GPUs
275 TByte memory
12.27 PFlops

JUWELS Booster

44,928 cores AMD EPYC Rome
3,744 NVIDIA A100 GPUs
629 TByte memory
73.02 PFlops

JURECA-DC

98,304 cores AMD EPYC Rome
768 NVIDIA A100 GPUs
443 TByte memory
18.51 PFlops

JUPITER

1st European Exascale Supercomputer
(2024)
> 1 EFlops

X-WiN
(2 x 100 GBit/s)

PRACE
(MD-VPN)

LOFAR
(8 x 10 GBit/s)

HIFIS (VPN)

Data Centre Network – 200 TBit/s connectivity (bandwidth)

Disk storage

155 PByte

Tape libraries

320 PByte

JUSUF

Neuroscience community
& others
26,240 cores AMD EPYC Rome
61 NVIDIA V100 GPUs
1.37 PFlops

QPACE3

Lattice QCD community
43,008 cores
48 TByte
1.8 PFlops

DEEP-EST

Technology prototype
2568 cores, 17.1 TByte,
150 TFlops
91 V100 GPUs, 2.9 TByte,
764 TFlops

HDF-ML

Machine-Learning community
720 cores
60 NVIDIA V100 GPUs
2.9 TByte
468 TFlops

JUMAX

PRACE-3IP PCP Pilot System
64 cores AMD EPYC Naples
Maxeler MPC-X with
8 MAX5 cards

Cluster systems and technology prototypes

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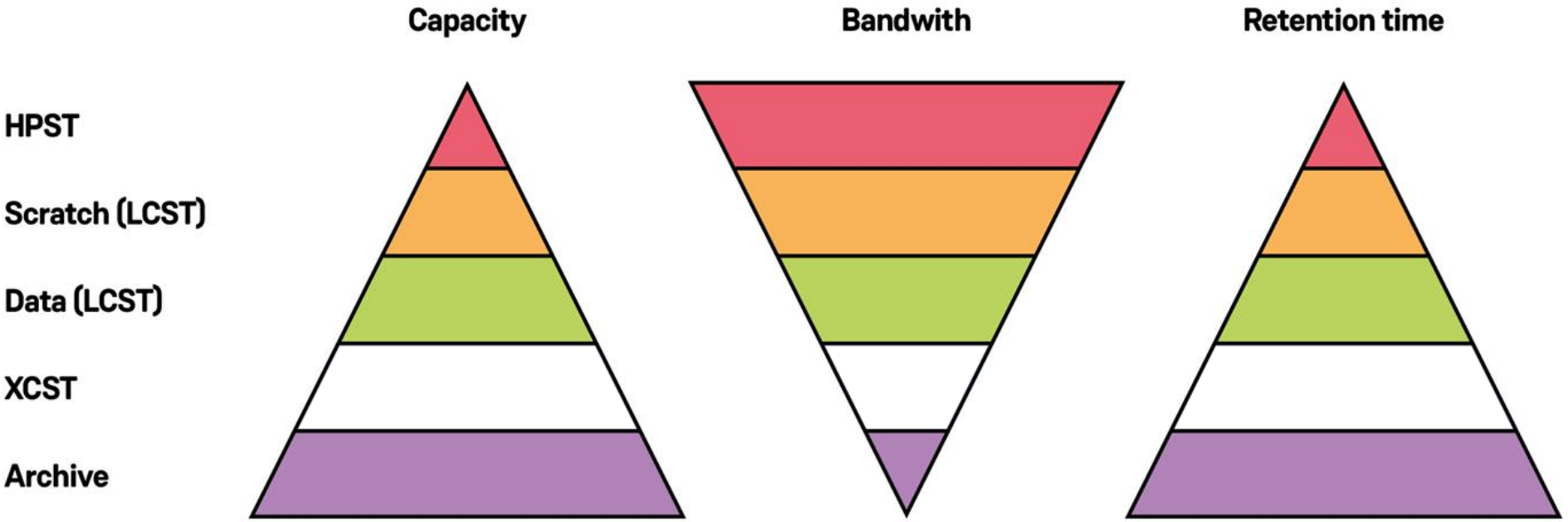
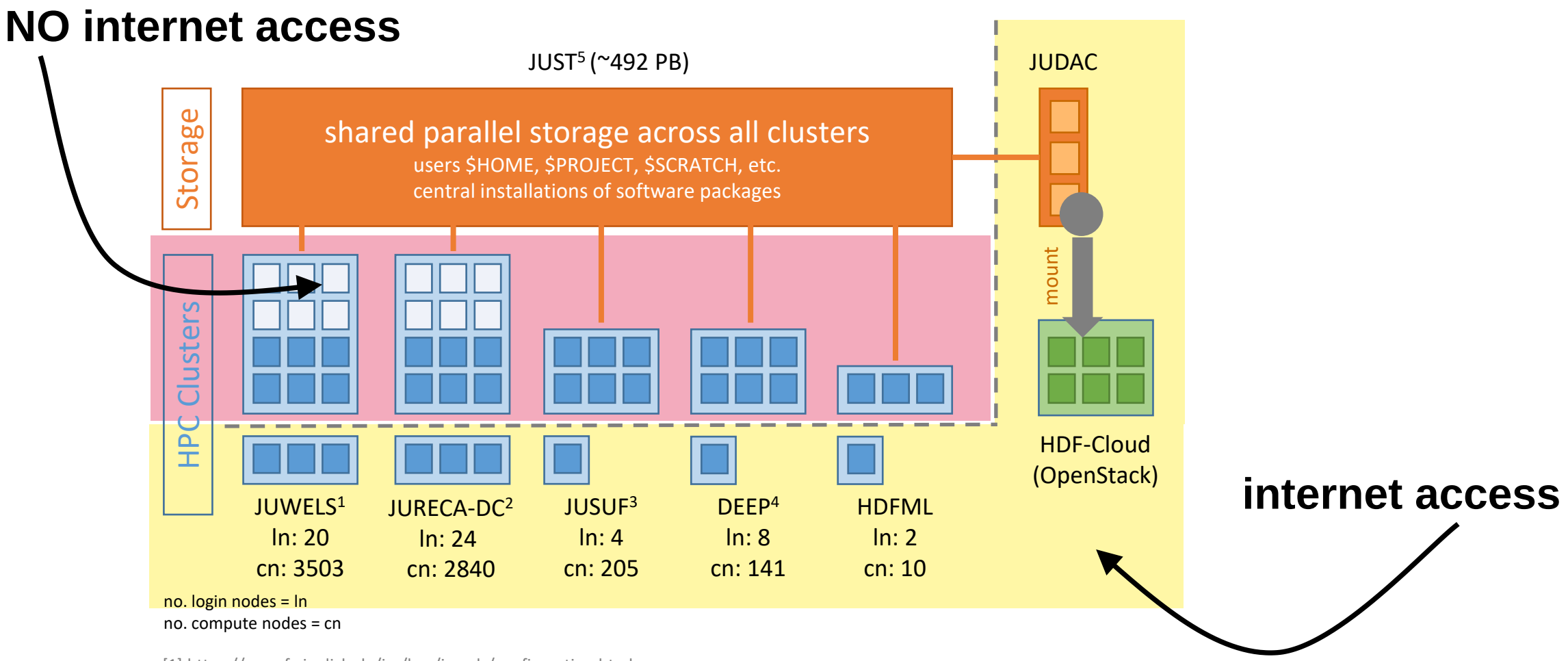
JUST (Juelich Storage cluster)

- 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. login nodes = ln
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/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

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ACCESS
TO COMPUTE RESOURCES
1. REGISTER & LOGIN

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PRE-ACCESS TODOS

1) Register & Login

- ✓ https://judoor.fz-juelich.de

2) Join the project „training2339“

- ✓ Wait to get joined by the project PI

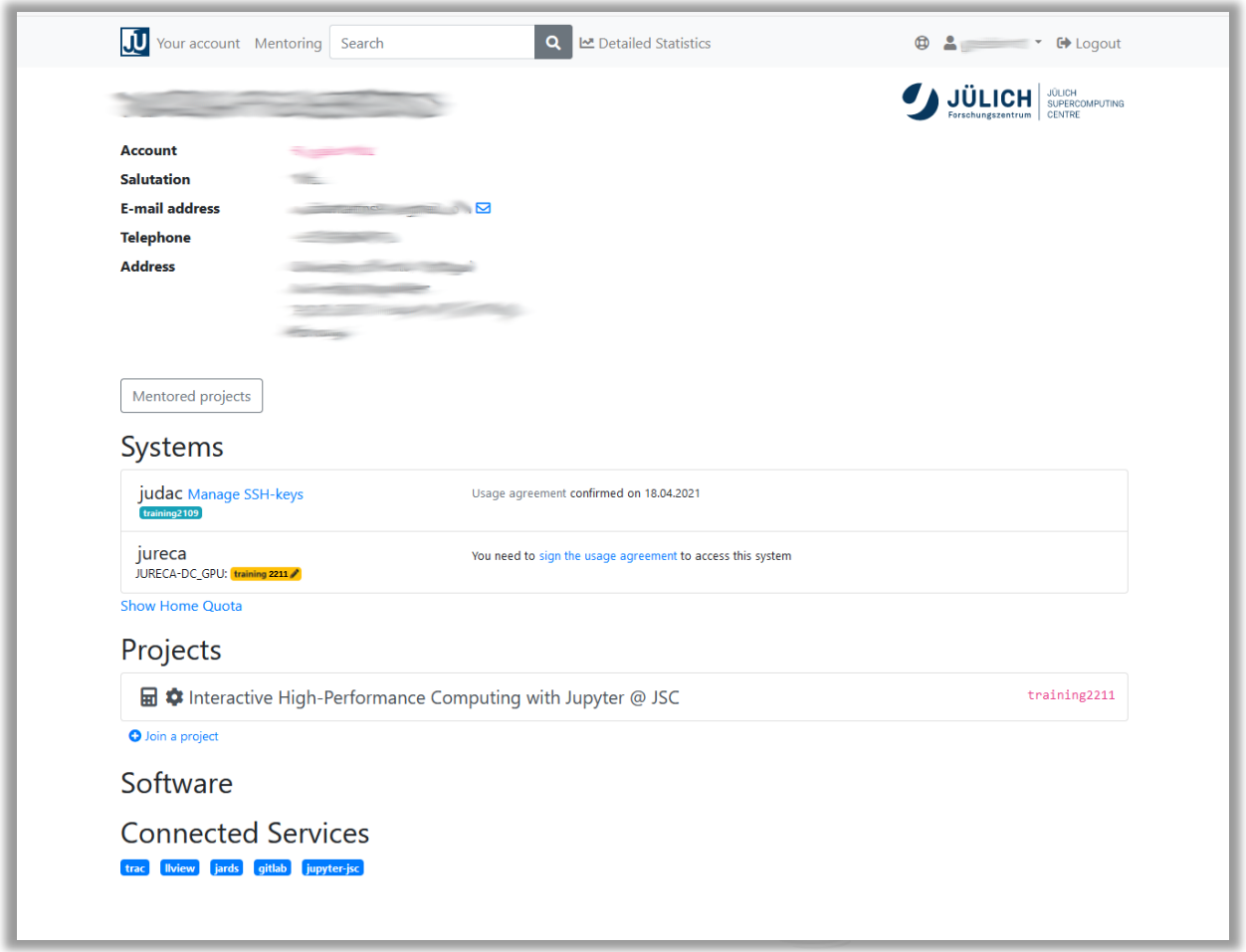
3) Sign usage agreement

- ✓ 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

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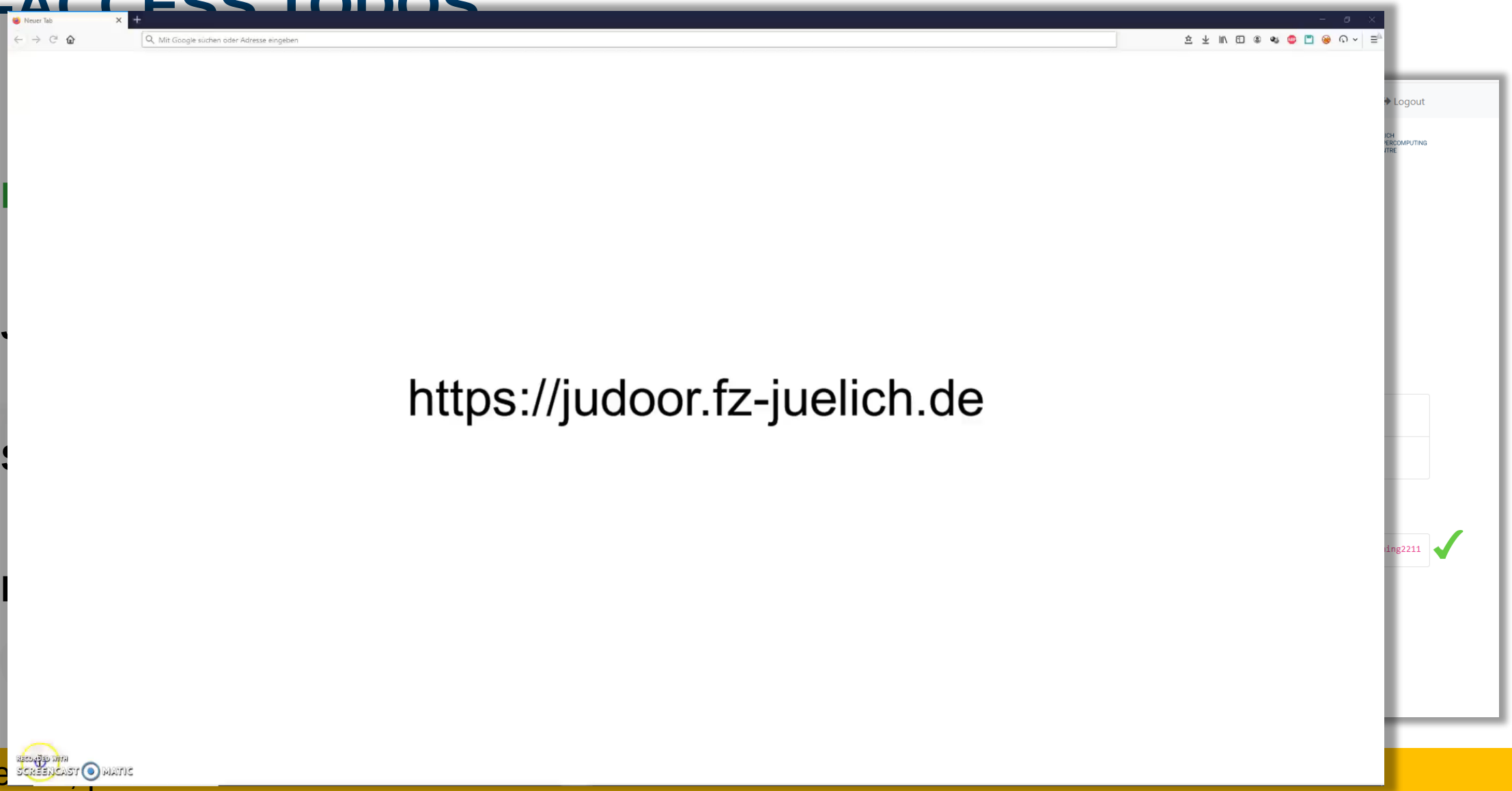

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ACCESS
TO COMPUTE RESOURCES
2. JOIN THE PROJECT

PRE-ACCESS TODOS

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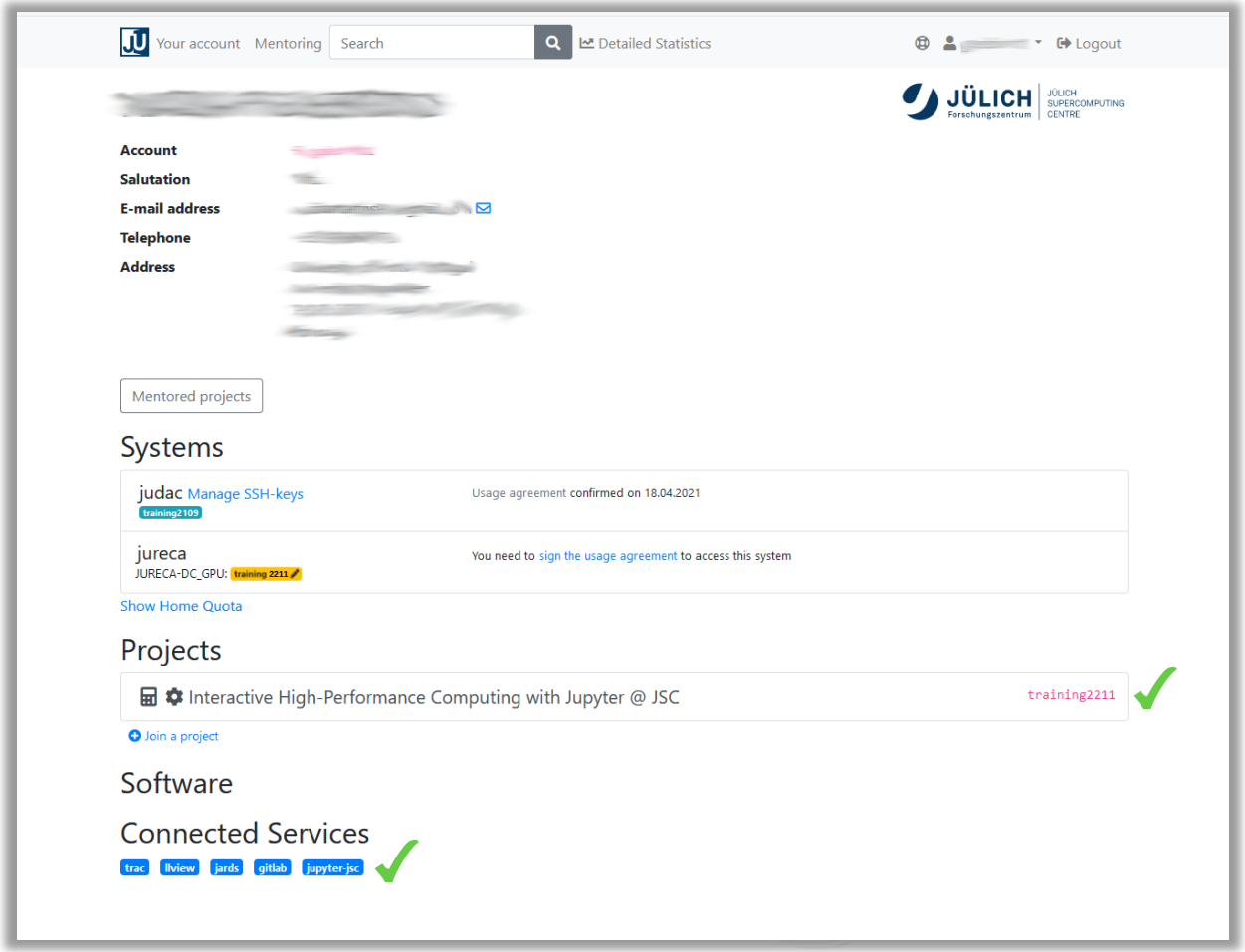

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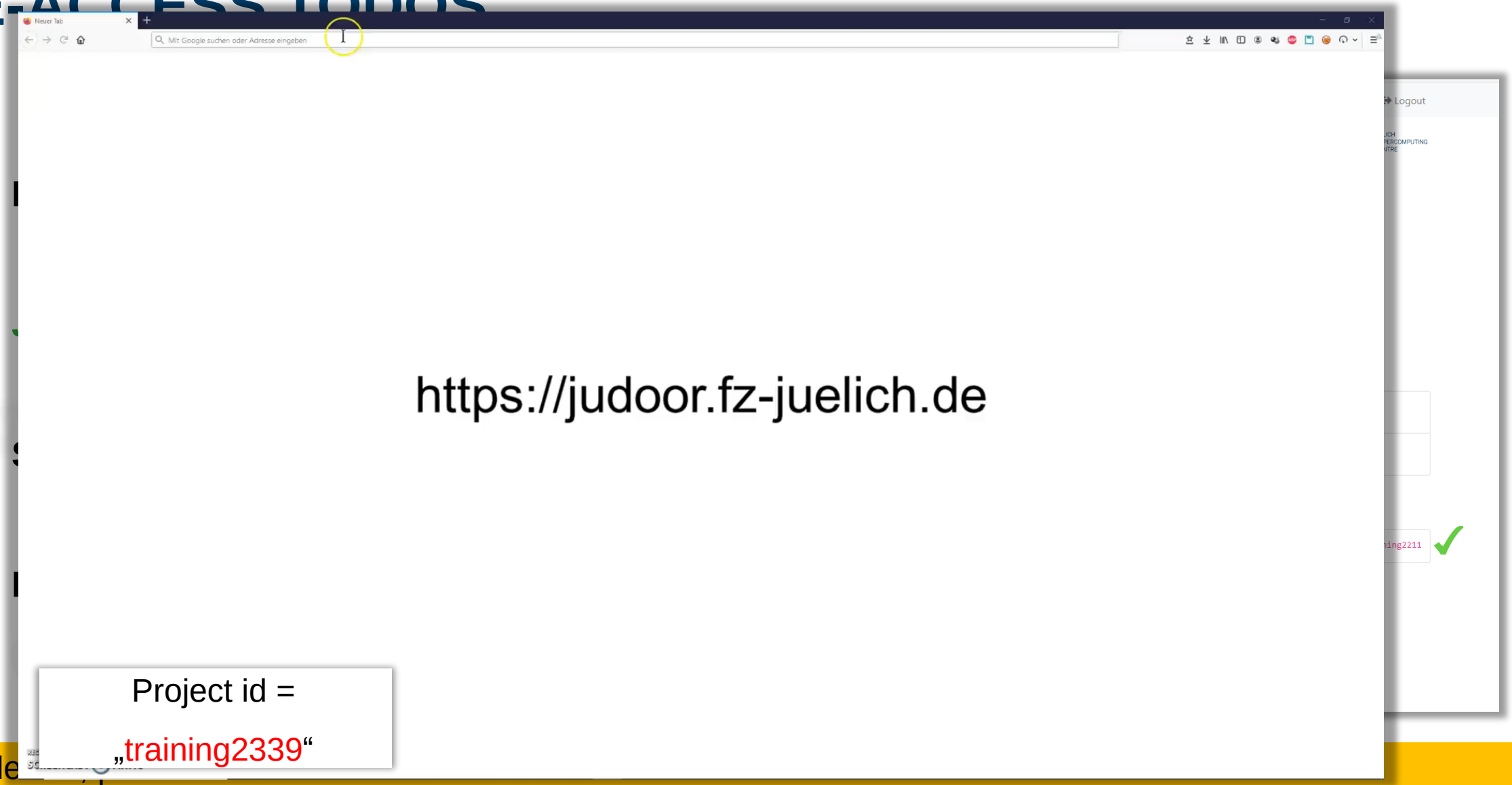

Project id =

„training2339“

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

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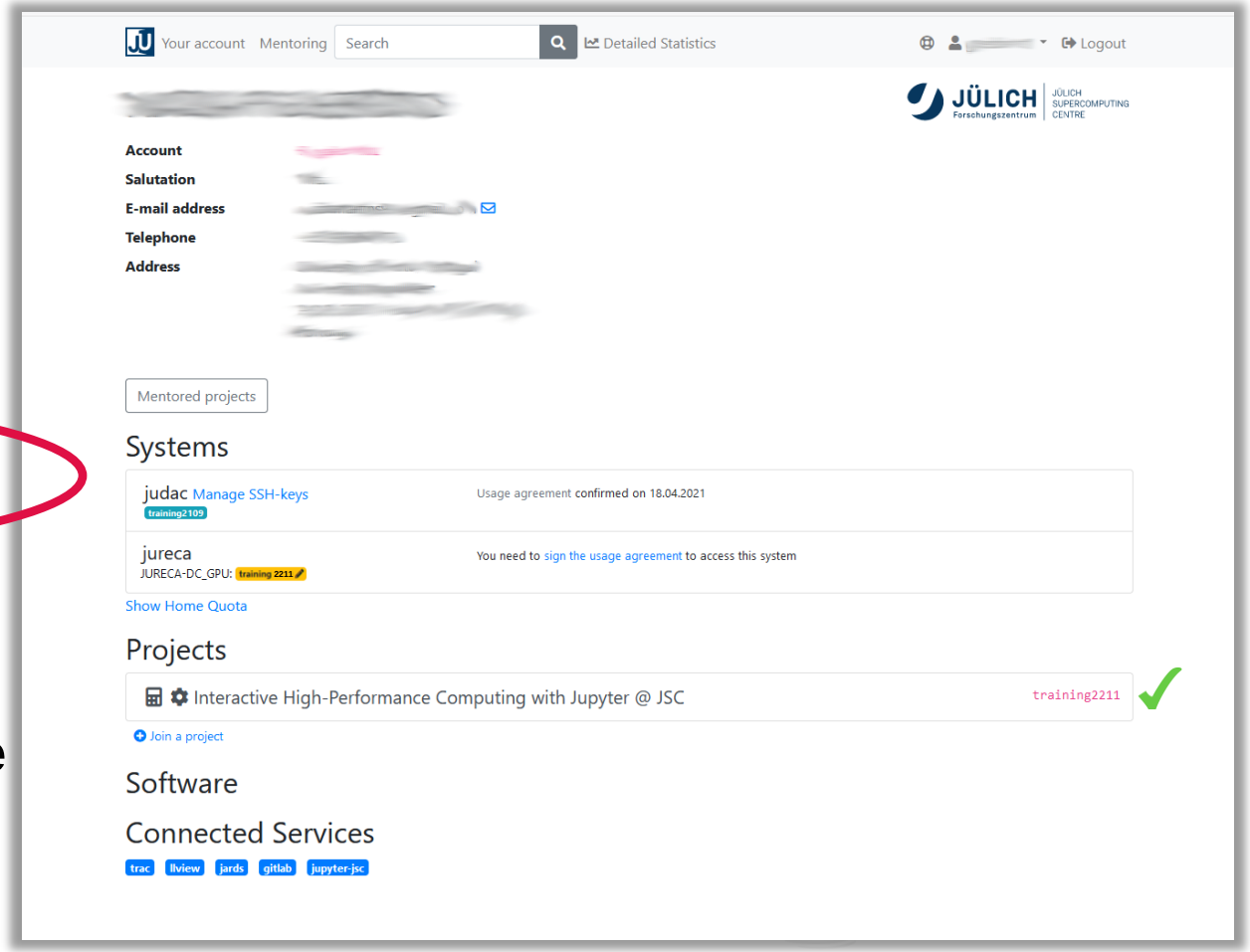

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ACCESS
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3. SIGN USAGE AGREEMENT

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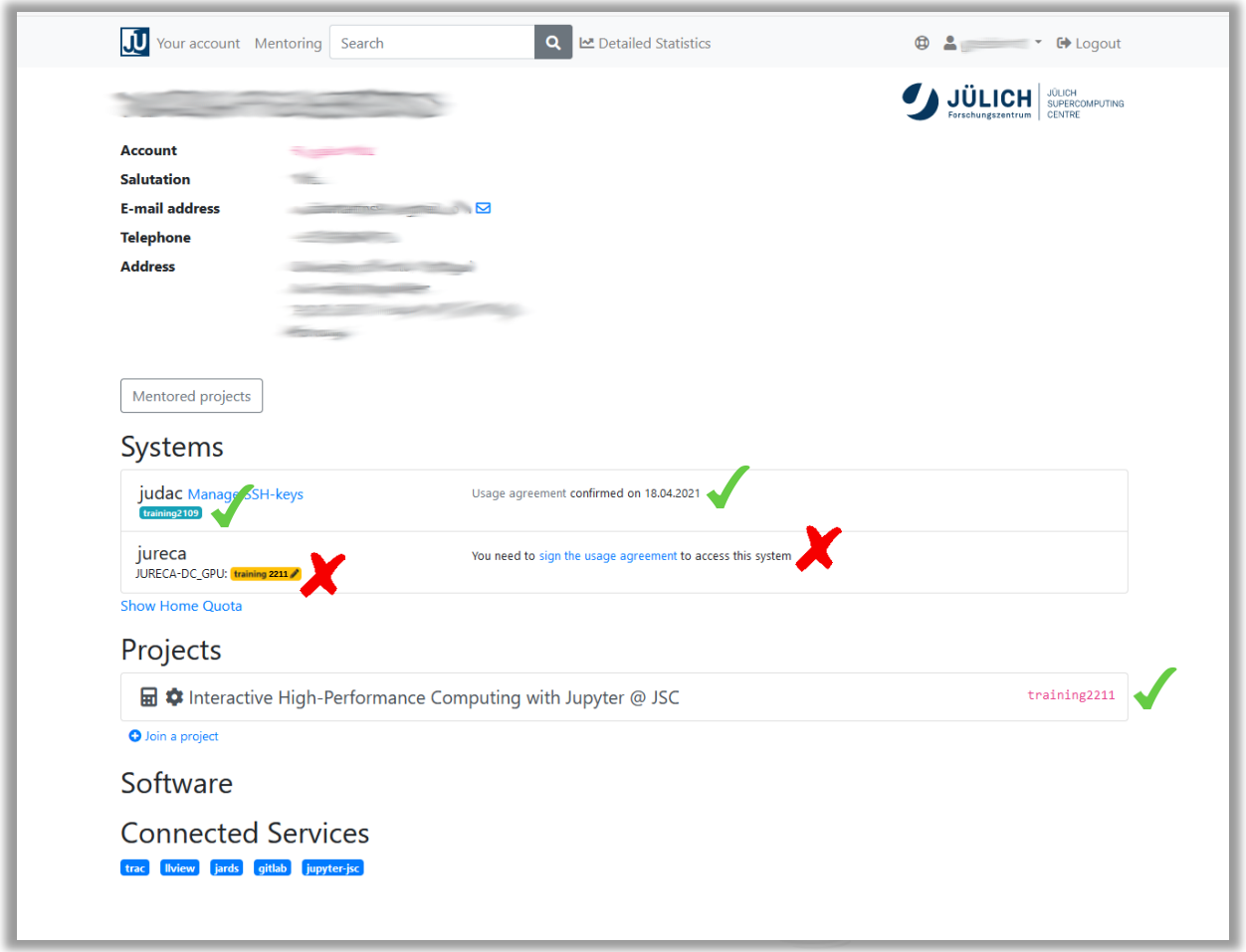

For more details, please visit
https://gitlab.jsc.fz-juelich.de/hedgedoc/S46PXGIuSiuMv1Vgw_UU_Q?view#Getting-Access

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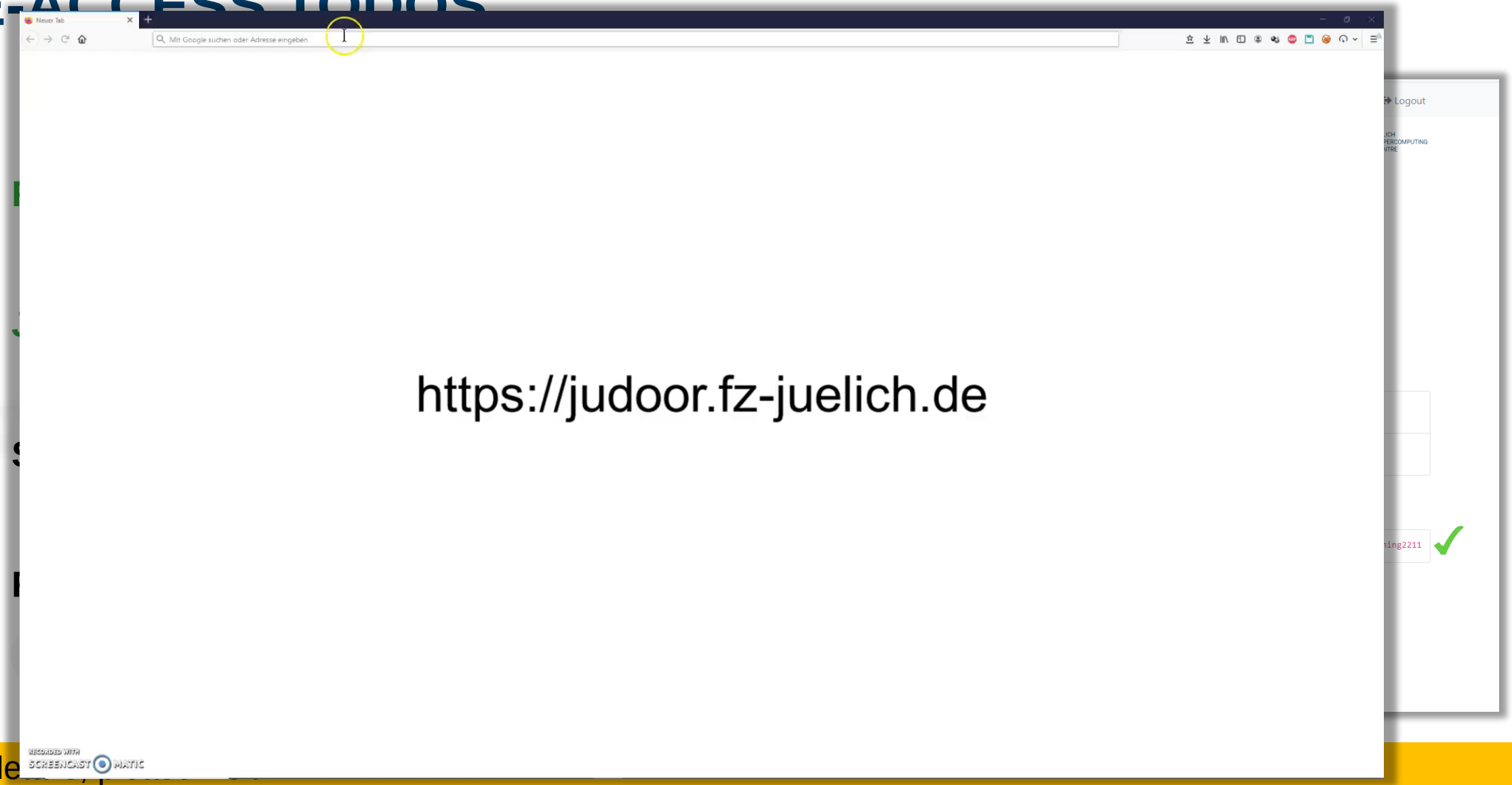

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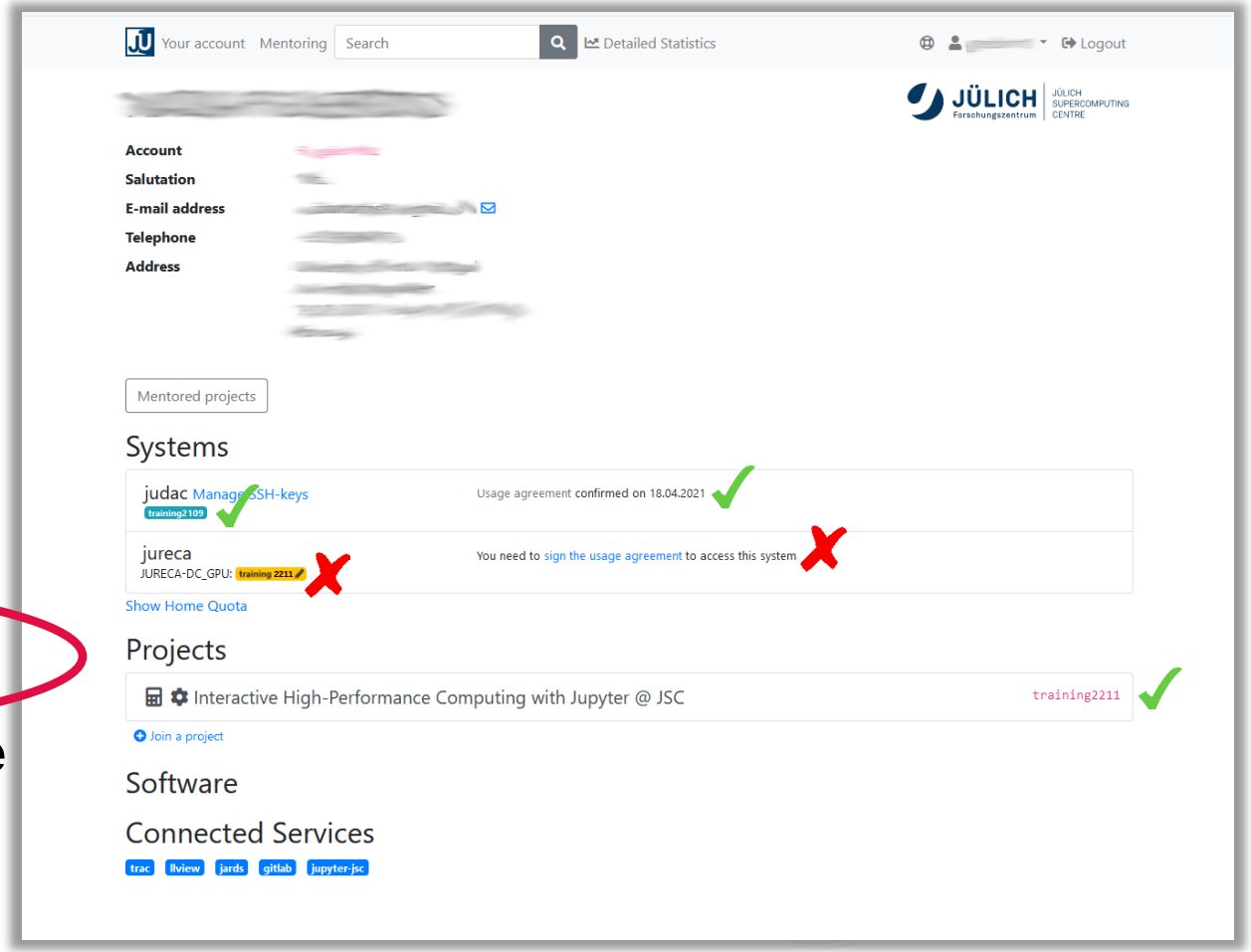

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ACCESS
TO COMPUTE RESOURCES
4. REQUEST ACCESS TO RESTRICTED SOFTWARE

PRE-ACCESS TODOS

1) Register & **Login**

- ✓ https://judoor.fz-juelich.de

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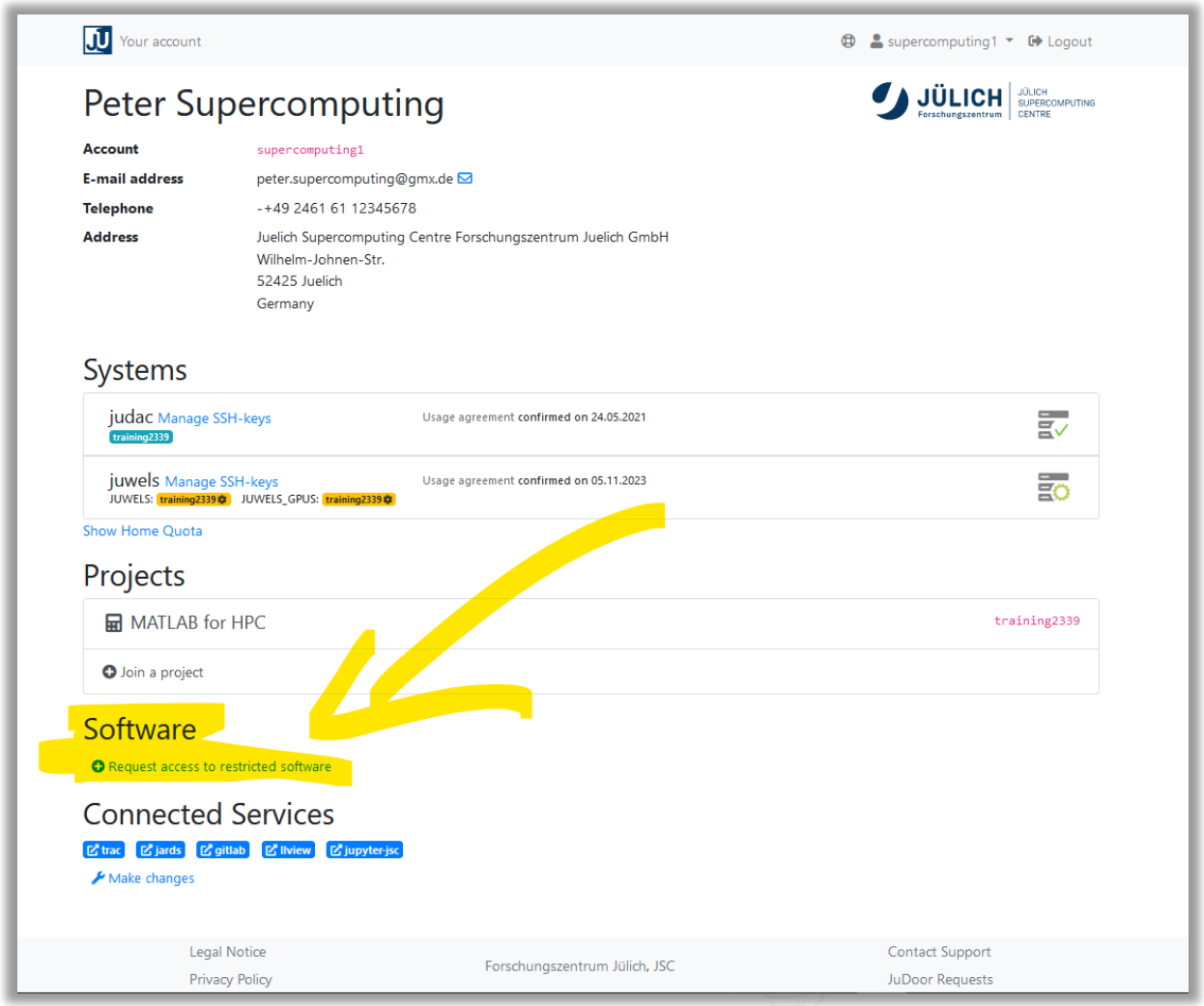
Waiting for access approval



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3) Sig
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✓
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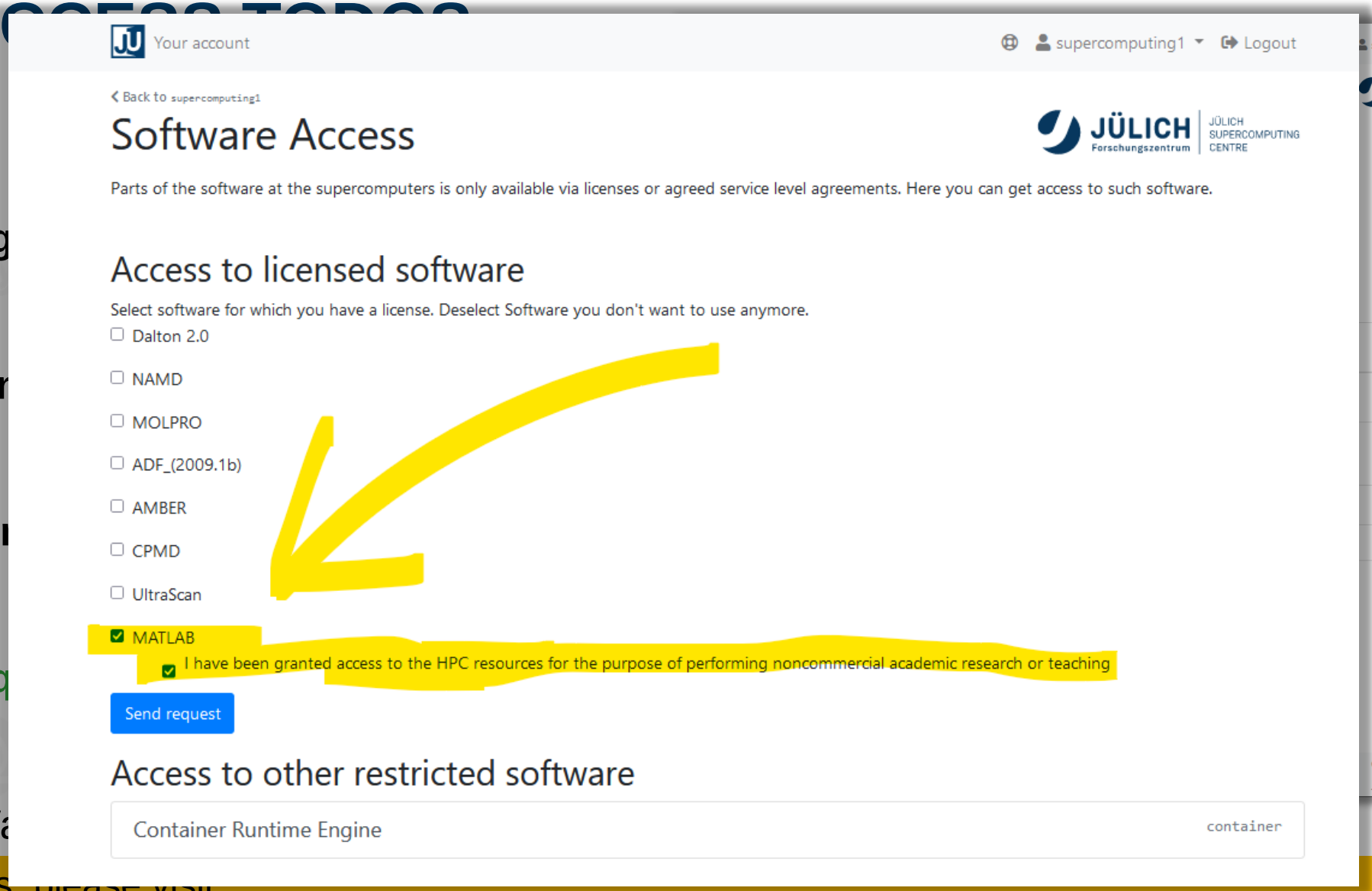

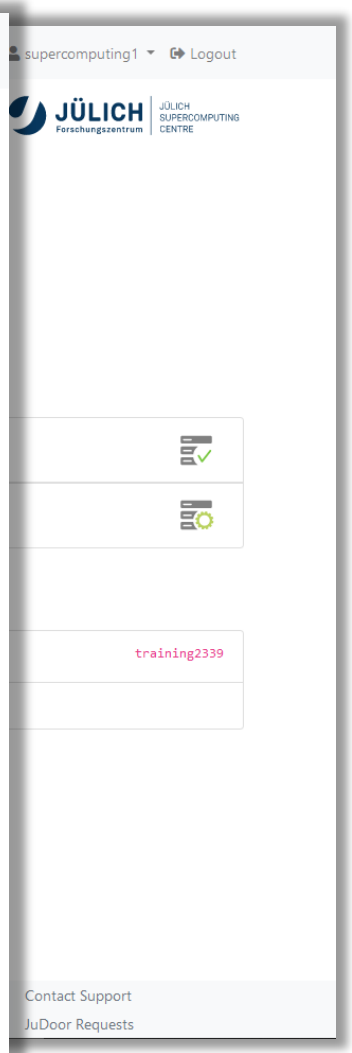

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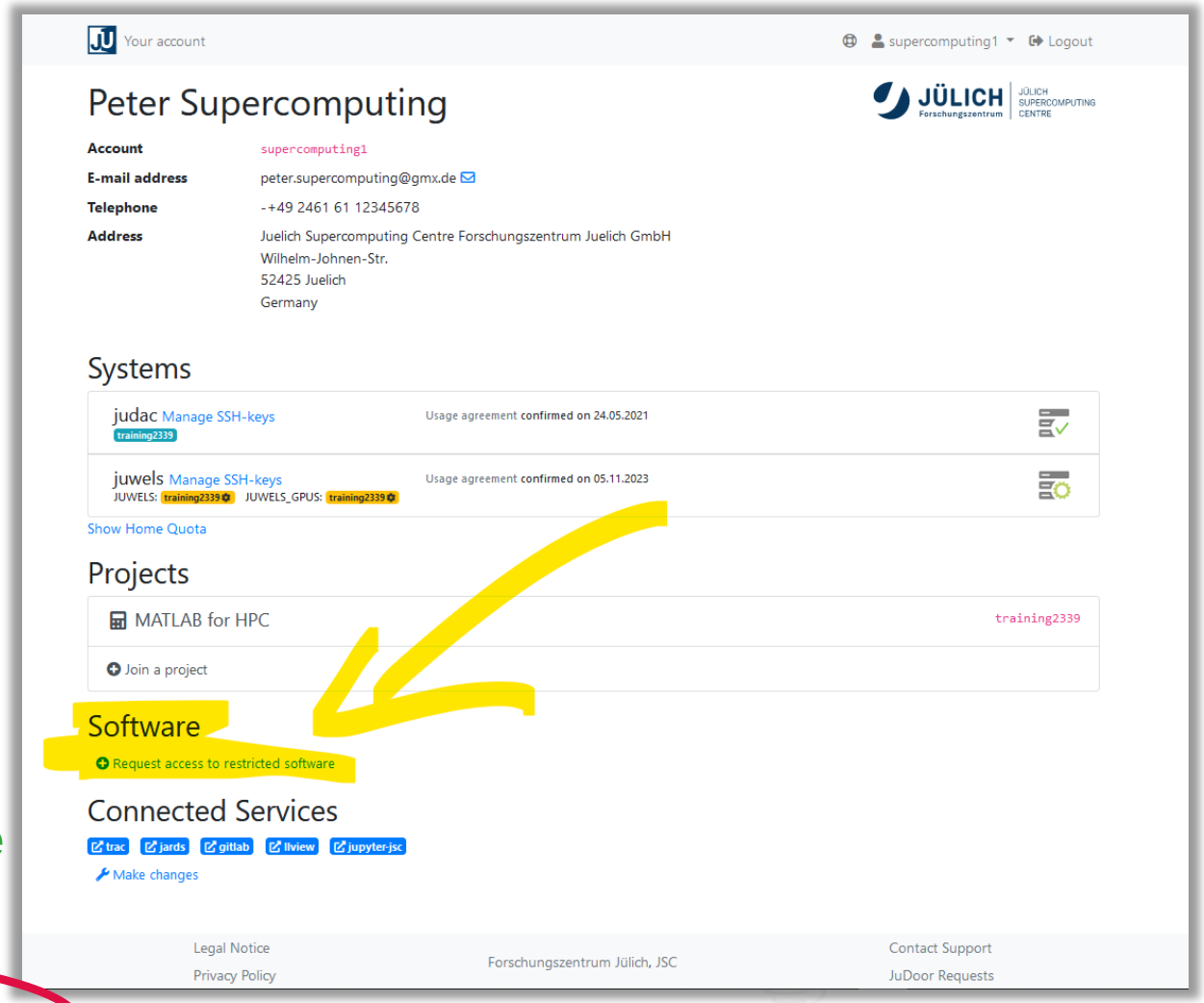

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ACCESS
TO COMPUTE RESOURCES
5. RESTER TO JUPYTER-JSC

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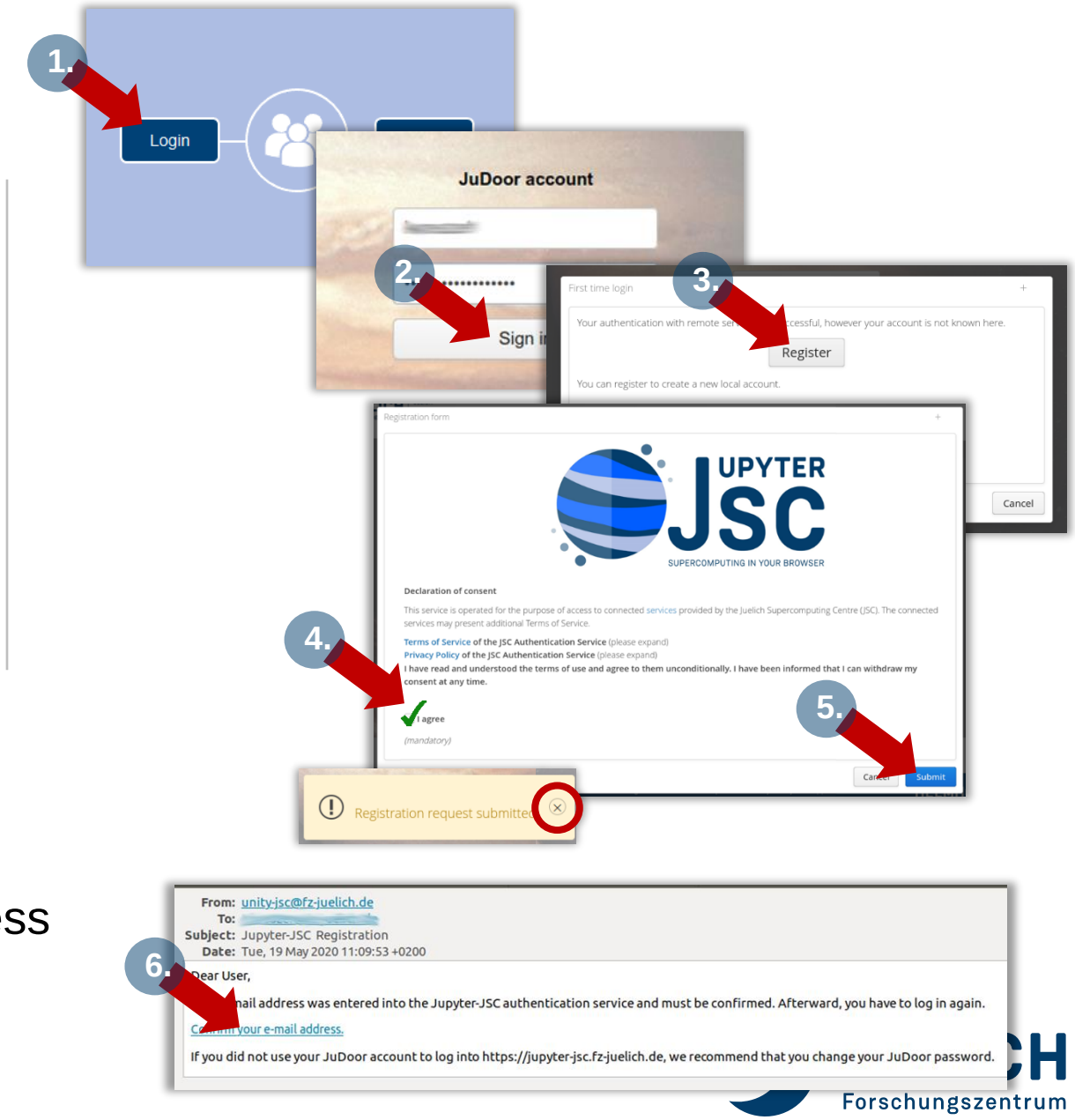
JUPYTER-JSC WEBSERVICE

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



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JUPYTER-JSC WEBSERVICE

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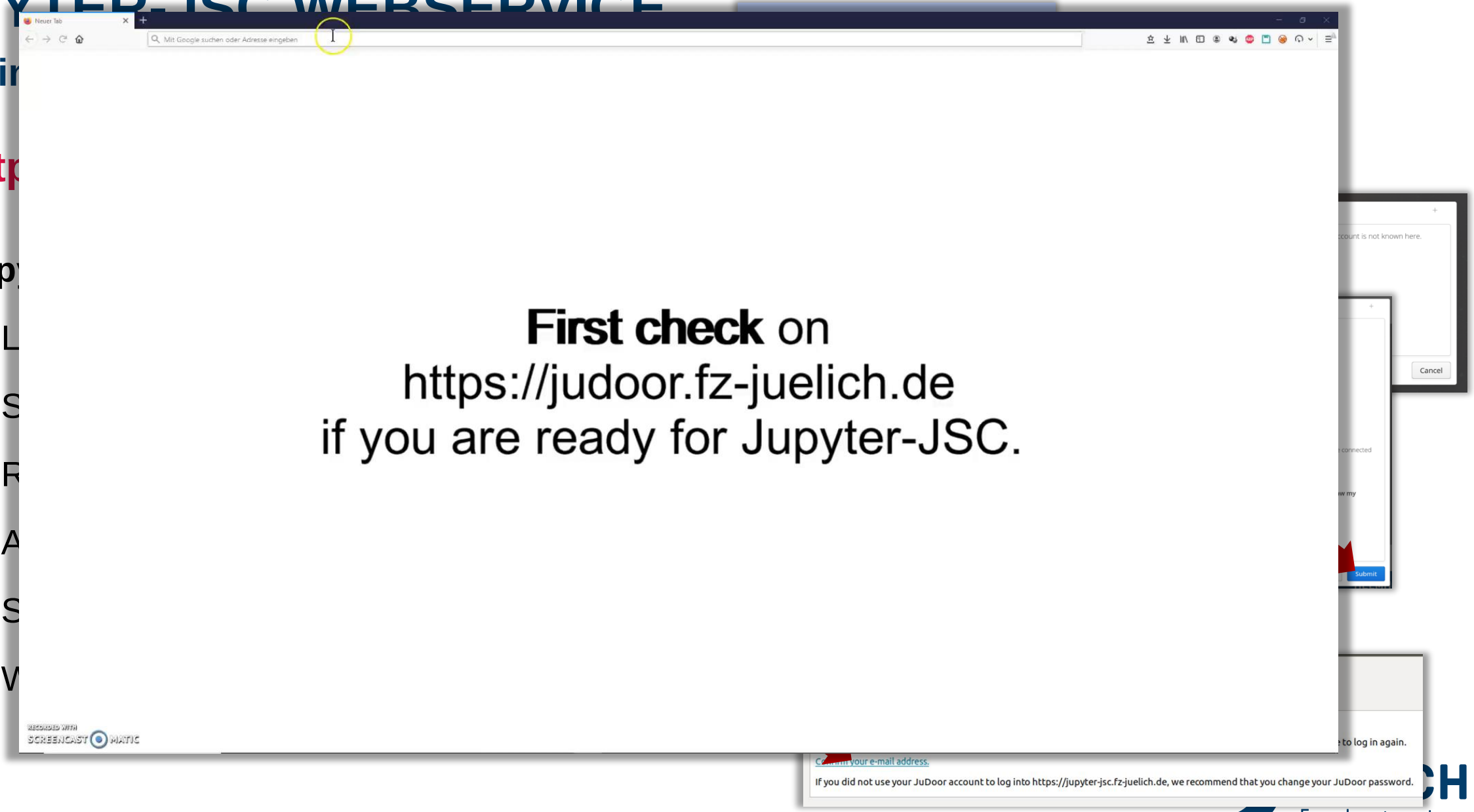

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ACCESS
TO COMPUTE RESOURCES
5. START WEB-UI

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JUPYTER-JSC WEBSERVICE

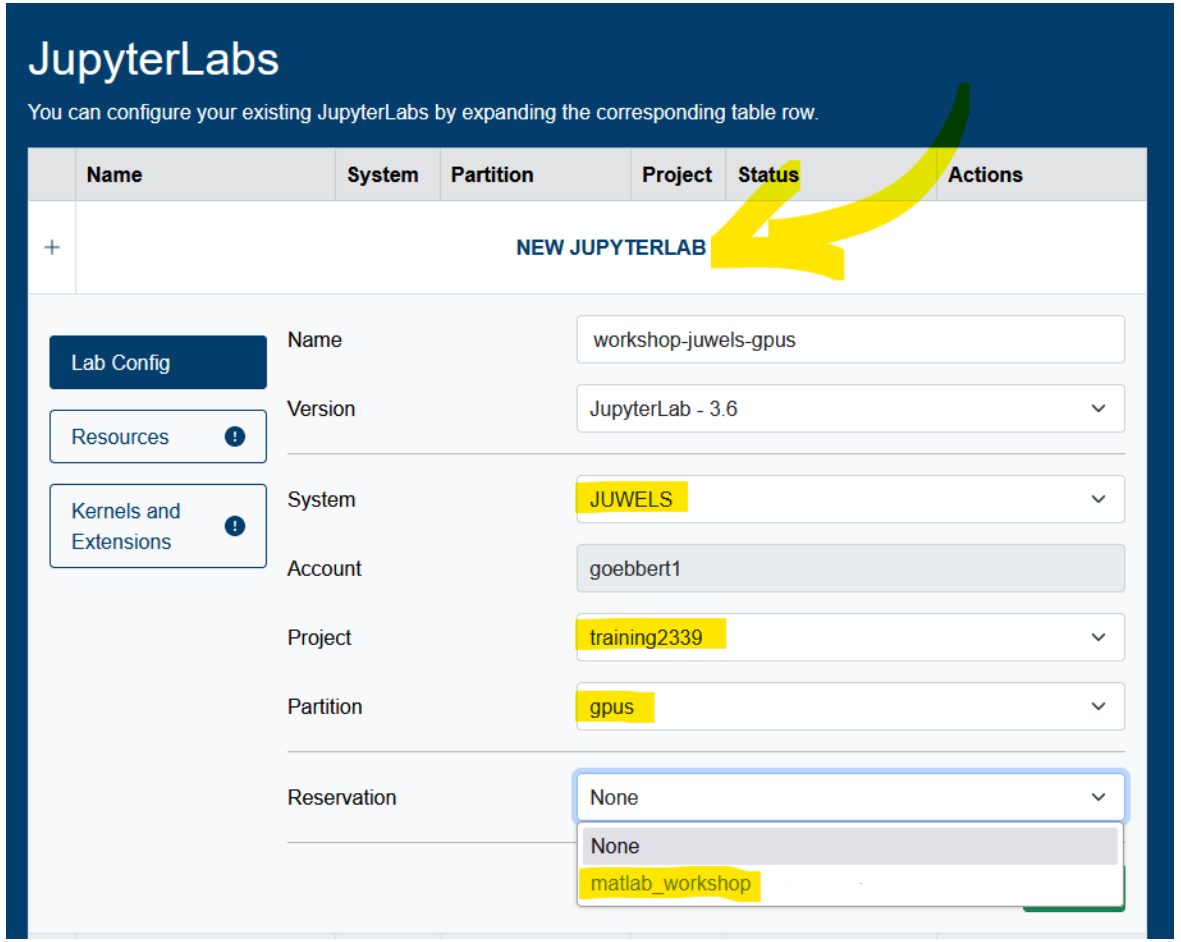
JupyterLab Configuration

Lab Config

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

Extra options

- Reservation
  matlab_workshop



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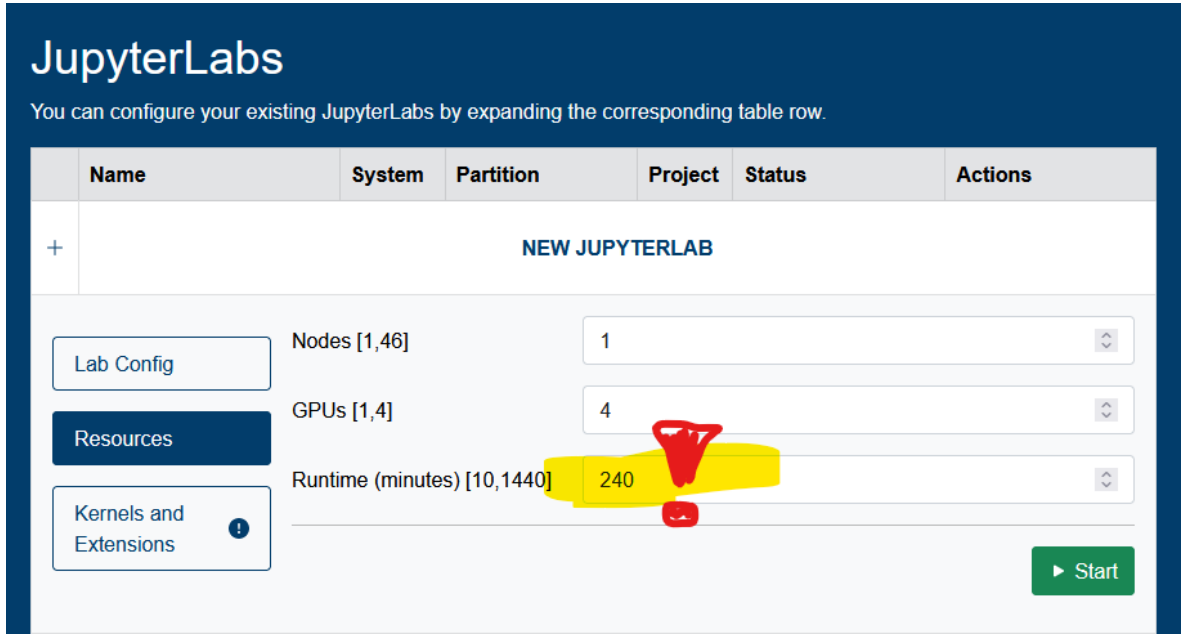
JUPYTER-JSC WEBSERVICE

JupyterLab Configuration

Resources

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



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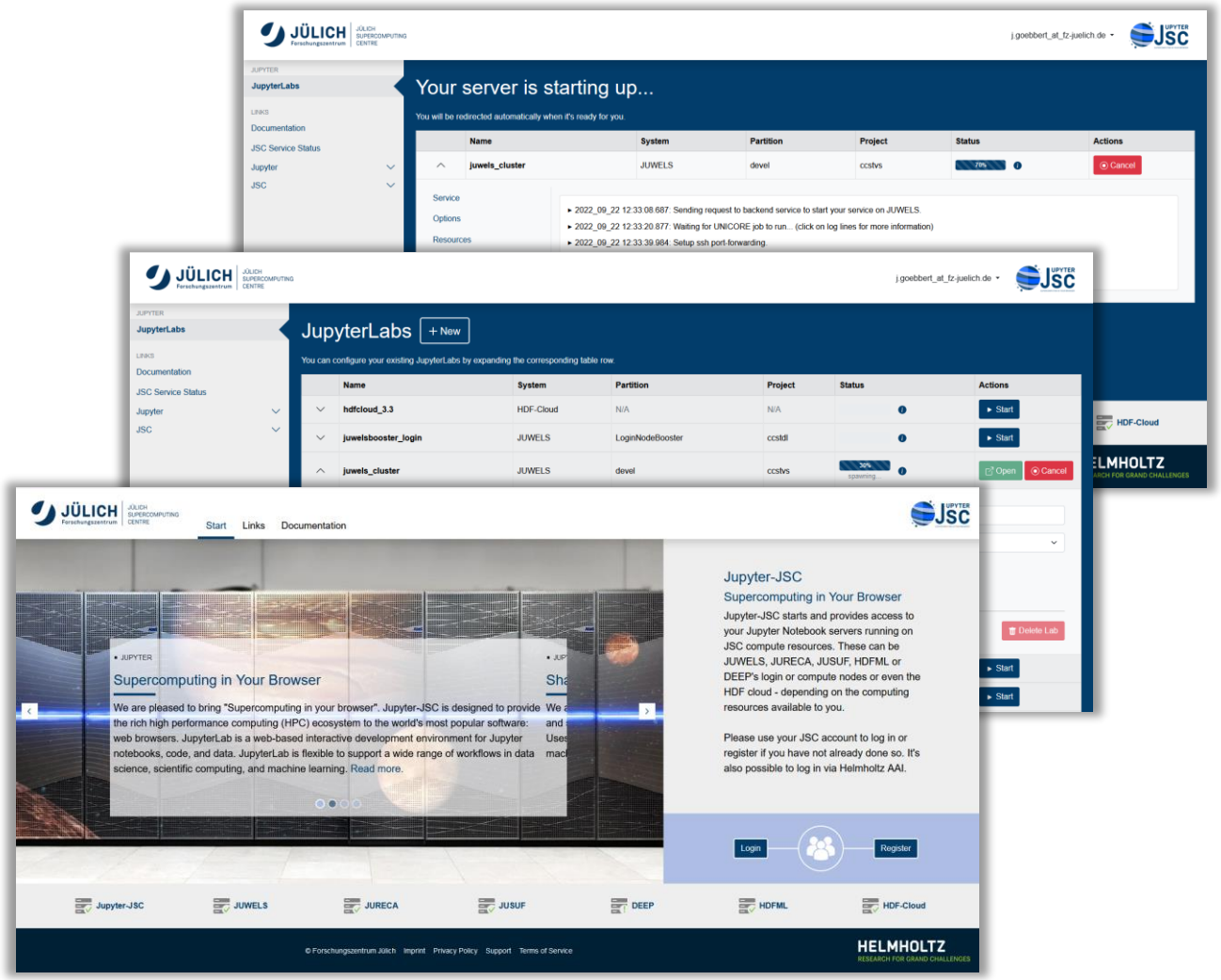
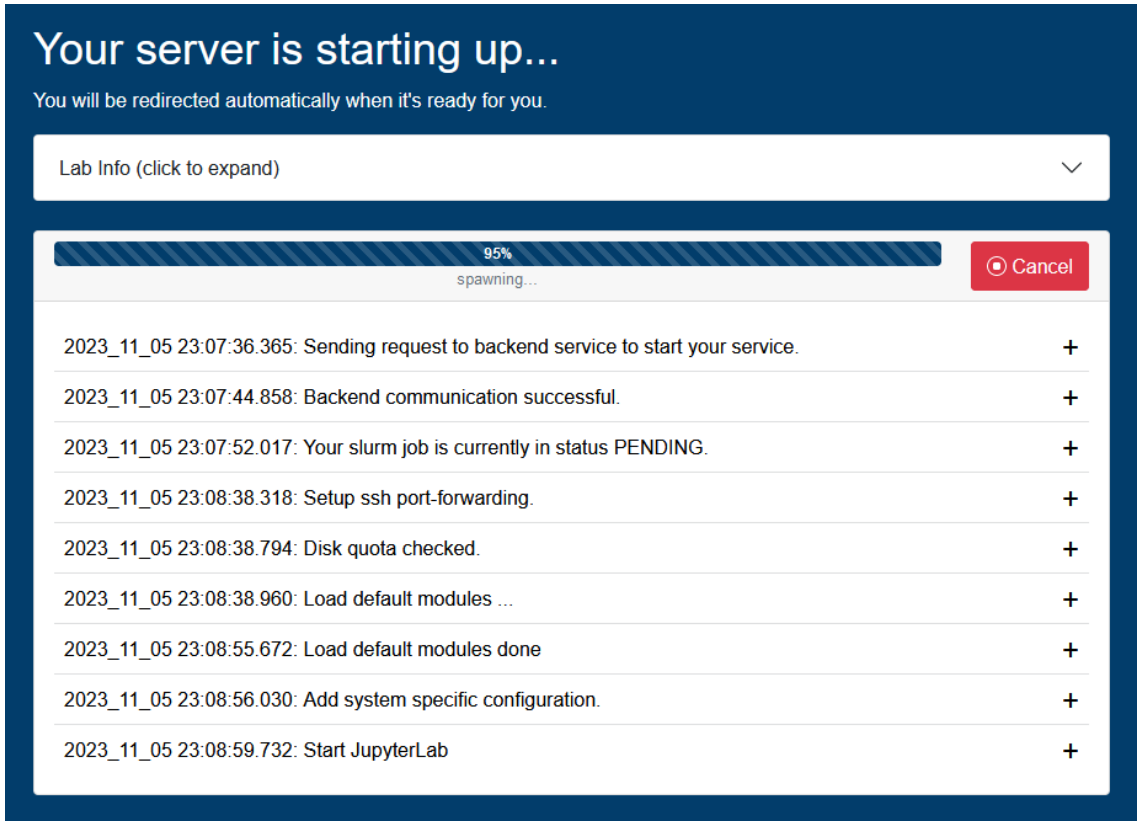
JUPYTER-JSC WEBSERVICE

Start your JupyterLab





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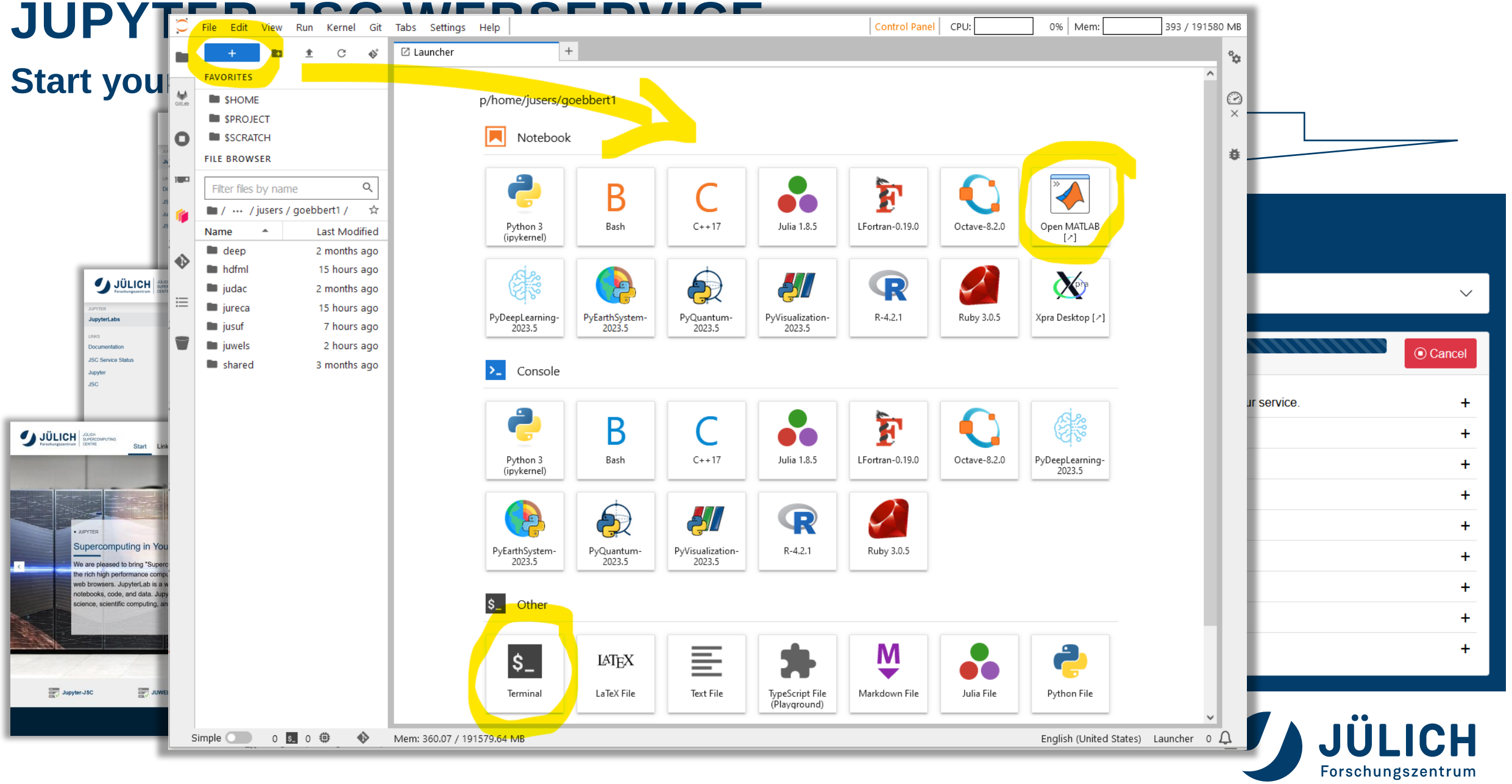
Start you



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