bw|HPC

KIT | NHR
National High-Performance Computing Center

Access Procedures: bwHPC Clusters + NHR@KIT

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KIT, SCC

Funding:
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MINISTERIUM FÜR WISSENSCHAFT, FORSCHUNG UND KUNST
Bundesministerium für Bildung und Forschung

Outline

- Registration Processes
  - bwUniCluster 3.0
  - HoreKa
  - bwForCluster
- Login Procedure
  - Virtual private network (VPN)
  - Two-factor authentication (2FA)
  - SSH - remote login client
  - Jupyter
- File Transfer & File storage
- FAQs

HPC Infrastructure in BaWü: Registration

- Bwunicluster 3.0
  - At tier (level) 3, Baden-Württemberg (BW) cluster for general purposes
  - **Simple** registration process

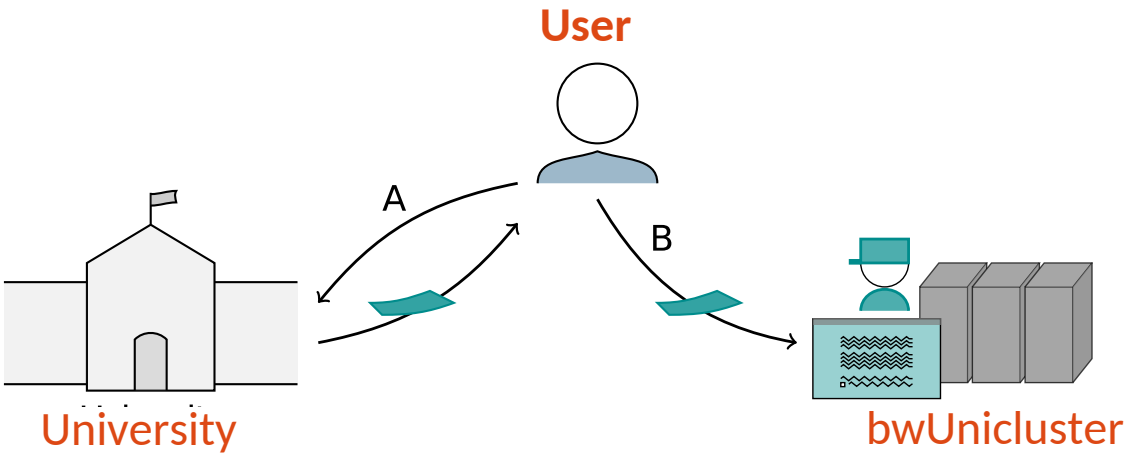
- HoreKa
  - At tier 2, national research cluster
  - Access process ensures that applications fulfill requirements of parallelization

- bwForCluster (JUSTUS 2, Helix, NEMO, BinAC)
  - Also at tier 3, BW research clusters
  - Architecture optimized for certain scientific communities
  - Access process ensures using the suitable cluster and enhances user support

Registration

Registration Process – bwUniCluster 3.0

- Access only for members of shareholder universities.
- More Details: https://wiki.bwhpc.de/e/Registration/bwUniCluster



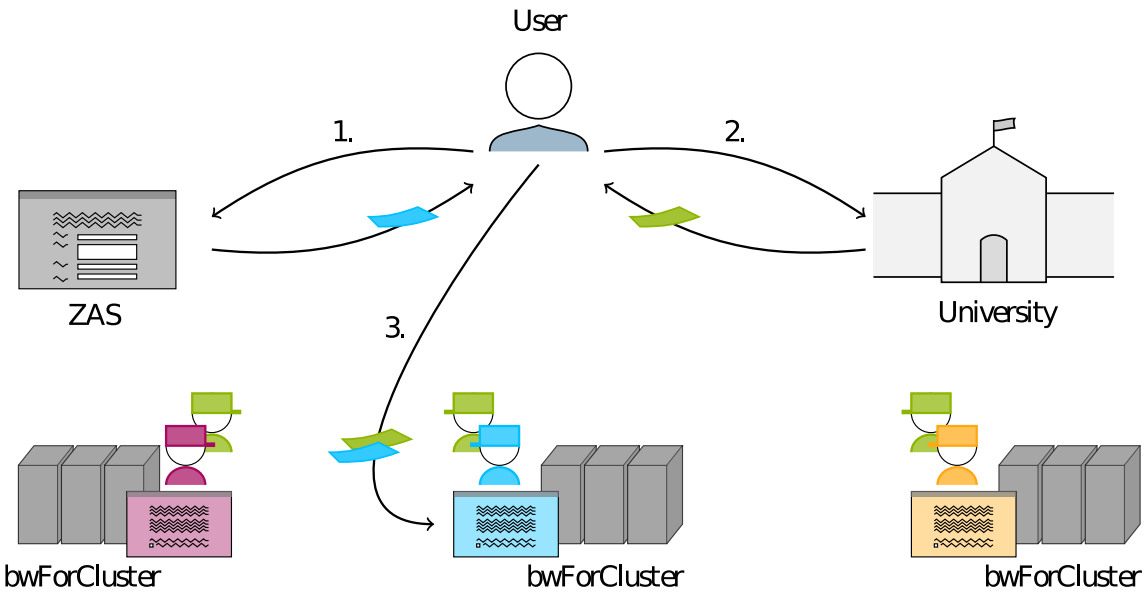
Step A: Obtainment of bwUniCluster entitlement

- Each university has its own entitlement granting policies!

Step B: Web registration at https://login.bwidm.de + questionnaire (https://zas.bwhpc.de/bwuni_questionnaire.php)

- Login via bwIDM with your university account, set service password and 2FA

Registration Process – bwForClusters (short version)



Step 1: Registration at „Central Application Site (ZAS)“

- Approval of Cluster Assignment Team (CAT)

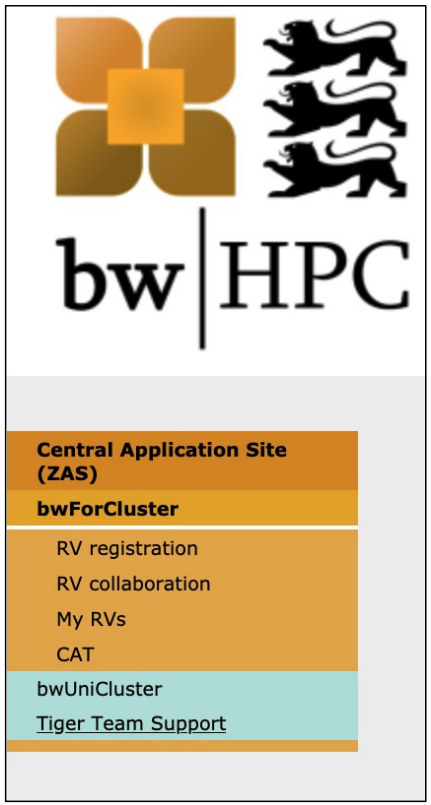
Step 2: Get bwForCluster entitlement by own university

Step 3: Web registration at designated bwForCluster site

e.g. https://login.bwidm.de , bwForCluster JUSTUS 2 (Computational Chemistry)

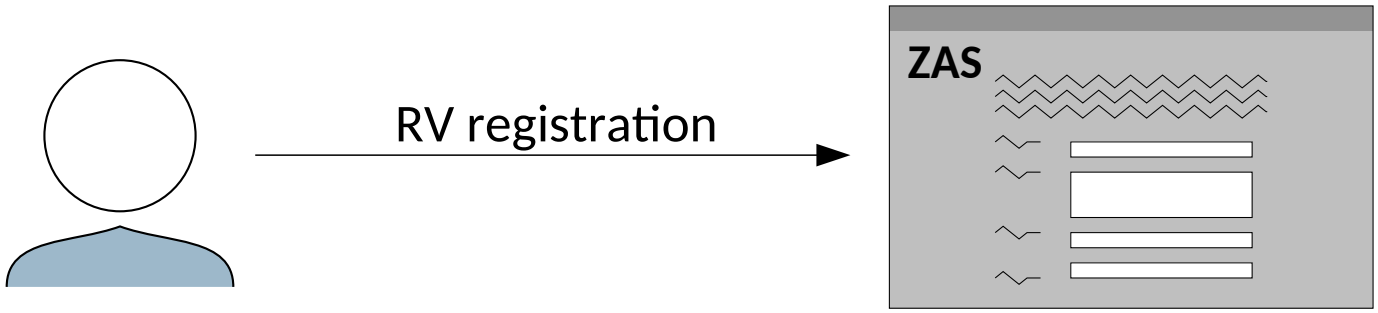
Central Application Site for bwHPC

zas.bwhpc.de

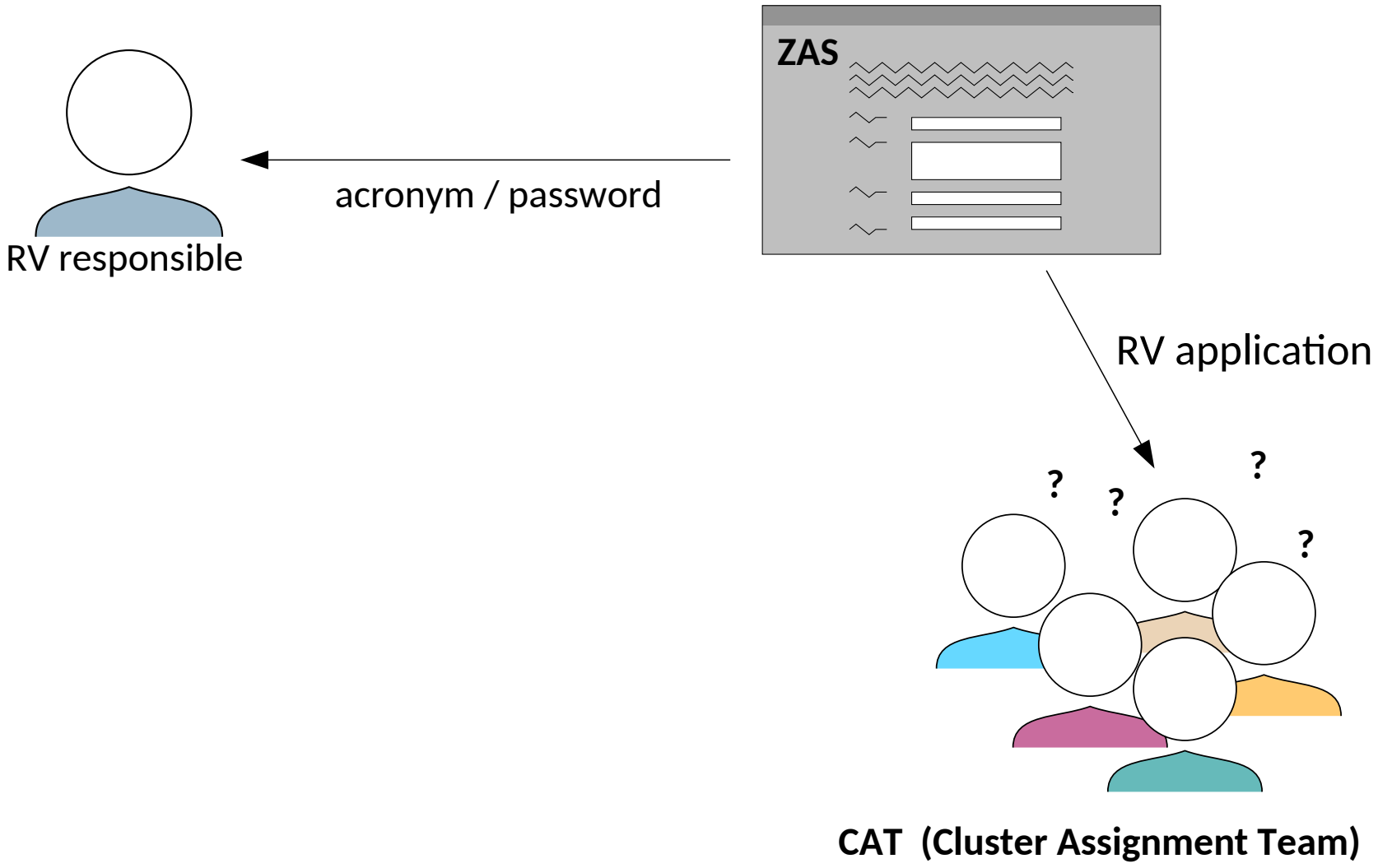


- Web interface of HPC clusters (in the state BW) to handle the user compute activities.
- Nomenclature:
  - RV = Planned compute activities (Rechenvorhaben).
  - RV Responsible: The person who does the registration of the RV (applicant)
  - Cluster Assignment Team: aka CAT; assigns to one fitting cluster according to the RV requirement.
  - RV collaboration = The team (managers and coworkers)
- An RV approval is valid
  - Only on one bwForcluster for a period of one year after the approval
  - For all team members

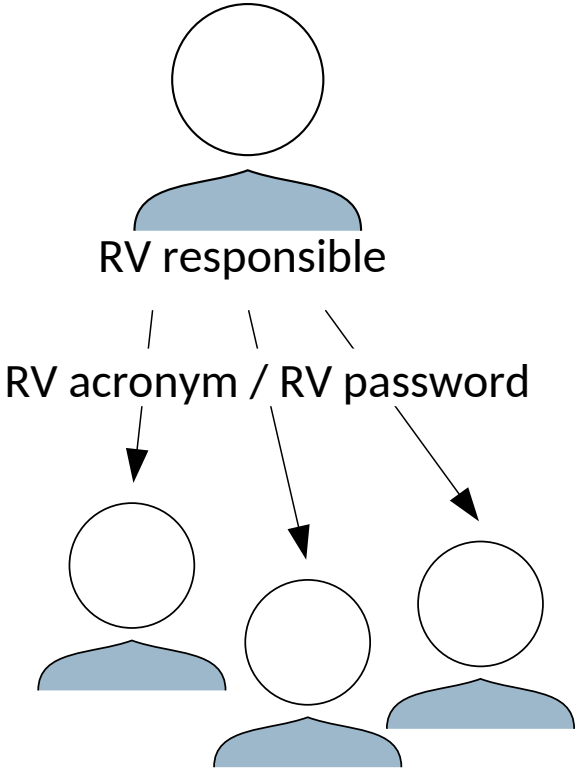
Registration Process: bwForCluster – Step 1a

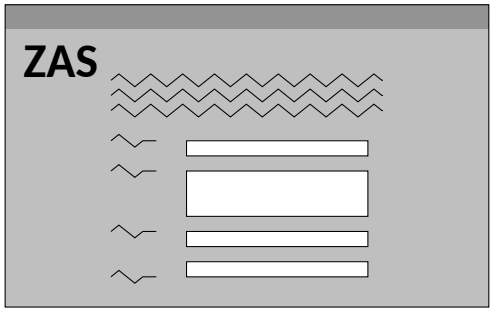


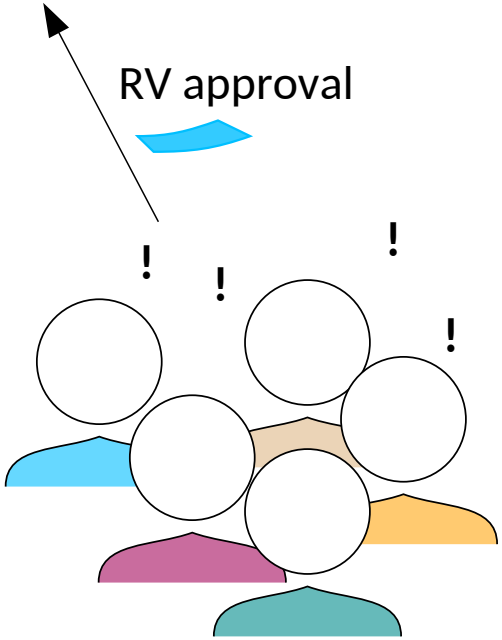
Registration Process: bwForClusters – Step 1b



Registration Process: bwForClusters Step 1c

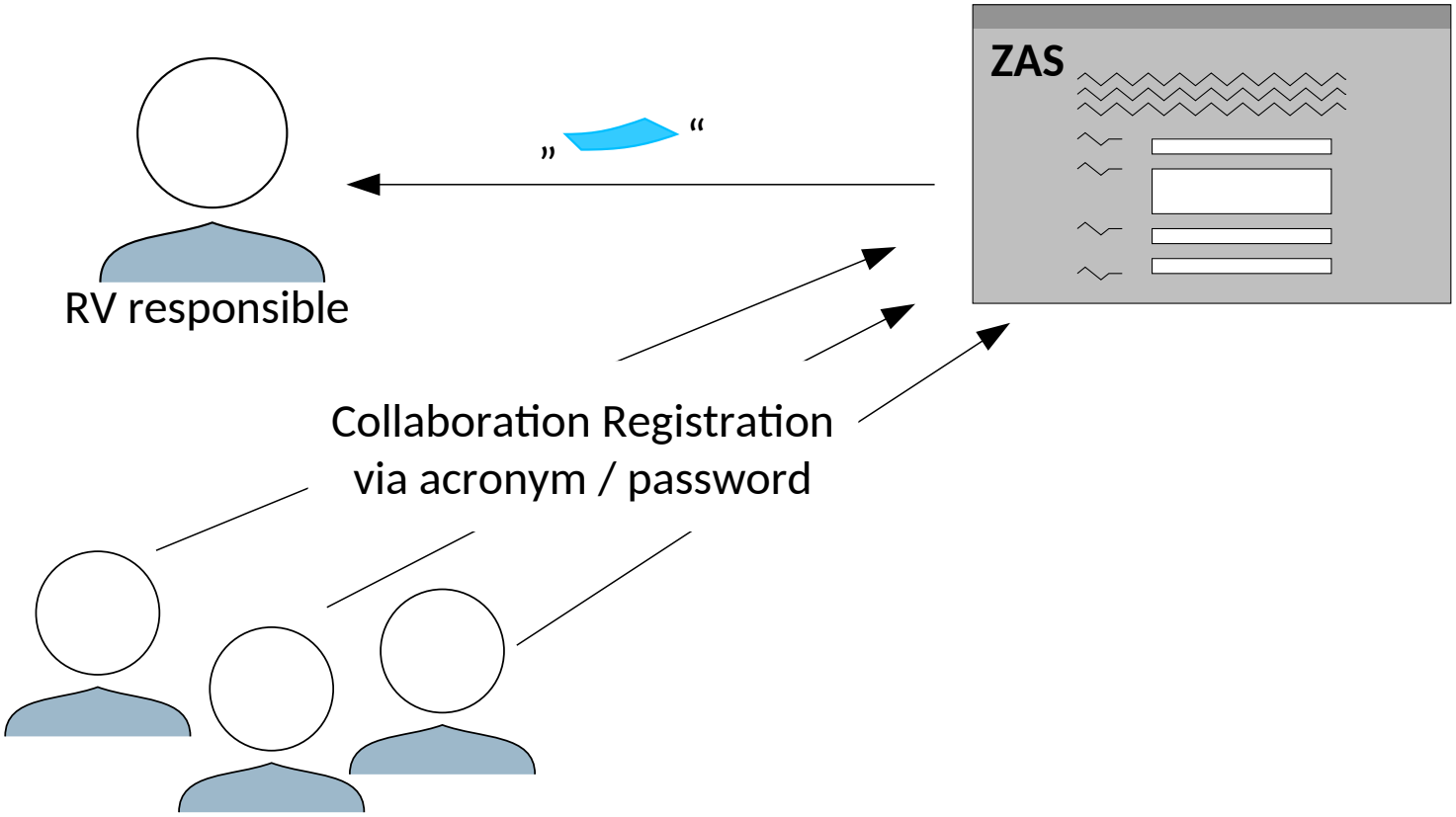




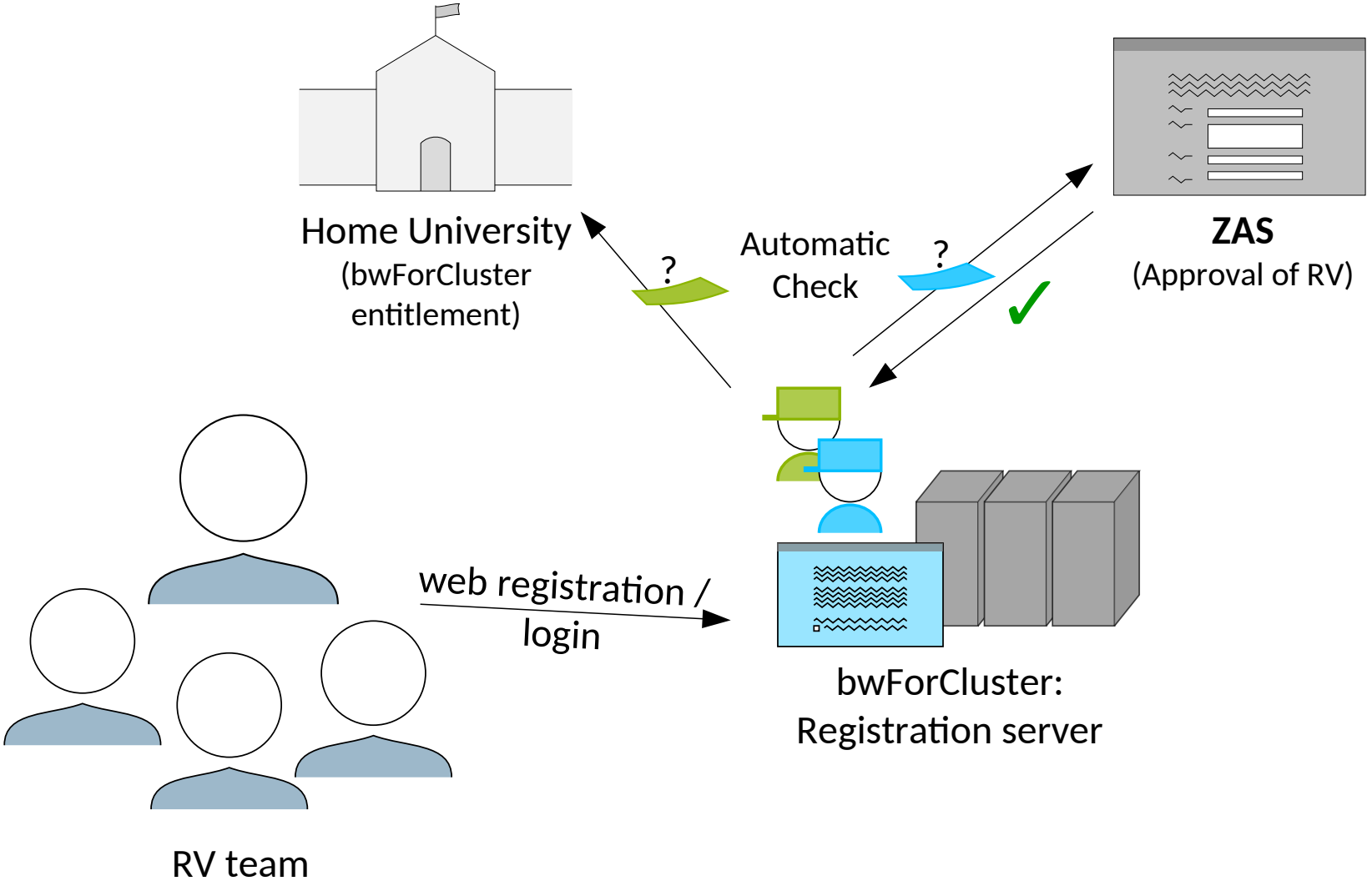


CAT (Cluster Assignment Team)

Registration Process: bwForClusters – Step 1d

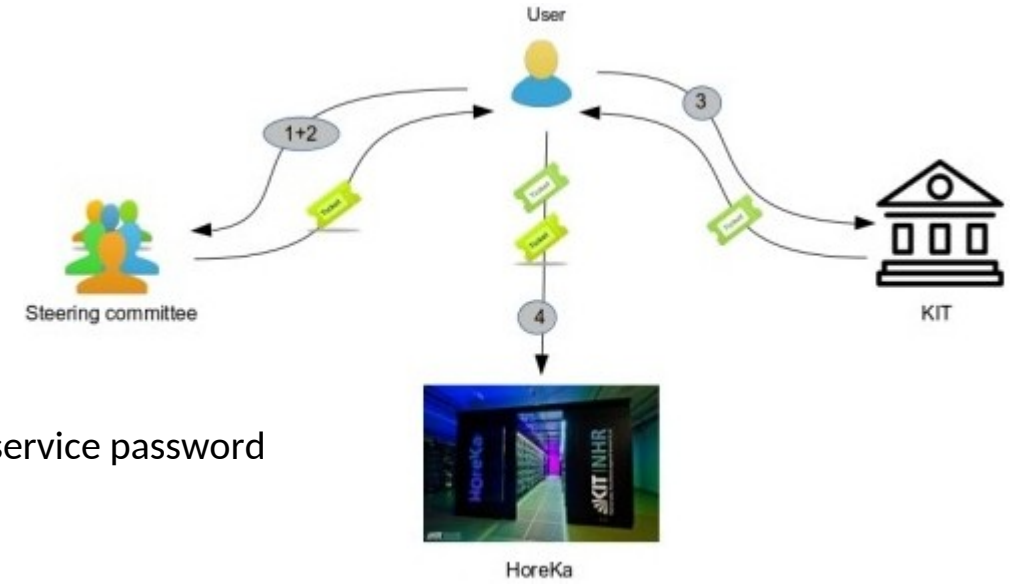


Registration Process: bwForClusters – Step 2 & 3



Registration Process – HoreKa

- Registration:
  1. Online Proposal Form (JARDS)
  2. Proposal is (peer) reviewed
  3. HoreKa access form
  4. Register on web page https://fels.scc.kit.edu
  5. Set a service password
  6. Login on HoreKa with OTP and service password



- **IMPORTANT:** A status report must be provided annually (10-15 pages)!
- More Info: https://www.nhr.kit.edu/userdocs/horeka/projects/

“Exercise”: Register and set password

https://fels.scc.kit.edu

https://login.bwidm.de

https://wiki.bwhpc.de/e/Registration/bwForCluster/Service

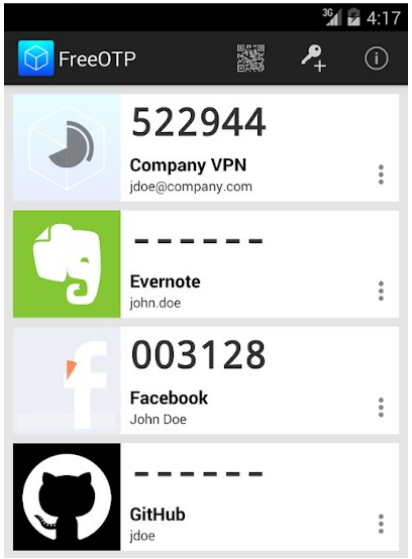
First Steps - 2FA

Two-Factor Authentication - 2FA (1)

- Besides your password you need a second factor,

  → the Time-dependent One-Time Password (TOTP), in order to log into any HPC system

- TOTPs can be generated by *Token*
  - an app on your smartphone or tablet, e.g.
    - FreeOTP for Android or iOS
    - Google Authenticator for Android or iOS
  - an app running on an additional PC / notebook, e.g.
    - Authy for Mac, Windows or Linux
  - a hardware token, e.g.
    - Yubikey



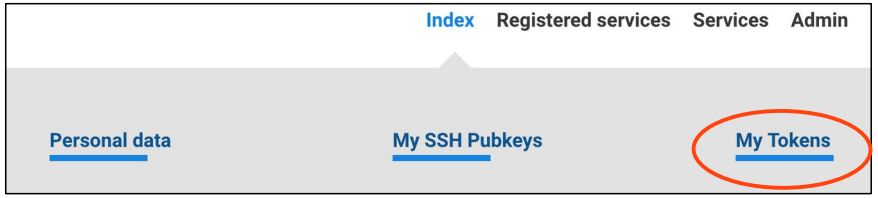
IMPORTANT: the device that generates the One-Time Passwords and the device for the cluster login **must not** be same!

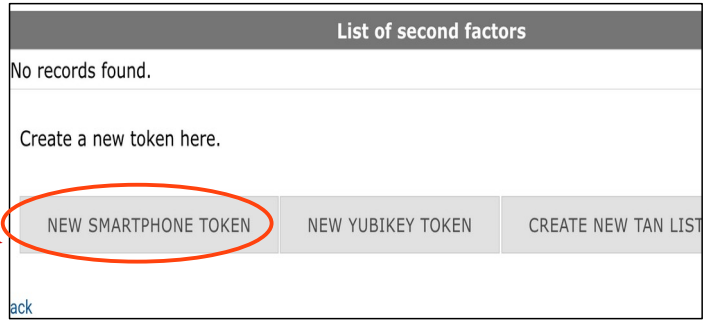
2FA: Registration of your token (1)

- Before usage:
  - Token has to be synchronized/registered with a central server

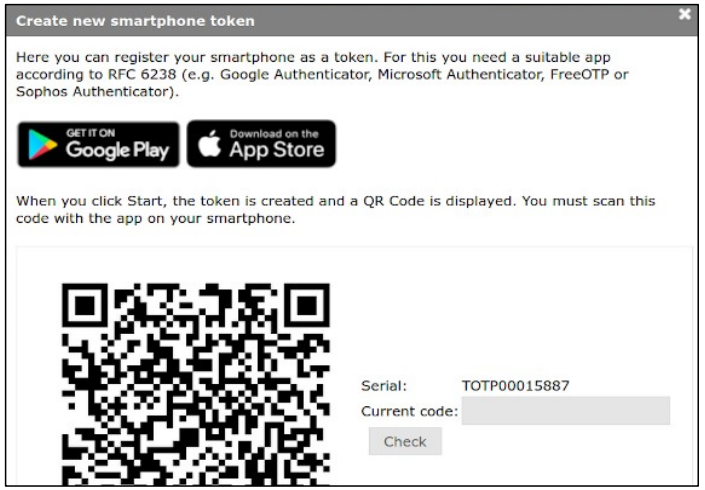
- 1. Login to
  - https://login.bwidm.de (BWUC3)
  - https://fels.scc.kit.edu (HoreKa)

  Go to „My Tokens“
- 2. Click on „New smartphone token“





3. A new windows opens.
Click on „Start“ to generate a new QR code.
This may take a while.

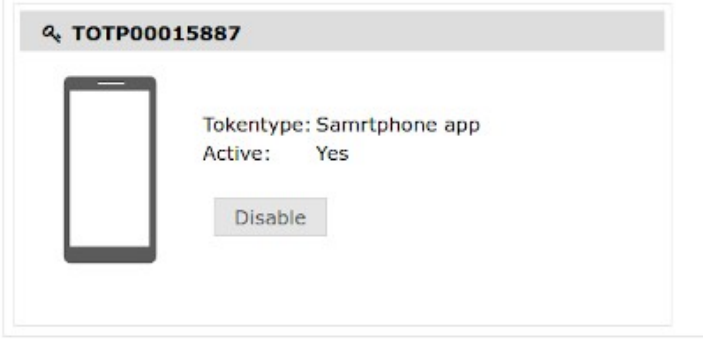


2FA: Registration of your token (2)

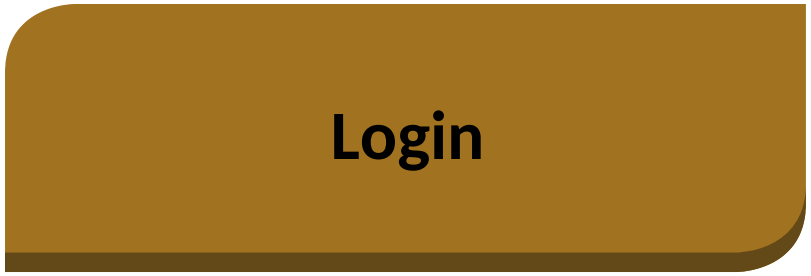
4. Scan QR code with your token app

- Once done, it generate an endless stream of (six-digit) values that can be used as a second value besides the normal account password.

5. Check your token, use „Check“, and compare list of active tokens under https://login.bwidm.de (bwUC3) / https://fels.scc.kit.edu (HoreKa)



6. Please register at least a Backup TAN list in addition to the hardware/software token if you only register a single token!


Login

Login Procedure - HoreKa

Virtual Private Network

- Cluster access is limited to IP addresses from the so-called BelWü networks
  - If outside: connect first via VPN to your home organisation

MS Windows

- **GUI:** MobaXterm, ~~PuTTY~~
- Connection via **SSH**

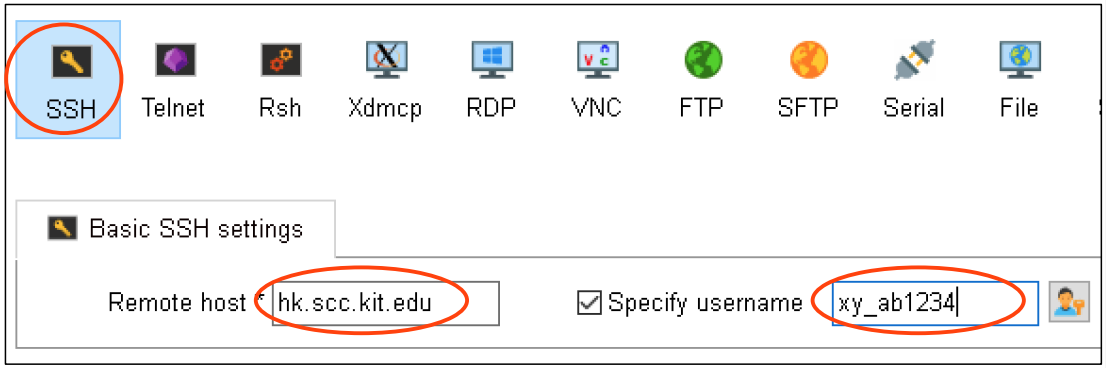
  UserID: ***prefix_username***

  Host, e.g. HoreKa:

  hk.scc.kit.edu

  or

  horeka.scc.kit.edu



Linux / macOS

- Command line interface (**CLI**): use terminal etc.

```
$ ssh -X xy_ab1234@hk.scc.kit.edu
```

Login Procedure – bwUniCluster 3.0

Virtual Private Network

- Cluster access is limited to IP addresses from the so-called BelWü networks
  - If outside: connect first via VPN to your home organisation

MS Windows

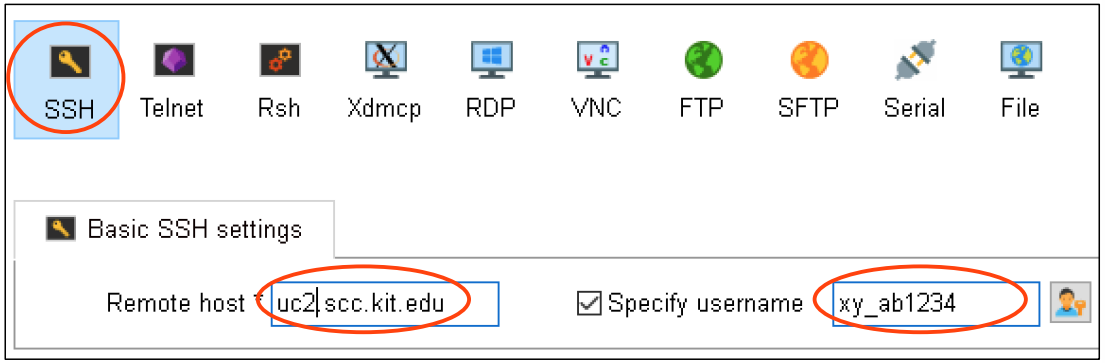
- **GUI:** MobaXterm, ~~PuTTY~~
- New Session

  Connection via **SSH**

  UserID: ***prefix*_username**

  Host, e.g. bwUniCluster:

  uc3.scc.kit.edu



Linux / macOS

- Command line interface (**CLI**): use terminal etc.

```
$ ssh -X xy_ab1234@uc3.scc.kit.edu
```

Login Procedure – bwUniCluster 3.0 and HoreKa

Virtual Private Network

- Cluster access is limited to IP addresses from the so-called BelWü networks
  - If outside: connect first via VPN to your home organisation

MS Windows

- **GUI:** MobaXterm, ~~PuTTY~~
- Connection via **SSH**

  UserID: ***prefix*_username**

  Host, e.g. bwUniCluster:

  uc3.scc.kit.edu

Linux / macOS

- Command line interface (**CLI**):

```
$ ssh -X xy_ab1234@uc3.scc.kit.edu
```

MS Windows

- **GUI:** MobaXterm, ~~PuTTY~~
- Connection via **SSH**

  UserID: ***prefix*_username**

  Host, e.g. HoreKa:

  hk.scc.kit.edu

  or

  horeka.scc.kit.edu

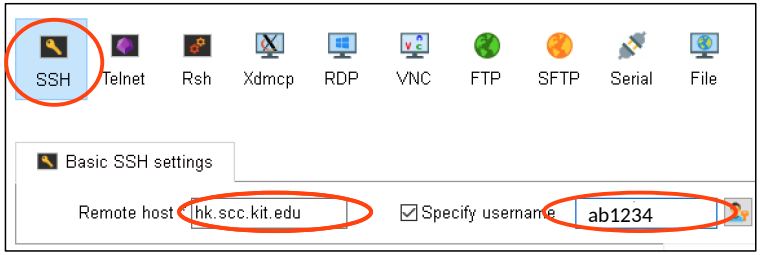
Linux / macOS

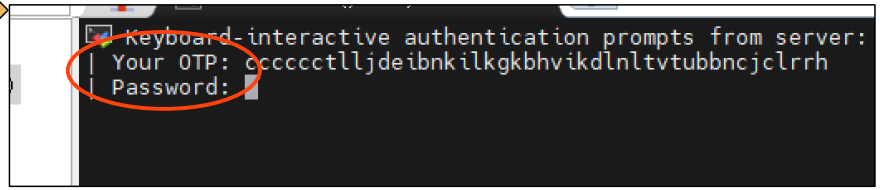
- Command line interface (**CLI**):

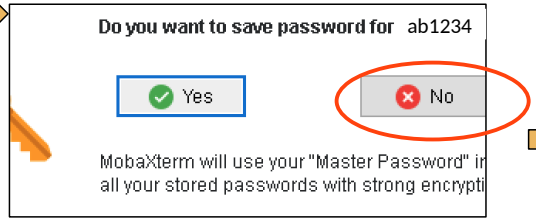
```
$ ssh -X xy_ab1234@hk.scc.kit.edu
```

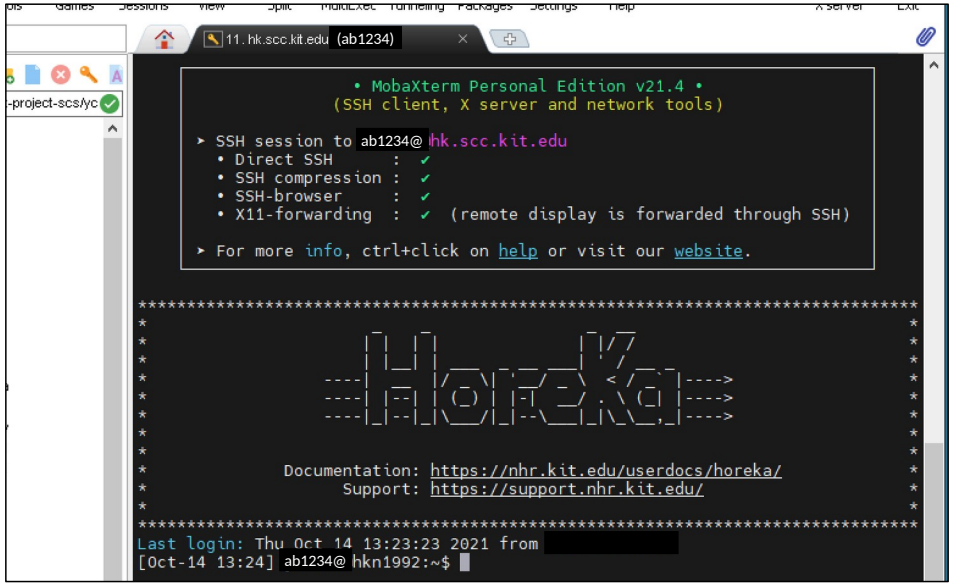
Login: GUI – MS Windows - HoreKa

- Preference: MobaXterm





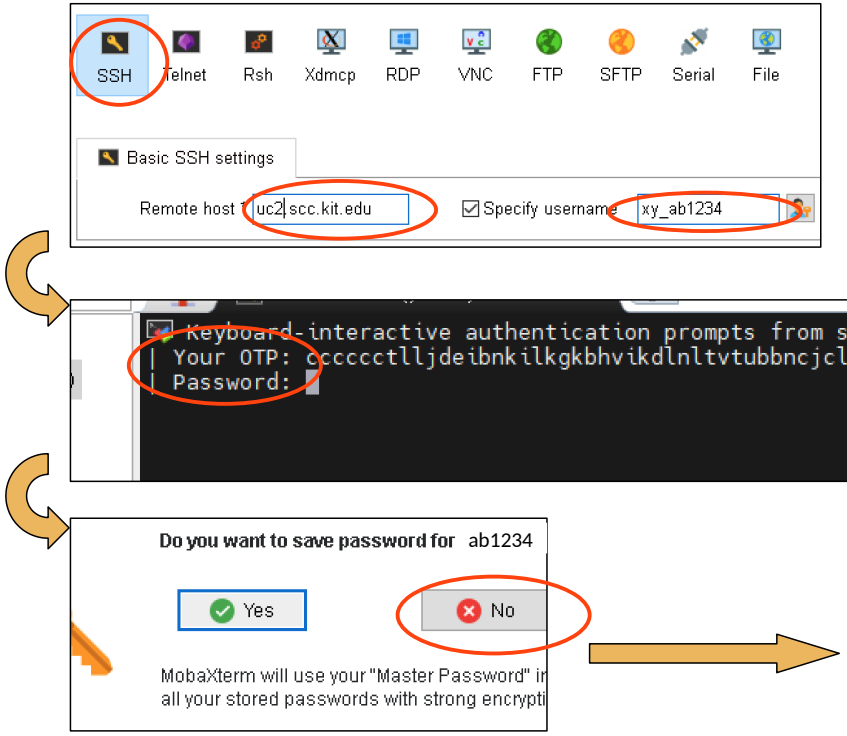




- Under „User Sessions“ double click on:
  - hk.scc.kit.edu (ab1234)
- Type in your OTP + Password
- Do not save password

Login: GUI – MS Windows – bwUniCluster 3.0

- Preference: MobaXterm



- Under „User Sessions“ double click on:
  - uc3.scc.kit.edu (ab1234)
- Type in your OTP + Password
- Do not save password

X11 Tunneling

- Run programs at the cluster, display the GUI at home.
- Linux / macOS

```
$ ssh -X xy_ab1234@hk.scc.kit.edu
```
enables X11 forwarding

```
$ ssh -Y xy_ab1234@hk.scc.kit.edu
```
enables trusted X11 forwarding

```
$ ssh -X -C xy_ab1234@hk.scc.kit.edu
```
adds compression to improve slow connections

- MS Windows
  - MobaXterm automatically starts X server

- BUT: For interacting with graphical applications on the Cluster better use:

  → Remote visualization

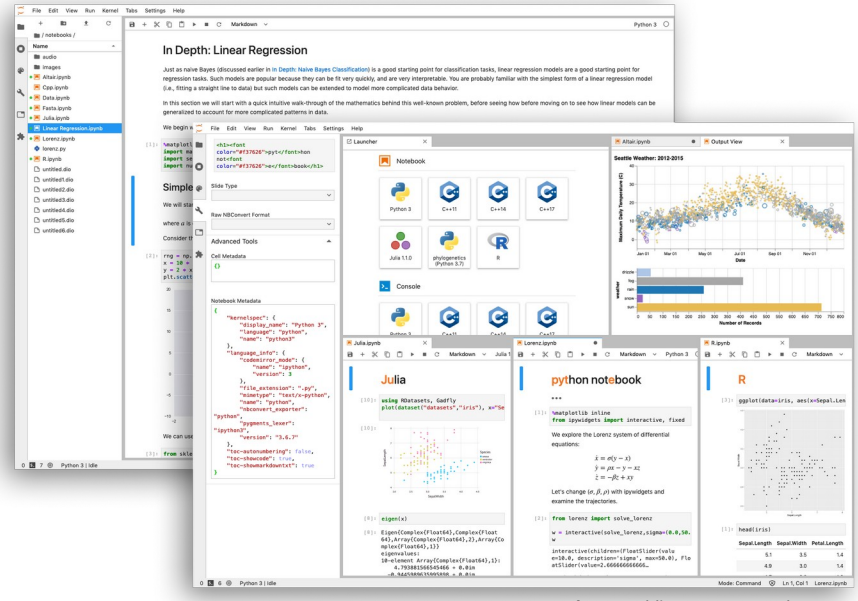
Jupyter

Jupyter

Interactive computing, teaching, prototyping

- HPC access with web browser

- **Jupyter notebook**
  - Executable code cells + any HTML element (text, images, videos, …)
- **JupyterLab**
  - Interactive development environment
  - Handling of multiple notebooks
- **JupyterHub**
  - Management of compute resources



https://jupyter.org/

Jupyter

Accessing JupyterLab @ KIT

- Accessible from within network of your home organization (VPN from home)
- Landing page
  - https://uc3-jupyter.scc.kit.edu
  - https://hk-jupyter.scc.kit.edu
  - https://haicore-jupyter.scc.kit.edu
- Login
  - Credentials of home organization
  - Second factor: TOTP
- Documentation
  - https://wiki.bwhpc.de/e/Jupyter_at_SCC
  - https://www.nhr.kit.edu/userdocs/jupyter/

File transfer

File transfer - Linux

- **`scp`** = OpenSSH secure file copy

```
Push: $ scp [options] SRC [USER@]HOST:DEST
Pull: $ scp [options]     [USER@]HOST:SRC  [DEST]
```

- **`rsync`** = fast file-copying tool
  - superior to scp, sending only the differences between the source files and the existing files in the destination

```
Push: $ rsync [options] SRC [USER@]HOST:DEST
Pull: $ rsync [options]     [USER@]HOST:SRC  [DEST]
```

- Example: Transfer a single file from your laptop to your HoreKa $HOME directory

```
$ echo 'Test file transfer' > transfer.txt
$ scp transfer.txt xy_ab1234@hk.scc.kit.edu:~

(xy_ab1234@hk.scc.kit.edu) Your OTP:
(xy_ab1234@hk.scc.kit.edu) Password:
transfer.txt                  100%   19     0.7KB/s   00:00
```

File transfer - Linux

- **`scp`** = OpenSSH secure file copy

```
Push: $ scp [options] SRC [USER@]HOST:DEST
Pull: $ scp [options]     [USER@]HOST:SRC  [DEST]
```

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```
Push: $ rsync [options] SRC [USER@]HOST:DEST
Pull: $ rsync [options]     [USER@]HOST:SRC  [DEST]
```

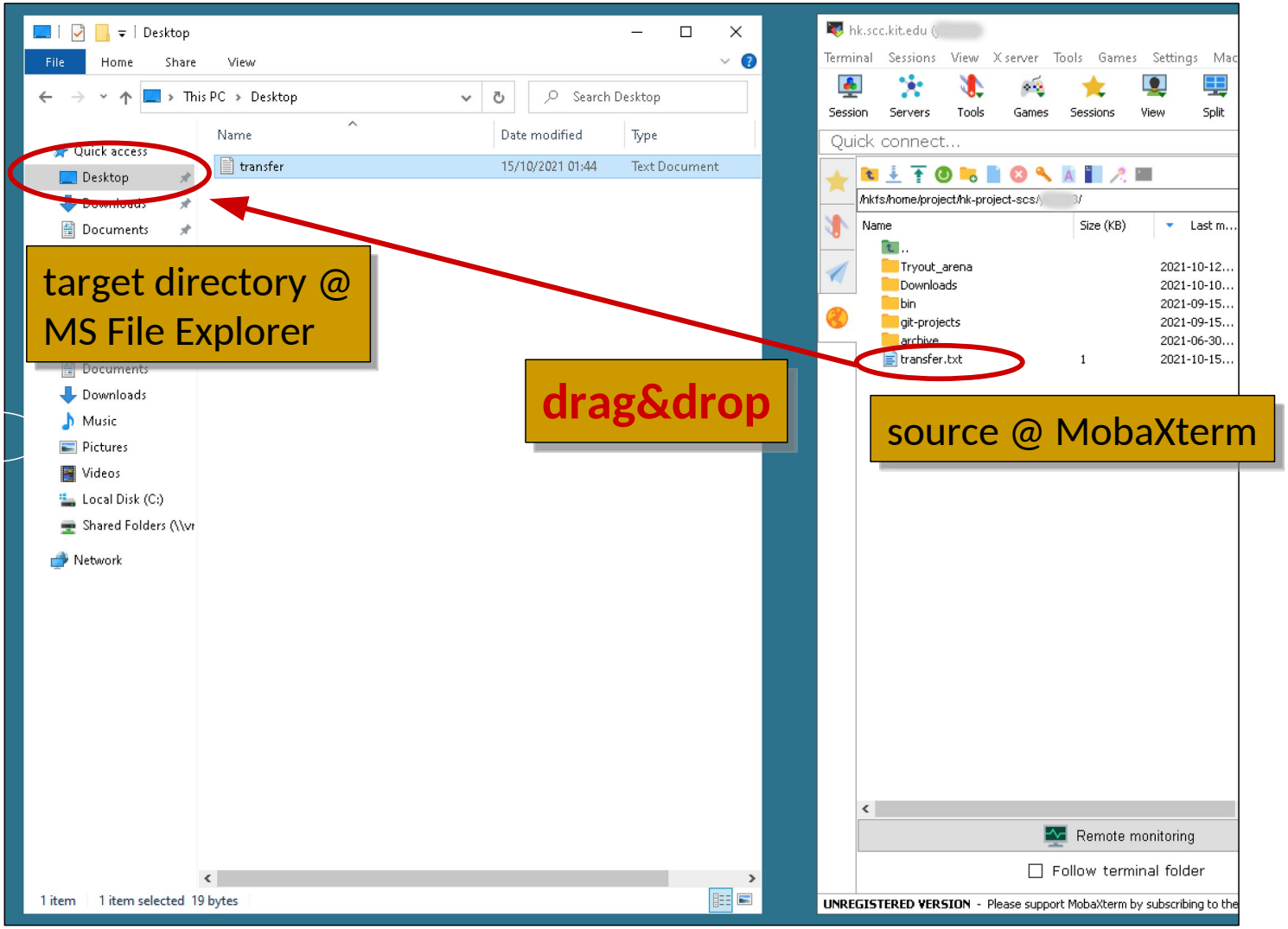
- Example: Transfer a single file from your laptop to your bwUC3 `$HOME` directory

```
$ echo 'Test file transfer' > transfer.txt
$ scp transfer.txt xy_ab1234@uc3.scc.kit.edu:~

(xy_ab1234@uc3.scc.kit.edu) Your OTP:
(xy_ab1234@uc3.scc.kit.edu) Password:
transfer.txt                  100%   19     0.7KB/s   00:00
```

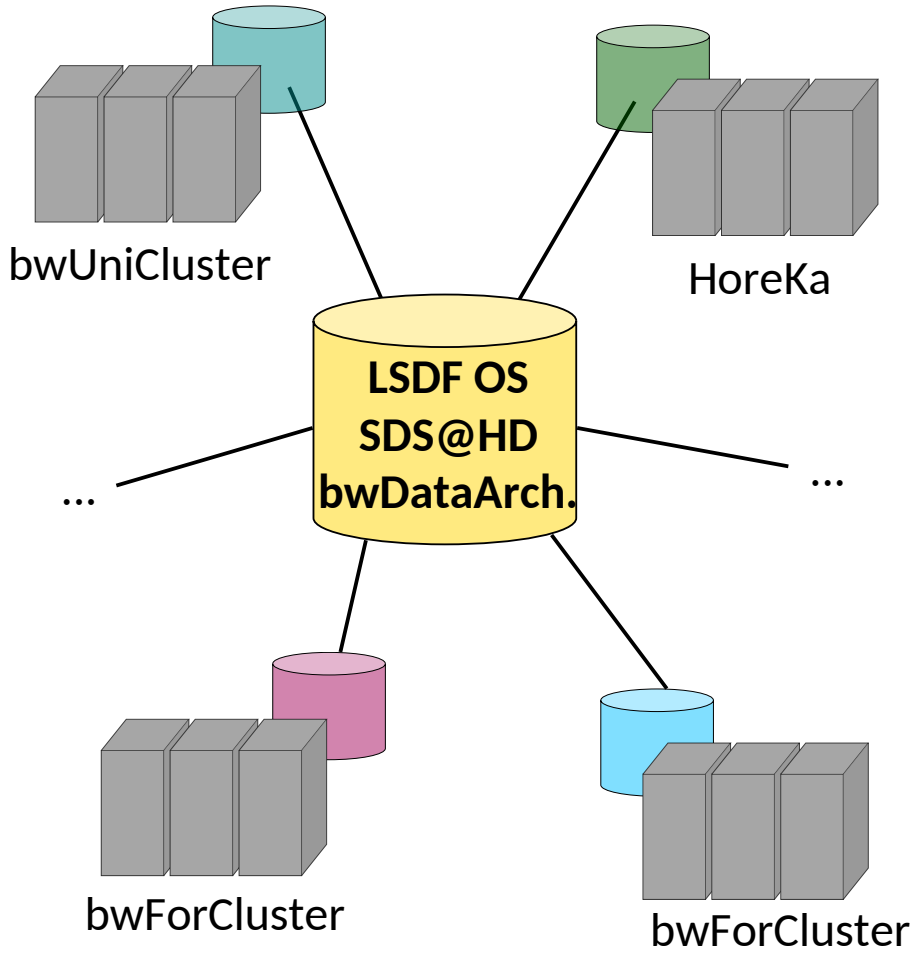
File transfer – MS Windows

- MobaXterm + MS File Explorer



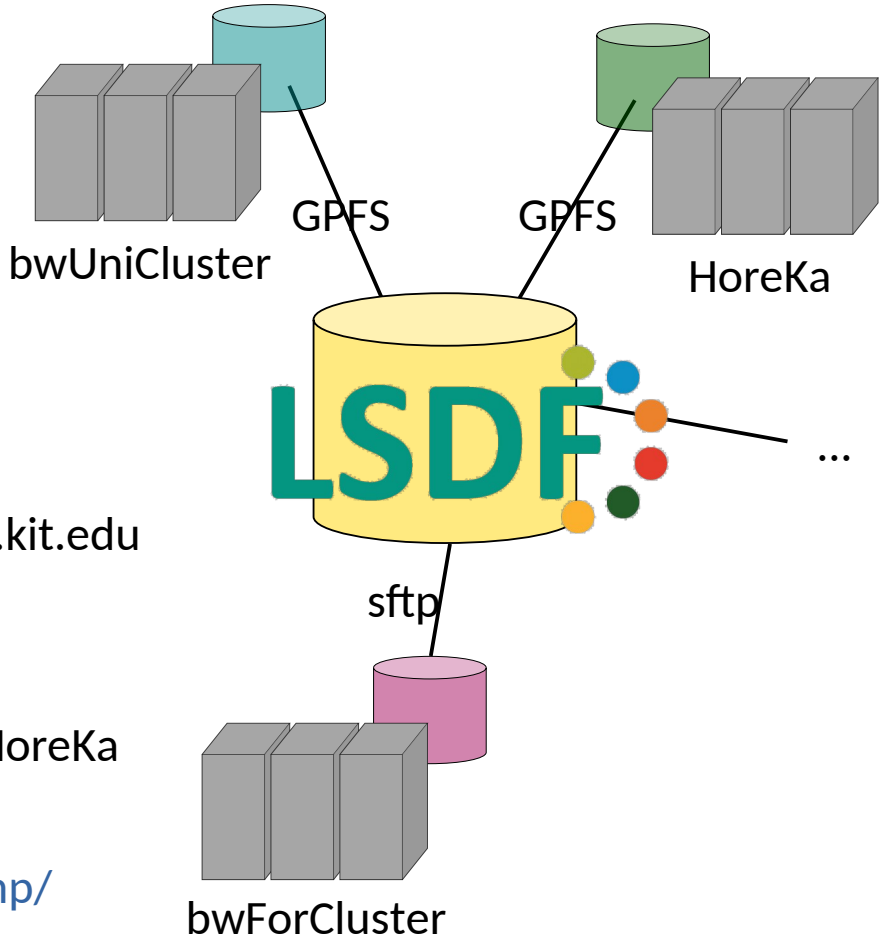
LSDF Online Storage (KIT)
SDS@HD
bwDataArchive

Additional storage for scientific data in BaWü



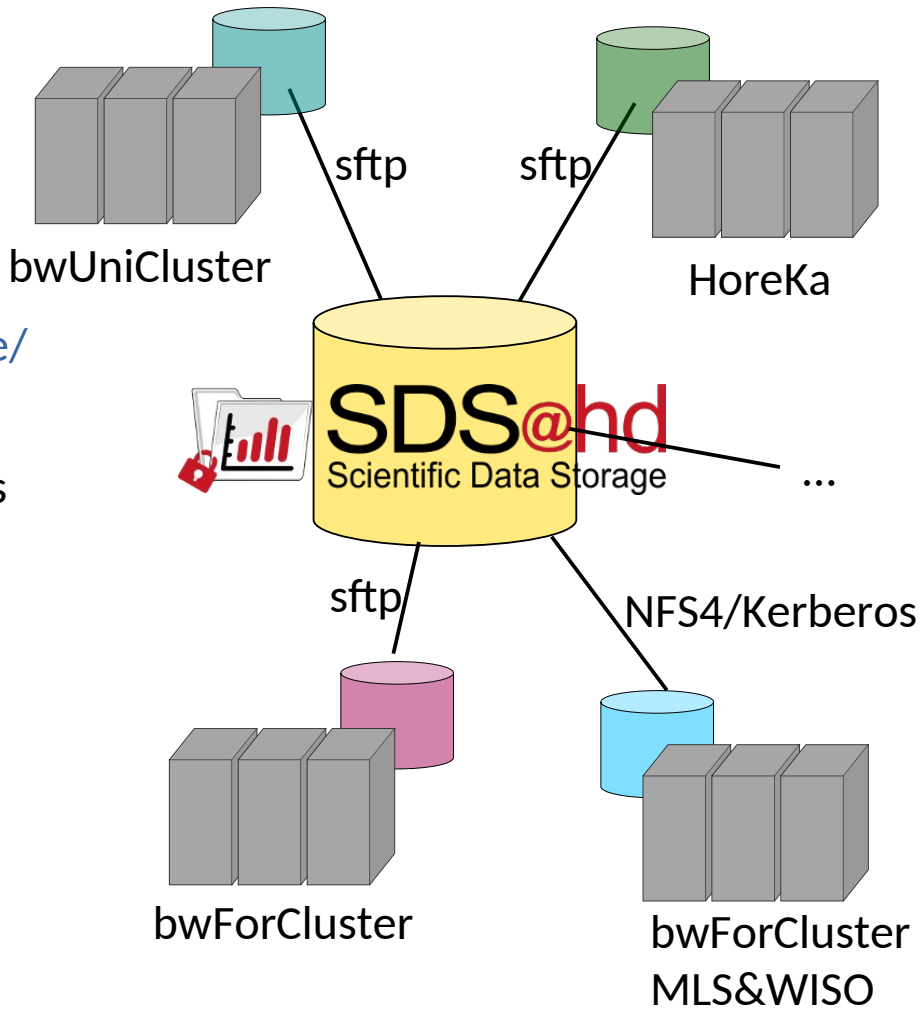
LSDF Online Storage (KIT)

- Central storage located at KIT
- 100GB Soft Limit/400 GB Hard Limit disk space per user
- Registration at
  https://bwidm.scc.kit.edu
- Hosts
  - Via NFS/CIFS: os.lsdf.kit.edu
  - Via SSH/SCP/SFTP: os-login.lsdf.kit.edu
- Transfer tools
  - scp, sftp, rsync, https, ...
- Direct mount on bwUniCluster and HoreKa
- Documentation at
  https://wiki.scc.kit.edu/lsdf/index.php/Category:LSDF_Online_Storage



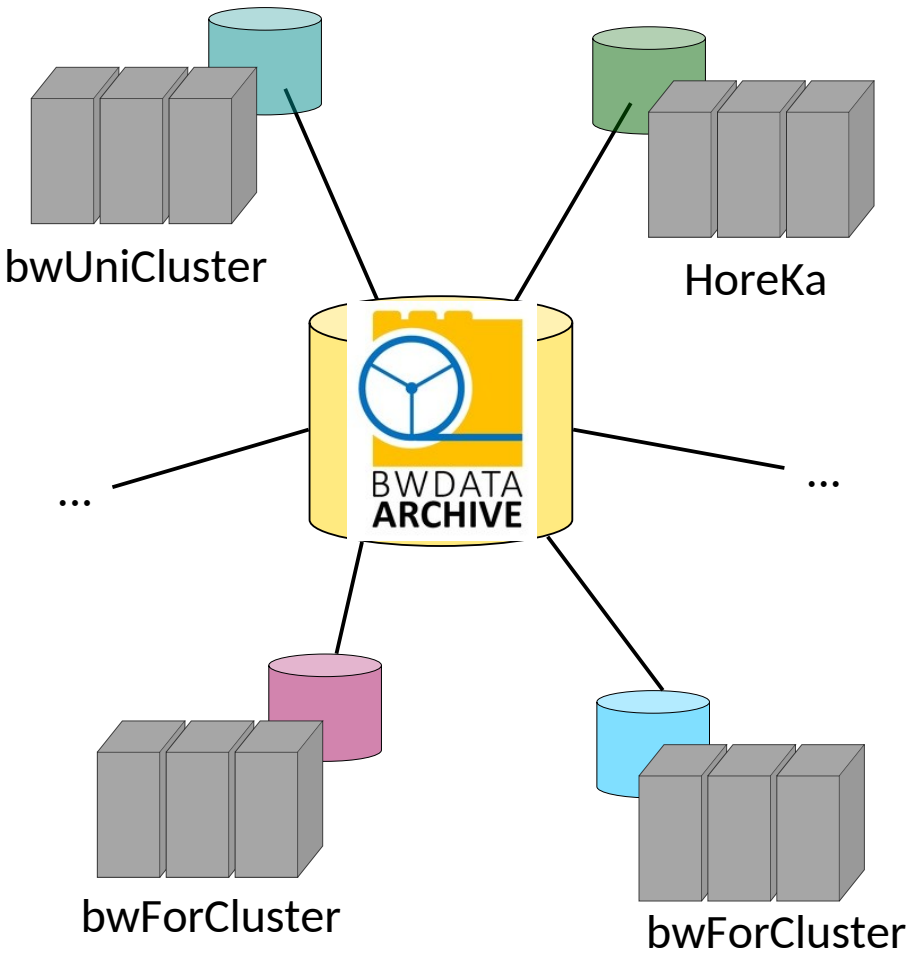
SDS@hd

- Central storage located at HD
- Capacity (March 2020): 11.2 PB
- Registration at
  https://bwservices.uni-heidelberg.de/
- Integration in bwIDM service
- Authentification with LDAP/Kerberos
- Hosts
  - NFSv4
  - SMB
  - sshfs
- Transfer tools
  - sftp
- Documentation at
  https://wiki.bwhpc.de/e/Category:Sds-hd



bwDataArchive

- Long-term data archiving of research data located at KIT
- Magnetic tape storage via HPSS
- Registration at https://www.rda.kit.edu/bwDA/
- Transfer tools
  - sftp
  - GridFTP
- Documentation at https://www.rda.kit.edu



FAQs

Frequently asked questions - bwUniCluster

More Info: https://wiki.bwhpc.de/e/BwUniCluster_3.0_Login#Troubleshooting

Issue: The "Your OTP:" prompt never appears and the connection hangs/times out instead

Likely cause: You are most likely not on a network from which access to the bwUniCluster 2.0 system is allowed. Please check if you might have to establish a VPN connection first.

Issue: The system asks for the One-Time Password multiple times

Likely cause: Make sure you are using the correct Software Token to generate the One-Time Password.

Issue: The system asks for the service password multiple times

Likely cause: Make sure you are using the service password set on bwIDM and not the password valid for your home institution. Unlike the bwUniCluster 1, the bwUniCluster 2.0 only accepts the service password.

Issue: There is an error message by the pam_ses_open.sh skript

Likely cause: Your account is in the "LOST_ACCESS" state because the entitlement is no longer valid, the questionaire was not filled out or there was a problem during the communication between your home institution and the central bwIDM system. Please try the following steps:

- Log into bwIDM, look for the bwUniCluster entry and click on **Registry info**. Your "Status:" should be "ACTIVE". If it is not, please wait for ten minutes since logging into the bwIDM causes a refresh and the problem might fix itself. If the status does not change to ACTIVE after a longer amount of time, please contact the support channels.
- If you have not filled out the questionaire, please do so on https://zas.bwhpc.de/shib/en/bwunicluster_survey.php and then wait for about ten minutes before attempting to log into the HPC system again.

Frequently asked questions - HoreKa

More Info: https://www.nhr.kit.edu/userdocs/horeka/faq/

The connection to HoreKa cannot be established.

Please note that you have to be connected to one of the trusted networks to be able to access HoreKa or HAICORE. If you are not on campus you have to establish a VPN connection to your institution first.

The "Your OTP:" prompt never appears and the connection hangs/times out instead.

The One-Time Password is not being accepted.

There are multiple possible reasons for this:

- The Token was not fully initialized. Please note that that after the QR code has been scanned, an OTP has to be generated and entered back into the web interface to confirm that the token works correctly.
- The One-Time Passwords are time-dependent. Please make sure that the local clock on your device is set correctly.
- Make sure you are using the correct Token to generate the OTP.

The service password is not being accepted.

Please keep in mind that the dedicated service password is different from the account password you are using to log into FeLS.

I have lost my token. Can I register a new one?

There is an error message by the pam_ses_open.sh script.

Your account is most likely in the "LOST_ACCESS" state because the entitlement is no longer valid or there was a problem during the communication between your home institution and the central bwIDM system. Please try the following steps:

Log into FeLS, look for the FH2 entry and click on Registry info. Your "Status:" should be "ACTIVE". If it is not, please wait for ten minutes since logging into the bwIDM causes a refresh and the problem might fix itself. If the status does not change to ACTIVE after a longer amount of time, please contact the support channels.