

Access Procedures: bwHPC Clusters + NHR@KIT

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ulm university universität
uulm



Outline

- Registration Processes
 - bwUniCluster 2.0
 - 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 2.0

- 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



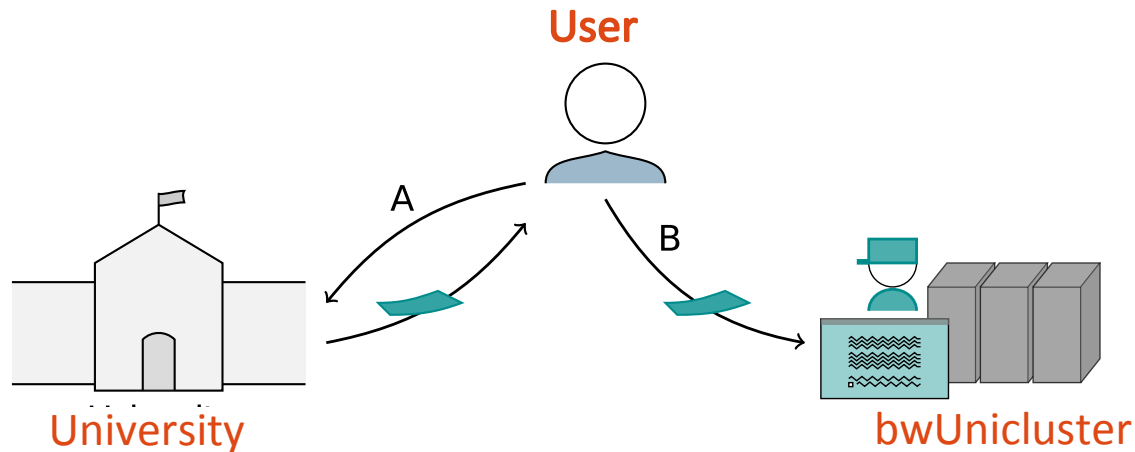
■ bwForCluster (JUSTUS 2, Helix, NEMO, BinAC)

- 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 2.0

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



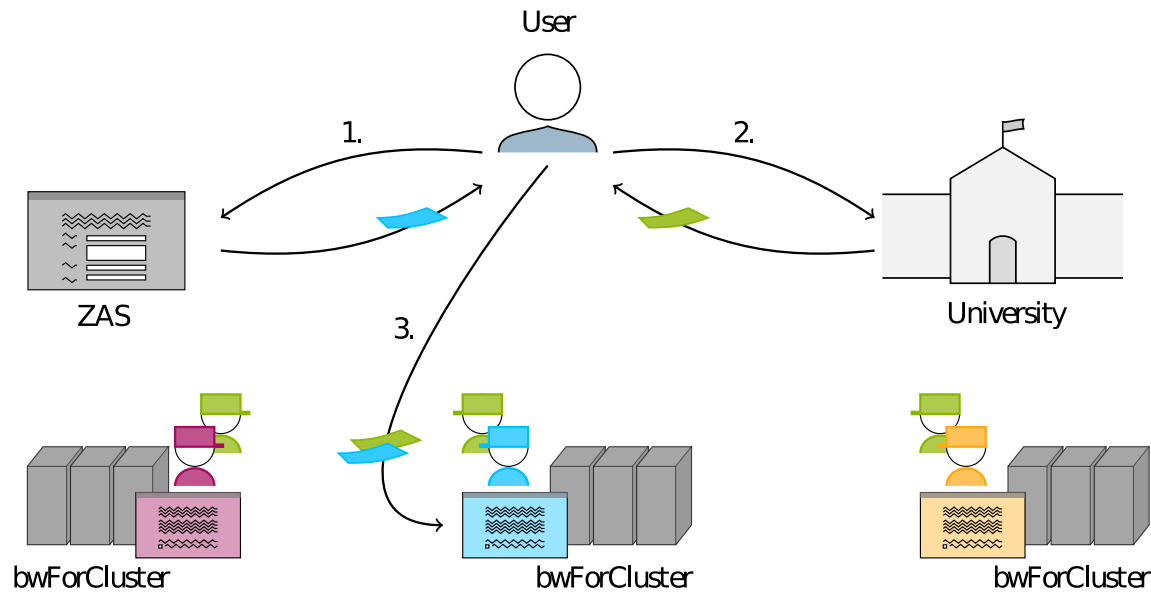
Step A: Obtainment of bwUniCluster entitlement

- 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

Registration Process – bwForClusters (short version)



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

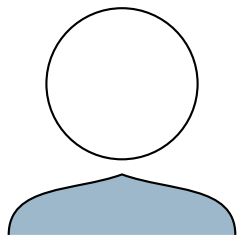
■ Approval  of Cluster Assignment Team (CAT)

Step 2: Get bwForCluster entitlement  by own university

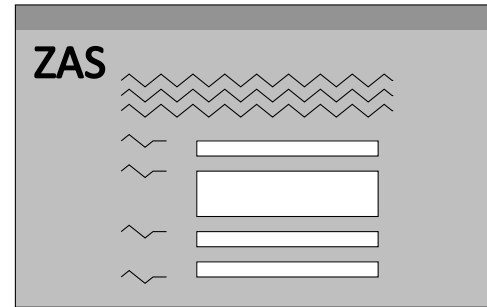
Step 3: Web registration at designated bwForCluster site

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

Registration Process: bwForCluster – Step 1a

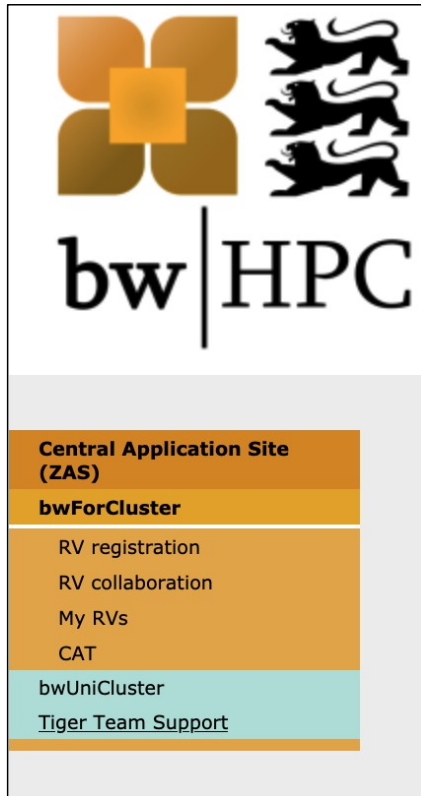


RV registration



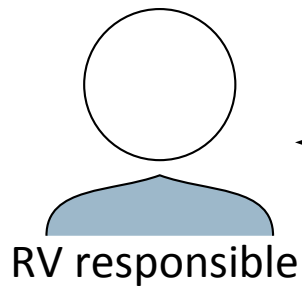
Central Application Site for bwHPC

zas.bwhpc.de

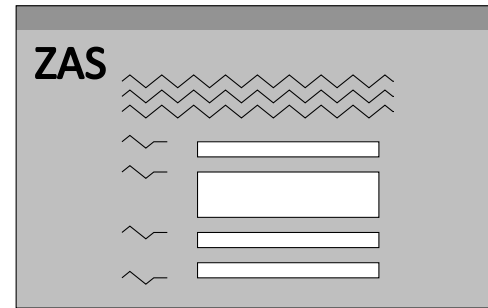


- Web interface of HPC clusters (in the state BW) to handle the user compute activities.
- Nomenclature:
 - RV = Planned compute activities (Rechenvorhaben).
 - RV Responsible: The person who does the registration of of the RV (applicant)
 - Cluster Assignment Team: aka CAT; assigns to one fitting cluster 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

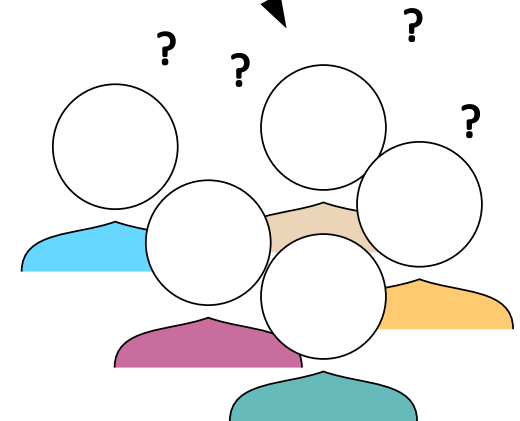
Registration Process: bwForClusters – Step 1b



← acronym / password

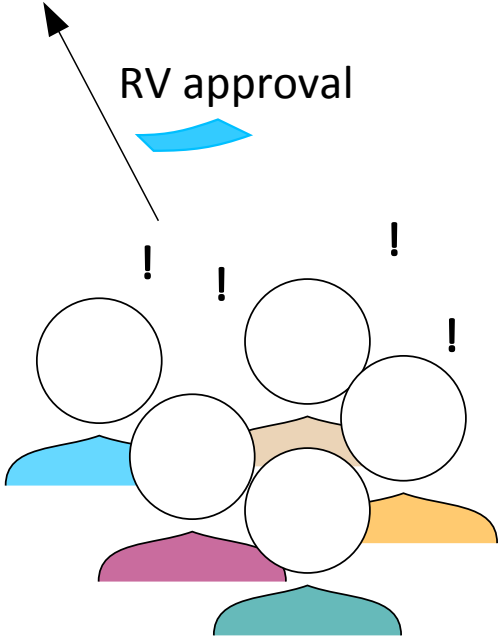
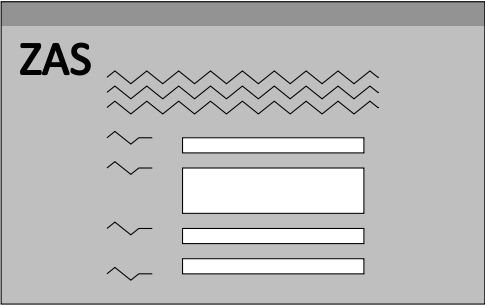
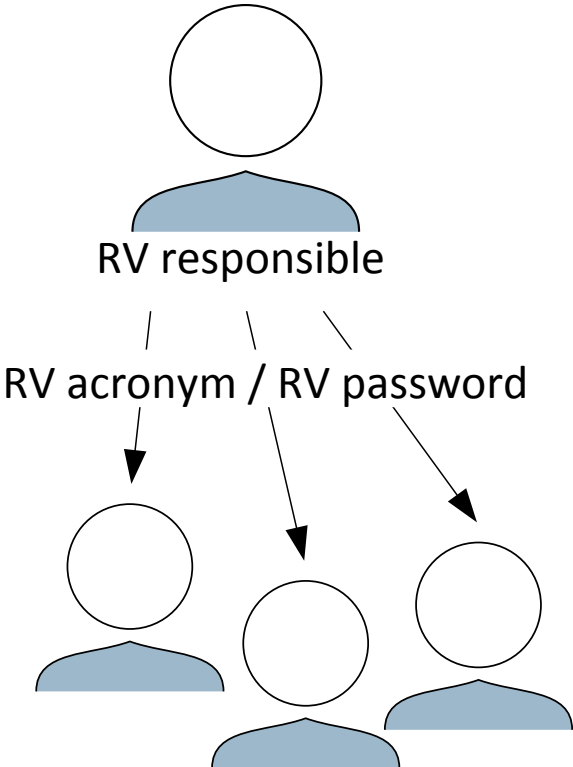


RV application



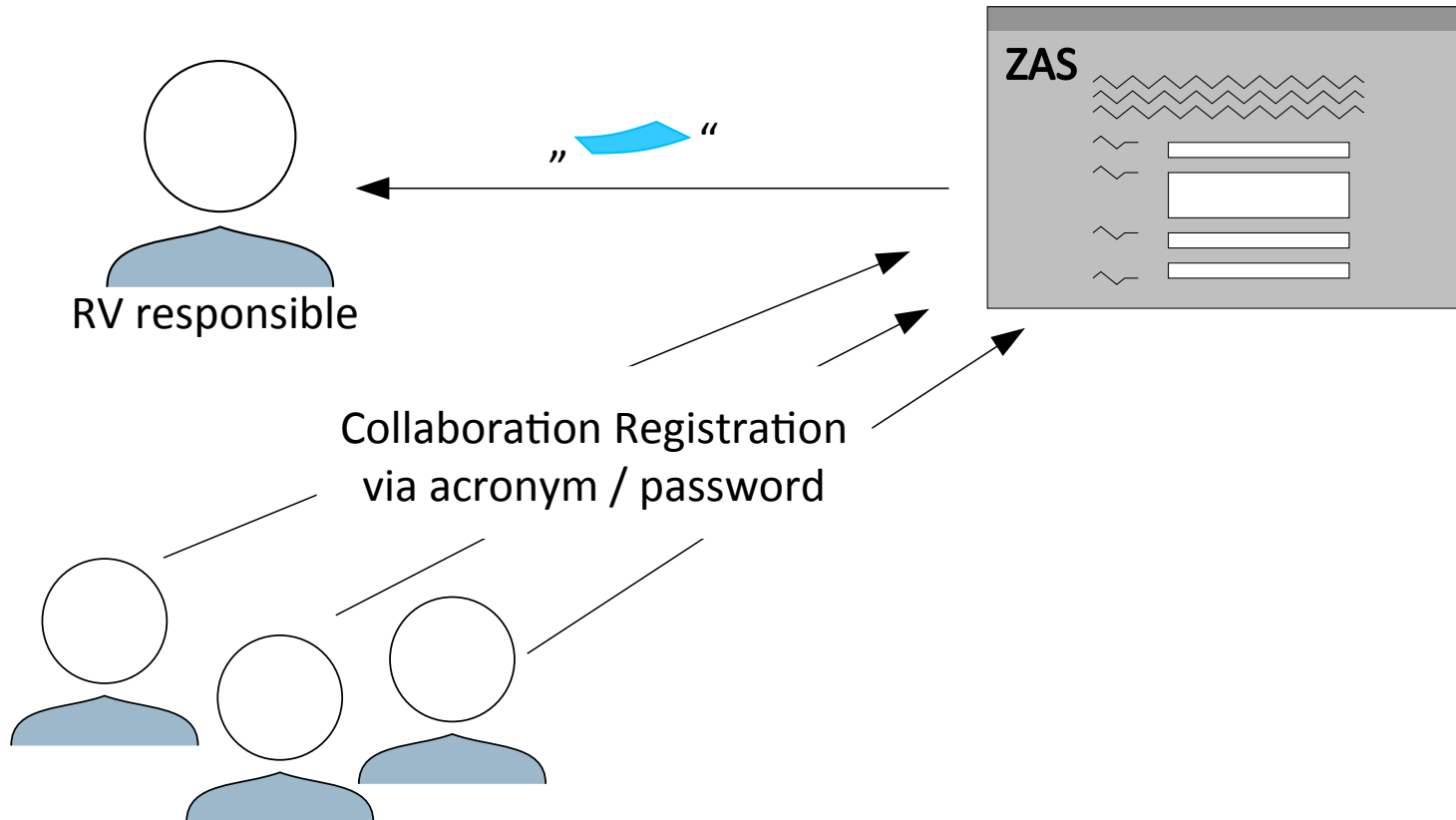
CAT (Cluster Assignment Team)

Registration Process: bwForClusters Step 1c

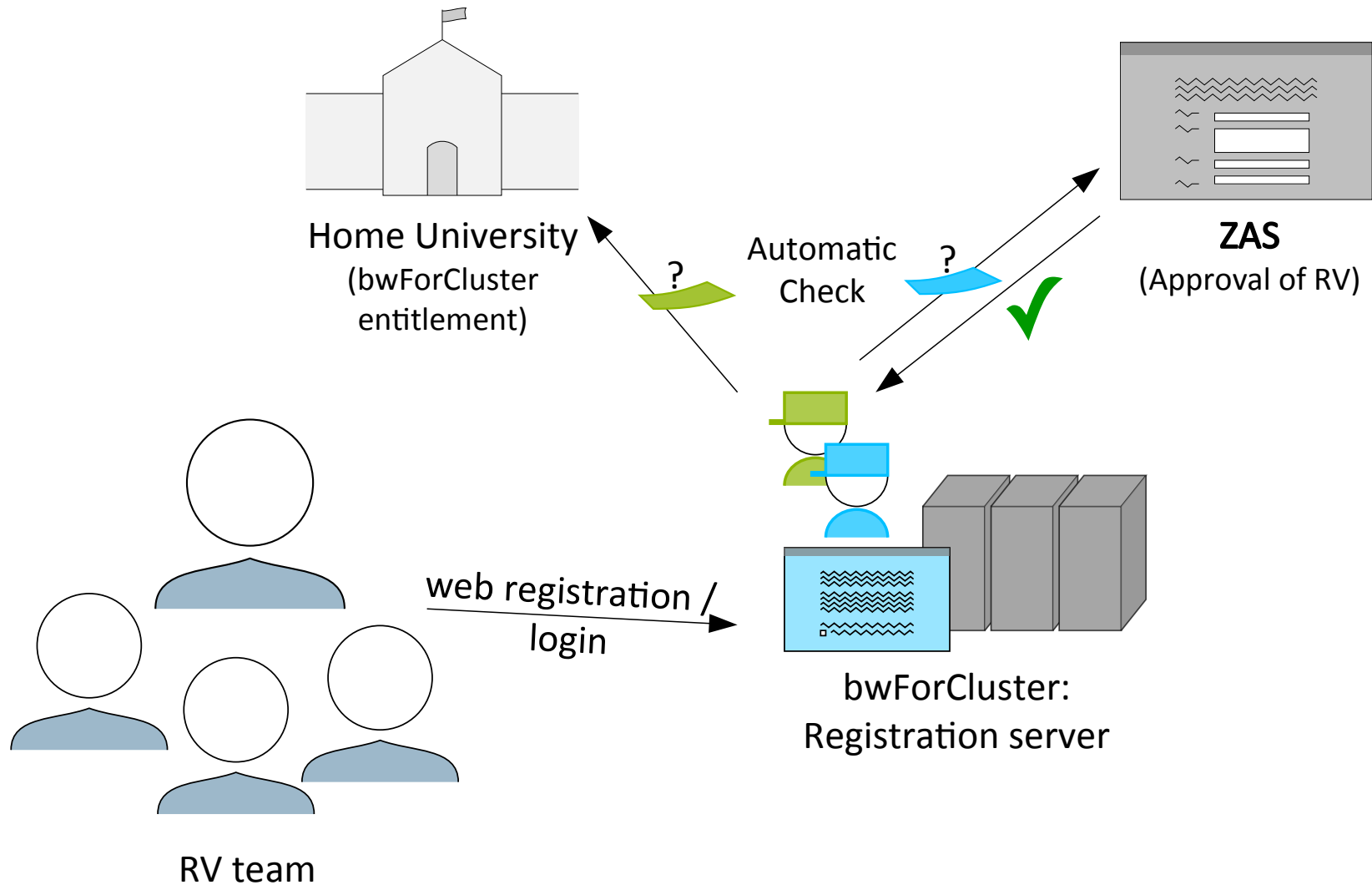


CAT (Cluster Assignment Team)

Registration Process: bwForClusters – Step 1a



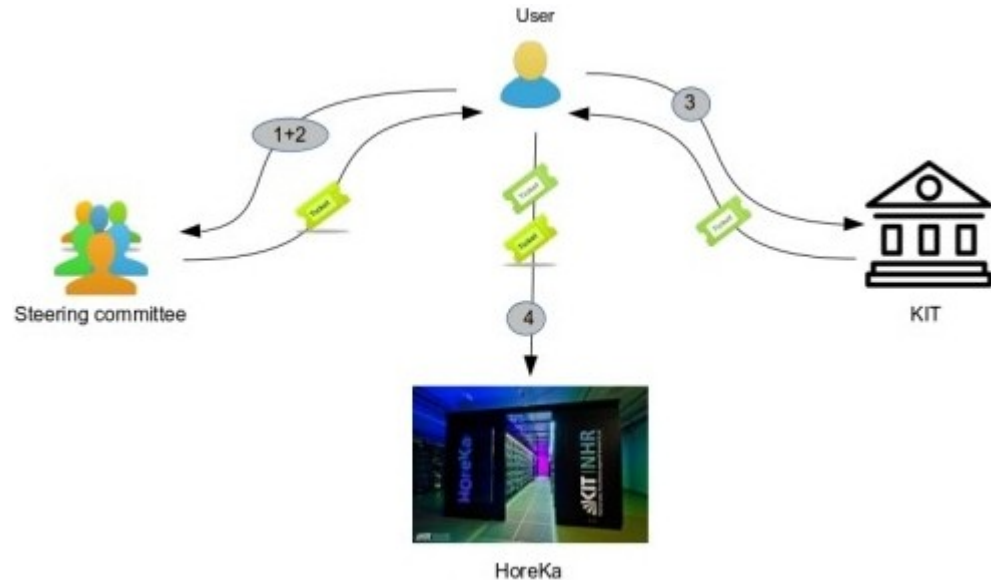
Registration Process: bwForClusters – Step 3



Registration Process – HoreKa

Registration:

1. Online Proposal Form (JARDS)
2. Peer reviewed proposal
3. HoreKa access form
4. Register on web page
<https://fels.scc.kit.edu>



Login:

■ @ HoreKa : `$ ssh <UserID>@hk.scc.kit.edu`

Auto logout

■ Variable “TMOUT” is set for 10 hours.

■ **IMPORTANT:** A status report must be provided annually (10-15 pages)!

Registration Process (2) – HoreKa

Ad 1:

- Fill Online Proposal Form on web page <https://jards.nhr.kit.edu/jards/dev/WEB/>
- Normal project (2-15 mill CPUh / 0.03-0.2 mill GPUh (peer reviewed) or
- Large project (15-70 mill CPUh / 0.2-1 mill GPUh (peer reviewed)
- Test project with unmodifiable 500000 CPUh / 5000 GPUh (review process by SCC)

Ad 2:

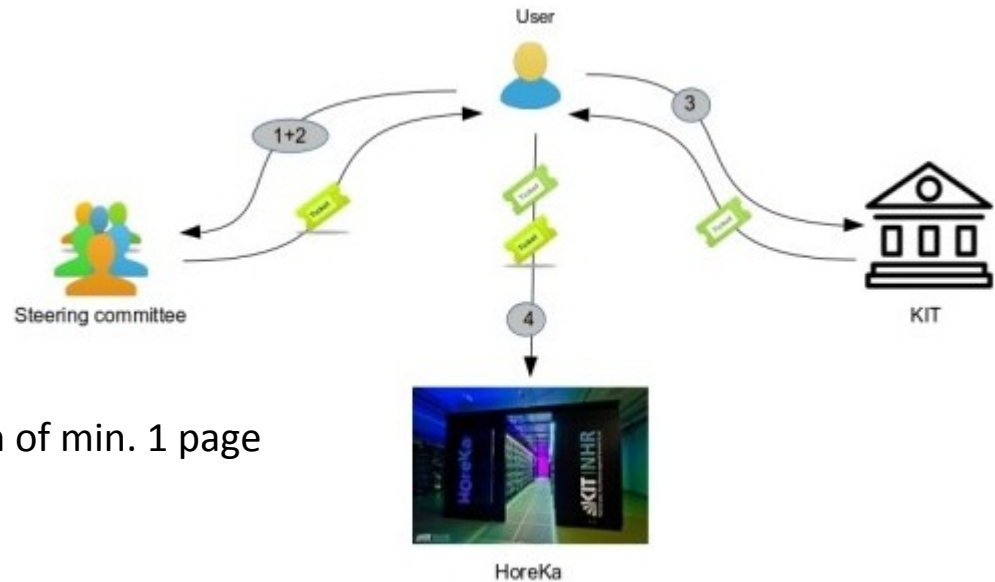
- Write an extended project description of min. 3 pages (N/L project) or
- an extended project description of min. 1 page (Test project)

Ad 3:

- Fill a HoreKa access form for each coworker (except for project manager)

Ad 4:

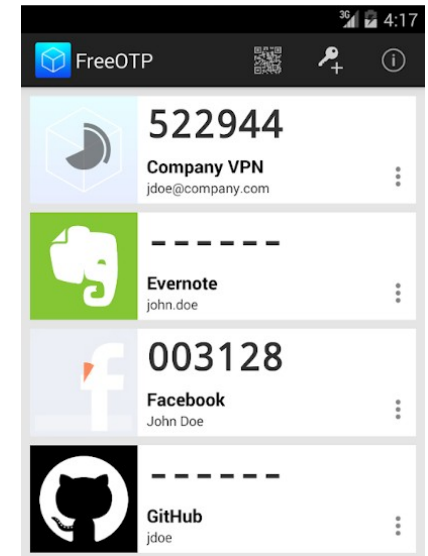
- Register on web page <https://fels.scc.kit.edu> for HoreKa and set a service password
- Login on HoreKa with OTP (2FA) and service password



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



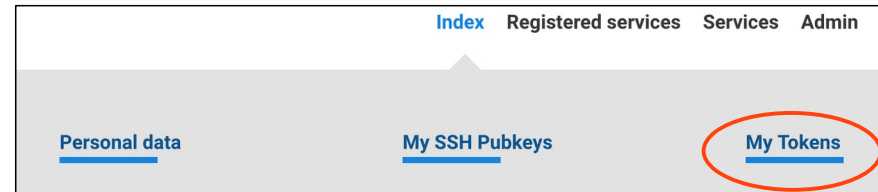
IMPORTANT: the device that generates the One-Time Passwords and the device for the cluster login **must not** be same!

2FA: Registration of your token (1)

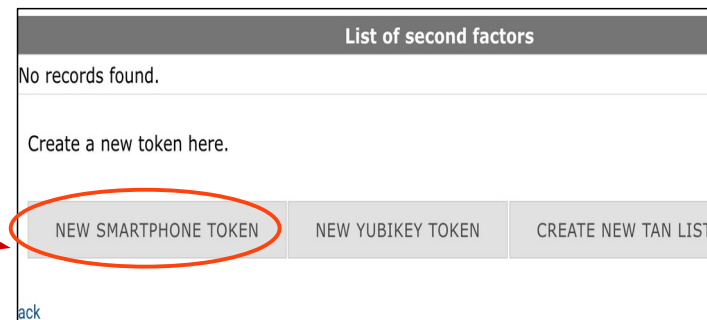
■ Before usage:

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

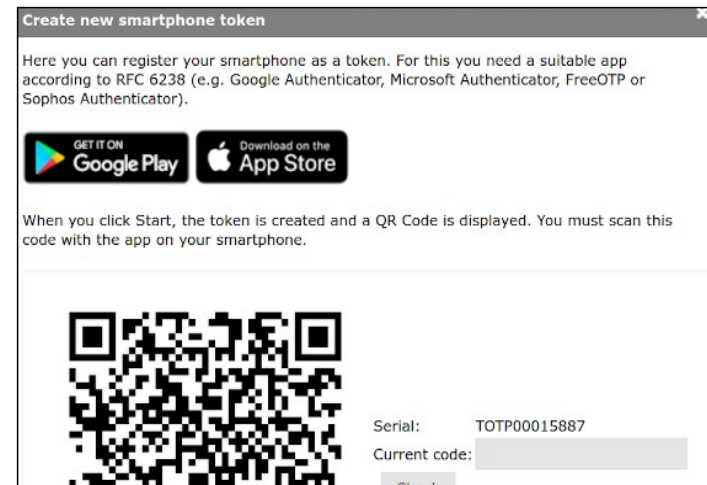
1. Login to <https://login.bwidm.de>
Go to „My Tokens“



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.

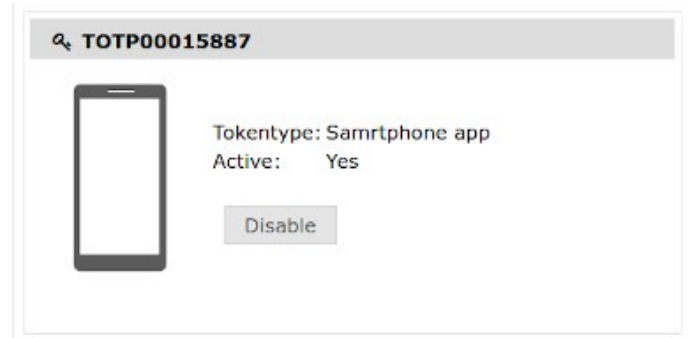


2FA: Registration of your token (2)

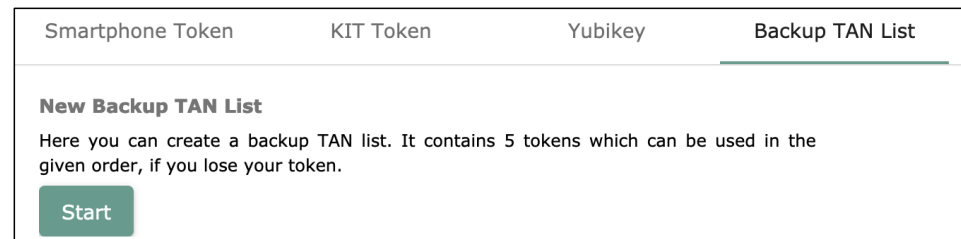
4. Scan QR code with your token app

- 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>



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

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**

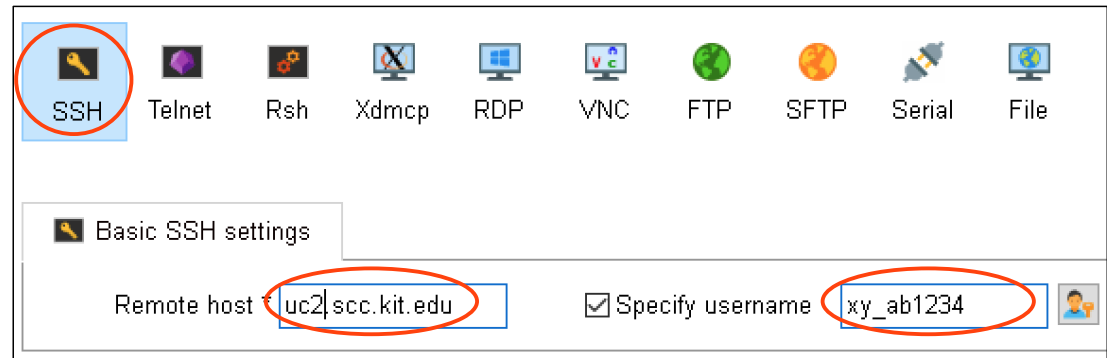
UserID: *prefix_username*

Host, e.g. HoreKa:

uc2.scc.kit.edu

or

bwunicluster.scc.kit.edu



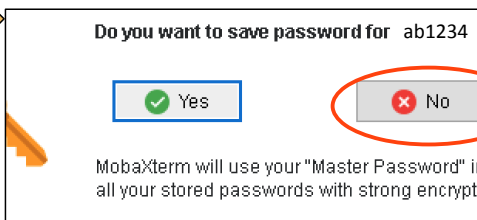
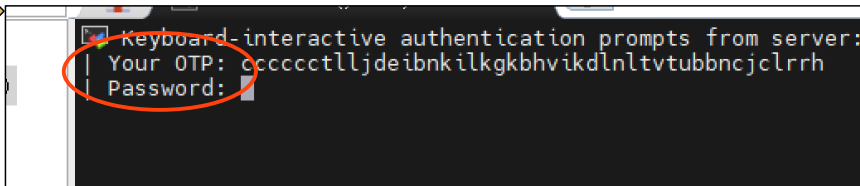
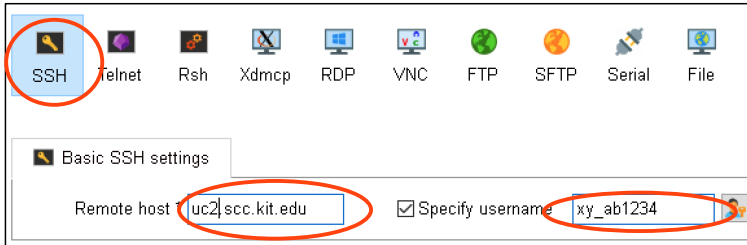
Linux / macOS

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

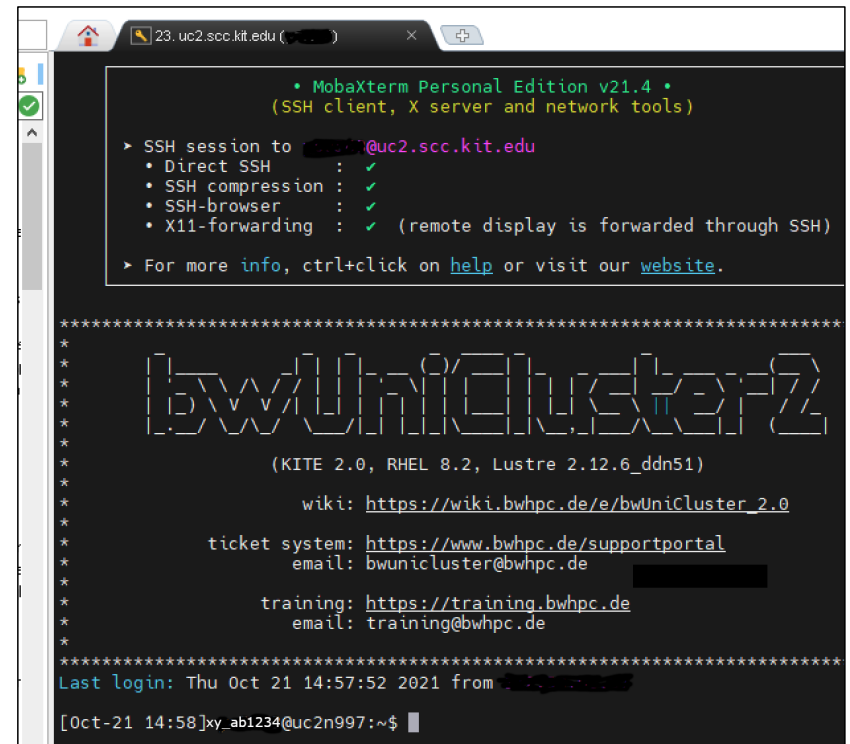
```
$ ssh -X xy_ab1234@uc2.scc.kit.edu
```

Login: GUI – MS Windows

Preference: MobaXterm



- Under „User Sessions“ double click on:
 - uc2.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
```

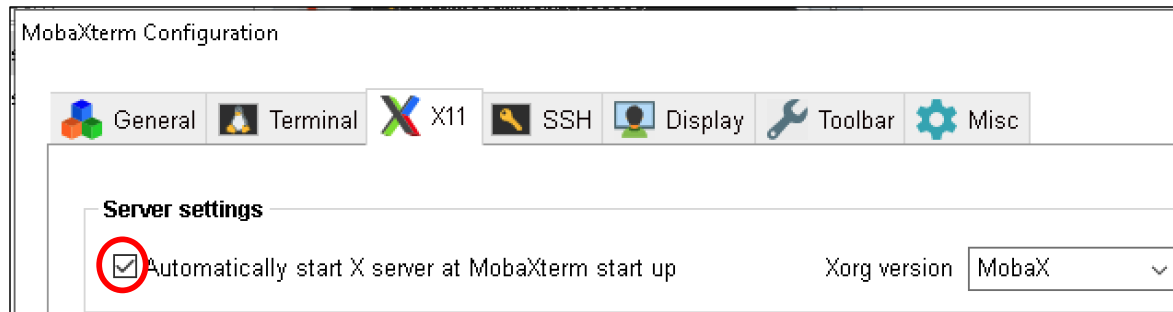
enables trusted X11 forwarding

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

adds compression to improve slow connections

■ MS Windows

- MobaXterm automatically starts X server



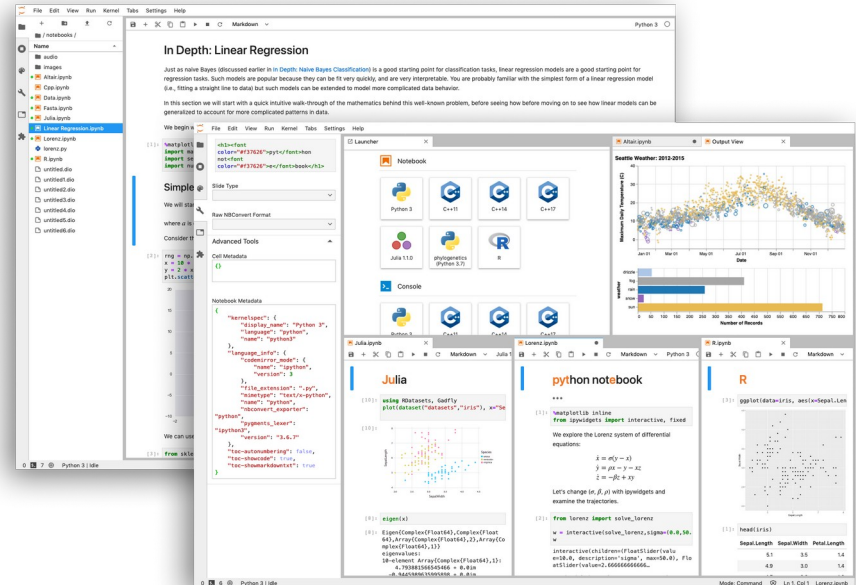
- BUT: For interacting with graphical applications on the Cluster better use:
→ [Remote visualization](#)

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://uc2-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 Cluster \$HOME directory

```
$ echo 'Test file transfer' > transfer.txt
$ scp transfer.txt xy_ab1234@uc2.scc.kit.edu:~
(xy_ab1234@uc2.scc.kit.edu) Your OTP:
(xy_ab1234@uc2.scc.kit.edu) Password:
transfer.txt                100%   19    0.7KB/s   00:00
```

File transfer – MS Windows

MobaXterm + MS File Explorer

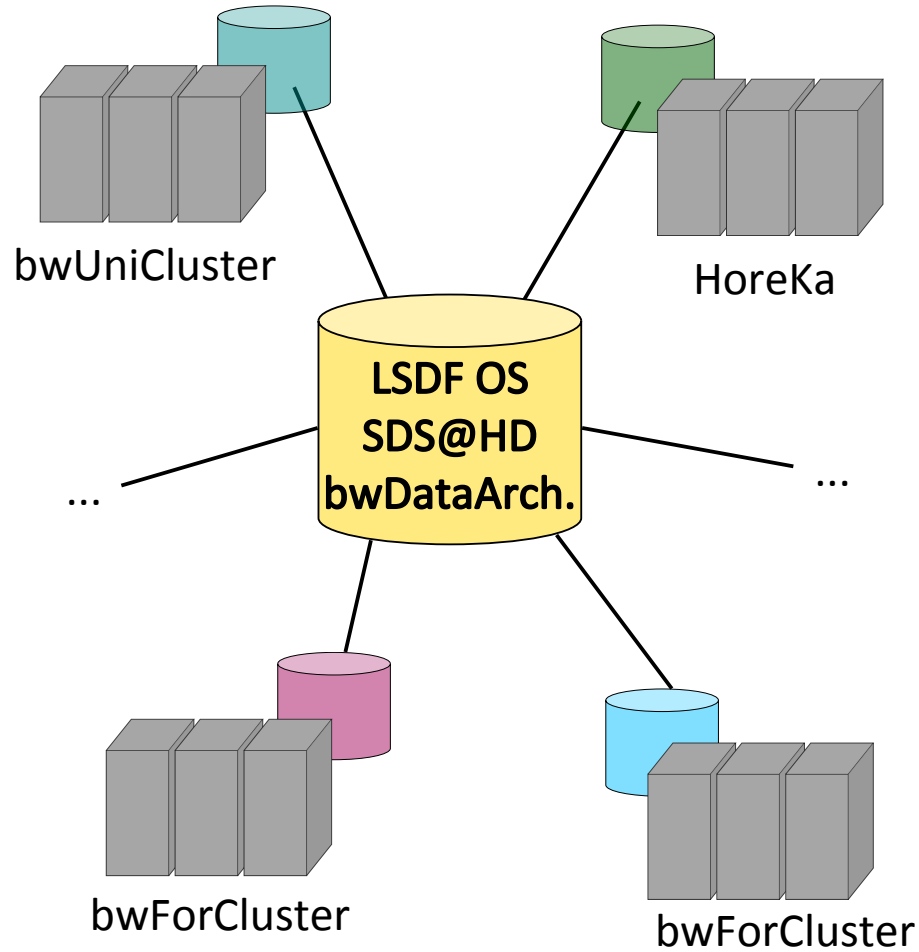
The image shows two windows side-by-side. The left window is MS File Explorer, showing the Desktop directory with a file named 'transfer'. The right window is MobaXterm, showing a remote directory with a file named 'transfer.txt'. A red arrow points from 'transfer.txt' in MobaXterm to 'transfer' in File Explorer. Three yellow callout boxes with red text provide instructions: 'target directory @ MS File Explorer' points to the Desktop folder in File Explorer; 'drag&drop' is in the center; 'source @ MobaXterm' points to 'transfer.txt' in MobaXterm.

Name	Date modified	Type
transfer	15/10/2021 01:44	Text Document

Name	Size (KB)	Last m...
..		
Tryout_arena		2021-10-12...
Downloads		2021-10-10...
bin		2021-09-15...
git-projects		2021-09-15...
archive		2021-06-30...
transfer.txt	1	2021-10-15...

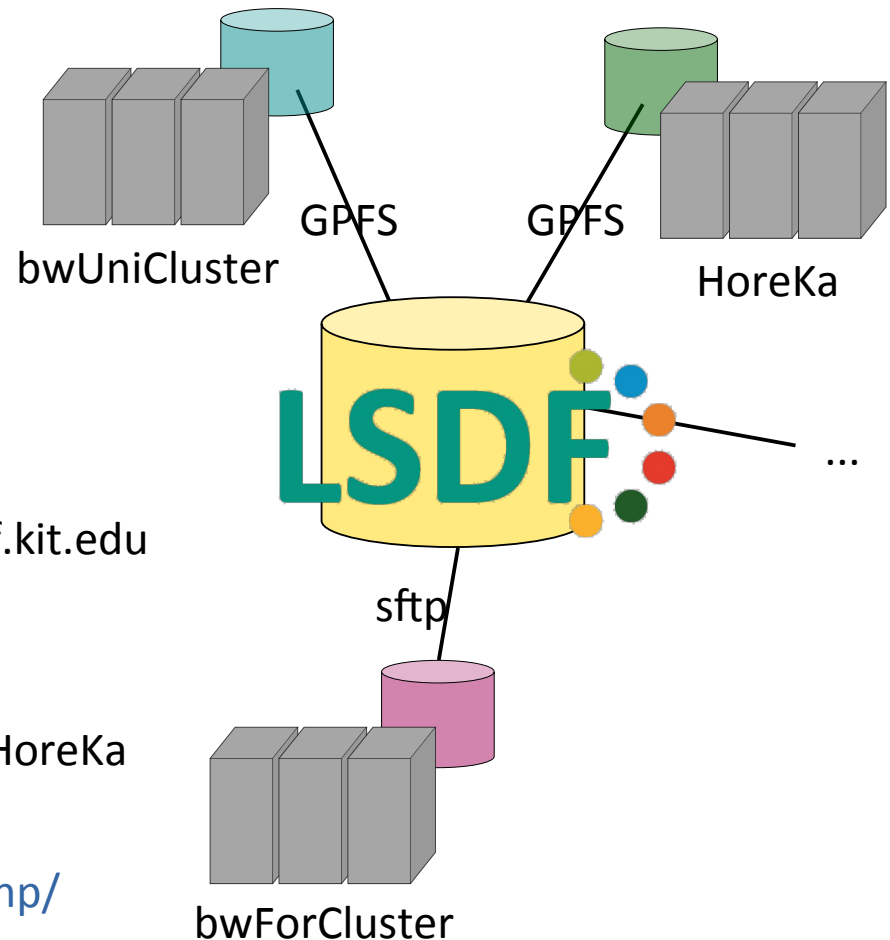
**LSDF Online Storage (KIT)
SDS@HD
bwDataArchive**

Additional storage for scientific data in BaWü



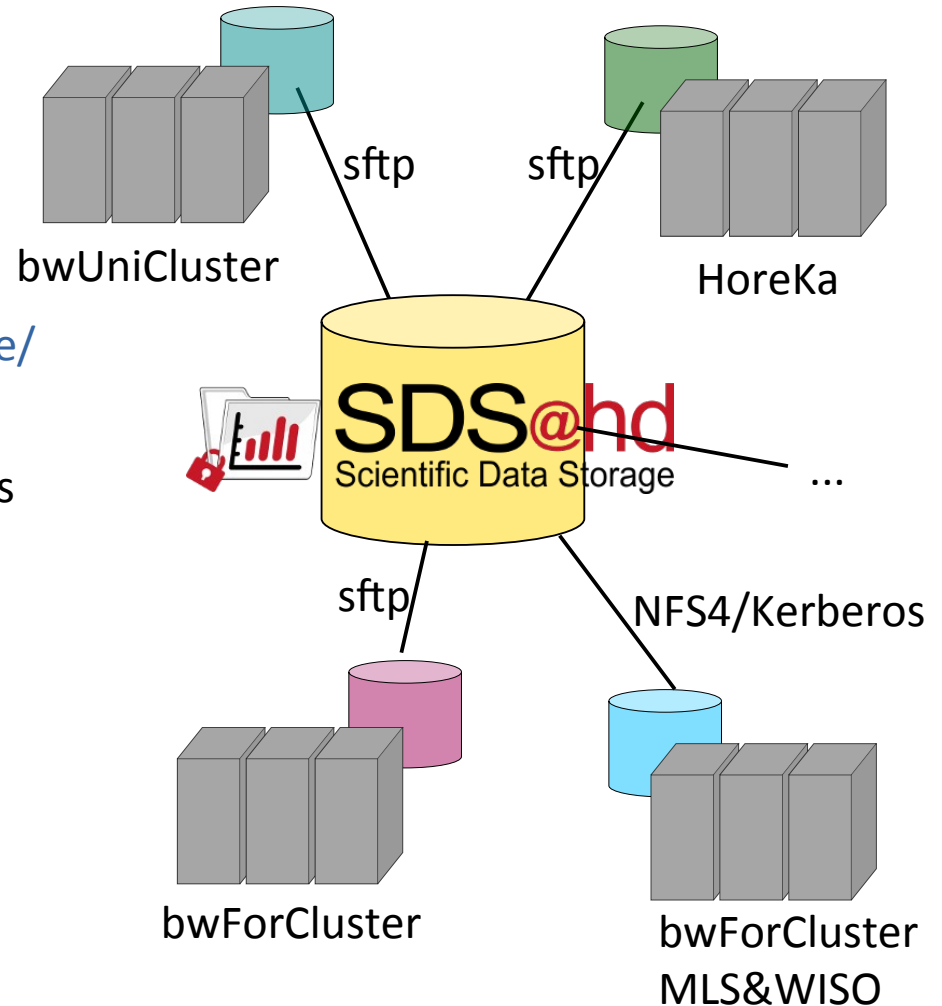
LSDF Online Storage (KIT)

- 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.lsd.f.kit.edu`
 - Via SSH/SCP/SFTP: `os-login.lsd.f.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



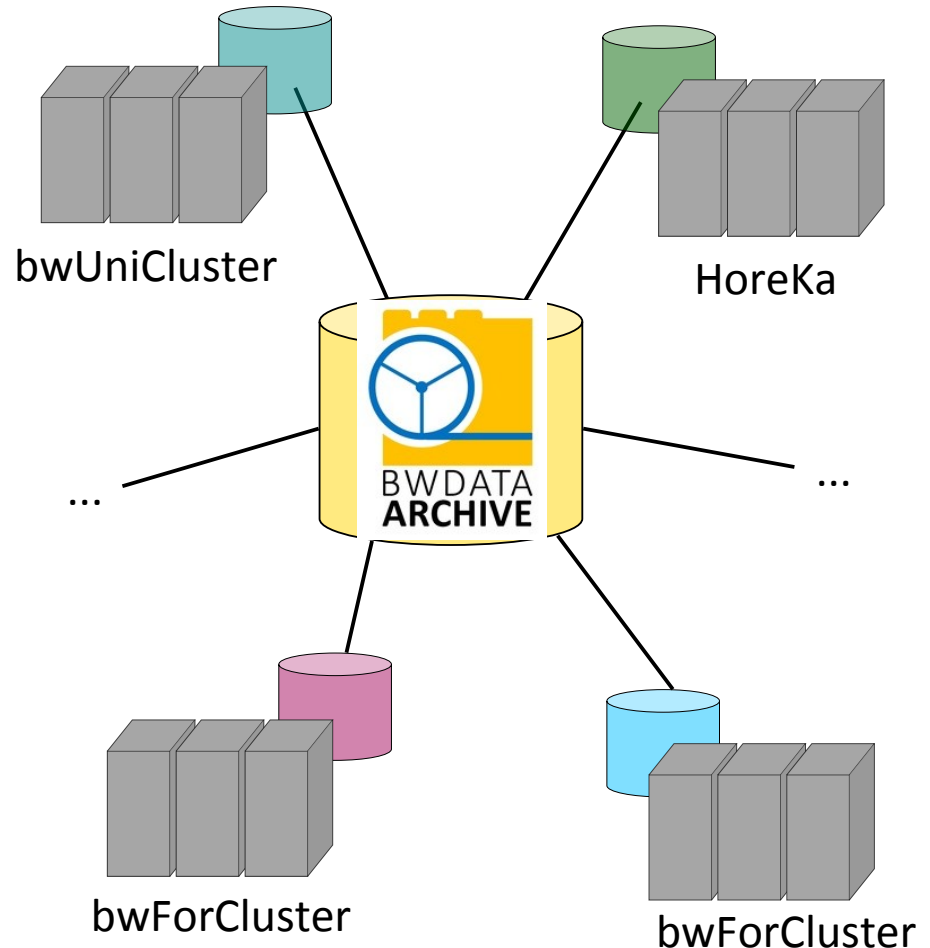
SDS@hd

- Central storage located at HD
- Capacity (March 2020): 11.2 PB
- Registration at <https://bwservices.uni-heidelberg.de/>
- Integration in bwIDM service
- Authentication 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: https://wiki.bwhpc.de/e/BwUniCluster_2.0_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 questionnaire 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 questionnaire, 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.