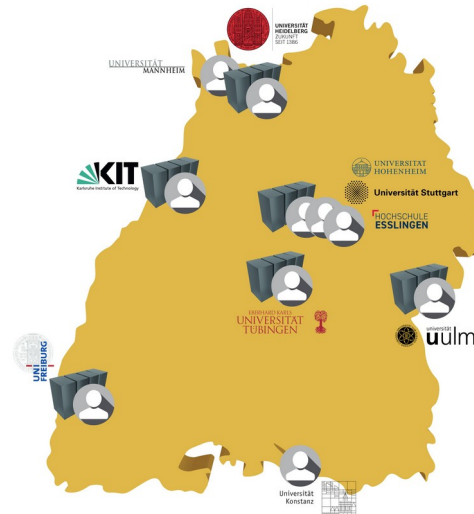


File Systems Introduction

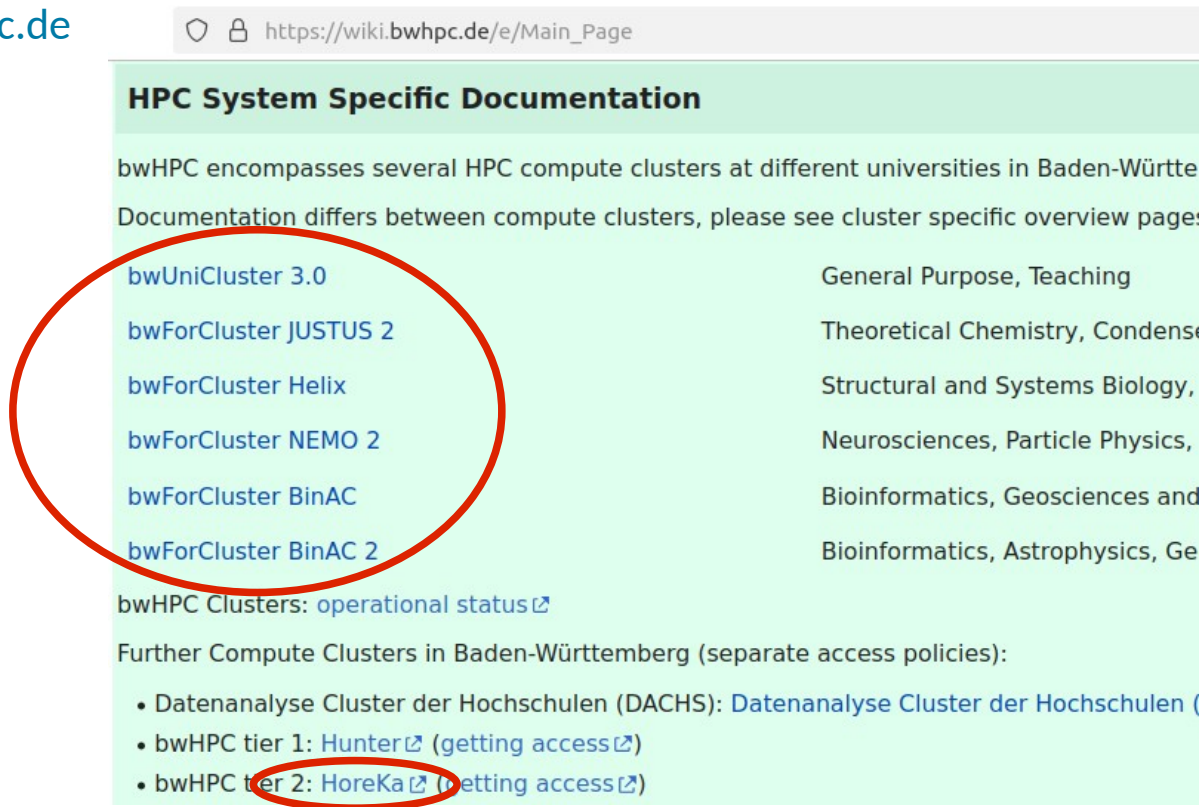
Roland Laifer
KIT, SCC



Reference: bwHPC Wiki

■ Most information given by this talk can be found at <https://wiki.bwhpc.de>

- select cluster
- then select File Systems



The screenshot shows the 'HPC System Specific Documentation' page on the bwHPC Wiki. A red circle highlights a list of compute clusters: bwUniCluster 3.0, bwForCluster JUSTUS 2, bwForCluster Helix, bwForCluster NEMO 2, bwForCluster BinAC, and bwForCluster BinAC 2. To the right of this list, various research areas are listed, such as General Purpose, Teaching, Theoretical Chemistry, Condensed Matter Physics, Structural and Systems Biology, Neurosciences, Particle Physics, Bioinformatics, Geosciences and Earth Sciences, and Bioinformatics, Astrophysics, Geophysics. Below the cluster list, there is a link to 'bwHPC Clusters: operational status' and a section for 'Further Compute Clusters in Baden-Württemberg (separate access policies)' which includes links to 'Datenanalyse Cluster der Hochschulen (DACHS)', 'bwHPC tier 1: Hunter', and 'bwHPC tier 2: HoreKa'. The 'HoreKa' link is also circled in red.

https://wiki.bwhpc.de/e/Main_Page

HPC System Specific Documentation

bwHPC encompasses several HPC compute clusters at different universities in Baden-Württemberg. Documentation differs between compute clusters, please see cluster specific overview pages:

bwUniCluster 3.0	General Purpose, Teaching
bwForCluster JUSTUS 2	Theoretical Chemistry, Condensed Matter Physics
bwForCluster Helix	Structural and Systems Biology, Bioinformatics
bwForCluster NEMO 2	Neurosciences, Particle Physics, Bioinformatics
bwForCluster BinAC	Bioinformatics, Geosciences and Earth Sciences
bwForCluster BinAC 2	Bioinformatics, Astrophysics, Geophysics

[bwHPC Clusters: operational status](#)

Further Compute Clusters in Baden-Württemberg (separate access policies):

- Datenanalyse Cluster der Hochschulen (DACHS): [Datenanalyse Cluster der Hochschulen \(DACHS\)](#)
- bwHPC tier 1: [Hunter](#) ([getting access](#))
- bwHPC tier 2: [HoreKa](#) ([getting access](#))

Material: Slides & Scripts

- <https://indico.scc.kit.edu/event/5221/>
- BwUniCluster 3.0: /opt/bwhpc/common/workshops/2025-10-21/
- HoreKa: /software/all/workshop/2025-10-21/

How to read the following slides

Abbreviation/Colour code	Full meaning
\$ command -option value	\$ = prompt of the interactive shell The full prompt may look like: user@machine:path\$ The command has been entered in the interactive shell session
<integer> <string>	<> = Placeholder for integer, string etc
foo, bar	Metasyntactic variables

How to use each File System (1)

- \$HOME = Home directory
 - Software, configuration files, final results
 - **Omit** heavy I/O
- Workspaces = Working directories with lifetime
 - Intermediate results, huge input/output data sets
 - Scratch data which needs to be shared between nodes
 - **Omit** small files, tiny block sizes, lots of metadata operations
 - If not possible to omit, KIT and HoreKa users can use [Workspaces on flash storage](#)
- \$TMPDIR = Separate file system on each node using local disks
 - Data is only available during job runtime on the local node
 - Possibly transfer data here within a batch job
 - **All** sorts of I/O **allowed**

How to use each File System (2)

- BeeOND = Private file system for batch job
 - Data is only available during job runtime on the batch job nodes
 - Possibly transfer data here within a batch job
 - **All** sorts of I/O **allowed**, only available on bwUniCluster 3.0 and HoreKa
- External storage
 - Archive scientific data, move data here when data sets become too large
 - Each organization has different solutions, examples are RDA or LSDF at KIT
 - **Use** huge files or compressed archives
- Summary
 - Use \$HOME for permanent data
 - Use workspaces for huge files and sequential I/O
 - Use \$TMPDIR or BeeOND with many (> 10000) small files or random I/O

\$HOME = Home directory

- \$HOME is visible on all nodes of a cluster
- Properties of \$HOME on different clusters

Cluster	Quota capacity limit	Quota file limit	Backup
JUSTUS 2	400 GB per user	2 mill. per user	Yes
Helix	200 GB per user	unlimited	Snapshots
NEMO 2	100 GB per user	unlimited	No
BinAC 2	40 GB per user	unlimited	Yes
BwUniCluster 3.0	500 GB per user also limit per organization	5 mill. per user	Yes
HoreKa	10 TB per project	10 mill. per project	Yes

\$HOME on bwUniCluster 3.0

■ HowTo goto:

```
$ cd $HOME
```

```
$ cd
```

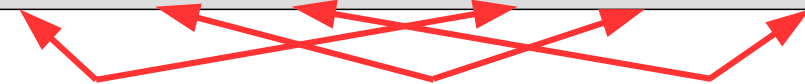
■ User's quota usage and limits:

```
$ lfs quota -uh $(whoami) $HOME
```

Disk quotas for usr ka_ab1234 (uid 9999):

Filesystem	used	quota	limit	grace	files	quota	limit	grace
/home/kit/ka_scc/ka_ab1234	22.59G	500G	550G	-	81408	5000000	5500000	-

current usage soft limit hard limit



■ Usage rate above soft limit for grace period (7 days) will only report a warning.

■ Organization quota usage and limits:

```
$ lfs quota -ph $(grep $(echo $HOME | sed -e "s|/[^/]*/[^/]*$||") \  
/pfs/data6/project_ids.txt | cut -f 1 -d\ ) $HOME
```

\$HOME / \$PROJECT on HoreKa

- \$HOME and \$PROJECT are identical if your account is member of one project
 - Otherwise to change to another project which will also modify \$PROJECT:

```
$ newgrp <another_project_group>
```

- Project group quota usage and limits:

- First start an interactive job (sometimes this step is not needed):

```
$ salloc -p dev_cpuonly -n 1 -t 20 --mem=500
```

- Show usage and limits of your project group on the \$HOME file system:

```
$ /usr/lpp/mmfs/bin/mmfsquota -j $PROJECT_GROUP --block-size G -C hkn.scc.kit.edu hkfs-home
```

		Block Limits				File Limits		
Filesystem	type	GB	quota	limit		files	quota	limit
home	FILESET	3467	10240	11264		4747501	10485760	11534336

current usage soft limit hard limit

Exercise 1: Show quotas

- Login to bwUnicluster 3.0 or HoreKa and show list of commands for exercises:

- BwUniCluster: `$ cat /opt/bwhpc/common/workshops/2025-10-21/pfs_commands.txt`

- HoreKa: `$ cat /software/all/workshop/2025-10-21/pfs_commands.txt`

- Use Cut & Paste to execute the first commands which show your quotas

Workspaces = Working directories with lifetime

■ **Workspace:** lifetime on allocated folder

- Available on all clusters, visible on all nodes of a cluster

- HowTo:

→ <https://wiki.bwhpc.de/e/Workspace>

\$ ws_allocate <i>foo</i> 10	Allocate workspace <i>foo</i> for 10 days
\$ ws_list	List your workspaces
\$ ws_find <i>foo</i>	Get absolute path of workspace <i>foo</i>
\$ ws_extend <i>foo</i> 5	Extend lifetime of your workspace <i>foo</i> by 5 days from now. Number of extensions depends on cluster.
\$ ws_release <i>foo</i>	Manually erase your workspace <i>foo</i>
\$ ws_... -F <i>ffuc</i> ...	Select non default workspace file system with -F (works for any command)

Properties of Workspaces on different clusters

Cluster	Capacity limit	File limit	Max lifetime	Max extensions
JUSTUS 2	20 TB per user	5 mill. per user	90 days	unlimited
Helix	10 TB per user	unlimited	30 days	10 times
NEMO 2	5 TB per user	1 mill. per user	100 days	99 times
BinAC	unlimited	unlimited	30 days	3 times
BwUniCluster 3.0	40 TB per user	20 mill. per user	60 days	3 times
HoreKa	250 TB per user	50 mill. per user	60 days	3 times

Exercise 2: Create workspace

■ Allocate two workspaces

```
$ ws_allocate ws01 30
Info: creating workspace.
/pfs/work9/workspace/scratch/myuser-ws01
remaining extensions : 3
remaining time in days: 30

$ ws_allocate -F ffuc ws_ssd 50
Info: creating workspace.
/pfs/work8/workspace/ffuc/scratch/myuser-ws_ssd
remaining extensions : 3
remaining time in days: 50
```

Exercise 3: List workspace

List workspaces

```
$ ws_list
id: ws_ssd
    workspace directory : /pfs/work8/workspace/ffuc/scratch/myuser-ws_ssd
    remaining time      : 49 days 23 hours
    creation time       : Wed Oct  6 18:59:11 2021
    expiration date     : Thu Nov 25 17:59:11 2021
    filesystem name     : pfs6wor8
    available extensions : 3
id: ws01
    workspace directory : /pfs/work9/workspace/scratch/myuser-ws01
    remaining time      : 29 days 23 hours
    creation time       : Wed Oct  6 18:55:17 2021
    expiration date     : Fri Nov  5 17:55:17 2021
    filesystem name     : pfs7wor9
    available extensions : 3
```

Exercise 4: Find workspace path

- Find workspace path and switch to it

```
$ ws_find ws01
/pfs/work9/workspace/scratch/myuser-ws01

$ ws_find -F ffuc ws_ssd
/pfs/work8/workspace/ffuc/scratch/myuser-ws_ssd

$ cd $(ws_find ws01)
$ pwd
/pfs/work9/workspace/scratch/myuser-ws01
```

Exercise 5: Release workspaces

Release workspaces

```
$ ws_release ws01
```

```
$ ws_release -F ffuc ws_ssd
```

```
$ ws_list
```