Karlsruher Institut für Technologie

7th HPC Café

04.07.2025

Agenda HPC Café – 04.07.2025

Topics for today:

- Cluster access and pitfalls
- Using (own/installed) software on cluster

As usual this format is meant to be interactive.
Don’t hesitate to ask questions!

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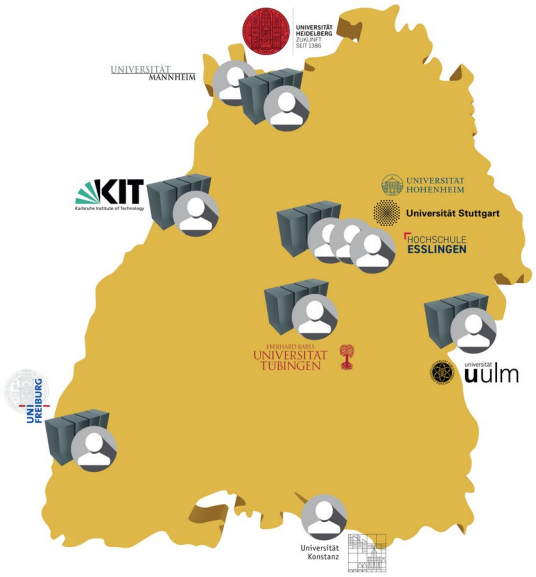
Cluster Access

HPC Café, 4.7.25



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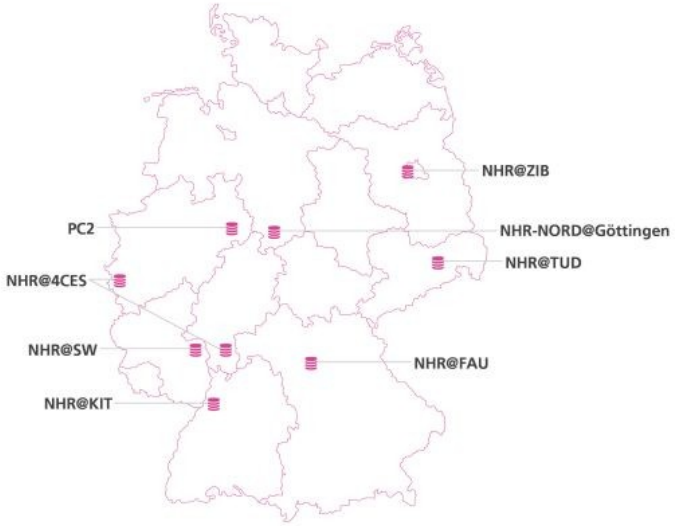


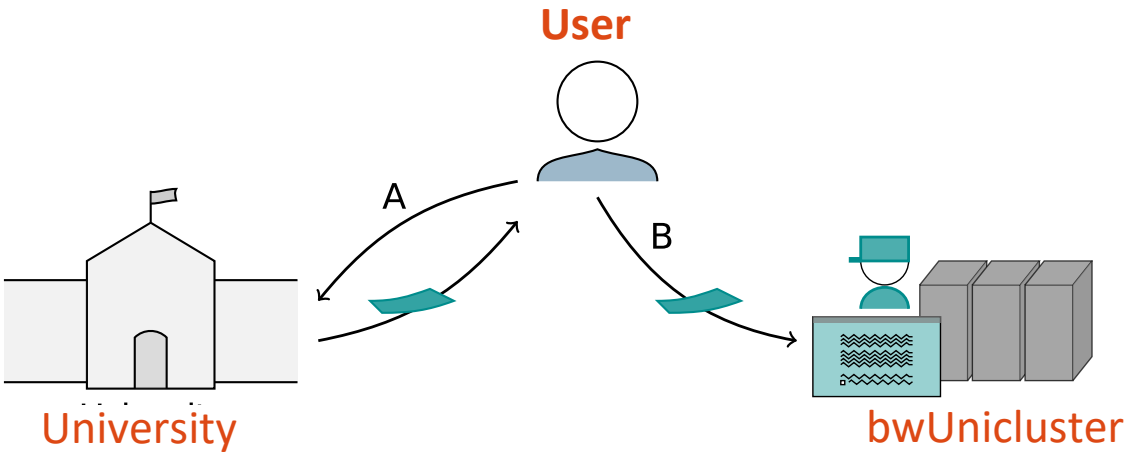
HPC Infrastructure at KIT: Registration

- 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

- HAICORE@KIT
  - Special AI resources within the Helmholtz Association

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

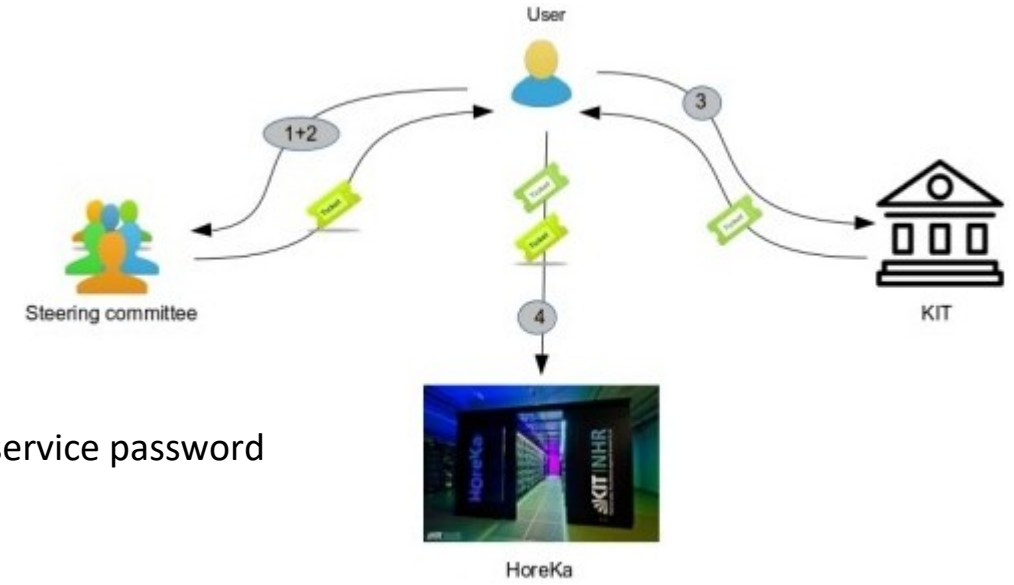
- Each university has its own entitlement granting policies!

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 – 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/

Registration Process – HAICORE

- Registration:
  1. Full Self Service for Helmholtz Members
     KIT Students require a KIT-Guest Account
  2. Login on web page
     https://fels.scc.kit.edu
  3. Register for Service HAICORE@KIT
  4. Set a service password
  5. Login on HAICORE@KIT with OTP and service password

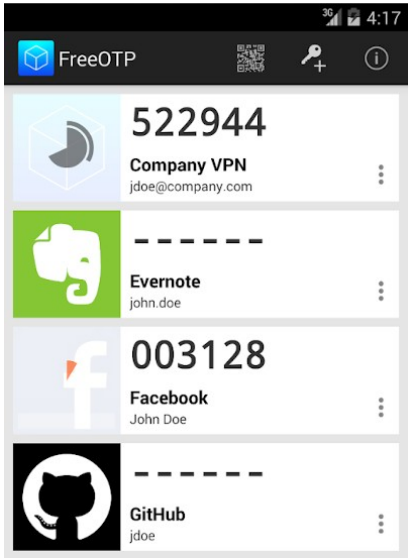
- More Info: https://www.nhr.kit.edu/userdocs/haicore/registration/

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

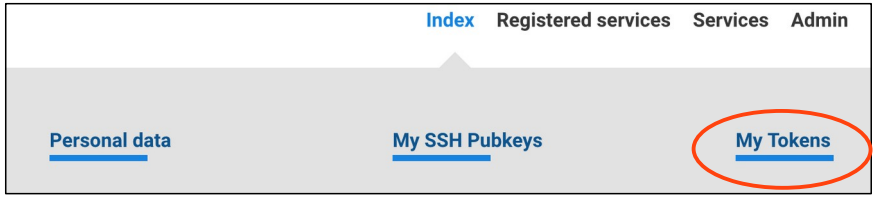
- TOTPs can be generated by *Token*
  - an app on your smartphone or tablet, e.g.
    - FreeOTP for Android or iOS
    - Google Authenticator for Android or iOS
  - an app running on an additional PC / notebook, e.g.
    - Authy for Mac, Windows or Linux
  - a hardware token, e.g.
    - Yubikey



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

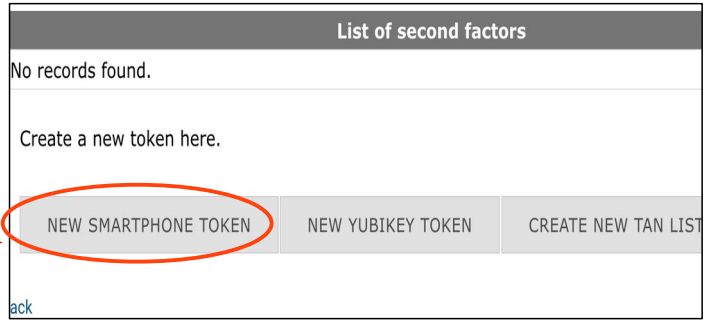
2FA: Registration of your token (1)

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

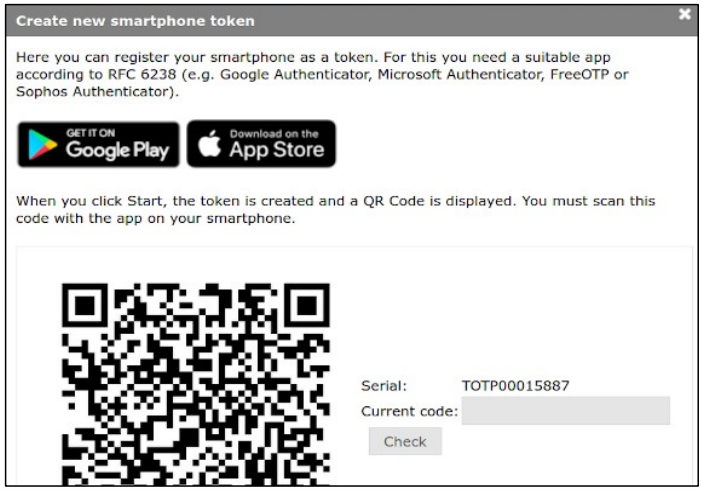


- 1. Login to
  - https://login.bwidm.de (BWUC3)
  - https://fels.scc.kit.edu (HoreKa)

  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.

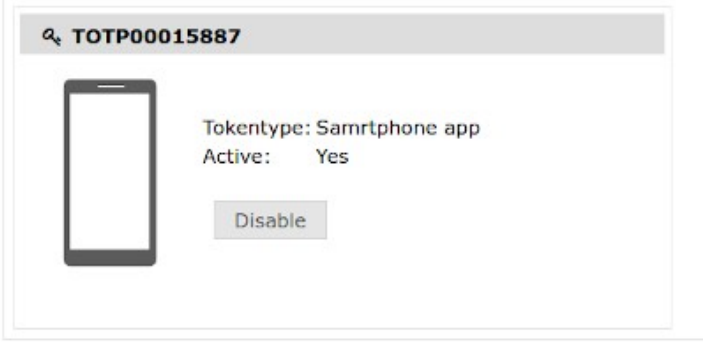


2FA: Registration of your token (2)

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 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
```

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/

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.

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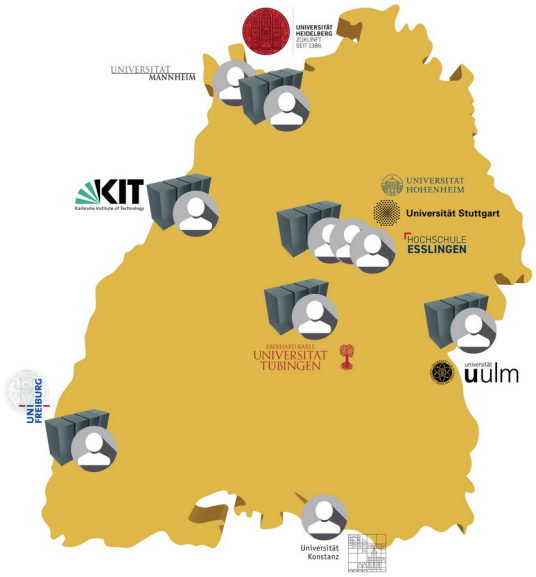
Software

HPC Café, 4.7.25



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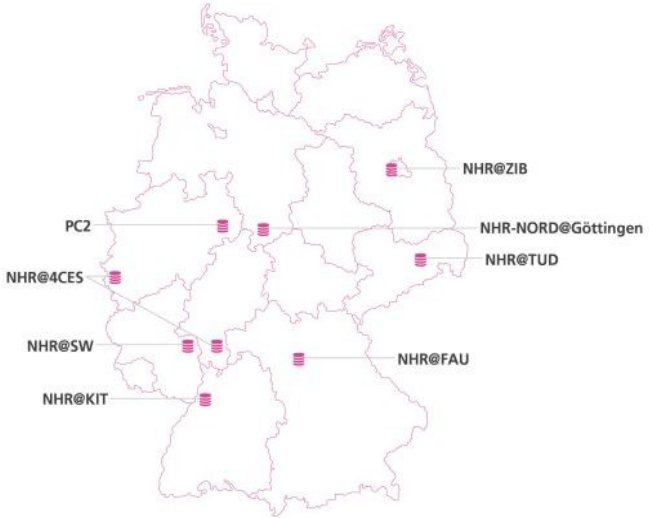

Software (=Environment) modules

By default manual setup of $PATH, $LD_LIBRARY_PATH … for

compilers, libraries and software packages etc.

→ Getting complicated if multiple versions of same software installed

Solution:

- dynamic modification of the session environment by

  → instruction sets stored in *modulefiles*

HowTo?

- *load* and *unload* instruction sets (= modulefiles)
- How to use modulefiles in general?

  ```
  $ module help
  ```

- More information:
  - about the tool in use: Lmod → https://lmod.readthedocs.io/en/latest/

modulefiles: available / search

- Display all **available** modulefiles (modules which can be loaded directly)

`$ module avail` = `$ ml av`

```
------------------------------------------------------ /opt/bwhpc/ka/modulefiles ------------------------------------------------------
   cae/abaqus/2024     cae/ansys/2023R2        cae/comsol/6.3       cae/starccm+/2310    cae/starccm+/2410
   cae/ansys/2022R1    cae/ansys/2024R1        cae/starccm+/2302    cae/starccm+/2402    cae/starccm+/2502     (D)
   cae/ansys/2023R1    cae/ansys/2025R1 (D)    cae/starccm+/2306    cae/starccm+/2406    math/mathematica/14.2

------------------------------------------------- /opt/bwhpc/common/modulefiles -------------------------------------------------
   cae/ansys/2024R2_no_license                lib/hdf5/1.14-gnu-14.2-serial
   cae/openfoam/v2406                         lib/hdf5/1.14-intel-2025.0-serial
   cae/openfoam/v2412                  (D)    lib/hdf5/1.14-llvm-19.1-serial
   compiler/aocc/5.0.0                        lib/hdf5/1.14-nvidia-24.9-serial
   compiler/gnu/11.4                          lib/hdf5/1.14-nvidia-25.1-serial         (D)
   compiler/gnu/14.2                   (D)    lib/icu4c/icu4c-77-1-gnu14.2
   compiler/intel/2025.0                      lib/netcdf/4.9-aocc-5.0.0-serial
   compiler/llvm/19.1                         lib/netcdf/4.9-gnu-11.4-serial
   cs/ollama/0.5.11                           lib/netcdf/4.9-gnu-14.2-serial
   devel/code-server/4.96.4            (E)    lib/netcdf/4.9-intel-2025.0-serial
   devel/cuda/11.8                            lib/netcdf/4.9-llvm-19.1-serial          (D)
   devel/cuda/12.8                     (D)    math/R/4.4.2
   devel/miniforge/24.11.0-python-3.12        math/julia/1.10.8                        (E)
   devel/python/3.11.7-gnu-11.4               math/julia/1.11.4                        (E,D)
   devel/python/3.11.7-gnu-14.2               math/matlab/R2024b
   devel/python/3.12.3-gnu-11.4               mpi/impi/2021.14-intel-2025.0
```

- Search: Display all **available** „compiler“ modulefiles

`$ module avail compiler`

```
------------------------------------------------- /opt/bwhpc/common/modulefiles -------------------------------------------------
   compiler/aocc/5.0.0         compiler/intel/2025.0                    toolkit/nvidia-hpc-sdk/25.1-byo-compiler
   compiler/gnu/11.4           compiler/llvm/19.1
   compiler/gnu/14.2    (D)    toolkit/nvidia-hpc-sdk/24.9-byo-compiler

  Where:
   D:  Default Module
```

modulefiles: categories & dependencies

- Module names already implicate dependencies:

  → **Category/softwarename/version_attributes-dependencies**

  e.g **devel/python/3.13.1-gnu-14.2**

  → python package version 3.13.1, compiled with GNU 14.2

- Categories:

`compiler/`	for compiler, e.g. intel, gnu, pgi, open64
`devel/`	for debugger, e.g. ddt, and development tools, e.g. cmake, itrac
`mpi/`	for MPI libraries, e.g. impi, openmpi, mvapich(2)
`numlib/`	for numerical libraries, e.g. Intel MKL, ACML, nag, gsl, fftw
`lib/`	for other libraries, e.g. netcdf, global array
`bio/`	for biology software, e.g. bowtie, abyss, mrbayes
`cae/`	for CAE software, e.g. ansys, abaqus, fluent
`chem/`	for chemistry software, e.g. gromacs, dacapo, turbomole
`math/`	for mathematics software, e.g. matlab, R
`phys/`	for physics software, e.g. geant4
`vis/`	for visualisation software, e.g. vmd, tigervnc

modulefiles: load / list

- Modulefiles are sorted in categories, software name and versions:

```
$ module load <category>/<software_name>/<version>
```

- Load a **default** software:

```
$ module load <category>/<software_name>
```

  - e.g. Intel compiler

```
$ module load compiler/intel mpi/impi
```

→ loads currently Intel compiler suite 2025.0

→ loads currently Intel-MPI 2021.14 for Intel compiler suite 2025.0

- Display all loaded modules

```
$ module list
```

=

```
$ ml
```

```
Currently Loaded Modules:
  1) compiler/intel/2025.0   2) mpi/impi/2021.14-intel-2025.0
```

modulefiles: load dependenices /conficts (1)

- **Dependencies**
  - e.g.: some applications require particular compiler libraries

```
$ module load devel/python/3.11.7-gnu-11.4
$ module list
```

```
Currently Loaded Modules:
  1) compiler/gnu/11.4   2) devel/python/3.11.7-gnu-11.4
```

autoloaded gnu compiler 11.4

- **Conflicts**:
  - a) load different software version in the same session, e.g. Intel:

```
$ module load compiler/gnu/11.4
$ module load compiler/gnu/14.2
```

```
The following have been reloaded with a version change:
  1) compiler/gnu/11.4 => compiler/gnu/14.2
```

  - b) load module with dependencies on other modules

```
$ module load compiler/gnu/14.2
$ module load devel/python/3.11.7-gnu-11.4
```

requires gnu compiler 11.4

```
The following have been reloaded with a version change:
  1) compiler/gnu/14.2 => compiler/gnu/11.4
```

modulefiles: unload/swap/purge

- To remove module *foo*:

  ```
  $ module unload foo
  ```

  → be aware that you might create inconsistencies

  ```
  $ module load mpi/impi/2021.14-intel-2025.0
  $ module unload compiler/intel/2025.0
  ```

  ```
  Lmod Warning:
  ------------------------------------------------------------
  The following dependent module(s) are not currently loaded:
  compiler/intel/2025.0 (required by: compiler/intel/2025.0)
  ------------------------------------------------------------
  ```

- Swap = remove + load

  e.g.: `$ module swap compiler/gnu compiler/intel`

  Removes loaded GNU version and loads default INTEL version

- To remove **ALL** modules at once:

  ```
  $ module purge
  ```

  ```
  $ module list
  No modules loaded
  ```

Private modulefiles

- Each user can create own modulefiles:

  e.g. modulefiles that adds path of own programs, $HOME/special, to $PATH

  → content of this modulefile *„mybin.lua“*

```
-- Own Lua modulefile to prepend $HOME/special to $PATH
--
prepend_path("PATH",  os.getenv("HOME") .. "/special")
```

  → place *„mybin.lua“* under $HOME/privatemodules

  → to make all own modules visible to “module avail” command, enter:

```
$ module use $HOME/privatemodules
```

  → note: own module have higher priority than systems ones

```
$ module avail

-- /home/kit/ka_scc/ka_ab1234/privatemodules --
   mybin
-------------------------------------------
```

- Remove own modules:

```
$ module unuse $HOME/privatemodules
```

And other Software?

- We do provide the option to easily use easybuild
  - Covers a lot of usecases
  - Over 4000 software packages
  - Details on how to use easybuild on the clusters:
    https://www.nhr.kit.edu/userdocs/horeka/software/#easybuild-modules
    https://wiki.bwhpc.de/e/BwUniCluster3.0/Software_Modules#EasyBuild_modules

And any other Software?

- If needed you can in principle compile any needed software yourself
  - Please note: we do not provide support for this

- A few things to note:
  - The clusters at the computing center are not like your own PC
    - You are not root, even if the “How-To” in the github repo you found assumes that
    - Do not blindly copy&paste commands you do not understand
    - Your home directory is not a local hard disk but a shared volume that is mounted over the network
  - Examples for things that do not work:
    - sudo apt install python-3.12
    - make && sudo make install
    - sudo <anything>