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Software Modules

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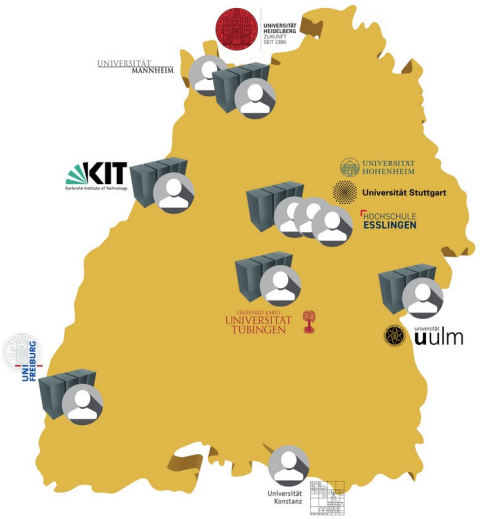

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Software (=Environment) modules

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

`$ module avail` = `$ ml av`

```
------------------------------------------ /opt/bwhpc/common/modulefiles/Core ------------------------------------------
   bio/freesurfer/6.0.0                          devel/python/3.8.6_intel_19.1
   bio/fsl/6.0.4                                 devel/python/3.10.0_gnu_11.1
   bio/nest/2.18.0                        (T)    devel/python/3.10.0_intel_19.1
   bio/nest/2.20.1                        (T,D)  devel/python/3.10.5_gnu_12.1                                  (D)
   cae/ansys/2022R1_no_license                   devel/python/3.10.5_intel_2021.4.0
   cae/ansys/2022R2_no_license                   devel/python/3.11.7_intel_2021.4.0
   cae/ansys/2024R2_no_license                   devel/python/3.12.3_gnu_13.3
   cae/cgns/3.4.1-intel-19.1                     devel/python/3.12.3_intel_2023.1.0
   cae/cgns/4.1.2-gnu-8.3                 (D)    devel/qiskit/1.1.2-py3.9.15
   cae/openfoam/v1812                            devel/recorder/2.3.3
   cae/openfoam/v2006                            devel/reports/20.0
   cae/openfoam/v2012-Prof                       devel/scorep/7.1-gnu-11.2-openmpi-4.1
   cae/openfoam/v2012                            devel/scorep/7.1-intel-2021.4.0-impi-2021.4.0
   cae/openfoam/v2112                            devel/scorep/7.1-intel-2021.4.0-openmpi-4.1
   cae/openfoam/v2206                            devel/scorep/7.1-llvm-12.0-openmpi-4.1                         (D)
   cae/openfoam/v2212                            devel/spindle/0.13
   cae/openfoam/v2306                            devel/swig/4.1.0
   cae/openfoam/v2312                     (D)    devel/tbb/2021.4.0
   cae/openfoam/v2406                            devel/tbb/2021.7.1                                             (D)
```

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

`$ module avail compiler`

```
------------------------------------------ /opt/bwhpc/common/modulefiles/Core ------------------------------------------
   compiler/gnu/8.5.0                  compiler/intel/2022.2.1_llvm        compiler/llvm/18.1                    (D)
   compiler/gnu/10.2                   compiler/intel/2022.2.1             compiler/pgi/2020
   compiler/gnu/13.3            (D)    compiler/intel/2023.1.0_llvm        toolkit/nvidia-hpc-sdk/21.2-byo-compiler
   compiler/gnu/14.1                   compiler/intel/2023.1.0      (D)    toolkit/nvidia-hpc-sdk/22.11-byo-compiler
   compiler/intel/2021.4.0_llvm        compiler/intel/2024.0_llvm          toolkit/nvidia-hpc-sdk/23.9-byo-compiler
   compiler/intel/2021.4.0             compiler/llvm/17.0
```

modulefiles: spider / search (1)

- Display all **possible** modulefiles

```
$ module spider
```

```
-----------------------------------------------------------------------------------------------------------
The following is a list of the modules and extensions currently available:
-----------------------------------------------------------------------------------------------------------
  bio/freesurfer: bio/freesurfer/6.0.0

  bio/fsl: bio/fsl/6.0.4

  bio/nest: bio/nest/2.18.0, bio/nest/2.20.1
    NEST is a command line tool for simulating neural networks

  cae/abaqus: cae/abaqus/2022, cae/abaqus/2023, cae/abaqus/2024

  cae/ansys: cae/ansys/2021R2, cae/ansys/2022R1_no_license, cae/ansys/2022R2_no_license, cae/ansys/2022R2, ...

  cae/cgns: cae/cgns/3.4.1-intel-19.1, cae/cgns/4.1.2-gnu-8.3

  cae/comsol: cae/comsol/6.0, cae/comsol/6.1, cae/comsol/6.2

  cae/cst: cae/cst/2022, cae/cst/2023, cae/cst/2024

  cae/openfoam: cae/openfoam/v1812, cae/openfoam/v2006, cae/openfoam/v2012-Prof, cae/openfoam/v2012, ...

  cae/paraview: cae/paraview/5.8, cae/paraview/5.9, cae/paraview/5.11, cae/paraview/5.11.2, ...

  cae/starccm+: cae/starccm+/2021.3, cae/starccm+/2022.6, cae/starccm+/2302, cae/starccm+/2306, ...

  cae/starcd: cae/starcd/2019.1.2
```

- Search: Display all **possible** „gnu compiler“ modulefiles

```
$ module spider compiler/gnu
```

```
-----------------------------------------------
  compiler/gnu:
-----------------------------------------------
     Versions:
        compiler/gnu/8.5.0
        compiler/gnu/10.2
        compiler/gnu/13.3
        compiler/gnu/14.1
```

modulefiles: spider / search (2)

- Display all **possible variants** of a modulefiles

```
$ module spider mpi/openmpi/5.0
```

```
----------------------------------------------
  mpi/openmpi: mpi/openmpi/5.0
----------------------------------------------

   You will need to load all module(s)
   on any one of the lines below before
   the "mpi/openmpi/5.0" module is available
   to load.

      compiler/gnu/.13.2
      compiler/gnu/13.3
      compiler/gnu/14.1
      compiler/intel/2023.1.0
      compiler/intel/2023.1.0_llvm
      compiler/intel/2024.0_llvm
      compiler/llvm/17.0
      compiler/llvm/18.1
```

modulefiles: help / whatis

- Show help of modulefiles, e.g. `$ module help chem/turbomole`

```
--Module Specific Help for "chem/turbomole/7.7.1" -------
---------------------------------------
| Loading Parallel version            |
---------------------------------------
* Code_words are: SMP (shared memory parallel) and
                  MPI (message passing interface)
* To load for e.g. SMP, execute:
     export PARA_ARCH=SMP
     module load chem/turbomole/7.7.1
...
...
---------------------------------------
| Support                             |
---------------------------------------
...
```

Version fallback is the defined default (here 7.6.1)

- Show short info modulefile

```
$ module whatis chem/turbomole
```

```
chem/turbomole/7.7.1    : Quantum chemistry package Turbomole version 7.7.1
```

modulefiles: show

- Show all instructions of modulefile

```
$ module show compiler/gnu/13
```

```
-------------------------------------------------------------------
   /opt/bwhpc/common/modulefiles/Core/compiler/gnu/13.lua:
-------------------------------------------------------------------
...
setenv("CC","/opt/gcc/13/bin/gcc")
setenv("CFLAGS","-O2 -march=native")
setenv("OMP_PROC_BIND","true")
...
prepend_path("PATH","/opt/gcc/13/bin")
prepend_path("LD_LIBRARY_PATH","/opt/gcc/13/lib64")
...
whatis("Sets up GCC C/C++/Fortran compiler version 13 in your environment...
help([[The GNU Compiler Collection includes front ends for C, C++,
Objective-C,Fortran, Java, Ada, and Go, as well as libraries for these
Languages (libstdc++, libgcj,...). GCC was originally written as the
compiler for the GNU operating system. The GNU system was developed
to be 100% free software, free in the sense that it respects the
user's freedom.

In case of problems, please https://support.nhr.kit.edu/
SCC support end: As soon as GNU compiler version 15 is available!
]])
prepend_path("MODULEPATH","/software/all/lmod/modulefiles/Compiler/gnu/13")
family("compiler")
```

Setting environment variables

Modifying environment variables

Content of printout functions

module show does NOT load the modulefile

modulefiles: show

- Show all instructions of modulefile

```
$ module show compiler/gnu/14.1
```

```
-------------------------------------------------------------------
   /opt/bwhpc/common/modulefiles/Core/compiler/gnu/14.1.lua:
-------------------------------------------------------------------
setenv("GNU_VERSION","14.1.0")
setenv("GNU_HOME","/opt/bwhpc/common/compiler/gnu/14.1.0")
setenv("GNU_BIN_DIR","/opt/bwhpc/common/compiler/gnu/14.1.0/bin")
...
prepend_path("PATH","/opt/bwhpc/common/compiler/gnu/14.1.0/bin")
prepend_path("LD_LIBRARY_PATH","/opt/bwhpc/common/compiler/gnu/14.1.0/lib64")
...
conflict("compiler/intel")
conflict("compiler/pgi")
whatis("GNU compiler suite version 14.1.0  (gcc, g++, gfortran,...
help([[This module provides the GNU compiler collection version 14.1.0
via commands gcc, g++, gfortran and gccgo. The GNU compiler has been build ...
...
cpp       - GNU pre processor
gcc       - GNU C compiler
g++       - GNU C++ compiler
gfortran - GNU Fortran compiler (Fortran 95/2003/2008 ...
...
In case of problems, submit a trouble ticket at
'https://bw-support.scc.kit.edu'.

The full version is: compiler/gnu/14.1.0
]])
```

Setting environment variables

Modifying environment variables

Conflict setup

module show does NOT load the modulefile

modulefiles: categories & dependencies

- Module names already implicate dependencies:

  → `Category/softwarename/version_attributes-dependencies`

  e.g `numlib/petsc/3.13.4-gnu-10.2-openmpi-4.1`

  → PETSc package version 3.13.4, compiled with GNU 10.2 and OpenMPI 4.1

- 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

Exercise 1

- 1. Find all modulefiles that start with „mpi“

Exercise 1 - Solution

- 1. Find all modulefiles that start with „mpi“

```
$ module -t -r spider '^mpi'
mpi/impi/2019
mpi/impi/2020
mpi/impi/2021.4.0
mpi/impi/2021.7.1
mpi/impi/2021.9.0
mpi/impi/2021.11
mpi/openmpi/default
mpi/openmpi/4.0
mpi/openmpi/4.1
mpi/openmpi/5.0
```

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 2023.1.0

→ loads currently Intel-MPI 2021.11 for Intel compiler suite 2023.1.0

- Display all loaded modules

```
$ module list
```

=

```
$ ml
```

```
Currently Loaded Modules:
  1) compiler/intel/2023.1.0   2) mpi/impi/2021.11
```

modulefiles: load dependenices /conficts (1)

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

```
$ module load numlib/gsl/2.6-gnu-10.2
$ module list
```

```
Currently Loaded Modules:
  1) compiler/gnu/10.2   2) numlib/gsl/2.6-gnu-10.2
```

autoloaded gnu compiler 10.2

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

```
$ module load compiler/gnu/10.2
$ module load compiler/gnu/13.3
```

```
The following have been reloaded with a version change:
  1) compiler/gnu/10.2 => compiler/gnu/13.3
```

  - b) load module with dependencies on other modules

```
$ module load compiler/gnu/13.3
$ module load numlib/gsl/2.6-gnu-10.2
```

```
The following have been reloaded with a version change:
  1) compiler/gnu/13.3 => compiler/gnu/10.2
```

requires gnu compiler 10.2

Exercise 2

- 1. Load latest OpenMPI with default INTEL compiler (Hint: Option ‚-d‘ to show only default version)

Exercise 2 - Solutions

- 1. Load latest OpenMPI with default INTEL compiler

```
$ module -d avail compiler/intel
compiler/intel/2023.1.0

$ module load compiler/intel/2023.1.0

$ module -r spider 'mpi/openmpi.*'
→ mpi/openmpi/5.0

$ module load mpi/openmpi/5.0
```

```
# Pitfall: Loading openmpi before compiler
$ module load mpi/openmpi/5.0

Lmod has detected the following error:
These module(s) or extension(s) exist but cannot be loaded as requested:
"mpi/openmpi/5.0"
   Try: "module spider mpi/openmpi/5.0" to see how to load the module(s).
```

modulefiles: unload/swap/purge

- To remove module *foo*:

```
$ module unload foo
```

→ be aware that you might create inconsistencies

```
$ module load numlib/gsl/2.6-gnu-10.2
$ module unload compiler/gnu/10.2
```

```
------------------------------------------------------------
The following dependent module(s) are not currently loaded:
compiler/gnu/10.2 (required by: numlib/gsl/2.6-gnu-10.2)
------------------------------------------------------------
```

- 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
```

Exercise 3

- 1. Determine system gcc version (without modulefile system)

- 2. Load newest gcc version (hint: newest → highest version number of compiler/gnu)

Exercise 3 - Solution

- 1. Determine system gcc version (without modulefile system)

```
$ module purge

$ module list
No modules loaded

$ gcc --version
gcc (GCC) 8.5.0 20210514 (Red Hat 8.5.0-18)
```

- 2. Load newest gcc version (hint: newest → highest version number of compiler/gnu)

```
$ module spider compiler/gnu

     Versions:
        compiler/gnu/8.5.0
        compiler/gnu/10.2
        compiler/gnu/13.3
        compiler/gnu/14.1

$ module load compiler/gnu/14.1
$ gcc --version
gcc (GCC) 14.1.0
```

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/scc/ab1234/privatemodules ----
   mybin
-------------------------------------------
```

- Remove own modules:

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