Software Modules

A. Baer, P. Weisbrod

KIT, SCC

Baden-Württemberg
Ministerium für Wissenschaft,
Forschung und Kunst

Software on bwUniCluster3.0, bwForClusters and HoreKa

- Software provided and maintained by bwHPC team
  - Available via Software Modules

- Software installed by users themselves
  - e.g. via installation in $HOME/Workspaces, containers, python, github/gitlab
  - see next talk for workflows to get required software

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/comsol/6.4    (D)    cae/starccm+/2410        cae/tecplot/2023r2
   cae/ansys/2025R1         cae/cst/2026             cae/starccm+/2502        math/mathematica/14.1
   cae/ansys/2025R2         cae/starccm+/2310        cae/starccm+/2506        math/mathematica/14.2     (D)
   cae/ansys/2026R1 (D)     cae/starccm+/2402        cae/starccm+/2510        optimization/gurobi/12.0.3
   cae/comsol/6.3           cae/starccm+/2406        cae/starccm+/2602 (D)

------------------------------------------------ /opt/bwhpc/common/modulefiles ---------------------------
--------------
   cae/ansys/2024R2_no_license                   lib/hdf5/1.14-llvm-19.1-serial
   cae/ansys/2025R2_no_license                   lib/hdf5/1.14-nvidia-24.9-nompi-openmpi-5.0
   cae/openfoam/v2012                            lib/hdf5/1.14-nvidia-24.9-nompi-serial
   cae/openfoam/v2112                            lib/hdf5/1.14-nvidia-25.1-nompi-openmpi-5.0
   cae/openfoam/v2212                            lib/hdf5/1.14-nvidia-25.1-nompi-serial              (D)
   cae/openfoam/v2406                            lib/icu4c/icu4c-77-1-gnu14.2
   cae/openfoam/v2412                            lib/libfyaml/0.9
   cae/openfoam/v2506                      (D)   lib/netcdf-fortran/4.6-aocc-5.0.0-openmpi-5.0
   cae/openfoam/6                                lib/netcdf-fortran/4.6-aocc-5.0.0-serial
   cae/openfoam/7                                lib/netcdf-fortran/4.6-gnu-11.4-openmpi-5.0
```

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

```
$ module avail compiler
```

```
------------------------------------ /opt/bwhpc/common/modulefiles -------------------------------------
   compiler/aocc/5.0.0          compiler/gnu/11.4            compiler/llvm/19.1
   compiler/aomp/21.0-1         compiler/gnu/14.2     (D)    toolkit/nvidia-hpc-sdk/24.9-byo-compiler
   compiler/aomp/22.0-1 (D)     compiler/intel/2025.0        toolkit/nvidia-hpc-sdk/25.1-byo-compiler
```

modulefiles: spider / search (1)

- Display all **possible** modulefiles

```
$ module spider
```

```
---------------------------------------------------------------------------------------------------------
The following is a list of the modules and extensions currently available:
---------------------------------------------------------------------------------------------------------
  cae/abaqus: cae/abaqus/2024

  cae/ansys: cae/ansys/2024R2_no_license, cae/ansys/2025R1, cae/ansys/2025R2_no_license, ...

  cae/comsol: cae/comsol/6.3, cae/comsol/6.4

  cae/cst: cae/cst/2026
    CST Studio Suite 2026 installation

  cae/openfoam: cae/openfoam/v2012, cae/openfoam/v2112, cae/openfoam/v2212, cae/openfoam/v2406, ...

  cae/starccm+: cae/starccm+/2310, cae/starccm+/2402, cae/starccm+/2406, cae/starccm+/2410, ...

  cae/tecplot: cae/tecplot/2023r2
    Tecplot 360 EX - visualization software for CFD and numerical simulation data

  chem/molden: chem/molden/7.3
```

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

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

```
---------------------------
  compiler/gnu:
---------------------------
     Versions:
        compiler/gnu/11.4
        compiler/gnu/14.2
```

modulefiles: spider / search (2)

- Some clusters (HoreKa, Helix, JUSTUS2) use hierarchical module system
- In hierarchical module system, availability depends on loaded modules
- 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/aocc/5.0.0
      compiler/gnu/12
      compiler/gnu/13
      compiler/gnu/14
      compiler/intel/2023.1.0
      compiler/intel/2023.1.0_llvm
      compiler/intel/2024.0_llvm
      compiler/intel/2025.1_llvm
      compiler/llvm/19.1
      toolkit/nvidia-hpc-sdk/23.9-nompi
      toolkit/nvidia-hpc-sdk/24.9-nompi
      toolkit/nvidia-hpc-sdk/25.3-nompi
```

modulefiles: help / whatis

- Show help of modulefiles, e.g. `$ module help cae/openfoam`

```
---- Module Specific Help for "cae/openfoam/v2506" ---
The OpenFOAM (Open Field Operation and Manipulation) CFD
Toolbox can simulate anything from complex fluid flows
...
Local documentation in:
   $FOAM_DOC_DIR
...
Online documentation in:
   https://wiki.bwhpc.de/e/OpenFoam
Homepage:
   https://www.openfoam.org
...
In case of problems, create a ticket at
'https://bw-support.scc.kit.edu/'
```

Version fallback is the defined default (here v2506)

- Show short info modulefile `$ module whatis cae/openfoam`

```
cae/openfoam/v2506  : Open Source CFD Toolbox OpenFOAM version v2506
```

modulefiles: show

- Show all instructions of modulefile

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

```
-------------------------------------------------------------------
   /software/all/lmod/modulefiles/Core/compiler/gnu/13.lua:
-------------------------------------------------------------------
...
setenv("CC","/opt/gcc/14/bin/gcc")
setenv("CFLAGS","-O2 -march=native")
setenv("OMP_PROC_BIND","true")
...
prepend_path("PATH","/opt/gcc/14/bin")
prepend_path("LD_LIBRARY_PATH","/opt/gcc/14/lib64")
...
whatis("Sets up GCC C/C++/Fortran compiler version 14 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/14")
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/14.2
```

```
-------------------------------------------------------------------
   /opt/bwhpc/common/modulefiles/Core/compiler/gnu/14.2.lua:
-------------------------------------------------------------------
setenv("GNU_VERSION","14.2.0")
setenv("GNU_HOME","/opt/bwhpc/common/compiler/gnu/14.2.0")
setenv("GNU_BIN_DIR","/opt/bwhpc/common/compiler/gnu/14.2.0/bin")
...
prepend_path("PATH","/opt/bwhpc/common/compiler/gnu/14.2.0/bin")
prepend_path("LD_LIBRARY_PATH","/opt/bwhpc/common/compiler/gnu/14.2.0/lib64")
...
conflict("compiler/intel")
conflict("compiler/pgi")
whatis("GNU compiler suite version 14.2.0  (gcc, g++, gfortran,...
help([[This module provides the GNU compiler collection version 14.2.0
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'.
...
]])
```

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 `devel/python/3.13.1-gnu-14.2`

  → python package version 3.13.1, compiled with GNU 14.2

- Possible categories (availability depends on cluster):

compiler/	bio/	phys/
devel/	cae/	vis/
econ/	chem/	system/
mpi/	cs/	dbdata
numlib/	math/	geo/
lib/	office/	toolkit/

- List of available software per cluster
  https://www.bwhpc.de/software.php

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/2021.14-intel-2025.0
mpi/openmpi/5.0-aocc-5.0.0
mpi/openmpi/5.0-gnu-11.4
mpi/openmpi/5.0-gnu-14.2
mpi/openmpi/5.0-intel-2025.0
mpi/openmpi/5.0-llvm-19.1
mpi/openmpi/5.0-nvidia-24.9-nompi
mpi/openmpi/5.0-nvidia-25.1-nompi
```

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 /conflicts (1)

Dependencies

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

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

autoloaded gnu compiler 11.4

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

modulefiles: load dependenices /conflicts (2)

- **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
```

Exercise 2

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

Exercise 2 - Solutions

- 1. Load latest OpenMPI with default GNU compiler

```
$ module -d avail compiler/gnu

compiler/gnu/14.2

$ module load compiler/gnu/14.2

$ module -r spider 'mpi/openmpi.*'
→ mpi/openmpi/5.0-gnu-14.2

$ module load mpi/openmpi/5.0-gnu-14.2
```

```
# Pitfall on clusters with hierarchical modules: 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 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:

```
$ 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) 11.4.1 20231218 (Red Hat 11.4.1-4)
```

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

```
$ module spider compiler/gnu

     Versions:
        compiler/gnu/11.4
        compiler/gnu/14.2

$ module load compiler/gnu/14.2
$ gcc --version
gcc (GCC) 14.2.0
```

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:

  → 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
```

EasyBuild modules

- On BwUniCluster3.0 beta-test to provide toolchains/scientific software built with EasyBuild
  - Add EasyBuild module paths to module environment:

```
$ source /opt/bwhpc/common/etc/easybuild/enable_eb_modules
```

  - Hide EasyBuild modules again:

```
$ source /opt/bwhpc/common/etc/easybuild/disable_eb_modules
```

  - More Information:
    https://wiki.bwhpc.de/e/BwUniCluster3.0/Software_Modules#EasyBuild_modules

- On HoreKa2 most software will be provided via EasyBuild