Software Modules

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www.bwhpc.de / www.nhr.kit.edu

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?

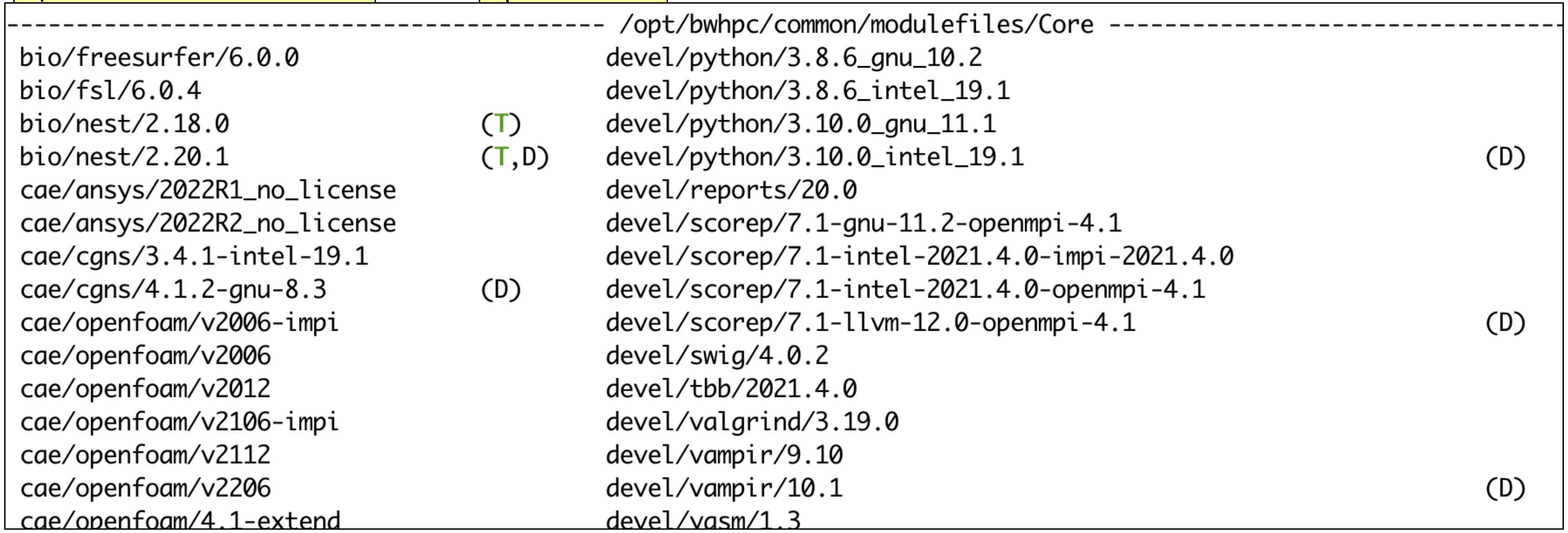
```
$ module help
```

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

modulefiles: available / search

- Display all **available** modulefiles

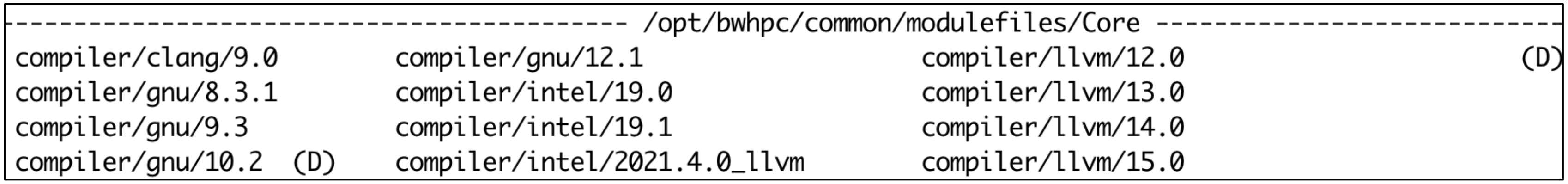
`$ module avail` = `$ ml av`



```
----------------------------------------- /opt/bwhpc/common/modulefiles/Core ------------------------------------
 bio/freesurfer/6.0.0                        devel/python/3.8.6_gnu_10.2
 bio/fsl/6.0.4                               devel/python/3.8.6_intel_19.1
 bio/nest/2.18.0                   (T)       devel/python/3.10.0_gnu_11.1
 bio/nest/2.20.1                   (T,D)     devel/python/3.10.0_intel_19.1                            (D)
 cae/ansys/2022R1_no_license                 devel/reports/20.0
 cae/ansys/2022R2_no_license                 devel/scorep/7.1-gnu-11.2-openmpi-4.1
 cae/cgns/3.4.1-intel-19.1                   devel/scorep/7.1-intel-2021.4.0-impi-2021.4.0
 cae/cgns/4.1.2-gnu-8.3            (D)       devel/scorep/7.1-intel-2021.4.0-openmpi-4.1
 cae/openfoam/v2006-impi                     devel/scorep/7.1-llvm-12.0-openmpi-4.1                    (D)
 cae/openfoam/v2006                          devel/swig/4.0.2
 cae/openfoam/v2012                          devel/tbb/2021.4.0
 cae/openfoam/v2106-impi                     devel/valgrind/3.19.0
 cae/openfoam/v2112                          devel/vampir/9.10
 cae/openfoam/v2206                          devel/vampir/10.1                                         (D)
 cae/openfoam/4.1-extend                     devel/vasm/1.3
```

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

`$ module avail compiler`



```
------------------------------------------ /opt/bwhpc/common/modulefiles/Core -------------------------------
 compiler/clang/9.0          compiler/gnu/12.1                 compiler/llvm/12.0                        (D)
 compiler/gnu/8.3.1          compiler/intel/19.0               compiler/llvm/13.0
 compiler/gnu/9.3            compiler/intel/19.1               compiler/llvm/14.0
 compiler/gnu/10.2   (D)     compiler/intel/2021.4.0_llvm      compiler/llvm/15.0
```

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/2020

  cae/ansys: cae/ansys/2020R2, cae/ansys/2021R2

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

  cae/comsol: cae/comsol/5.6

  cae/cst: cae/cst/2020

  cae/lsdyna: cae/lsdyna/9.3.1, cae/lsdyna/12.0.0

  cae/openfoam: cae/openfoam/v2006-impi, cae/openfoam/v2006, cae/openfoam/v2012, cae/openfoam/v2106-impi, ...
```

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

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

```
-----------------------------------------
  compiler/gnu:
-----------------------------------------
     Versions:
        compiler/gnu/8.3.1
        compiler/gnu/9.3
        compiler/gnu/10.2
        compiler/gnu/10.3
        compiler/gnu/11.1
        compiler/gnu/11.2
```

modulefiles: spider / search (2)

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

```
$ module spider mpi/openmpi/4.1
```

```
----------------------------------------------
  mpi/openmpi: mpi/openmpi/4.1
----------------------------------------------

   You will need to load all module(s)
   on any one of the lines below before
   the "mpi/openmpi/4.0" module is available
   to load.

      compiler/gnu/10.2
      compiler/gnu/11.2
      compiler/gnu/12.1
      compiler/intel/19.1
      compiler/intel/2021.4.0
      compiler/intel/2021.4.0_llvm
      compiler/llvm/15.0
      compiler/pgi/2020
```

modulefiles: help / whatis

- Show help of modulefiles, e.g.

```
$ module help chem/turbomole
```

```
--Module Specific Help for "chem/turbomole/7.6.1" -------
--------------------------------------
| 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/7.6.1
...
...
--------------------------------------
| Support                            |
--------------------------------------
...
```

Version fallback is the defined default (here 7.6.1)

- Show short info modulefile

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

```
chem/turbomole/7.6.1    : Quantum chemistry package Turbomole version 7.6.1
```

modulefiles: show

- Show all instructions of modulefile

```
$ module show compiler/gnu/11
```

```
----------------------------------------------------------------
   /opt/bwhpc/common/modulefiles/Core/compiler/gnu/11.lua:
----------------------------------------------------------------
...
setenv("CC","/opt/gcc/11/bin/gcc")
setenv("CFLAGS","-O2 -march=native")
setenv("OMP_PROC_BIND","true")
...
prepend_path("PATH","/opt/gcc/11/bin")
prepend_path("LD_LIBRARY_PATH","/opt/gcc/11/lib64")
...
whatis("Sets up GCC C/C++/Fortran compiler version 11 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 contact: Hartmut Häfner <hartmut.haefner@kit.edu>
SCC support end: As soon as GNU compiler version 13 is available!
]])
```

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/11.2
```

```
----------------------------------------------------------------
   /opt/bwhpc/common/modulefiles/Core/compiler/gnu/11.2.lua:
----------------------------------------------------------------
setenv("GNU_VERSION","11.2.0")
setenv("GNU_HOME","/opt/bwhpc/common/compiler/gnu/11.2.0")
setenv("GNU_BIN_DIR","/opt/bwhpc/common/compiler/gnu/11.2.0/bin")
...
prepend_path("PATH","/opt/bwhpc/common/compiler/gnu/11.2.0/bin")
prepend_path("LD_LIBRARY_PATH","/opt/bwhpc/common/compiler/gnu/11.2.0/lib64")
...
conflict("compiler/intel")
conflict("compiler/pgi")
whatis("GNU compiler suite version 11.2.0  (gcc, g++, gfortran,...
help([[This module provides the GNU compiler collection version 11.2.0
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'.

The full version is: compiler/gnu/11.2.0
]])
```

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-4.0`

  → PETSc package version 3.13.4, compiled with GNU 10.2 and OpenMPI 4.0

- 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/openmpi/default
mpi/openmpi/4.0
mpi/openmpi/4.1
```

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 2022.2.1

→ loads currently Intel-MPI 2021.7.1 for Intel compiler suite 2022.2.1

- Display all loaded modules

```
$ module list
```

=

```
$ ml
```

```
Currently Loaded Modules:
  1) compiler/intel/2022.2.1   2) mpi/impi/2021.7.1
```

modulefiles: load dependenices /conficts (1)

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

```
$ module load numlib/gsl/2.6-intel-19.1
$ module list
```

```
Currently Loaded Modules:
  1) compiler/intel/19.1   2) numlib/gsl/2.6-intel-19.1
```

Autoloaded Intel-Suite 19.1

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

```
$ module load compiler/intel/19.1
$ module load compiler/intel/2021.4.0
```

```
The following have been reloaded with a version change:
  1) compiler/intel/19.1 => compiler/intel/2021.4.0
```

  - b) load module with dependencies on other modules

```
$ module load compiler/intel/2021.4.0
$ module load numlib/gsl/2.6-intel-19.1
```

Requires Intel-Suite 19.1

```
The following have been reloaded with a version change:
  1) compiler/intel/2021.4.0 => compiler/intel/19.1
```

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/2022.2.1

$ module load compiler/intel/2022.2.1

$ module -r spider 'mpi/openmpi.*'
→ mpi/openmpi/4.1

$ module load mpi/openmpi/4.1
```

```
# Pitfall: Loading openmpi before compiler
$ module load mpi/openmpi/4.1

Lmod has detected the following error:
These module(s) or extension(s) exist but cannot be loaded as requested:
"mpi/openmpi/4.1"
   Try: "module spider mpi/openmpi/4.1" 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-intel-19.1
$ module unload compiler/intel/19.1
```

```
-------------------------------------------------------------
The following dependent module(s) are not currently loaded:
compiler/intel/19.1 (required by: numlib/gsl/2.6-intel-19.1)
-------------------------------------------------------------
```

- Swap = remove + load

e.g.:

```
$ module swap compiler/gnu compiler/intel
```

Removes default GNU version and loads default INTEL version

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

```
$ module purge
```

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

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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 8.5.0-10)
```

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

```
$ module spider compiler/gnu

     Versions:
        compiler/gnu/8.3.1
        compiler/gnu/9.3
        ...
        compiler/gnu/12.1
        compiler/gnu/13.2

$ module load compiler/gnu/13.2
$ gcc --version
gcc (GCC) 13.2.0
```

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:

```
$ 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
```