Software Environment on CLAIX

HPC Intro 2024

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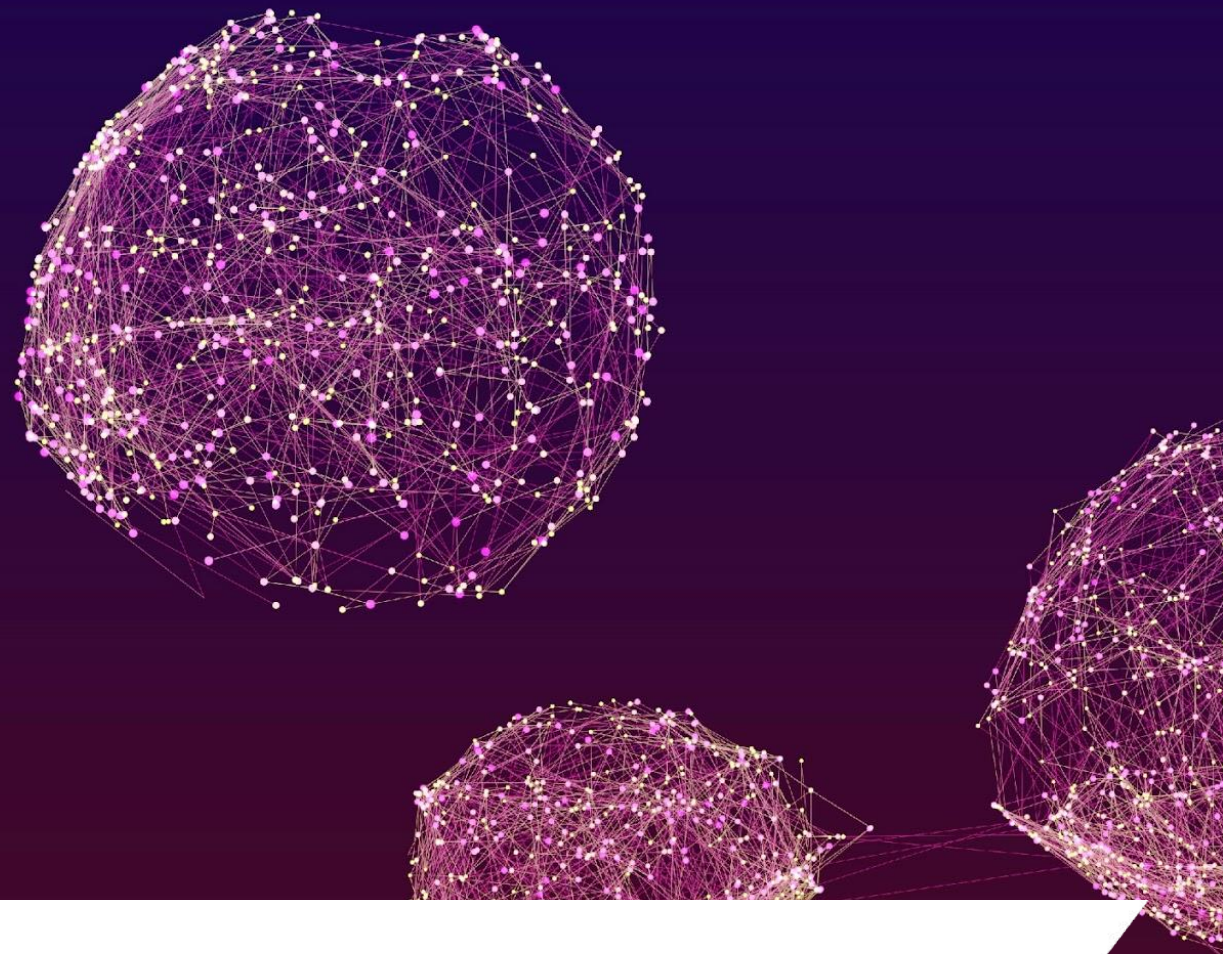

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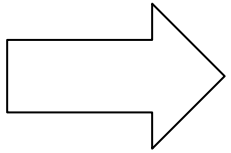
Module system

```
export PATH=/opt/intel/bin:$PATH
make CC=icc CXX=icpc FC=ifort
```

```
export PATH=/opt/gcc/bin:$PATH
make CC=gcc CXX=g++ FC=gfortran
```



```
make
```

```
export PATH=/opt/clang/bin:$PATH
make CC=clang CXX=clang++ FC=flang
```

- Simplifies usage of software
  - different versions of same software
  - conflicting software, e.g. different compilers
- Software hidden behind modules
  - Handles conflicts & dependencies
  - Adjusts environment variables

Listing loaded modules

```
$ module list

Currently Loaded Modules:
  1) GCCcore/.11.3.0          (H,C)   5) numactl/2.0.14       9) imkl-FFTW/2022.1.0
  2) zlib/1.2.12                      6) UCX/1.12.1          10) intel/2022a        (TC)
  3) binutils/2.38                    7) impi/2021.6.0  (M)
  4) intel-compilers/2022.1.0 (C)     8) imkl/2022.1.0  (m)

  Where:
   TC:          Toolchain, comprising a compiler, possibly an MPI implementation, and optional mathematical libraries
   C:           Compiler
   M:           MPI implementation
   m:           mathematical libraries
   H:           Hidden Module
```

Software usable “at the moment”

Showing currently available modules

```
$ module avail
   ABAQUS/2017                                 iimpi/2020a                      (TC)
   ABAQUS/2018                                 iimpi/2020b                      (TC)
   ABAQUS/2019                                 iimpi/2021a                      (TC)
   ABAQUS/2020                                 iimpi/2021b                      (TC)
   ABAQUS/2021                                 iimpi/2022a                      (TC,D)
   ABAQUS/2022                                 iimpi/2022b                      (TC)
   ABAQUS/2023                          (D)    iimpi/2023a                      (TC)
   Advisor/2023.0.0                            iimpi/2023b                      (TC)
   ANSYS/2021R2-test                           ImageNet/ILSVRC2012
   ANSYS/2021R2                                ImageNet/Winter21_whole          (D)
...
```

Only shows modules loadable with currently loaded modules

Case sensitive

```
$ module avail CMake
   CMake/3.21.1    CMake/3.22.1    CMake/3.23.1    CMake/3.24.3    CMake/3.26.3 (D)
```

Loading modules

```
$ module load intel-compilers/2023.1.0

[INFO] Module intel-compilers/2023.1.0 loaded.

[INFO] Module numactl/2.0.14 loaded.


Inactive Modules:

  1) UCX/1.12.1     2) imkl-FFTW/2022.1.0     3) impi/2021.6.0


Due to MODULEPATH changes, the following have been reloaded:

  1) numactl/2.0.14


The following have been reloaded with a version change:

  1) GCCcore/.11.3.0 => GCCcore/.12.3.0     3) intel-compilers/2022.1.0 => intel-compilers/2023.1.0

  2) binutils/2.38 => binutils/2.40         4) zlib/1.2.12 => zlib/1.2.13

$ module list

  1) imkl/2022.1.0 (m)    3) GCCcore/.12.3.0 (H,C)   5) binutils/2.40                 7) numactl/2.0.14

  2) intel/2022a   (TC)   4) zlib/1.2.13             6) intel-compilers/2023.1.0 (C)
```

Modules no longer available with newly loaded module

Automatically (re)load dependencies of newly loaded module

Module hierarchy

```
$ module avail

------------------------------------------ MPI dependent Modules ------------------------------------------
   AlphaFold/2.3.1-CUDA-11.7.0              netCDF/4.9.0
   Biopython/1.79                           networkx/2.6.3
…
---------------------------------------- Compiler dependent Modules ----------------------------------------
   ACTC/1.1                               libsndfile/1.1.0
   at-spi2-atk/2.38.0                     LibTIFF/4.3.0
…
------------------------------------------------ Core Modules ------------------------------------------------
   ABAQUS/2017                                 iimpi/2020a                    (TC)
   ABAQUS/2018                                 iimpi/2020b                    (TC)
…
```

Independent of any other modules (no dependencies)

Toolchains

```
$ module load GCC OpenMPI

[INFO] Module GCC/11.3.0 loaded.

[INFO] Module OpenMPI/4.1.4 loaded.


Lmod is automatically replacing "impi/2021.6.0" with "OpenMPI/4.1.4".


Lmod Warning:

-------------------------------------------------------------------------------------------------

The following dependent module(s) are not currently loaded: imkl-FFTW/2022.1.0 (required by: intel/2022a),

impi/2021.6.0 (required by: intel/2022a)

-------------------------------------------------------------------------------------------------

Inactive Modules:

  1) imkl-FFTW/2022.1.0
```

Cannot use two MPI implementations simultaneously

Toolchains

Includes GCC & OpenMPI

```
$ module switch intel foss
[INFO] Module zlib/1.2.12 loaded.
[INFO] Module binutils/2.38 loaded.
[INFO] Module numactl/2.0.14 loaded.
[INFO] Module foss/2022a loaded.
$ module list
  1) GCCcore/.11.3.0   (H,C)   7) OpenSSL/1.1       13) OpenMPI/4.1.4      (M)  19) foss/2022a     (TC)
  2) GCC/11.3.0        (TC)    8) libevent/2.1.12   14) OpenBLAS/0.3.20          20) zlib/1.2.12
  3) XZ/5.2.5                  9) UCX/1.12.1        15) FlexiBLAS/3.2.0          21) binutils/2.38
  4) libxml2/2.9.13           10) libfabric/1.15.1  16) FFTW/3.3.10              22) numactl/2.0.14
  5) libpciaccess/0.16        11) PMIx/4.1.2        17) FFTW.MPI/3.3.10
  6) hwloc/2.7.1              12) UCC/1.0.0         18) ScaLAPACK/2.2.0-fb
```

- Defines a set of modules
- Included modules are (un)loaded when (un)loading the toolchain

Switching modules may leave some inactive modules loaded

➢ Undesired side-effects

➢ Purge before loading completely different module version / toolchain

```
$ module purge

$ module load foss
[INFO] Module foss/2022a loaded.
```

User module collections

```
$ module purge

$ module load foss CMake Ninja Autotools CUDA Boost Python

$ module save dev
```

```
$ ssh login18-1

$ module restore dev
```

No manual `purge` needed

- Convenient when having fixed environments for different projects
- Better alternative to (un)loading in shell config (`zshrc`, `bashrc`)
  - Should be avoided, might lead to login problems

Finding modules

```
$ module avail CMake

   CMake/3.21.1    CMake/3.22.1    CMake/3.23.1    CMake/3.24.3    CMake/3.26.3 (D)
```

Case insensitive

```
$ module spider cmake
    Description:
      CMake, the cross-platform, open-source build system. CMake is a family of tools designed to build, test
      and package software.
     Versions:
        CMake/3.15.3
        CMake/3.16.4
        CMake/3.18.4
        CMake/3.20.1
        CMake/3.21.1
        CMake/3.22.1
        CMake/3.23.1
        CMake/3.24.3
        CMake/3.26.3
        CMake/3.27.6
```

Find out dependencies of specific version

```
$ module spider CMake/3.27.6

    You will need to load all module(s) on any one of the lines below before the "CMake/3.27.6" module is available to load.

      GCCcore/.13.2.0
```

Module categories

```
$ module category

---------------------------------------------- List of Categories ----------------------------------------------

cfd  chem  devel  io  material  math  perf  tools
```

```
$ module category chem

------------------------------------------------- chem -------------------------------------------------------

CP2K  (4)   GAMESS-US (1)   ORCA  (2)   QuantumESPRESSO (3)   VASP (2)

CREST (1)   Gaussian  (7)   PETSc (2)   Siesta          (1)   xtb  (3)
```

Module overview

```
$ module overview

---------------------------------------------- MPI dependent Modules ----------------------
ABINIT          (4)   GAMESS-US (1)   mpi4py         (1)   OpenBabel (1)   SciPy-bundle (1)   Wa
CGAL            (1)   HDF5      (7)   mpiP           (1)   OpenMX    (1)   Score-P      (5)
...

------------------------------------------- Compiler dependent Modules --------------------------------------------
ACTC              (1)   Ghostscript          (2)   libdwarf      (1)   METIS           (1)   Qhull        (1)
at-spi2-atk       (1)   giflib               (1)   libelf        (1)   MPC             (1)   Qt5          (2)
...

---------------------------------------------------- Core Modules ----------------------------------------------------
ABAQUS        (7)    Dymola     (1)    gomkl           (3)   iompi        (4)   Mathematica   (2)   STAR-CCM+    (6)
Advisor       (1)    EasyBuild  (8)    gompi           (8)   itac         (2)   MATLAB        (9)   Tcl          (1)
...

------------------------------------------------ Container Image Modules ------------------------------------------------
datascience-notebook (2)   PyTorch (1)   rapids (1)   tensorflow (1)   TensorFlow (1)
```

As `spider` command, independent of currently loaded modules

Prefer provided software over own installations

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Provided software

- Configured and tuned for CLAIX
  - Compiled for host architecture with AVX512 etc.
  - Make use of GPUs if available
  - ➢ Better performance
- Has probably already been tested
  - Should work out-of-the-box
  - ➢ Less effort for you and supportive staff

Examples

- Especially Python packages via `pip`
- `TensorFlow, PyTorch, Horovod, NumPy, SciPy`
  - Available as ordinary modules or containers

Advise

- Search via `module spider <name>`
- Search under help.itc.rwth-aachen.de

```
$ module load TensorFlow
[INFO] You can access the TensorFlow image via $TENSORFLOW_IMAGE
$ apptainer exec -nv $TENSORFLOW_IMAGE <command>
```

Enable CUDA/GPU support

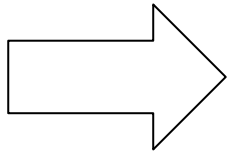
Environment variables

Only works with specific `intel` toolchain

```
$ icc \
 -qopenmp \
-L/cvmfs/software.hpc.rwth.de/Linux/RH8/x86_64/intel/skylake_avx512/software/FFTW/3.3.10-intel-2022a \
 -lfftw3 \
 main.c
```

Only works with specific `foss` toolchain

```
$ gcc \
 -fopenmp \
-L/cvmfs/software.hpc.rwth.de/Linux/RH8/x86_64/intel/skylake_avx512/software/FFTW/3.3.10-GCC-11.3.0 \
 -lfftw3 \
 main.c
```



Works with any `intel` & `foss` toolchain

```
$ $CC \
 $FLAGS_OPENMP \
 -L$EBROOTFFTW/lib \
 -lfftw3 \
 main.c
```

`$EBROOT<module>` always refers to base directory of loaded `<module>`

- Write version- and toolchain-independent scripts
  - Use environment variables if possible
  - Avoid hardcoding names, versions, paths etc.

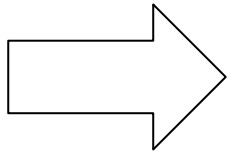
Compiling MPI programs

Only works with Intel MPI

```
$ make \
 CC=mpiicc \
 CXX=mpicpc \
 FC=mpiifort
```

Only works with Open MPI

```
$ make \
 CC=mpicc \
 CXX=mpicxx \
 FC=mpifort
```



Works with Intel & Open MPI on CLAIX

```
$ make \
 CC=$MPICC \
 CXX=$MPICXX \
 FC=$MPIFC
```

Summary

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Key takeaways

- Module system: simplifies management & usage of different software/versions
- Use toolchains (set of modules) when possible
- Prefer provided software over own installations
- Use environment variables in scripts instead of hardcoded names, paths etc. where possible

Commands

- `module list`
- `module (un)load <module>`
- `module avail [<module>]` (case sensitive)
- `module spider <module>` (case insensitive)
- `module switch <module1> <module2>`
- `module purge`
- `module overview`
- `module category [<category>]`

Environment variables

- Compiler: CC, CXX, FC
- MPI: MPICC, MPICXX, MPIFC
- Misc.: FLAGS_OPENMP, FLAGS_FAST
- Generic: EBROOT<module>

More information & help

- help.itc.rwth-aachen.de
- lmod.readthedocs.io/en/latest/010_user.html (user guide for the module system)
- servicedesk@itc.rwth-aachen.de