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Tutorial: BwUniCluster 3.0/HoreKa Modules

In this tutorial we will learn about modules and how to utilize them on the BwUniCluster or HoreKa.

1. What are modules?

Modules are means by which the user can access and use the software installed on the BwUniCluster or HoreKa such as widely used compilers and software. In order to use a specific programm or software (e.g. OpenFOAM) the user has to load the corresponding module during their session. It is an excellent concept that allows the users to immediately load and use any version of OpenFOAM that is currently installed (currently 15 versions from 3 vendors in April 2024 on the bwUniCluster). User do not need to do any installation!

2. How to find and load specific module?

You can view the list of all available modules using the following command:

\$> module av

or

\$> module spider openfoam

The modules can be then loaded by using the following command:

\$> module load [name of the module]

For example:

\$> module load cae/openfoam/v2112

The compiler then generates the following response:

In the contrast of the contras

source \$FOAM_INIT

or simply:

 Together with the OpenFOAM v2112 also the corresponding compilers and MPI packages (with which the OpenFOAM was compiled) are automatically loaded:

\$> module list

returns: Currently Loaded Modules (could differ depending on the supercomputer): 1) compiler/gnu/12.1 2) mpi/openmpi/4.1 3) cae/openfoam/v2112

After initializing OpenFOAM we can use it like we would on a personal computer. However, we need to remember that <u>a module initialized this way can only be used in the</u> <u>current terminal window</u>, i.e. opening a second terminal does not mean that the modules loaded on the first terminal will be available in the second one! The same is valid for the compute nodes – before running OpenFOAM on a compute node we have to load the modules anew. In order to use a module on the computing node we need to load it using the batch job command (in blue). For example (the job-example here is <u>not parallel</u>):

#SBATCH --partition dev_cpu // dev_cpu_il or dev_cpuonly (HoreKa) #SBATCH --nodes=1

#SBATCH --mem=8000mb #SBATCH --job-name=MyFirstParallelJob module purge module load cae/openfoam/v2112

source \$FOAM INIT

#SBATCH --time=00:30:00

#SBATCH --nodes=1 #SBATCH --ntasks=1

pimpleFoam

3. How to remove installed modules (in order to load others)?

To see what modules you have currently loaded (some of them are loaded automatically when you login) use the command:

\$> module list

In order to remove the already loaded modules (all of them) we can use the following command:

\$> module purge

To remove only one module, e.g. the module system/ssh_wrapper/0.1 use:

\$> module unload system/ssh_wrapper/0.1