Tutorial: BwUniCluster 2.0/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 (eg. OpenFOAM) the user has to load in the corresponding module during their session.

2. How to find and load specific module?

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

$> module av

or

$> module spider openfoam

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

$> module load [name of the module]

For example:

$> module load cae/openfoam/v2106-impi

The compiler then generates the following response:

//
Don't forget to initialize OpenFOAM with:

source $FOAM_INIT

or simply:

foamInit
//

After initializing OpenFOAM we can use it like we would on a personal computer. However, we need to remember that a module initialized this way can only be used on the current terminal i.e. opening a second terminal does not mean that the modules loaded on the first terminal will be availible 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-examle here is not parallel):

```
///////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////
#!/bin/bash

#SBATCH --partition dev_single
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --time=00:30:00
#SBATCH --mem=8000mb
#SBATCH --job-name=MyFirstParallelJob

module purge
module load  cae/openfoam/v2106-impi
source $FOAM_INIT

pimpleFoam
///////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////
```

3. How to remove installed modules?

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