Software modules on bwUniCluster

bwHPC support team Hohenheim

Installed software on bwUniCluster

- There is a software stack installed on bwUniCluster that can be directly used you (which are called modules)

- You get the whole list of modules with the command

```
$ module avail
```

- Modules are organized in categories, show all modules within a category:

```
$ module avail <category>
```

bio *Biology*	**cae** *Computer-aided engineering*	**chem** *Chemistry*	**compiler** *multiple compilers*
devel *Devel tools, e.g. cuda, cmake, JRE*	**math** *Julia, Matlab, R*	**mpi** *Parallelisation*	**numlib** *Numerical libraries*
phys *Physics*	**vis** *Visualisation*		**system, jupyter, lib**

Installed software on bwUniCluster - homepage

The software installed on the bwUniCluster (and on the other Tier 3 bwHPC clusters) are also listed on https://www.bwhpc.de/software.php

Information on modules

- “Module address”: specifies the specific module, there can be multiple versions. Example: The newest R version has “address” math/R/4.1.2

- Get more information on how to load module, first steps, <u>examples</u>, ... (so a short manual)

```
$ module spider <module address>
```

- You can also use

```
$ module spider <key>
```

to get all modules (+ basic information) that include the key
(key = module category, short name (e.g. python),...)

<u>Exercises</u>:
- Pick a module and check its manual
- Use **module spider <key>** with a key of your choice

Working with modules

- Load a module (loaded ⇨ commands from module run everywhere)

```
$ module load <module address>
```

- Some modules have dependencies, `module spider <module address>` shows them (this means you just have to load additional modules)

- Unload a module

```
$ module unload <module address>
```

- List all modules loaded by you, unload all modules

```
$ module list
$ module purge
```

Modules are loaded on ALL nodes: once loaded, they also are available in batch jobs

How to install further software

- You can install programs by yourself unless they need root user rights
- You can clone git repositories into your directories
- If you run into any trouble: Open a ticket at the support & help desk
  https://bw-support.scc.kit.edu

Example: Installing packages for the statistical computation software R

- A good number of packages is preinstalled (more than in standard R)
- Within R, check with *installed.packages*
- You can install further packages within R as usual (e.g. via *install.packages*)

Of course: you need to load the R module first (via **module load**)

Example: Module parbatch

Let’s look at the module parbatch, which simply takes many (serial) jobs and runs them in parallel

```
$ module load parbatch
```

Get more information via

```
$ module spider parbatch
```

We learn here that there are examples in a dedicated directory (gets set when module is loaded)

```
$ cd  $PARBATCH_EXA_DIR
```

Let’s have a look!

Exercise: Open R on bwUniCluster

- Start R on the command line via
  $ R
- In R, quit R by
  > q()

Exercise: This only works after a R module is loaded

- Load a (the?) R module, launch and quit R
- Locate example scripts for R