

17th HPC Café

02.07.2026



Agenda HPC Café – 02.07.2026

Topics for today:

- **Focus Topic: Easybuild - or how to use modules and own modules on bwUniCluster 3.0 and HoreKa 2**
- Discussion and open floor

As usual this format is meant to be interactive.
Don't hesitate to ask questions!

Easybuild - or how to use modules and own modules on bwUniCluster 3.0 and HoreKa 2

Sven Trautmann (SCC)



Time for Discussion

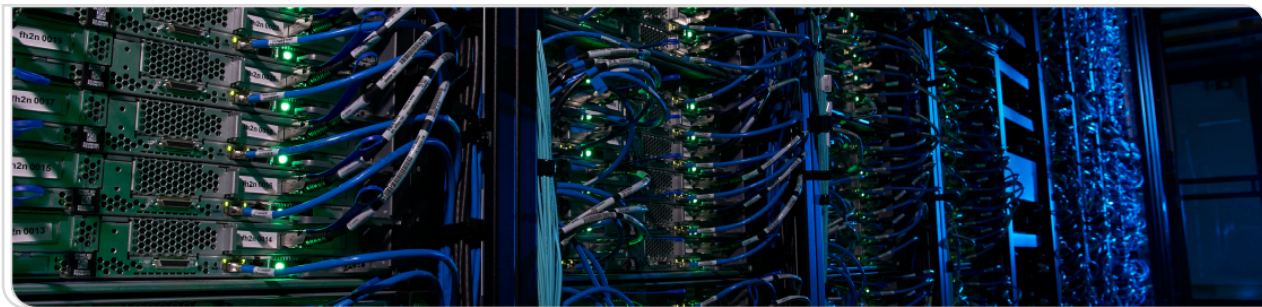


Next HPC Café

- Next HPC Café planned for **3 September 2026, 10 am**
- Reminder: regular timeslot for the HPC Café
 - Every **first Thursday of the month 10:00 am**
 - Summerbreak in August
- As always, open to hear ideas for topics and talks, from ...
 - Yourself
 - Colleagues and collaborators
 - Also just expressions for “topics of interest”

HPC Cafe: EasyBuild on bwUniCluster 3.0 and HoreKa 2

Sven Trautmann | 2026-07-02



Software on bwUniCluster 3.0 and HoreKa

- On bwUniCluster 3.0
 - Software is provided by multiple sites
 - best effort, people are busy doing other things
- HoreKa
 - Ancient hand-made build system based on make and rpm spec files
 - Big software matrix (compilers/MPI implementations/scientific libraries)
 - more compilers (NVIDIA, AMD, LLVM)
 - Many problems to get all combinations to build, e.g. Intel compiler needs convincing to work on AMD CPUs, C/C++/Fortran standards ...
 - Not enough checks and time to check
 - Minor updates have broken things in the past
 - other SCC teams provide additional software

What's new on HoreKa 2?

- HoreKa 2.0 will have
 - CPU nodes with AMD ZEN5 architecture
 - GPU nodes with NVIDIA ARM CPUs and NVIDIA GPUs (Grace/Hopper)
 - Some HoreKa nodes
 - AMD nodes with ZEN4 architecture and NVIDIA GPUs
 - Intel CPU node with NVIDIA GPUs
 - Maybe some more Intel CPU nodes
- From a software point-of-view
 - Need to support multiple architectures (x86_64, aarch64)
 - Software needs to be compiled on different machines
 - 2nd architecture almost doubles the effort

How to improve the situation?

- provide less software?
- Have staff dedicated to user software?
- use and contribute to available solutions
 - EasyBuild
 - EESSI
 - Spack

Why EasyBuild?

■ Pro

- Some experience in software team
- It's European, many contributors from all over Europe (e.g. NL, BE, SE, UK, DE, FI, CH)
- It's being used by many big HPC systems like LUMI and Jupiter (EESSI uses EasyBuild)
- Switching from HoreKa2 to a bigger system will be easier for the users
- The job scheduler can be used to build software (even the whole stack) in parallel over many nodes
- Commercial software packages can be integrated, some already are

■ Contra

- It's not perfect, some patching required
- Module naming scheme is different
- Not all compiler/MPI combinations are available

Why not something else?

- Why not Spack?
 - No experience in software team
 - Module naming scheme seems odd
 - Description language is pure Python
 - It's not European
- Why not EESSI (yet)?
 - [European Environment for Scientific Software Installations](#) (EESSI pronounced as easy)
 - uses EasyBuild
 - needs an additional file system (CernVM-FS) on all nodes
 - needs local proxies to provide better performance
 - limited number of supported architectures and packages

EasyBuild basics

- [EasyBuild](#) is a community driven software to provide a reproducible way to build software on computer systems
- Not limited to HPC, you can use EasyBuild on your laptop
- Most community members are from Europe and several HPC sites are actively developing and updating the software.
- EasyBuild is implemented in Python.
- EasyConfig files (file extension `.eb`) are used to describe the build process.
- [easyconfigs Github repository](#)
- EasyBuild tries to be as independent of the underlying operating system as possible
- Loading a module will automatically load all the dependent lower level modules and the output of `module list` will be rather long

Module load example

- loading the gnuplot module, will load 79 modules in total

```
[user@host ~]$ module load gnuplot  
[user@host ~]$ module list
```

Currently Loaded Modules:

1) GCCcore/14.3.0	41) giflib/5.2.2-GCCcore-14.3.0
2) ncurses/6.5-GCCcore-14.3.0	42) libwebp/1.5.0-GCCcore-14.3.0
3) bzip2/1.0.8-GCCcore-14.3.0	43) libde265/1.0.16-GCCcore-14.3.0
4) zlib/1.3.1-GCCcore-14.3.0	44) x265/4.1-GCCcore-14.3.0
5) libpng/1.6.50-GCCcore-14.3.0	45) Gdk-Pixbuf/2.42.12-GCCcore-14.3.0
...	
39) libdeflate/1.24-GCCcore-14.3.0	79) gnuplot/6.0.3-GCCcore-14.3.0
40) LibTIFF/4.7.0-GCCcore-14.3.0	

User software on SCC HPC systems

- HoreKa 2
 - Lmod will be the default and only module system
 - make sure to convert tc1 modules
 - as before `module load anyModule` will load the default (which usually means latest version of `anyModule`)
 - a specific version can be requested
- bwUniCluster 3.0
 - will not have EasyBuild as default for now
 - maybe EESSI is the next step
- we have been testing EasyBuild for a while but there will be growing pains, sorry

Where to get more information, try EasyBuild?

- on bwUniCluster 3.0 and HoreKa EasyBuild is already available
- optional feature which needs to be enabled
- We provide a basic documentation
 - [bwHPC wiki](#)
 - [HoreKa documentation](#)
- There are plenty of good tutorials available
 - [Official EasyBuild tutorial](#)
 - [LUMI tutorials](#)

Want to build software with EasyBuild?

- Set up your own EasyBuild module tree, parallel to the central one
- Build and test your software
- Let us know, if it should be made available to all users
- Give it a try, it's not rocket surgery

Thank you!

Comments?

Questions?