

How to use spack – solving the dependency problem

Building your model with netcdf-fortran (modules)

\$ module load netcdf-fortran/4.5.3-openmpi-4.1.2-intel-2021.5.0

- Problem: long list of dependencies like MPI, hdf5, parallel-netcdf and netcdf-c not accessible with the module system
- Solution: use spack to list them all

```
$ module show netcdf-fortran/4.5.3-openmpi-4.1.2-intel-2021.5.0 $ spack find -dp /k6xq5g
```



How to use spack – module vs. spack

- Module system is easy to use but does not help much for building your own software
 - Users need to set compilation and linking commands
 - Might lead to unstable binaries, which depend on the loaded modules at runtime
- Spack is more complex but allows to build packages with stable dependencies
 - Linking paths are written into the binaries so they know where to look for their needed libraries
 - Software can be build completely in user-space -> user can be more independent of the software tree (similar to conda)



How to use spack – build your own package (I)

Example: you want an older CDO version

 Create your own installation directory and set up the spack config accordingly:

docs.dkrz.de/doc/levante/code-development/building-with-spack.html

Check the existing compilers

\$ spack compilers

Check the available cdo versions

\$ spack info cdo



How to use spack – build your own package (II)

 Select compiler and version and check what spack would build

\$ spack spec -I cdo@1.9.2 %gcc

- Since spack is designed for HPC centers, using MPI is default. Can be disabled to speed up building process
 - \$ spack spec -I cdo@1.9.2 %gcc ^fftw~mpi ^hdf5~mpi ^eccodes
- If everything looks ok, start the build
 - \$ spack install cdo@1.9.2 %gcc ^fftw~mpi ^hdf5~mpi ^eccodes