Managing HPC Application Software with SPACK@LRZ

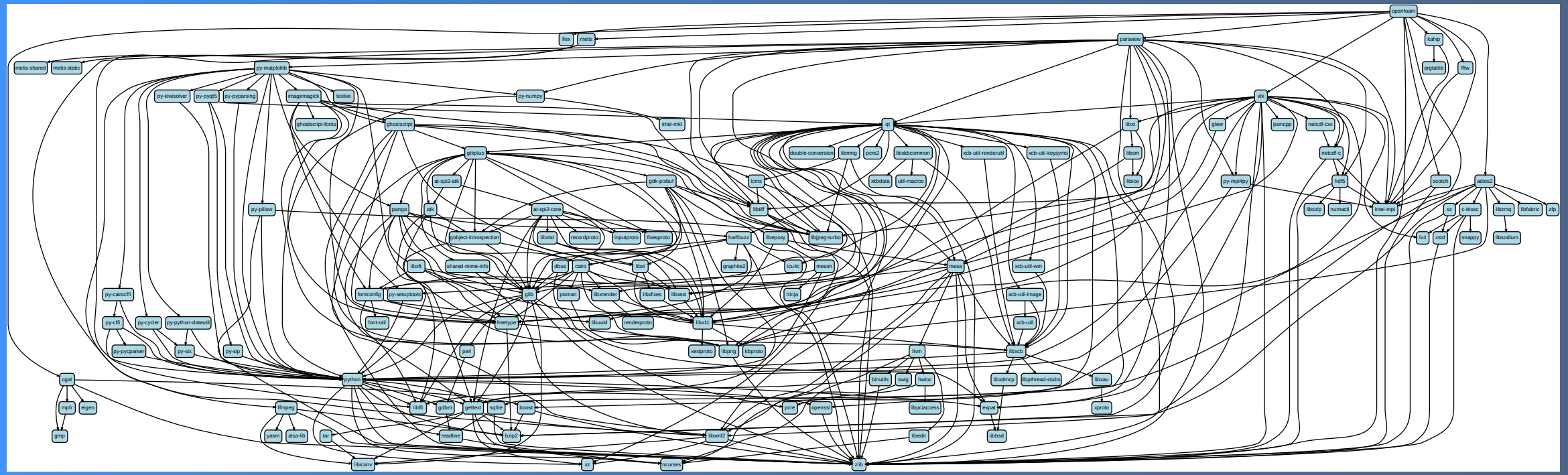
Leibniz-Rechenzentrum | 09.06.2021 | Gilbert Brietzke

Motivation: How to manage the dependency-hell?

- A high-level application may just be the „tip of an iceberg“ when considering a feature-rich configuration of the software with all it‘s dependencies
- Example: OpenSource CFD-Package OpenFOAM

e.g.: feature-rich OpenFOAM incl. vtk & paraview

140 dependencies



Spack is a flexible package manager targeted at HPC-systems

- Spack available at github ‚ready to use'
  few prerequisits only:
  - a basic python,
  - make and a c/c++-compiler
  - tar/gzip/bzip2/xz
  - patch + git + curl
  - pgp (for gnupg2 commands only)

In principle it may be as simple as:

```
git clone https://github.com/spack/spack.
. spack/share/spack/setup.env.sh
spack install <package-spec>
```

NOTE: doing like this is fine but you are on your own … needs some experience with configuring and compiling software in many circumstances

However - we do support spack in user-space via a module called **user_spack**
(with pre-installed and -configured spack)

```
spack install <package-spec>
# e.g.:
spack install hdf5
spack install hdf5%gcc@9.3.0+fortran+hl
spack install hdf5 ^openmpi
```

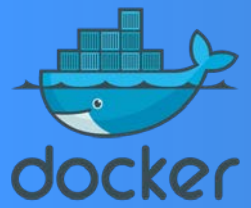
- Spack may install many different variants of the same package:
  - Built different package-versions
  - Built with different compilers
  - Built with different MPI-implementations
  - Built with different build-options

- Installation locations are seperated via unique hashes
  -> installations may peacefully coexist

Spack is one of the many package-managers

- Functional Cross-Platform Package Managers:
  e.g Nix (NixOs), Gnu Guix (Gnu Guix Linux) … use hashes in install-dirs
- Build-from-source Package Managers
  e.g. HomeBrew/LinuxBrew
- Package Managers for specific scripting languages
  e.g. Pip (Python), NPM (Javascript)
- Easy Build:
  installation framework for managing scientific software on HPC-systems: less flexible for experimental build-combinations
- Conda:
  popluar binary package managers for Python and R (but also for other rpm–like packaging in user-space). Easy to use.
  In general no architecture optimized binaries, not targeted at HPC

Containers



- Containers provide a great way to reproduce and distribute an already-built software stack
- In cloud Machines this may be a good choice
- But: who builds the container for your project on a specific HPC-machine?
  - What about MPI?
  - What about well performing parallel-IO
- ! For sofisticated scientific projects on specific HPC-machines this often isn‘t a trivial task!
- `spack containerize` -command may help you with building containers using spack
- This short-talk is not on container. But just to mention:
  We do support Containers at LRZ (at present mostly by Charliecloud-containers)

From manual single package installations to automated stack builds

In the past at LRZ …

- Software stack on LRZ HPC-systems used to be provided via the module system in a non-orchestrated way with hand-written TCL-files to make installations available: applications/libraries/tools /compilers

Limitations:

- Non-transparent or oblique conflicts and/or dependencies of packages
- Non-transparent package-configs and build-variants
- Builds often not reproducible (documentation issue)

Since recently at LRZ …

- Spack compiled software provided for many open-source packages

Advantages:

- **Spack Builds** are **self-documenting:**

  -> Package-builds are typically **reproducible**

- Spack-compiler wrappers inject compiler-flags for the target-architecture -> **optimized** software stack
- Installation of many package-variants do not disturb each other -> many packages may **peacefully coexist**
- Installation (fetch/configure/build/install/module-create) of the software is **automized**

Spack in user-space:
chaining existing installations into your own Spack environment

1. We do privide compiled software with support via environment–modules (the classical way ~>300 modules)

2. NEW + Experimental (work in progress):
module load user_spack
We provide compiled software via spack-chaining

- For experienced users:
  - may use spack via `module load user_spack` that provides a preconfigured spack
  - making use of already installed packages via spack chaining of upstream-location (lrzs/sys/spack/x/y)

-> avoids recompiling low level packages in many situations
-> has working defaults configurated for some essential dependencies (e.g. MPI)

- **Simple Example 1 – install (missing) package libvdwxc:**

```
cm2login3~>module list
Currently Loaded Modulefiles:
 1) admin/1.0    2) tempdir/1.0    3) lrz/1.0    4) spack/21.1.1
cm2login3~>module load user_spack
executing /lrz/sys/spack/user/release/21.1.1/bin/../spack/share/spack/setup-env.sh
cm2login3~>spack spec -lI libvdwxc
Input spec
--------------------------------
 -   libvdwxc

Concretized
--------------------------------
 -   duakorn  libvdwxc@0.4.0%gcc@8.4.0+mpi~pfft arch=linux-sles15-haswell
[^]  ve6ybks      ^fftw@3.3.8%gcc@8.4.0+mpi~openmp~pfft_patches precision=double,f
loat arch=linux-sles15-haswell
[^]  cyojcvv          ^intel-mpi@2019.8.254%gcc@8.4.0 arch=linux-sles15-haswell

cm2login3~>spack install libvdwxc
[+] /dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/intel-mpi/2019.8.254-gc
c-cyojcvv
[+] /dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/intel-mpi/2019.8.254-gc
c-cyojcvv
[+] /dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/fftw/3.3.8-gcc-ve6ybks
[+] /dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/fftw/3.3.8-gcc-ve6ybks
==> Installing libvdwxc
==> No binary for libvdwxc found: installing from source
==> libvdwxc: Executing phase: 'autoreconf'
==> libvdwxc: Executing phase: 'configure'
==> libvdwxc: Executing phase: 'build'
==> libvdwxc: Executing phase: 'install'
[+] /dss/dsshome1/          /spack/opt/linux-sles15-haswell/libvdwxc/0.4.0-gcc-8.4
.0-duakorn
```

Spack in user-space: chaining existing installations into your own Spack environment

NEW + Experimental (work in progress):
module load user_spack

Example 2: create your own new package inside your own repository.

e.g. libgeotiff
Recently moved to github, version that comes built-in-spack is too old for your purpose

```
cm2login3~>spack create -n libgeotiff -N mine-15.4 https://github.
com/OSGeo/libgeotiff/releases/download/1.6.0/libgeotiff-1.6.0.tar.
gz
==> Using specified package name: 'libgeotiff'

==> This package looks like it uses the cmake build system
==> Created template for libgeotiff package
==> Created package file: /dss/dsshome1/(          /spack/repos/min
e-15.4/packages/libgeotiff/package.py
```

```
# See the Spack documentation for more information on packaging.
# ----------------------------------------------------------------------------

from spack import *


class Libgeotiff(CMakePackage):
    """FIXME: Put a proper description of your package here."""

    # FIXME: Add a proper url for your package's homepage here.
    homepage = "https://www.example.com"
    url      = "https://github.com/OSGeo/libgeotiff/releases/download/1.6.0/libgeotiff-1.6.0.tar.gz"

    # FIXME: Add a list of GitHub accounts to
    # notify when the package is updated.
    # maintainers = ['github_user1', 'github_user2']

    version('1.6.0', sha256='9311017e5284cffb86f2c7b7a9df1fb5ebcdc61c30468fb2e6bca36e4272ebca')
    version('1.5.1', sha256='f9e99733c170d11052f562bcd2c7cb4de53ed405f7acdde4f16195cd3ead612c')
    version('1.4.3', sha256='b8510d9b968b5ee899282cdd5bef13fd02d5a4c19f664553f81e31127bc47265')

    # FIXME: Add dependencies if required.
    # depends_on('foo')

    def cmake_args(self):
        # FIXME: Add arguments other than
        # FIXME: CMAKE_INSTALL_PREFIX and CMAKE_BUILD_TYPE
        # FIXME: If not needed delete this function
        args = []
        return args


-UU-:----F1  package.py     All L1     (Python) ----------------------------------------------------
```

Add the missing stuff: here at least the dependencies need to be specified

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    version('1.6.0', sha256='9311017e5284cffb86f2c7b7a9df1fb5ebcdc61c30468fb2e6bca36e4272ebca')
    version('1.5.1', sha256='f9e99733c170d11052f562bcd2c7cb4de53ed405f7acdde4f16195cd3ead612c')
    version('1.4.3', sha256='b8510d9b968b5ee899282cdd5bef13fd02d5a4c19f664553f81e31127bc47265')

    depends_on('jpeg')
    depends_on('libtiff')
    depends_on('proj')
    depends_on('zlib')

    def cmake_args(self):
        # FIXME: Add arguments other than
        # FIXME: CMAKE_INSTALL_PREFIX and CMAKE_BUILD_TYPE
        # FIXME: If not needed delete this function
        args = []
        return args
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E.g. libgeotiff
Recently moved to github, version that comes built in spack is too old for your purpose

Depending on the complexity the package Implementing package.py

- may be very easy
- may become more difficult

But in many cases it is doable

```
cm2login3~>spack spec -lINt libgeotiff
Input spec
--------------------------------
 -   [    ]  .libgeotiff

Concretized
--------------------------------
 -   cprryjt  [    ]  mine-15.4.libgeotiff@1.6.0%gcc@8.4.0 build_type=RelWithDebInfo arch=linux-sles15-haswell
[^]  fi3lvva  [b   ]      ^builtin.cmake@3.16.5%gcc@8.4.0~doc+ncurses+openssl+ownlibs~qt patches=1c540040c7e203
dd8e27aa20345ecb07fe06570d56410a24a266ae570b1c4c39 arch=linux-sles15-haswell
[^]  6qhv5ta  [bl  ]          ^fixes015x.ncurses@6.2%gcc@8.4.0~symlinks+termlib arch=linux-sles15-haswell
[^]  cfijkws  [b   ]              ^builtin.pkgconf@1.7.3%gcc@8.4.0 arch=linux-sles15-haswell
[^]  jpko756  [bl  ]          ^builtin.openssl@1.1.1g%gcc@8.4.0+systemcerts arch=linux-sles15-haswell
[^]  bhpjih4  [b  t]              ^builtin.perl@5.30.3%gcc@8.4.0+cpanm+shared+threads arch=linux-sles15-haswell
[^]  szzheyp  [bl  ]                  ^builtin.gdbm@1.18.1%gcc@8.4.0 arch=linux-sles15-haswell
[^]  3kfx6pu  [bl  ]                      ^builtin.readline@8.0%gcc@8.4.0 arch=linux-sles15-haswell
[^]  m2bfsoy  [bl  ]              ^builtin.zlib@1.2.11%gcc@8.4.0+optimize+pic+shared arch=linux-sles15-haswell
[^]  fvj645l  [bl  ]      ^builtin.libjpeg-turbo@2.0.4%gcc@8.4.0 arch=linux-sles15-haswell
[^]  q7vii4v  [b   ]          ^builtin.nasm@2.14.02%gcc@8.4.0 arch=linux-sles15-haswell
[^]  zltgjjg  [bl  ]      ^builtin.libtiff@4.0.10%gcc@8.4.0 arch=linux-sles15-haswell
[^]  mz5q6pl  [bl  ]          ^builtin.xz@5.2.5%gcc@8.4.0 arch=linux-sles15-haswell
[^]  qrrrav5  [bl  ]      ^builtin.proj@6.3.1%gcc@8.4.0 arch=linux-sles15-haswell
[^]  ophpcos  [bl  ]          ^builtin.sqlite@3.31.1%gcc@8.4.0+column_metadata+fts~functions~rtree arch=linux-s
les15-haswell

cm2login3~>spack install libgeotiff
[+] /dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/pkgconf/1.7.3-gcc-cfijkws
```

```
[+] /dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/libtiff/4.0.10-gcc-zltgjjg
==> Installing libgeotiff
==> No binary for libgeotiff found: installing from source
==> libgeotiff: Executing phase: 'cmake'
==> libgeotiff: Executing phase: 'build'
==> libgeotiff: Executing phase: 'install'
[+] /dss/dsshome1/          spack/opt/linux-sles15-haswell/libgeotiff/1.6.0-gcc-8.4.0-cprryjt
```

Spack: a few words on dynamic linking

Priority-ordering of dynamic linking:

1. LD_PRELOAD
2. RPATH
3. LD_LIBRARY_PATH
4. RUNPATH

Spack uses RPATH as default:

- pathes where to find libraries are coded into the executables & libraries
- executables and libraries are functional without setting up einvironment:
  - -> the binaries know where to look for their dependency-libraries

installed libgeotiff as example here:

```
cm2devel~>ldd $HOME/spack/opt/linux-sles15-haswell/libgeotiff/1.6.0-gcc-8.4.0-cprryjt/bin/makegeo
        linux-vdso.so.1 (0x00007fffa35da000)
        libtiff.so.5 => /dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/libtiff/4.0.10-gcc-zltgjjg/lib/libtiff.so.5 (0x00007f301adcd000)
        libproj.so.15 => /dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/proj/6.3.1-gcc-qrrrav5/lib/libproj.so.15 (0x00007f301a910000)
        libc.so.6 => /lib64/libc.so.6 (0x00007f301a555000)
        libwebp.so.6 => /usr/lib64/libwebp.so.6 (0x00007f301a2f7000)
        liblzma.so.5 => /dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/xz/5.2.5-gcc-mz5q6pl/lib/liblzma.so.5 (0x00007f301a0d1000)
        libjpeg.so.62 => /dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/libjpeg-turbo/2.0.4-gcc-fvj645l/lib64/libjpeg.so.62 (0x00007f30
        libz.so.1 => /dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/zlib/1.2.11-gcc-m2bfsoy/lib/libz.so.1 (0x00007f3019c23000)
        libm.so.6 => /lib64/libm.so.6 (0x00007f30198eb000)
        libsqlite3.so.0 => /dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/sqlite/3.31.1-gcc-ophpcos/lib/libsqlite3.so.0 (0x00007f30195d
        libdl.so.2 => /lib64/libdl.so.2 (0x00007f30193cf000)
        libpthread.so.0 => /lib64/libpthread.so.0 (0x00007f30191b0000)
        libstdc++.so.6 => /dss/dsshome1/lrz/sys/spack/release/21.1.0/opt/x86_64/gcc/8.4.0-gcc-656wch7/lib64/libstdc++.so.6 (0x00007f3018e27000)
        libgcc_s.so.1 => /dss/dsshome1/lrz/sys/spack/release/21.1.0/opt/x86_64/gcc/8.4.0-gcc-656wch7/lib64/libgcc_s.so.1 (0x00007f3018c0f000)
        /lib64/ld-linux-x86-64.so.2 (0x00007f301b047000)
cm2devel~>readelf -d $HOME/spack/opt/linux-sles15-haswell/libgeotiff/1.6.0-gcc-8.4.0-cprryjt/bin/makegeo

Dynamic section at offset 0x4dc8 contains 28 entries:
  Tag        Type                         Name/Value
 0x0000000000000001 (NEEDED)             Shared library: [libtiff.so.5]
 0x0000000000000001 (NEEDED)             Shared library: [libproj.so.15]
 0x0000000000000001 (NEEDED)             Shared library: [libc.so.6]
 0x000000000000000f (RPATH)              Library rpath: [/dss/dsshome1/lrz/sys/spack/release/21.1.0/opt/x86_64/gcc/8.4.0-gcc-656wch7/lib:/dss/d
rz/sys/spack/release/21.1.0/opt/x86_64/gcc/8.4.0-gcc-656wch7/lib64:/dss/dsshome1/0D/di34faf/spack/opt/linux-sles15-haswell/libgeotiff/1.6.0-gcc
rryjt/lib:/dss/dsshome1/0D/di34faf/spack/opt/linux-sles15-haswell/libgeotiff/1.6.0-gcc-8.4.0-cprryjt/lib64:/dss/dsshome1/lrz/sys/spack/release/
t/haswell/libtiff/4.0.10-gcc-zltgjjg/lib:/dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/xz/5.2.5-gcc-mz5q6pl/lib:/dss/dsshome1/lrz/sys/
ease/21.1.1/opt/haswell/zlib/1.2.11-gcc-m2bfsoy/lib:/dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/proj/6.3.1-gcc-qrrrav5/lib:/dss/dssh
sys/spack/release/21.1.1/opt/haswell/sqlite/3.31.1-gcc-ophpcos/lib:/dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/readline/8.0-gcc-3kfx
dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/ncurses/6.2-gcc-6qhv5ta/lib:/dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/libjpe
.0.4-gcc-fvj645l/lib64:/dss/dsshome1/0D/di34faf/spack/opt/linux-sles15-haswell/libgeotiff/1.6.0-gcc-8.4.0-cprryjt/lib:/dss/dsshome1/0D/di34faf/
/linux-sles15-haswell/libgeotiff/1.6.0-gcc-8.4.0-cprryjt/lib64:/dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/readline/8.0-gcc-3kfx6pu/
dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/sqlite/3.31.1-gcc-ophpcos/lib:/dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/libjpeg-
.4-gcc-fvj645l/lib64:/dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/zlib/1.2.11-gcc-m2bfsoy/lib:/dss/dsshome1/lrz/sys/spack/release/21.
aswell/ncurses/6.2-gcc-6qhv5ta/lib:/dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/xz/5.2.5-gcc-mz5q6pl/lib:/dss/dsshome1/lrz/sys/spack/
1.1.0/opt/x86_64/gcc/8.4.0-gcc-656wch7/lib/gcc/x86_64-pc-linux-gnu/8.4.0]
 0x000000000000000c (INIT)               0x401aa8
 0x000000000000000d (FINI)               0x403844
 0x0000000000000019 (INIT_ARRAY)         0x604d10
 0x000000000000001b (INIT_ARRAYSZ)       8 (bytes)
 0x000000000000001a (FINI_ARRAY)         0x604d18
 0x000000000000001c (FINI_ARRAYSZ)       8 (bytes)
 0x0000000000000004 (HASH)               0x400278
```

Spack in user-space:
chaining existing installation into your own spack environment

```
cm2login3~>module load hdf5/1.8.22-gcc8-impi
Autoloading numactl/2.0.12-gcc8

Loading hdf5/1.8.22-gcc8-impi
  Loading requirement: numactl/2.0.12-gcc8
cm2login3~>spack spec -lI $HDF5_SPEC
Input spec
--------------------------------
[^]  hdf5@1.8.22%gcc@8.4.0+cxx~debug+fortran+hl~java+mpi+pic+shared+szip+threadsafe api=none a
[^]      ^intel-mpi@2019.8.254%gcc@8.4.0 arch=linux-sles15-haswell
[^]      ^libszip@2.1.1%gcc@8.4.0 arch=linux-sles15-haswell
[^]      ^numactl@2.0.12%gcc@8.4.0 arch=linux-sles15-haswell
[^]      ^zlib@1.2.11%gcc@8.4.0+optimize+pic+shared arch=linux-sles15-haswell

Concretized
--------------------------------
[^]  3lmvxrf  hdf5@1.8.22%gcc@8.4.0+cxx~debug+fortran+hl~java+mpi+pic+shared+szip+threadsafe a
[^]  cyojcvv      ^intel-mpi@2019.8.254%gcc@8.4.0 arch=linux-sles15-haswell
[^]  o62frdt      ^libszip@2.1.1%gcc@8.4.0 arch=linux-sles15-haswell
[^]  wz47lgr      ^numactl@2.0.12%gcc@8.4.0 arch=linux-sles15-haswell
[^]  m2bfsoy      ^zlib@1.2.11%gcc@8.4.0+optimize+pic+shared arch=linux-sles15-haswell

cm2login3~>spack spec -lI hdf5@1.8.22%gcc@8.4.0+cxx+debug+fortran+hl~java+mpi+pic+shared+szip+
Input spec
--------------------------------
 -   hdf5@1.8.22%gcc@8.4.0+cxx+debug+fortran+hl~java+mpi+pic+shared+szip+threadsafe

Concretized
--------------------------------
 -   4exl2a5  hdf5@1.8.22%gcc@8.4.0+cxx+debug+fortran+hl~java+mpi+pic+shared+szip+threadsafe a
[^]  cyojcvv      ^intel-mpi@2019.8.254%gcc@8.4.0 arch=linux-sles15-haswell
[^]  o62frdt      ^libszip@2.1.1%gcc@8.4.0 arch=linux-sles15-haswell
[^]  wz47lgr      ^numactl@2.0.12%gcc@8.4.0 arch=linux-sles15-haswell
[^]  jns7liw          ^autoconf@2.69%gcc@8.4.0 arch=linux-sles15-haswell
[^]  6vxvnrt              ^m4@1.4.18%gcc@8.4.0+sigsegv patches=3877ab548f88597ab2327a2230ee048
aswell
[^]  gv36h32                  ^libsigsegv@2.12%gcc@8.4.0 arch=linux-sles15-haswell
[^]  bhpjih4              ^perl@5.30.3%gcc@8.4.0+cpanm+shared+threads arch=linux-sles15-haswel
[^]  szzheyp                  ^gdbm@1.18.1%gcc@8.4.0 arch=linux-sles15-haswell
[^]  3kfx6pu                      ^readline@8.0%gcc@8.4.0 arch=linux-sles15-haswell
[^]  6qhv5ta                          ^ncurses@6.2%gcc@8.4.0~symlinks+termlib arch=linux-sles1
[^]  cfijkws                              ^pkgconf@1.7.3%gcc@8.4.0 arch=linux-sles15-haswell
[^]  zzoup2h          ^automake@1.16.2%gcc@8.4.0 arch=linux-sles15-haswell
[^]  4nya677          ^libtool@2.4.6%gcc@8.4.0 arch=linux-sles15-haswell
[^]  m2bfsoy      ^zlib@1.2.11%gcc@8.4.0+optimize+pic+shared arch=linux-sles15-haswell
```

NEW + Experimental (work in progress):
module load user_spack

Example 3:

Install existing installation in a different variant: here -- with debug-option: +debug

Spack-generated environment modules at LRZ provide a variable <package>_SPEC that holds location of the input/concretized spack-spec dumped in a yaml-file: spec.yaml

One may use this to see details of the installation behind the module: via the spack spec -command

Spack in user-space: chaining existing installation into your own spack environment

```
cm2login3~>module unload hdf5/1.8.22-gcc8-impi numactl/2.0.12-gcc8
cm2login3~>spack install hdf5@1.8.22%gcc@8.4.0+cxx+debug+fortran+hl~java+mpi+pic+shared+szip+threadsafe
[+] /dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/intel-mpi/2019.8.254-gcc-cyojcvv
[+] /dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/intel-mpi/2019.8.254-gcc-cyojcvv
[+] /dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/libszip/2.1.1-gcc-o62frdt
```

```
[+] /dss/dsshome1/lrz/sys/spack/release/21.1.1/opt/haswell/numactl/2.0.12-gcc-wz47lgr
==> Installing hdf5
==> No binary for hdf5 found: installing from source
==> hdf5: Executing phase: 'autoreconf'
==> hdf5: Executing phase: 'configure'
==> hdf5: Executing phase: 'build'
==> hdf5: Executing phase: 'install'
[+] /dss/dsshome1/        /spack/opt/linux-sles15-haswell/hdf5/1.8.22-gcc-8.4.0-4exl2a5
```

```
cm2login3~>ls spack/opt/linux-sles15-haswell/hdf5/1.8.22-gcc-8.4.0-4exl2a5/lib*
libhdf5.a               libhdf5_fortran.so.10      libhdf5hl_fortran.a          libhdf5_hl.so.10.2.3
libhdf5_cpp.a           libhdf5_fortran.so.10.0.7  libhdf5hl_fortran.la         libhdf5.la
libhdf5_cpp.la          libhdf5_hl.a               libhdf5_hl_fortran.so        libhdf5.settings
libhdf5_cpp.so          libhdf5_hl_cpp.a           libhdf5hl_fortran.so         libhdf5.so
libhdf5_cpp.so.16       libhdf5_hl_cpp.la          libhdf5hl_fortran.so.10      libhdf5.so.10
libhdf5_cpp.so.16.0.1   libhdf5_hl_cpp.so          libhdf5hl_fortran.so.10.0.6  libhdf5.so.10.4.0
libhdf5_fortran.a       libhdf5_hl_cpp.so.11       libhdf5_hl.la
libhdf5_fortran.la      libhdf5_hl_cpp.so.11.1.3   libhdf5_hl.so
libhdf5_fortran.so      libhdf5_hl_fortran.a       libhdf5_hl.so.10
```

NEW + Experimental (work in progress):
module load user_spack

Example 3 from previous slide continued

Spack self documenting artifacts

`.spack` directory in all installation-paths:
-> usefull information from installation process is available

Lets inspect this for our own hdf5 installation :

```
cm2login3~>ls spack/opt/linux-sles15-haswell/hdf5/1.8.22-gcc-8.4.0-4exl2a5/.spack/
```

```
archived-files
install_manifest.json
repos
spack-build-env.txt
spack-build-out.txt
spack-configure-args.txt
spec.yaml
cm2login3~>
```

- `archived-files`contains log of configure-phase (if avail)
- `repos` contains all procedures (package.py‘s) used for installation (package + all deps)
- `spack-build-env.txt` -- dump of environment during installation
- `spack-build-out.txt` -- dump of output-stream from installation
- `spack-configure-args` -- dump of configure arguments
- `spec.yaml` -- dictionary with input and concretized spack-specs

Spack commands (subset) that may be usefull for your work

```
query packages:
  list            list and search available packages
  info            get detailed information on a
                  particular package
  find            list and search installed packages

build packages:
  install         build and install packages
  uninstall       remove installed packages
  dev-build       developer build: build from code
                  in current working directory
  spec            show what would be installed,
                  given a spec

container:
  containerize    creates recipes to build images
                  for different container runtimes
environments:
  env               manage virtual environments
```

```
create packages:
  create          create a new package file
  edit            open package files in $EDITOR

system:
  compilers       list available compilers

user environment:
  load            add package to the user
                  environment
  module          manipulate module files
  unload          remove package from the user
                  environment
configuration:
  config          get and set configuration options
  repo            manage package source repositories
```

Automated stack builds with Spack: Improving our documentation

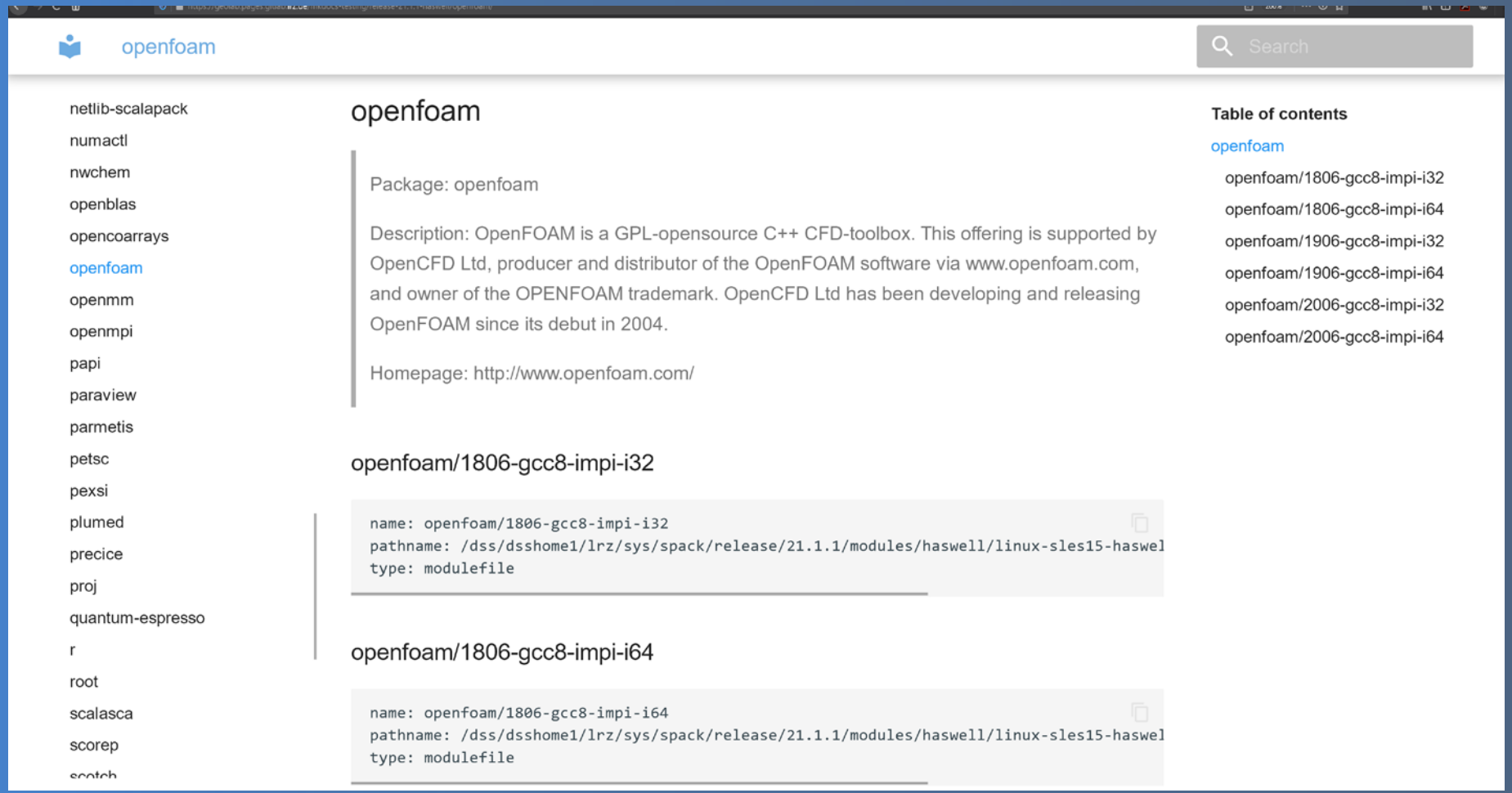
Work in Progress:

- evaluating auto-generated documentation for a **basic** or an advanced view

  Basic

… with basic info on what‘s installed

  - Package info
  - installed versions
  - url to homepage

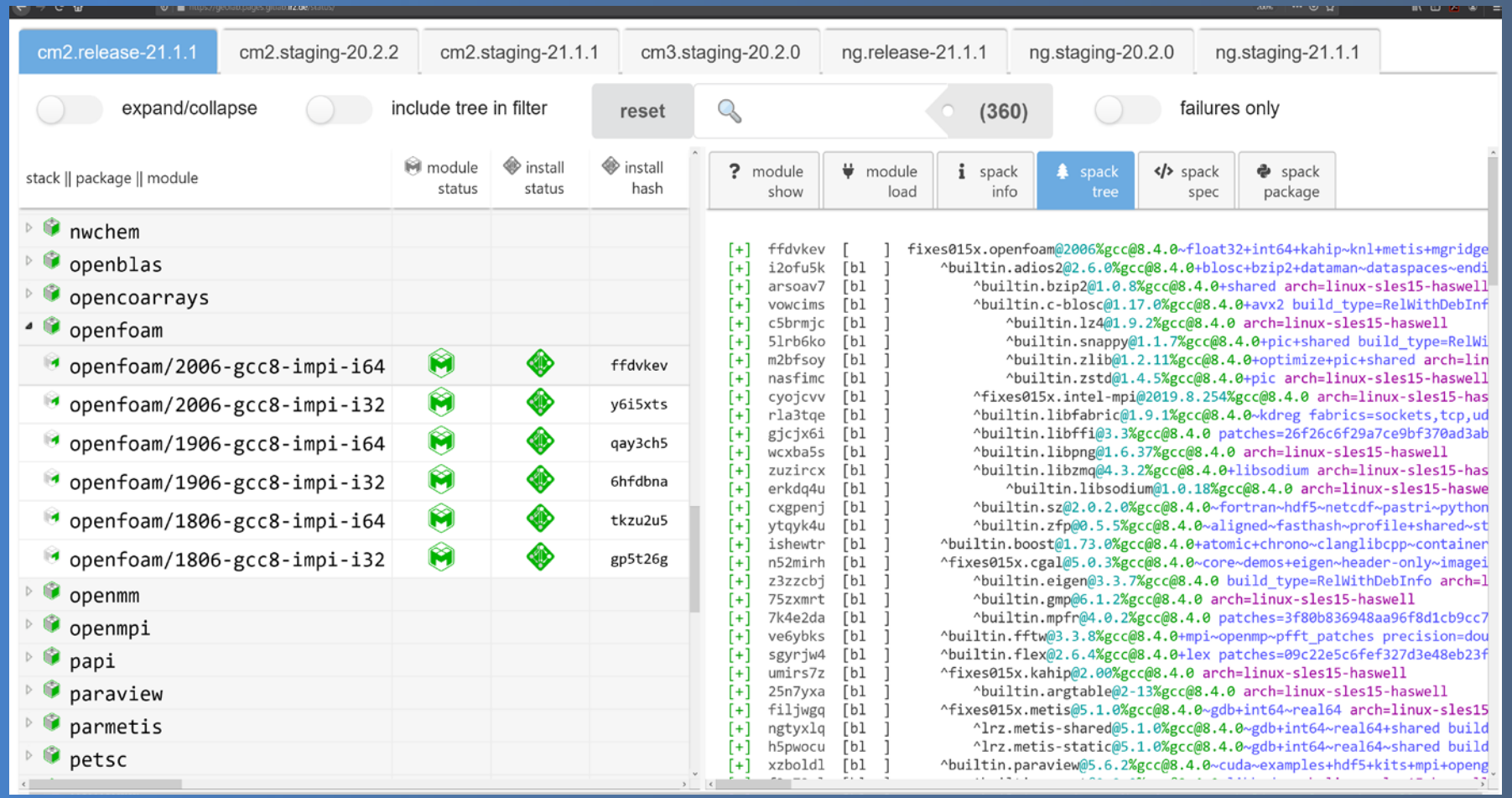


Automated stack builds with Spack: Improving Transparency

Work in Progress:

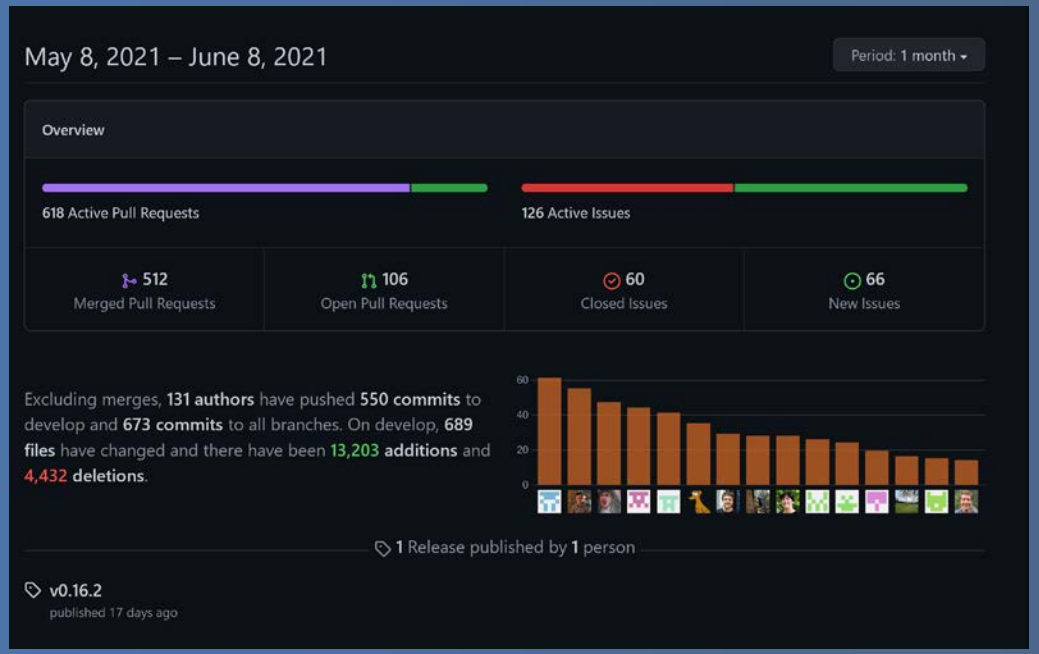
- evaluating auto-generated documentation for a basic or an **advanced** view
- Advanced:

  … with details on installations:
  - installed package
  - dependencies
  - package configuration
  - reference to external docs
  - reference to source origin



Spack is open-source with many community contributions

- Spack has excellent documentation: https://spack.readthedocs.io/en/v0.15.4/
- Spack community gives strong support via slack https://slack.spack.io/
- Spack repository is hosted on github: https://github.com/spack/spack
  - Spack is under heavy development
    - spack-developers
    - application-developers
    - domain-scientists
    - HPC-support-staff
    - hardware-vendors
- Consider yourself becoming part of the community:
  - Contributing and benefitting from



- LRZ Documentation on spack in user-space (updates pending) https://doku.lrz.de/display/PUBLIC/Building+software+in+user+space+with+spack