ICC Theory Lunch 13th July 2020

Starting promptly at 13:05!

News - Shaun
Virgo database update – John
DiRAC day update – Adrian
BlueField update – Ali
COSMA8 update – Ali
RSE Effort update – Ali
SPACK – Ali

Spack

Alternative to modules

ICC Theory Lunch
13th July 2020
Alastair Basden

What is Spack?

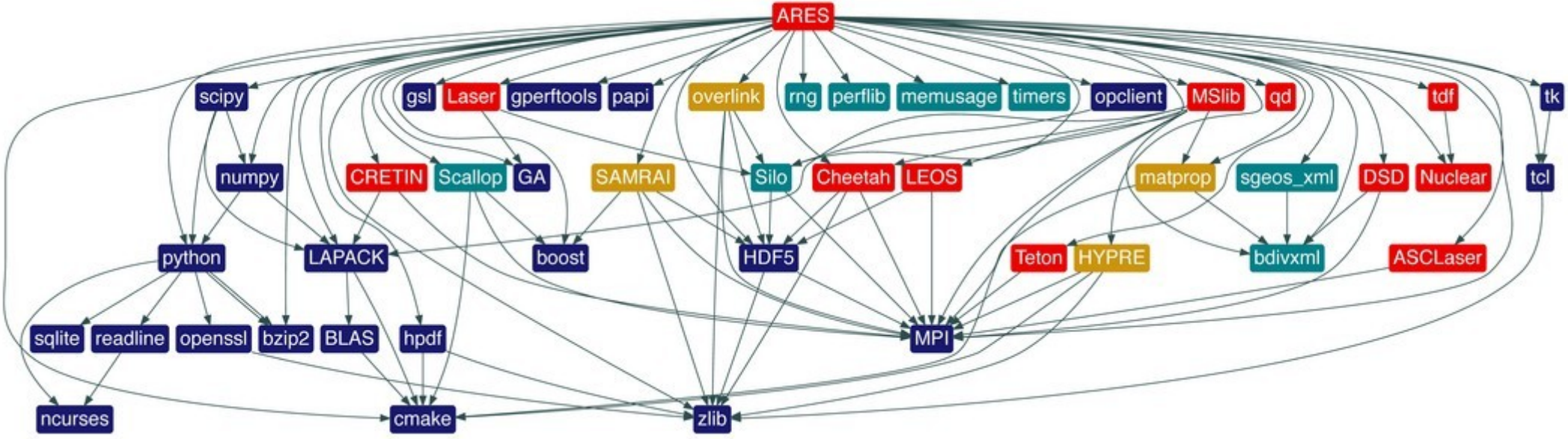
- Provides an alternative to the module environment
  - A flexible package manager for HPC
  - Understands dependencies, architectures, compilers, versions, etc
    - Easy to reinstall on a new system / with a new compiler / with an updated library
  - Automates installation of known packages
    - Allows fine tuning of libraries and parameters
    - Uses an internal dependency graph
- Developed by LLNL
  - Active development community
  - Not a finished product

What does it solve?

- Setting up modules is unwieldy
  - Compiling a new package for every combination of compiler and MPI
    - Multiple compiler releases per year
  - Not easy to summarise which packages work with which compilers etc
  - We also don’t currently optimise modules for machine architecture

Dependencies

- An intelligent set of dependencies
  - If a package doesn't exist on the system it will be downloaded and compiled
    - Also if a new version is required or for a different architecture



Using spack on COSMA

- Currently “at risk”
  - i.e. in test phase
    - Will likely remain here for a while
  - Please help to test, make suggestions, new packages, etc.
- module load spack
  - Currently only provides information

```
[dc-basd1@login7b [cosma7] ~]$ module load spack
cosma
Please souce one of --depending on your shell--:
source /cosma/local/spack/2020.06/spack/share/spack/setup-env.sh
source /cosma/local/spack/2020.06/spack/share/spack/setup-env.csh
Then activate the environment you want, e.g.:
spack env list
spack env activate cosma
[dc-basd1@login7b [cosma7] ~]$
[dc-basd1@login7b [cosma7] ~]$ source /cosma/local/spack/2020.06/spack/share/spack/setup-env.sh
[dc-basd1@login7b [cosma7] ~]$ spack env list
==> 1 environments
    cosma
[dc-basd1@login7b [cosma7] ~]$ spack env activate cosma
[dc-basd1@login7b [cosma7] ~]$
```

Advisable to module purge first

spack env activate

- Activate an environment
  - Currently, only 1 environment
    - “cosma-avx512”
      - Suitable for swift example on cosma7
  - Others will be added in due course
    - Open to suggestions
- Loads all the packages within this environment
  - Others can be seen with `spack env list`
- Note: Might give a permission denied error:
  - Just ls the affected directory and try again!
- Unload with `spack env deactivate`
  - Or `despactivate`

```
[dc-basd1@login7b [cosma7] ~]$ spack env activate cosma-avx512
==> Error: [Errno 13] Permission denied: '/cosma/local/spack/0.15/spack/var/spack/environments/cosma-avx512/.spack-env'
[dc-basd1@login7b [cosma7] ~]$ ls /cosma/local/spack/0.15/spack/var/spack/environments/cosma-avx512/.spack-env
logs  repos  transaction_lock  view
[dc-basd1@login7b [cosma7] ~]$ spack env activate cosma-avx512
```

Alternative use

- Once the setup-env.sh has been activated, modules produced by spack can be loaded in the usual way:

```
[dc-basd1@login7b [cosma7] ~]$ source /cosma/local/spack/2020.06/spack/share/spack/setup-env.sh
[dc-basd1@login7b [cosma7] ~]$ module av
------------------------------------------------------------------------------ /cosma/local/spack/2020.06/spack/share/spack/modules/linux-centos7-sandybridge -------------------------------------------------------------------------------
bzip2-1.0.6-gcc-9.3.0-xjjtbzb   fftw-3.3.8-gcc-9.3.0-s6reoht       gsl-2.5-gcc-9.3.0-nnobo2w       metis-5.1.0-gcc-9.3.0-zv54qge     openssl-1.0.2g-gcc-9.3.0-hnm5pq2     python-3.7.7-gcc-9.3.0-lsv3wn6     xz-5.5.2-gcc-9.3.0-lotrjvx
cmake-3.11.4-gcc-9.3.0-dhr3dlv  gdbm-1.18.1-gcc-9.3.0-qdlvyql      hdf5-1.10.6-gcc-9.3.0-uky4dgk   ncurses-5.9.14-gcc-9.3.0-gefdfxa  parmetis-4.0.3-gcc-9.3.0-b4tcare     readline-6.2.11-gcc-9.3.0-hsjp23u  zlib-1.2.7-gcc-9.3.0-whmwsvq
expat-2.1.0-gcc-9.3.0-xj5gqdt   gettext-0.19.8.1-gcc-9.3.0-i4s3ijv  libffi-3.0.13-gcc-9.3.0-mi2khs7  openmpi-4.0.3-gcc-9.3.0-qg5cmx5   pkg-config-0.27.1-gcc-9.3.0-sbxdaps  sqlite-3.31.1-gcc-9.3.0-p4v4uby

------------------------------------------------------------------------------ /cosma/local/Modules/modulefiles/mpi ------------------------------------------------------------------------------
hpcx-mt/2.2     intel_mpi/2018  intel_mpi/2019-update1  intel_mpi/2019-update3  intel_mpi/2020          openmpi/3.0.1(default)  openmpi/4.0.3
intel_mpi/2017  intel_mpi/2019  intel_mpi/2019-update2  intel_mpi/2019-update4  intel_mpi/2020-update1  openmpi/4.0.1           openmpi/20190429

---------------------------------------------------------------------------- /cosma/local/Modules/modulefiles/compilers -----------------------------------------------------------------------------
aocc/1.3.0  cuda/10.1               gnu_comp/8.2.0  gnu_comp/9.3.0   intel_comp/2018(default)  intel_comp/2019          intel_comp/2019-update2  intel_comp/2019-update4  intel_comp/2020-update1
aocc/2.0.0  gnu_comp/7.3.0(default)  gnu_comp/9.1.0  intel_comp/2017  intel_comp/2018-update2  intel_comp/2019-update1  intel_comp/2019-update3  intel_comp/2020          pgi/2019-1910
```

```
[dc-basd1@login7b [cosma7] ~]$ module load fftw-3.3.8-gcc-9.3.0-s6reoht
```

spack find

- `spack find`
  - Lists all the packages available in the current environment
  - These are already “loaded”

```
[dc-basd1@login7b [cosma7] ~]$ spack find
==> In environment cosma-avx512
==> Root specs
-- linux-centos7-skylake_avx512 / gcc@9.3.0 ----------------------
fftw%gcc@9.3.0   gsl%gcc@9.3.0   parmetis%gcc@9.3.0   py-h5py%gcc@9.3.0   py-matplotlib%gcc@9.3.0   py-numpy%gcc@9.3.0   py-scipy%gcc@9.3.0   python%gcc@9.3.0

==> 58 installed packages
-- linux-centos7-skylake_avx512 / gcc@9.3.0 ----------------------
autoconf@2.69    gdbm@1.18.1     libjpeg-turbo@2.0.4  nasm@2.14.02     pkgconf@1.7.3            py-nose@1.3.7            py-setuptools@46.1.3     xz@5.2.5
automake@1.16.2  gettext@0.20.2  libpciaccess@0.13.5  ncurses@6.2      py-cached-property@1.5.1 py-numpy@1.19.0          py-setuptools-scm@4.1.2  zlib@1.2.11
bzip2@1.0.8      gsl@2.5         libpng@1.6.37        numactl@2.0.12   py-cycler@0.10.0         py-pillow@7.0.0          py-six@1.14.0
cmake@3.17.3     hdf5@1.10.6     libsigsegv@2.12      openblas@0.3.10  py-cython@0.29.16        py-pkgconfig@1.5.1       python@3.7.7
diffutils@3.7    hwloc@1.11.11   libtool@2.4.6        openmpi@3.1.6    py-h5py@2.10.0           py-pybind11@2.5.0        readline@8.0
expat@2.2.9      libbsd@0.10.0   libxml2@2.9.10       openssl@1.0.2g   py-kiwisolver@1.1.0      py-pyparsing@2.4.2       sqlite@3.31.1
fftw@3.3.8       libffi@3.3      m4@1.4.18            parmetis@4.0.3   py-matplotlib@3.2.2      py-python-dateutil@2.8.0 tar@1.32
freetype@2.10.1  libiconv@1.16   metis@5.1.0          perl@5.30.3      py-mpi4py@3.0.3          py-scipy@1.5.0           util-macros@1.19.1
```

```
[dc-basd1@login7b [cosma7] ~]$ spack find fftw
==> In environment cosma-avx512
==> Root specs
-- linux-centos7-skylake_avx512 / gcc@9.3.0 ----------------------
fftw%gcc@9.3.0   gsl%gcc@9.3.0   parmetis%gcc@9.3.0   py-h5py%gcc@9.3.0   py-matplotlib%gcc@9.3.0   py-numpy%gcc@9.3.0   py-scipy%gcc@9.3.0   python%gcc@9.3.0

==> 1 installed package
-- linux-centos7-skylake_avx512 / gcc@9.3.0 ----------------------
fftw@3.3.8
```

spack compilers

- Lists available compilers

```
[dc-basd1@login7b [cosma7] ~]$ spack compilers
==> Available compilers
-- clang centos7-x86_64 -------------------------------------------
clang@8.0.0  clang@7.0.0  clang@aocc2.0.0

-- gcc centos7-x86_64 ---------------------------------------------
gcc@9.3.0  gcc@9.1.0  gcc@8.2.0  gcc@7.3.0  gcc@7.3.0  gcc@4.8.5  gcc@4.8.5  gcc@4.4.7

-- intel centos7-x86_64 -------------------------------------------
intel@2018        intel@19.1.1.217  intel@19.0.3.199  intel@19.0.1.144  intel@18.0.2
intel@20.0.1.217  intel@19.1.0.166  intel@19.0.3.199  intel@19.0.1.144
intel@20.0.0.166  intel@19.0.4.243  intel@19.0.2.187  intel@18.0.2
```

spack list

- To see what packages are available for install
  - Note - not what is currently installed
    - Use `spack find` for that

```
[dc-basd1@login7b [cosma7] ~]$ spack list | wc -l
4338
[dc-basd1@login7b [cosma7] ~]$
```

spack arch

- Gets the current architecture

```
[dc-basd1@login7b [cosma7] ~]$ spack arch
linux-centos7-skylake_avx512
```

spack spec

- Get specifications of an installed package
  - i.e. how it has been compiled

```
[sfw@login5a spack]$ spack spec fftw
Input spec
--------------------------------
fftw

Concretized
--------------------------------
fftw@3.3.8%gcc@9.3.0+mpi~openmp~pfft_patches precision=double,float arch=linux-centos7-sandybridge
    ^openmpi@3.1.6%gcc@9.3.0~atomics~cuda~cxx~cxx_exceptions+gpfs~java~legacylaunchers~memchecker~pmi~sqlite3+static~thread_mu
ulers=none arch=linux-centos7-sandybridge
        ^hwloc@1.11.11%gcc@9.3.0~cairo~cuda~gl~libudev+libxml2~netloc~nvml+pci+shared arch=linux-centos7-sandybridge
            ^libpciaccess@0.13.5%gcc@9.3.0 arch=linux-centos7-sandybridge
                ^libtool@2.4.6%gcc@9.3.0 arch=linux-centos7-sandybridge
                    ^m4@1.4.18%gcc@9.3.0+sigsegv patches=3877ab548f88597ab2327a2230ee048d2d07ace1062efe81fc92e91b7f39cd00,fc9b
99f09828d793b853c8 arch=linux-centos7-sandybridge
                        ^libsigsegv@2.12%gcc@9.3.0 arch=linux-centos7-sandybridge
                ^pkgconf@1.7.3%gcc@9.3.0 arch=linux-centos7-sandybridge
                ^util-macros@1.19.1%gcc@9.3.0 arch=linux-centos7-sandybridge
            ^libxml2@2.9.10%gcc@9.3.0~python arch=linux-centos7-sandybridge
                ^libiconv@1.16%gcc@9.3.0 arch=linux-centos7-sandybridge
                ^xz@5.2.5%gcc@9.3.0 arch=linux-centos7-sandybridge
                ^zlib@1.2.11%gcc@9.3.0+optimize+pic+shared arch=linux-centos7-sandybridge
            ^numactl@2.0.12%gcc@9.3.0 arch=linux-centos7-sandybridge
                ^autoconf@2.69%gcc@9.3.0 arch=linux-centos7-sandybridge
                    ^perl@5.30.3%gcc@9.3.0+cpanm+shared+threads arch=linux-centos7-sandybridge
                        ^gdbm@1.18.1%gcc@9.3.0 arch=linux-centos7-sandybridge
                            ^readline@8.0%gcc@9.3.0 arch=linux-centos7-sandybridge
                                ^ncurses@6.2%gcc@9.3.0~symlinks+termlib arch=linux-centos7-sandybridge
                ^automake@1.16.2%gcc@9.3.0 arch=linux-centos7-sandybridge
```

```
[dc-basd1@login7b [cosma7] ~]$ spack spec gsl
Input spec
--------------------------------
gsl

Concretized
--------------------------------
gsl@2.5%gcc@9.3.0~external-cblas arch=linux-centos7-skylake_avx512
```

Spack location

- Gets the installed location of a package

```
[dc-basd1@login7b [cosma7] ~]$ spack location -i gsl
/cosma/local/spack/2020.06/spack/opt/spack/linux-centos7-sandybridge/gcc-9.3.0/gsl-2.5-nnobo2w7qupe4uwzcr4cssvz4pwnirdw
```

spack info

- Provides information about packages

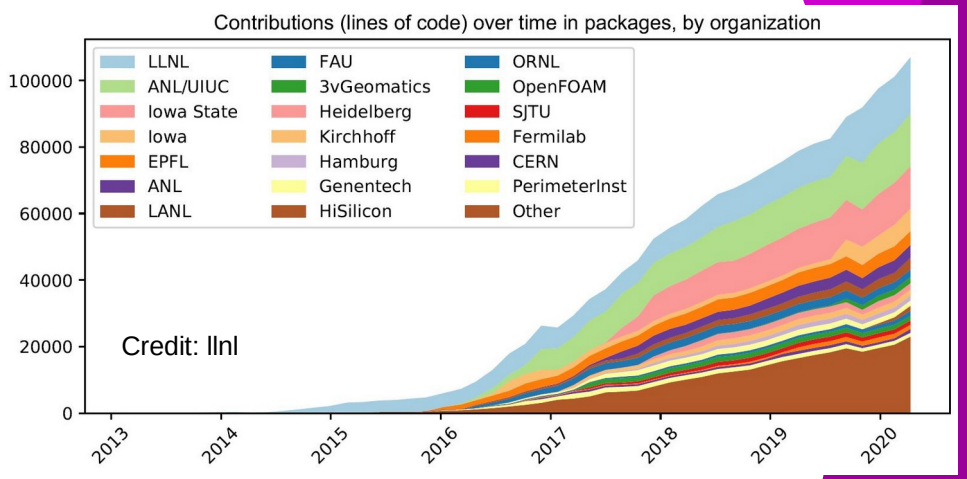
```
[dc-basd1@login7b [cosma7] ~]$ spack info fftw
AutotoolsPackage:   fftw

Description:
    FFTW is a C subroutine library for computing the discrete Fourier
    transform (DFT) in one or more dimensions, of arbitrary input size, and
    of both real and complex data (as well as of even/odd data, i.e. the
    discrete cosine/sine transforms or DCT/DST). We believe that FFTW, which
    is free software, should become the FFT library of choice for most
    applications.

Homepage: http://www.fftw.org

Tags:
    None

Preferred version:
    3.3.8        http://www.fftw.org/fftw-3.3.8.tar.gz

Safe versions:
    3.3.8        http://www.fftw.org/fftw-3.3.8.tar.gz
    3.3.7        http://www.fftw.org/fftw-3.3.7.tar.gz
    3.3.6-pl2    http://www.fftw.org/fftw-3.3.6-pl2.tar.gz
    3.3.5        http://www.fftw.org/fftw-3.3.5.tar.gz
    3.3.4        http://www.fftw.org/fftw-3.3.4.tar.gz
    2.1.5        http://www.fftw.org/fftw-2.1.5.tar.gz

Variants:
    Name [Default]              Allowed values          Description
    ========================    ====================    ============================================

    mpi [on]                    on, off                 Activate MPI support
    openmp [off]                on, off                 Enable OpenMP support.
    pfft_patches [off]          on, off                 Add extra transpose functions for PFFT
                                                        compatibility
    precision [float,double]    float, long_double,     Build the selected floating-point precision
                                double, quad            libraries

Installation Phases:
    autoreconf    configure    build    install

Build Dependencies:
    autoconf  automake  libtool  mpi

Link Dependencies:
    mpi

Run Dependencies:
    None

Virtual Packages:
    fftw@3: provides fftw-api@3
    fftw@2.1.5 provides fftw-api@2
```

spack install/add

- Spack can be used to add/install new packages
  - c.f. Python virtual envs
  - But please don’t unless you are absolutely sure
  - It creates lots of files
  - Each package may have lots of dependencies
  - Your file system space will quickly fill up
  - Please ask us to install instead!

Notes

- Spack is a work in progress
- Actively developed by the largest HPC systems
- Likely to have bugs and “features’
- Usage on COSMA might change as we learn
  - Perhaps a “spack working group” would be an idea!



Summary

- Spack makes package management easier
  - Can automatically install for multiple compilers/mpis.
- module load spack
- source /cosma/local/spack/2020.06/spack/share/spack/setup-env.sh
- spack env activate cosma
- spack find
- Load compiler/mpi – required since these were imported into spack
  - (gcc is not an installed package within spack)
  - module load gnu_comp/9.3.0
  - module load open_mpi/4.0.3
  - This may change – the compiler/mpi might become part of spack in the future
- See cosma-support web pages for (relatively) up to date details