



COSMA modules

Explaining the module environment

ICC Theory Lunch

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Introduction to COSMA

- The COSmology MACHine
 - Now in its 7th Generation
- Part of a national facility: DiRAC
 - Now in its 2.5yth Generation(!)
- 3 active facilities: COSMA5, COSMA6, COSMA7
 - COSMA5 belongs to ICC
 - COSMA6/7 are DiRAC funded and operated

COSMA HPC

- Large number of compute nodes (computer servers)
- Fast interconnect (network)
- Large parallel file systems
 - Hundreds of disks and tens of servers all working together
- Login nodes
 - Job queue system
 - Precompiled software “modules”

COSMA5

- 2012
- ~320 nodes
 - 2 processors → 16 cores per node
 - 128GB RAM
- 2.5PB storage
 - Being replaced by a 0.65PB storage plus tape
- 40Gbit/s interconnect

COSMA6

- Arrived 2016 (second hand)
- Identical hardware to COSMA5
- 2.5PB storage
 - Being replaced

COSMA7

- 2018
- 452 nodes
 - Two processors → 28 cores per node
 - 512GB RAM
- 3.1PB storage
- 100Gbit/s interconnect
- Also other services (e.g. mad01)

Accessing COSMA

- See www.dur.ac.uk/cosma

COSMA Modules

- Rationale: Users have different needs and requirements
 - Compilers, tools, libraries, middleware
- Separate the software into “modules”

Module commands

- `module av [ailable]`
 - lists all the modules available on the system
- `module li [st]`
 - lists the currently loaded modules
- `module lo [ad] MODULE`
 - e.g. `module load gnu_comp`
- `module unload MODULE / module switch MODULE MODULE`
- `module purge`
 - removes all modules
- `module show MODULE`
 - provides basic information about the module

Current modules (4/10/19)

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

----- /cosma/local/Modules/modulefiles/compiler -----
aocc/1.3.0  gnu_comp/7.3.0(default)  gnu_comp/9.1.0  intel_comp/2018(default)  intel_comp/2019  intel_comp/2019-update2  intel_comp/2019-update4
aocc/2.0.0  gnu_comp/8.2.0          intel_comp/2017  intel_comp/2018-update2  intel_comp/2019-update1  intel_comp/2019-update3

----- /cosma/local/Modules/modulefiles/libraries -----
arctic/oct2018  fftw/3.3.7(default)  hdf5/1.8.20  jemalloc/5.1.0  multine/est/oct2018  parallel_hdf5/1.10.3cosma5  qt/5.11.1
bison/3.4.1     fftw/3.3.7cosma5    hdf5/1.10.2  libffi/3.2.1   netcdf/4.6.1         parallel_hdf5/1.10.5  sundials/3.1.1
boost/1_67_0    fgsl/1.2.0          hdf5/1.10.3(default)  llvm/5.0.2     openblas/0.3.6      parmetis/4.0.3(default)  vtk/8.1.1
cfitsio/3.450  gnu-parallel/20181122  hdf5/1.10.5  llvm/7.0.0     openexr/2.2.1       parmetis/4.0.3-64bit  wcslib/6.2
curl/7.61.0    grib_api/1.28.0     Healpix/3.40  mesa/18.1.4    parallel_hdf5/1.8.20  parmetis/4.0.3cosma5
eccodes/2.12.0  gsl/2.4(default)    hwloc/1.11.11  metis/5.1.0   parallel_hdf5/1.8.20cosma5  pgplot/5.2.2
fftw/2.1.5     gsl/2.5             hypre/2.11.2  metis/5.1.0-64bit  parallel_hdf5/1.10.3(default)  pnetcdf/1.10.0

----- /cosma/local/Modules/modulefiles/tools -----
advisor/2019-update4  cosma/2018  idl/8.0  mplayer/1.3.0  python/3.6.5  singularity/3.0.1  valgrind/3.13.0
allinea/ddt/18.1.2   ffmpeg/4.0.2  imagemagick/7.0.8-9  muse/2.4.1  python/intelpython2  sm/2_4_36  vim/jan2019
anaconda3/5.2.0     gadgetviewer/1.0.7  inspector/2019-update4  nasm/2.13  python/intelpython3  starlink/2018A  vtune/2019-update4
anaconda3/5.3.1     gadgetviewer/1.0.9  itac/2019-update4  oprofile/1.3.0  pythonconda3/4.5.4  svn/1.10.2  wcstools/3.9.5
bbcp/20190508      go/1.11.14  java/jdk1.8.0_181  paraview/5.5.2  R/3.5.1  swig/3.0.12  yasm/1.3.0
cloudy/17.01       gperftools/2.6.1  lenstool/7.0  pyHST/nov2018  rsyncLustre/3.1.0  texlive/20181109  yorick/a3972ff
cmake/3.11.4       hdfview/2.14.0  lenstool/20180809-svn  python/2.7.15(default)  scalasca/2.4  utils/201805

----- /cosma/local/Modules/modulefiles/MAD -----
casa/5.1.2
```

Module load

- Does not actually load anything!
- Changes environment variables
 - e.g PATH, LIBRARY_PATH, CC, etc
 - See which ones using “module show”

Module show gsl

/cosma/local/Modules/modulefiles/libraries/gsl/2.4:

```
module-whatis    loads the gsl environment
prepend-path     PATH /cosma/local/gsl/2.4/bin
prepend-path     PKG_CONFIG_PATH /cosma/local/gsl/2.4/lib/pkgconfig
prepend-path     LD_RUN_PATH /cosma/local/gsl/2.4/lib
prepend-path     --delim { } LDFLAGS -Wl,-rpath=/cosma/local/gsl/2.4/lib
prepend-path     --delim { } LDFLAGS -L/cosma/local/gsl/2.4/lib
prepend-path     --delim { } OMPI_LDFLAGS -Wl,-rpath=/cosma/local/gsl/2.4/lib
prepend-path     --delim { } OMPI_LDFLAGS -L/cosma/local/gsl/2.4/lib
prepend-path     --delim { } MPI_CC_OPTIONS {-L/cosma/local/gsl/2.4/lib -Wl,-rpath=/cosma/local/gsl/2.4/lib}
prepend-path     --delim { } MPI_CXX_OPTIONS {-L/cosma/local/gsl/2.4/lib -Wl,-rpath=/cosma/local/gsl/2.4/lib}
prepend-path     --delim { } MPI_F90_OPTIONS {-L/cosma/local/gsl/2.4/lib -Wl,-rpath=/cosma/local/gsl/2.4/lib}
prepend-path     --delim { } MPI_F77_OPTIONS {-L/cosma/local/gsl/2.4/lib -Wl,-rpath=/cosma/local/gsl/2.4/lib}
prepend-path     CMAKE_LIBRARY_PATH /cosma/local/gsl/2.4/lib
prepend-path     LIBRARY_PATH /cosma/local/gsl/2.4/lib
prepend-path     --delim { } CPPFLAGS -I/cosma/local/gsl/2.4/include
prepend-path     --delim { } OMPI_CPPFLAGS -I/cosma/local/gsl/2.4/include
prepend-path     --delim { } MPI_CC_OPTIONS -I/cosma/local/gsl/2.4/include
prepend-path     --delim { } MPI_CXX_OPTIONS -I/cosma/local/gsl/2.4/include
prepend-path     CMAKE_INCLUDE_PATH /cosma/local/gsl/2.4/include
prepend-path     CPATH /cosma/local/gsl/2.4/include
conflict         gsl
-----
```

Module dependencies

- Some modules depend on others
- e.g. to use parallel HDF5, you need an MPI module loaded
- `module load parallel_hdf5`

A compiler must be chosen before loading the `parallel_hdf5` module.

Please load one of the following compiler modules:

`gnu_comp/7.3.0`

`gnu_comp/9.1.0`

`intel_comp/2018`

`intel_comp/2019`

Module versions

- `module av gnu_comp`

```
----- /cosma/local/Modules/modulefiles/compilers -----  
gnu_comp/7.3.0(default)  gnu_comp/8.2.0  gnu_comp/9.1.0
```

- You can specify which to use, or just use the default one
 - e.g. `module load gnu_comp` will give you gcc 7.3.0
 - In some cases, the default will be the newest module
 - In other cases it will be one known to be stable

If you need a new module:

- Just ask cosma-support@durham.ac.uk

Typical combinations

- intel_comp with intel_mpi
- gnu_comp with open_mpi

Python modules

- (not “Python modules”)
- python/2.7.15, python/3.6.5, python/intelpython2, python/intelpython3, pythonconda/4.5.2, anaconda3/5.2.0, anaconda3/5.3.1
- Each of these will contain different “Python modules”
 - Depending on what has been requested
- You can also install “Python modules” in your local account
 - Good if you’re the only person likely to use them, or if you want them updated regularly
- python/2.7.15 and python/3.6.5 have the most modules installed

Modules with SLURM

- Put a module purge, and then module load...
 - within your SLURM submission script
- You have a record of which modules were used
- You always start from the same place

Summary

- Modules simplify your development environment
- But cannot be used on COSMA during downtime...!