EasyBuild at University of Melbourne

5th EasyBuild User Meeting

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EasyBuild History at Uni. of Mel.

- Research Computing Services at University of Melbourne started using EasyBuild since 2016
- EasyBuild is used for our HPC (spartan), which include 190 cloud nodes, 116 CPU nodes, 85 GPU nodes (p100 v100)
- We introduced our own toolchain in 2018

  spartan_gcc (gcc, OpenMPI, OpenBLAS, FFTW, ScaLAPACK)

  spartan_intel (icc, ifort, OpenMPI, imkl,)
- We improved our EasyBuild with Hierarchy at end of 2019

Old Building System

jzhang8@spartan-login2:~

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```
------------------------------------------------------------------- /usr/local/easybuild/modules/all -------------------------------------------------------------------
   ABAQUS/6.14.2-linux-x86_64                                              SWIG/3.0.11-goolf-2015a-Python-2.7.12
   ABAQUS/2017-hotfix-1721                                    (D)          SWIG/3.0.11-intel-2016.u3-Python-2.7.9
   ABINIT/8.0.8b-GCC-4.9.2                                                 SWIG/3.0.11-intel-2016.u3-Python-2.7.11
   ABINIT/8.0.8b-GCC-4.9.3                                                 SWIG/3.0.11-intel-2016.u3-Python-2.7.12
   ABINIT/8.0.8b-intel-2016.u3                                (D)          SWIG/3.0.12-GCC-6.2.0-Python-3.7.1
   ABRicate/0.8.7-spartan_intel-2017.u2                                    SWIG/3.0.12-intel-2017.u2-Python-2.7.13
   ABySS/1.5.2-goolf-2015a                                                 SWIG/3.0.12-intel-2017.u2-Python-3.6.1
   ABySS/1.9.0-goolf-2015a                                                 SWIG/3.0.12-intel-2018.u4-Python-3.6.4
   ABySS/2.0.2-goolf-2015a                                    (D)          SWIG/3.0.12-spartan_gcc-6.2.0-Python-2.7.13
   ACTC/1.1-intel-2016.u3                                                  SWIG/3.0.12-spartan_gcc-6.2.0-Python-3.7.3
   ADMIXTURE/1.3.0                                                         SWIG/3.0.12-spartan_gcc-8.1.0-Python-3.7.3
   AFNI/linux_openmp_64-intel-2016.u3-20180104                             SWIG/3.0.12-spartan_intel-2017.u2-Python-2.7.13
   AFNI/linux_openmp_64-spartan_intel-2017.u2-20180521                     SWIG/3.0.12-spartan_intel-2017.u2-Python-3.6.4                                  (D)
   AFNI/linux_openmp_64-spartan_intel-2017.u2-20190219        (D)          SaTScan/9.6
   ANSYS_CFD/18.1                                                          Sablotron/1.0.3-goolf-2015a
   ANSYS_CFD/19.0                                             (D)          Sagemath/8.1
   ANTLR/2.7.7-intel-2016.u3                                               Salmon/0.11.3
   ANTLR/2.7.7-intel-2017.u2                                  (D)          ScaLAPACK/2.0.2-gompi-2015a-OpenBLAS-0.2.14-LAPACK-3.5.0
   ANTs/2.2.0-goolf-2015a                                                  ScaLAPACK/2.0.2-gompi-2016b-OpenBLAS-0.2.18-LAPACK-3.5.0
   ANTs/2.2.0-intel-2016.u3                                                ScaLAPACK/2.0.2-gompi-2017a-OpenBLAS-0.2.19-LAPACK-3.7.0
   ANTs/2.3.1-spartan_gcc-6.2.0                               (D)          ScaLAPACK/2.0.2-gompi-2017b-OpenBLAS-0.2.20
   APR-util/1.5.4-GCC-4.9.2                                                ScaLAPACK/2.0.2-gompi-2018.u1-OpenBLAS-0.2.20
   APR-util/1.6.1-GCC-6.2.0                                                ScaLAPACK/2.0.2-gompic-2017.01-OpenBLAS-0.2.20-LAPACK-3.7.0
   APR-util/1.6.1-spartan_intel-2017.u2                       (D)          ScaLAPACK/2.0.2-spartan_gompi-GCC-6.2.0-OpenMPI-3.0.0-OpenBLAS-0.2.19-LAPACK-3.7.0
   APR/1.5.2-GCC-4.9.2                                                     ScaLAPACK/2.0.2-spartan_gompi-GCC-6.2.0-OpenMPI-3.1.0-cuda9.2-OpenBLAS-0.2.19-LAPACK-3.7.0
   APR/1.7.0-GCC-6.2.0                                                     ScaLAPACK/2.0.2-spartan_gompi-GCC-8.1.0-OpenMPI-3.1.0-OpenBLAS-0.2.19-LAPACK-3.7.0          (D)
   APR/1.7.0-spartan_intel-2017.u2                            (D)          ScientificPython/2.9.4-goolf-2015a-Python-2.7.10
   ARAGORN/1.2.36-GCC-4.9.2                                                ScientificPython/2.9.4-intel-2016.u3-Python-2.7.9
   AST/0.0.2-intel-2018.u4-Python-3.6.4                                    ScientificPython/2.9.4-intel-2016.u3-Python-2.7.10
   ATK/2.18.0-intel-2016.u3                                                ScientificPython/2.9.4-intel-2016.u3-Python-2.7.11                              (D)
   ATK/2.24.0-GCC-4.9.2                                                    Scipion/1.2-GCC-6.2.0-CUDA-9.0
   ATK/2.24.0-GCC-6.2.0                                                    Scipion/1.2-GCC-6.2.0-CUDA-9                                                    (D)
   ATK/2.24.0-intel-2016.u3                                                Scipion/1.2-GCC-6.2.0
   ATK/2.24.0-intel-2017.u2-GCC-5.4.0-CUDA8                                Scipion/1.2.1-GCC-6.2.0-CUDA-9.0
   ATK/2.24.0-intel-2017.u2                                                Scipion/1.2.1-GCC-6.2.0-CUDA-9.1
   ATK/2.30.0-intel-2017.u2                                                Score-P/2.0.1-goolf-2015a
   ATK/2.30.0-intel-2018.u4                                   (D)          Seaborn/0.8.1-intel-2017.u2-Python-2.7.11
   ATLAS/3.10.1-GCC-4.9.2-LAPACK-3.5.0                                     Seqtk/1.3-r106-foss-2017b
   ATLAS/3.10.1-GCC-5.4.0-LAPACK-3.5.0                                     Seqtk/1.3-r106-GCCcore-6.4.0
   ATLAS/3.10.1-GCC-6.2.0-LAPACK-3.5.0                                     Seqtk/1.3-r106-intel-2017.u2
   ATLAS/3.10.1-gompi-2015a-LAPACK-3.4.2                                   Seqtk/1.3-r106-spartan_gcc-6.2.0
lines 1-43
```

New Building System

```
jzhang8@build:~
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------------------------------------------------------------------------ System Modules -------------------------------------------------------------------------
   EasyBuild/latest    EasyBuild/4.0.1 (D)    showq/0.15   (L,D)    spartan/2016-03-parallel          unimelb-mf-clients/current    web_proxy/1.0 (D)
   EasyBuild/3.9.3     showq/0.12             slurm/latest (L)      spartan/2016-03          (L,D)    web_proxy/latest

--------------------------------------------------------- Compiler: gcc 8.3.0 OpenMPI: 3.1.4 ----------------------------------------------------------
   arpack-ng/3.7.0                ftgl/2.1.3-rc5                      matplotlib/2.2.4-python-3.7.4          scalapack/2.0.2                    (D)
   bamm/2.5.0                     gl2ps/1.4.0                         matplotlib/3.1.1-python-3.7.4    (D)   scipy-bundle/2019.03
   beagle-lib/3.0.2               gnuplot/5.2.6                (D)    metis/5.1.0                      (D)   scipy-bundle/2019.10-python-2.7.16
   boost.python/1.64.0            graphicsmagick/1.3.31               ncdf4/1.16.1-r-3.6.0                   scipy-bundle/2019.10-python-3.7.4
   boost/1.64.0                   gtdb-tk/0.3.2-python-2.7.16         netcdf/4.7.1                           scipy-bundle/2019.10               (D)
   boost/1.71.0            (D)    hdf5/1.10.5                         openfoam/v1906                         scotch/6.0.9
   cgal/4.14.1-python-3.7.4       hmmer/3.2.1                         openfoam/6                       (D)   sleuth/0.30.0-r-3.6.0
   eman2/2.3-python-2.7.16        ipython/5.8.0-python-2.7.16         paraview/5.6.2-python-3.7.4-mpi        suitesparse/5.4.0-metis-5.1.0
   fastani/1.1                    jags/4.3.0                          pkgconfig/1.5.1-python-3.7.4     (D)   tkinter/3.7.4                      (D)
   fasttree/2.1.10                kallisto/0.45.1                     pyopengl/3.1.3b2-python-2.7.16         udunits/2.2.26                     (D)
   fftw/3.3.8              (D)    libglu/9.0.1                 (D)    qrupdate/1.1.2                         valgrind/3.14.0
   fltk/1.3.4                     littlecms/2.9                (D)    r-bundle-bioconductor/3.9-r-3.6.0      vtk/8.2.0-python-3.7.4
   freeglut/3.0.0          (D)    mariadb-connector-c/2.3.7           r/3.6.0
   fsl/6.0.1-python-3.7.4         matplotlib/2.2.4-python-2.7.16      samtools/1.9

------------------------------------------------------------------- Compiler: gcc 8.3.0 -------------------------------------------------------------------
   clapack/3.2.1       cuda/10.1.243       openblas/0.3.7       p7zip/16.02    texinfo/6.6  (D)    ucx/1.7.x-nocuda
   cmake/3.16.1  (D)   fastani/1.2   (D)    openmpi/3.1.4  (D)   phast/1.5      texlive/2019 (D)

------------------------------------------------------ Compiler: gcc-cuda 8.3.0-10.1.243 OpenMPI: 3.1.4 -------------------------------------------------------
   fftw/3.3.8    scalapack/2.0.2    scipion/2.0-cuda-10.1

--------------------------------------------------------- Compiler: gcc-cuda 8.3.0-10.1.243 ----------------------------------------------------------
   openmpi/3.1.4

------------------------------------------------------------------ Compiler: gcccore 8.2.0 ------------------------------------------------------------------
   binutils/2.31.1    bison/3.0.5    flex/2.6.4 (D)    help2man/1.47.7    m4/1.4.18 (D)    zlib/1.2.11 (D)

------------------------------------------------------------------ Compiler: gcccore 8.3.0 ------------------------------------------------------------------
   autoconf/2.69                          harfbuzz/2.4.0              libxft/2.3.2                   protobuf/3.7.1
   automake/1.16.1                        help2man/1.47.8      (D)    libxml++/2.40.1                pyqt5/5.12.1-python-2.7.16
   autotools/20180311                     hwloc/1.11.12               libxml2/2.9.9                  python/2.7.16
   bazel/1.1.0                            hwloc/2.0.3          (D)    libxrender/0.9.9               python/3.7.4               (D)
   binutils/2.32                   (D)    icu/65.1                    libxslt/1.1.33                 qhull/2015.2
   bison/3.3.2                     (D)    imagemagick/7.0.8-46        littlecms/2.9                  qt5/5.13.1
   bsddb3/6.2.6                           inputproto/2.3.2            llvm/9.0.0                     qwt/6.1.4
   bzip2/1.0.8                            intltool/0.51.0             m4/1.4.18                      re2c/1.2.1
lines 1-43
```

Old VS New

	Old	New
Software	1000+	200+
EB Version	3.7.1	4.0.1
Name Scheme	No	Yes

- Currently, the default building system for user still old. We are going to migrate to new one this year
- Existing software will stay, but all new request will use the new system

New Building System 1

- EasyBuild version 4.0.1, RHEL 7.7 and python 2.7
- Naming Scheme: hierarchical_lowercase_mns.py

  all modules in our new system are lowercase to make it easier for researchers

  add following line to easybuild.cfg

  module-naming-scheme = HierarchicalLowercaseMNS

  https://github.com/ASVO-TAO/easybuild-framework/blob/develop/easybuild/tools/module_naming_scheme/hierarchical_lowercase_mns.py

New Building System 2

- Due to we still have some old node which doesn’t support avx512, so we add ‘optarch=GCC:mno-avx512f -mno-avx512pf -mno-avx512er -mno-avx512cd;Intel:xAVX2’ in easybuild.cfg to stop use avx512 everywhere
- Lmod, we also changed MasterControl.lua and Master.lua to meet the hierarchy we have

New Building System 3

- Python:

  Installed python from EasyBuild Upstream

  Installed python-bare which doesn’t include any python packages (we encourage user to install there own python packages by pip install –user or virtualenv

Challenges

- Installing software as a single user, much of which we can just copy/paste from Easybuilders Github. Does any sites encourage users to use Easybuild on their own?
- Keeping Python/R packages up to date. How often?
- Have sites decided to make a Python module with all packages based on IntelPython?
- Dealing with CUDA/cudNN version changes
- Install Tensorflow from package or wheel?

Questions

Lev is asking Kenneth that due to recent reaction to some Python upgrade if you are considering shifting EasyBuild scripts to bash shell scripts.

Questions? Suggestions?
Thank You