building software with ease

SC'15 BoF lightning talk

Getting Scientific Software Installed: Tools & Best Practices

November 17th 2015

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“Please install this software on the cluster?”

Scientists focus on the *science* of the software they produce,

not on build procedure, portability, …

This makes building/installing (lots of) scientific software **painful**:

very time-consuming, error-prone, hard to get right, …

Common issues:

- non-standard build tools
- incomplete build procedure
  e.g., no install step
- interactive scripts
- hardcoded parameters
- poor/outdated documentation
- …

Lots of duplication of work across HPC sites!

EasyBuild: building software with ease

http://hpcugent.github.io/easybuild

EasyBuild is a *software build and installation framework*.

- written in **Python 2**
- started in 2009, in-house for ~2.5 years, **GPLv2** since 2012
- **stable API** since EasyBuild v1.0 (Nov'12), latest is v2.4.0
- continuously enhanced and extended, thoroughly tested
- *release early, release often strategy* (major version every 6-8 weeks)
- development is highly **community-driven**

Using EasyBuild

0) Easily install EasyBuild by bootstrapping it:

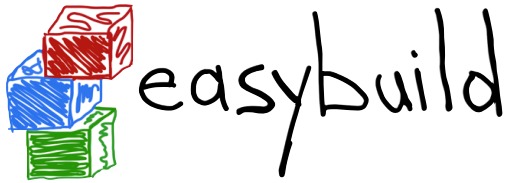
```
$ curl -O http://hpcugent.github.io/easybuild/bootstrap_eb.py
$ python bootstrap_eb.py <prefix>
```

1) Set module path, load EasyBuild module, basic configuration:

```
$ module load EasyBuild
$ export EASYBUILD_PREFIX=<prefix>
$ export MODULEPATH=<prefix>/modules/all:$MODULEPATH
```

2) Example: build WRF & all deps using Intel compilers/libraries:

```
$ eb WRF-3.6.1-intel-2015a-dmpar.eb --robot
$ module av WRF
  WRF/3.6.1-intel-2015a-dmpar
```



Key features

- requires **Linux**/x86(_64), experimental Cray support, Linux/POWER in the works
- supports **various compilers** & MPI/BLAS/LAPACK/FFT **libraries**
- robust **framework** providing supporting functionality
- thorough **logging** of executed build/install procedure
- **archiving** of build specifications
- very **dynamic design**: plugin support for new compiler/MPI/software package
- **generates module files** (Tcl or Lua), supports using Tcl/C & Lmod module tools
- support for using a *custom module naming scheme* you define yourself
- **fully autonomous builds**, build logging, automagical dependency resolution, ...
- supports **over 730** different (scientific) software packages & libraries
- well documented: http://easybuild.readthedocs.org
- thriving **community**: actively contributing, driving development

EasyBuild community drives most new features, so *get involved!*

EasyBuild community

***10th** EasyBuild hackathon*

November 11-13th 2015, TACC at Austin

Ghent University & VSC sites (Belgium)

University of Luxembourg

The Cyprus Institute

University of Basel (Switzerland)

IMP/IMBA (Austria)

Jülich Supercomputer Centre (Germany)

CSCS (Switzerland)

Bayer (Germany)

Ottawa Hospital Research Inst. (Canada)

NeSI / Univ. of Auckland (New Zealand)

Univ. of Colorado Boulder (US)

University of Wyoming (US)

Texas A&M (US)

& (many?) more…

+ support from NVIDIA, TACC (Lmod), …

easybuild

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Do you want to know more?

website: https://hpcugent.github.io/easybuild

GitHub: https://github.com/hpcugent/easybuild*[-framework*|*-easyblocks*|*-easyconfigs]*

PyPi: https://pypi.python.org/pypi/easybuild*[*-framework|-easyblocks|-easyconfigs*]*

mailing list: *easybuild@lists.ugent.be*

Twitter: *@easy_build*

YouTube: *search for "EasyBuild intro", "EasyBuild WRF"*

IRC: *#easybuild on* freenode.net