



EasyBuild

past, present, and future

Kenneth Hoste
HPC-UGent, Ghent University, Belgium
kenneth.hoste@ugent.be

http://users.ugent.be/~kehoste/EasyBuild_20160127.pdf

January 27th 2016 – 1st EasyBuild User Meeting – Ghent (Belgium)
<https://github.com/hpcugent/easybuild/wiki/1st-EasyBuild-User-Meeting>

HPC-UGent in a nutshell



<http://www.ugent.be/hpc> – <http://www.vscenrum.be>

- HPC team at central IT dept. of Ghent University (Belgium)
- 9+1 team members: 1 manager, ~3 user support, ~6 sysadmin
- 4+1 Tier2 clusters + one Tier1 cluster (8.5k cores)
- ~1.5k user accounts, across all scientific domains
- tasks: hardware, system administration, user support/training, ...
- member of Flemish Supercomputer Centre (VSC)
 - virtual centre, collaboration between Flemish university associations



A little bit of history

- created in summer of 2009 by Stijn De Weirdt @ HPC-UGent
- end of 2010: I 'inherit' EasyBuild
- developed in-house until Apr'12: first public release (v0.5)
- Nov'12 (SC'12): **EasyBuild v1.0.0**
- Jul'13 (v1.6.0): support for using Lmod
- May'14 (v1.13.0): support for '--from-pr'
- Jul'14 (v1.14.0): support for hierarchical module tree
- Dec'14: <http://easybuild.readthedocs.org>
- Mar'15: **EasyBuild v2.0.0**
- Apr'15 (v2.1.0): support for module files in Lua syntax
- Dec'15 (v2.5.0): support for '--extended-dry-run'/'-x'

Easybuild v2.6.0

- released Tue Jan 26th 2016
- (experimental) support for '--new-pr' and '--update-pr'
- better isolation w.r.t. installing Python packages (badly needed)
- 'foss/2016a' and 'intel/2016a' common toolchains
- support for installing GCC 5.3.0, DOLFIN 1.6.0, numba, PGI
- support for 799 different software packages
- 34 different compiler toolchains
- includes 5,093 (example) easyconfig files

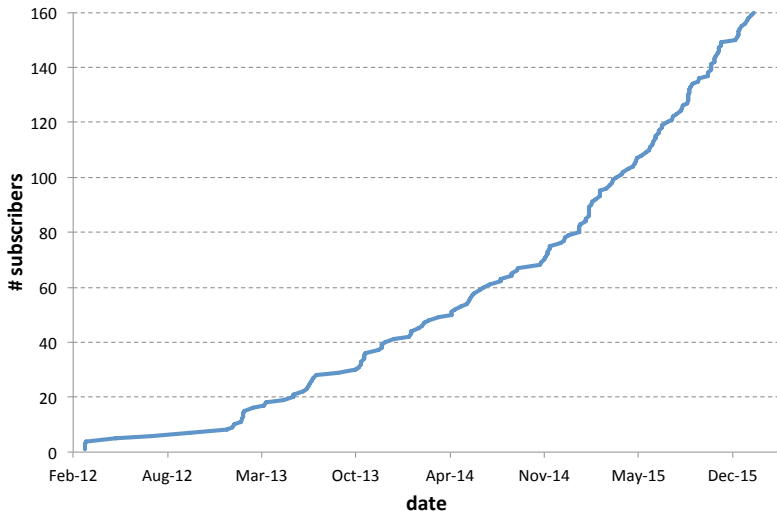
--new-pr lowers bar for contributing back

- submit pull requests to central GitHub repository from eb CLI
- for now, only pull requests to easyconfigs repository are supported
- automagically renames/relocates easyconfig files
- takes into account policy/guidelines for pull requests
- implementation is dry run-aware (-D, -x)
- marked *experimental* for now
 - requires 'manual' setup (GitPython & keyring, GitHub token)
 - including patch files is not supported yet
 - plan is to extend it to also easyblocks & EasyBuild framework itself
 - interface may slightly change before considered stable
 - should incorporate a style check + minimal run of unit test suite

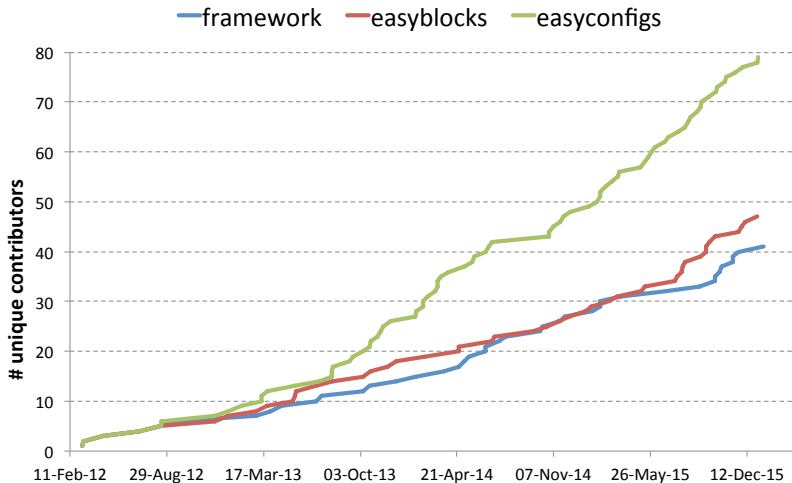
Community by numbers

- 6 '*Getting Scientific Software Installed*' BoF sessions at ISC/SC
- 10 two/three-day EasyBuild hackathons (+ user meeting)
- ~20 'active' souls on the #easybuild IRC channel
- a couple of dozen of HPC sites using it around the world
- 43 EasyBuild conference calls
- 159 subscribers to the EasyBuild mailing list
- framework: 900 merged closed PRs (45 open)
- easyblocks: 596 merged PRs (45 open)
- easyconfigs: 1,636 merged PRs (295 open)

EasyBuild mailing list



EasyBuild contributors



More manpower/automation needed

- automated style check, especially for easyconfig PRs
- '--new-pr'/'--update-pr' helps to enforce policies
- more 3rd party testing
- pledge for dedicated man hours by (large) sites active in community
- hierarchical way of handling contributions
- more 'aggressive' policy on closing PRs?

WIP features/enhancements

- (even) better GitHub integration
 - ‘--new-pr’/‘--update-pr’ also for easyblocks & framework
 - only submit/update PR if automated ‘code’ style check passes
 - easy way to install/test GitHub token (‘--install-github-token’)
- RPATH support
 - cfr. dedicated conf call
 - update from Rob?
- performance improvements
 - use ‘python -0’ in ‘eb’ wrapper: 2-3x speedup improvement
 - make EasyBuild ‘zip-safe’, enables installation of zipped ‘.egg’
 - better integration with Lmod: avoid setting \$LMOD_IGNORE_CACHE
- more (automatically generated) documentation
 - several WIP PRs by Caroline awaiting attention... (Fotis?)

Easyconfig files in YAML syntax (.yeb)

- (slightly) easier to read/write for humans
- same syntax as other similar projects (Spack, conda, HashDist, ...)
- properly parsed (as opposed to using 'exec')
- (experimental) support implemented by intern
- current status: roughly on-par with .eb format
- intention is to:
 - extend current format to also support 'fat' easyconfigs
 - support (validated) conversion from .eb to .yeb
 - support merging multiple .eb files into a single 'fat' .yeb file
 - flesh out .yeb parser as a stand-alone library (libyeb)?
- (current half-implemented 'format v2' is not going anywhere)

http://easybuild.readthedocs.org/en/latest/Writing_yeb_easyconfig_files.html

Subtoolchain-aware dependency resolution

- `--robot` should also consider subtoolchains
- significantly helps in avoiding clutter in module tree
- example:
 - build/install Python 2.7.11 with `foss/2016a`
 - requires `zlib 1.2.8` as a dependency (no toolchain specified)
 - dependency resolution mechanism should consider (in order):
 - `zlib/1.2.8` (*maybe?*)
 - `zlib/1.2.8-GCC-4.9.3-2.25`
 - `zlib/1.2.8-gompi-2016a`
 - `zlib/1.2.8-foss-2016a`
- experimental support by Alan, cfr. `--minimal-subtoolchains`
- consider dummy toolchain with `--add-dummy-to-minimal-toolchains`
- consider already existing modules with `--use-existing-modules`

Python 3?

- make EasyBuild work reliably in Python 3.x environment
 - prefer 'python2' over 'python'
 - check Python version, exit with clear error message if needed
 - done: bootstrap script, 'eb' wrapper
 - todo:
 - generic easyblock for Python packages (PythonPackage)
 - EasyBuildMeta easyblock
 - stand-alone scripts
 - anything else?
- make EasyBuild Python 3 compatible; different options:
 - mixed codebase (Python 2.6+ and Python 3.2+ compatible)
 - port to (only) Python 3
- latter is (still) not worth the effort (yet)
- Python 2.x ('python2') is not going to disappear anytime soon

Easybuild v3.0 (very early outlook)

- remove support for currently deprecated functionality
 - stop raising `EasyBuildError` with `log.error`
- YAML easyconfig format as default/recommended format
 - with retained support for current `.eb` format
- enhanced eb CLI to specify what to install (Spack-like?)
- subtoolchain-aware dependency resolution enabled by default
- RPATH by default?
- dropped support for old toolchains (goal`f`, iqac`m1`, ictce v3.x)
- (Python 3 support)