5 Years of Getting Scientific Software Installed Using

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http://hpcugent.github.io/easybuild
http://easybuild.readthedocs.io

GHENT UNIVERSITY http://www.ugent.be/hpc

https://www.vscentrum.be Vlaams Supercomputer Centrum

HPC-UGent

GHENT UNIVERSITY

- part of central IT department of Ghent University (Belgium)
- centralised scientific computing services, training & support
- for researchers of UGent, industry & knowledge institutes
- member of Flemish Supercomputer Centre (VSC)
  https://www.vscentrum.be/

VSC Vlaams Supercomputer Centrum

- core values:
  empowerment - centralisation - automation - collaboration

whoami

- Masters & PhD in Computer Science from Ghent University (Belgium)
- joined HPC-UGent team in October 2010
- main tasks: user support & training, software installations
- inherited maintenance of EasyBuild in 2011
- slowly also became lead developer & release manager
- big fan of loud music & FOSS (Free & Open Source Software)

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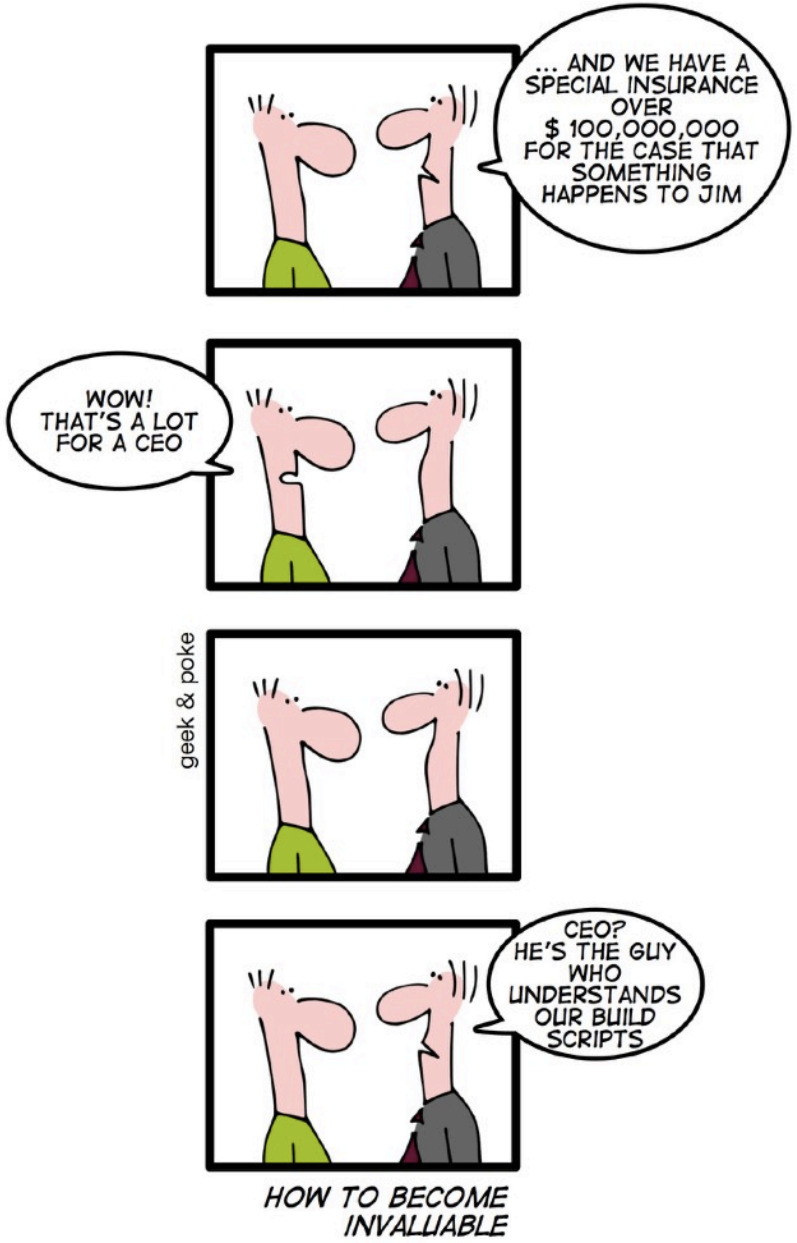
Getting Scientific Software Installed

Installation of scientific software is a tremendous problem for HPC sites all around the world.

- ideally built from source (performance is key)
- tedious, time-consuming, frustrating,
  sometimes simply not worth the (manual) effort...
- huge burden on HPC user support teams
  - over 25% of support tickets at HPC-UGent,
    but consumes *way* more time...
- very little collaboration among HPC sites (until recently)



http://geekandpoke.typepad.com/geekandpoke/2010/05/how-to-become-invaluable.html

Common issues with scientific software

Researchers focus on the *science* behind the software they implement,
and care little about tools, build procedure, portability, ...

Scientists are not software developers or sysadmins (nor should they be).

"If we would know what we are doing, it would not be called 'research'."

This results in:

- use of non-standard build tools (or broken ones)
- incomplete build procedure, e.g., no configure or install step
- interactive installation scripts
- hardcoded parameters (compilers, libraries, paths, . . .)
- poor/outdated/missing/incorrect documentation

Prime example: WRF

Weather Research and Forecasting Model (http://www.wrf-model.org)

- dozen dependencies: netCDF (C, Fortran), HDF5, tcsh, JasPer, ...
- known issues in last release are (only) documented on website
- no patch file provided, infrequent bugfix releases
- interactive '`configure`' script, options change between versions
- resulting configuration file '`configure.wrf`' needs work:
  fix hardcoded settings (compilers, libraries, . . .), tweaking of options
- custom ‘compile’ script (wraps around ‘make’)
  building in parallel is broken without fixing the Makefile
- no actual installation step

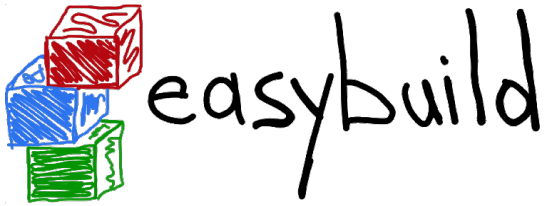
What about existing software installation tools?

- package managers: yum (RPMs), apt-get (.deb), ...
- Homebrew (Mac OS X), http://brew.sh/ ; Linuxbrew, http://brew.sh/linuxbrew/
- Portage (Gentoo), http://wiki.gentoo.org/wiki/Project:Portage
- pkgsrc (NetBSD & (a lot) more), http://pkgsrc.org/
- Nix, http://nixos.org/nix ; GNU Guix, https://www.gnu.org/s/guix

Existing tools are not well suited to scientific software and HPC systems.

Common problems:

- usually poor support for old/multiple versions and/or to have builds side-by-side
- not flexible enough to deal with idiosyncrasies of scientific software
- little support for scientific software, non-GCC compilers, MPI, ...



- website: http://hpcugent.github.io/easybuild/
- documentation: http://easybuild.readthedocs.io
- **framework to build & install scientific software on HPC clusters**
- implemented in Python 2, lead development by HPC-UGent
- Free & Open Source Software (GPLv2)
- supports different compilers & MPI libraries, **> 1,200 different software packages**, ...
- **active & helpful worldwide community**

5 years of (stable) EasyBuild

- in-house development at HPC-UGent since 2009
  - originally created by Stijn De Weirdt (tech lead at HPC-UGent)
- first public release in April 2012 (EasyBuild v0.5)
- **first stable release in November 2012, during SC'12 (EasyBuild v1.0)**
- initial intention was to get feedback, but a community emerged around it quickly...
- frequent stable releases since then (latest: EasyBuild v3.2.1, May 12th 2017)
- development is highly community-driven: bug reports, feature requests, contributions

Supported software

http://easybuild.readthedocs.io/en/latest/version-specific/Supported_software.html

- EasyBuild v3.2.1 supports installing **over 1,200 software packages**
  - including CP2K, NAMD, NWChem, OpenFOAM, QuantumESPRESSO, WRF, WPS, ...
  - also a lot of bioinformatics software is supported out of the box...
  - in addition: ~1,000 of R libraries, Python packages, Perl modules, X11 libraries, ...
- diverse toolchain support:
  - compilers: GCC, Intel, Clang, PGI, IBM XL, Cray
  - MPI libraries: OpenMPI, Intel MPI, MPICH, MPICH2, MVAPICH2, ...
  - BLAS/LAPACK libraries: Intel MKL, OpenBLAS, ATLAS, ACML, Cray LibSci, ...

Some EasyBuild terminology

http://easybuild.readthedocs.io/en/latest/Concepts_and_Terminology.html

- **EasyBuild framework**
  - core of EasyBuild: Python modules & packages
  - provides supporting functionality for building and installing software
- **easyblock**
  - a Python module that serves as a build script, 'plugin' for the EasyBuild framework
  - implements a (generic) software build/install procedure
- **easyconfig file** (*.eb): build specification; software name/version, compiler toolchain, etc.
- **(compiler) toolchain***:* set of compilers with accompanying libraries (MPI, BLAS/LAPACK, . . .)
- **extensions***:* additional libraries/packages/modules for a particular applications (e.g., Python, R)

Feature highlights (1)

- fully **autonomously** building and installing (scientific) software
  - automatic dependency resolution
  - automatic generation of module files (Tcl or Lua syntax)
- thorough **logging** of executed build/install procedure
- **archiving** of easyconfigs and patches
- highly **configurable**, via config files/environment/command line
- **dynamically extendable** with additional easyblocks, toolchains, etc.

Feature highlights (2)

- support for **custom module naming schemes** (incl. hierarchical)
- **transparency** via support for 'dry run' installation
- **comprehensively tested**: lots of unit tests, regression testing, ...
- actively developed, frequent stable releases
- **collaboration** between various HPC sites large & small
- worldwide **community**

What EasyBuild is (not)

EasyBuild is ***not***:

- YABT (Yet Another Build Tool); it doesn't replace tools like `make` (it wraps around them)
- a replacement for your favourite package manager (`yum`, `apt-get`, ...)
- a magic solution to all your (software installation) problems...

What EasyBuild is (not)

EasyBuild is:

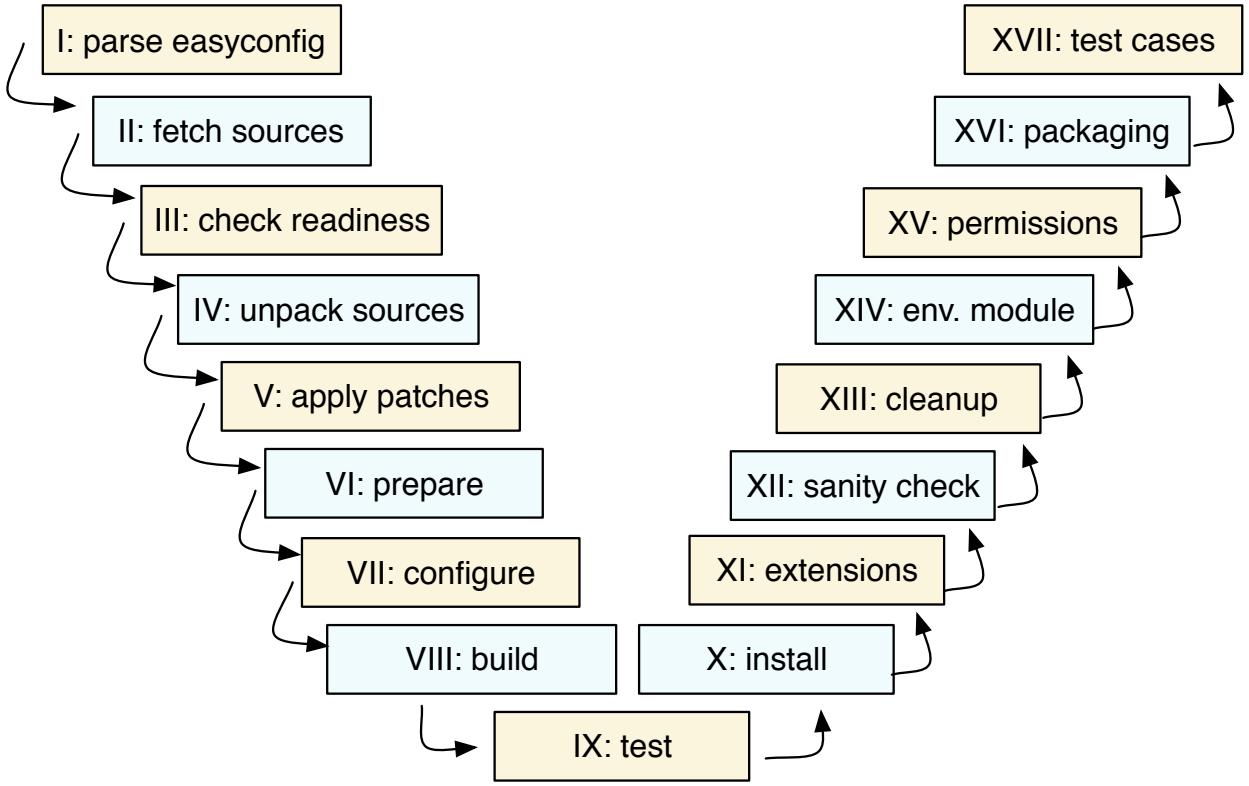
- a **uniform interface** that wraps around software installation procedures
- a huge **time-saver**, by automating tedious/boring/repetitive tasks
- a way to provide a **consistent software stack** to your users
- an **expert system** for software installation on HPC systems
- a **platform for collaboration** with HPC sites world-wide
- a way to **empower users to self-manage their software stack** on HPC systems

Example output of using 'eb' command

```
$ eb GCC-4.9.3.eb
== temporary log file in case of crash /tmp/eb-GyvPHx/easybuild-U1TkEI.log
== processing EasyBuild easyconfig GCC-4.9.3.eb
== building and installing GCC/4.9.3...
== fetching files...
== creating build dir, resetting environment...
== unpacking...
== patching...
== preparing...
== configuring...
== building...
== testing...
== installing...
== taking care of extensions...
== postprocessing...
== sanity checking...
== cleaning up...
== creating module...
== permissions...
== packaging...
== COMPLETED: Installation ended successfully
== Results of the build can be found in the log file /opt/easybuild/software/GCC/4...
== Build succeeded for 1 out of 1
== Temporary log file(s) /tmp/eb-GyvPHx/easybuild-U1TkEI.log* have been removed.
== Temporary directory /tmp/eb-GyvPHx has been removed.
```

Step-wise installation procedure

EasyBuild performs a step-wise installation procedure for each software



- download sources (best effort)
- set up build directory & environment
  - unpack sources (& apply patches)
  - load modules for toolchain & deps
  - define toolchain-related env vars (`$CC`, `$CFLAGS`, ...)
- configure, build, (test), install, (extensions)
- perform a simple sanity check on installation
- generate module file

each step can be customised via easyconfig parameters or an easyblock

Easyconfig files as build specifications

http://easybuild.readthedocs.io/en/latest/Writing_easyconfig_files.html

- **simple text files including a set of easyconfig parameters** (in Python syntax)
- some are mandatory: software name/version, toolchain, metadata (homepage, descr.)
- other commonly used parameters:
  - easyblock to use
  - list of sources & patches
  - (build) dependencies
  - options for configure/build/install commands
  - files and directories that should be present (sanity check)

Example easyconfig file

```
name = 'WRF'
version = '3.8.0'

buildtype = 'dmpar'  # custom parameter for WRF
versionsuffix = '-' + buildtype  # part of module name

homepage = 'http://www.wrf-model.org'
description = "Weather Research and Forecasting (WRF) Model"

toolchain = {'name': 'intel', 'version': '2016b'}

source_urls = ['http://www.mmm.ucar.edu/wrf/src/']
sources = ['%(name)sV%(version_major_minor)s.TAR.gz']
patches = ['WRF-%(version)s_known_problems.patch']

builddependencies = [('tcsh', '6.20.00')]
dependencies = [
    ('JasPer', '2.0.10'),
    ('netCDF', '4.4.1'),
    ('netCDF-Fortran', '4.4.4'),
]
```

Example easyconfig file

software name and version

software metadata

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Example easyconfig file

software name and version

software metadata

toolchain name & version

sources & patches

list of (build) dependencies

note: all versions are *fixed*!

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]
```

Example easyconfig file

software name and version

build variant (specific to WRF)
('dmpar': distributed, MPI)

software metadata

toolchain name & version

sources & patches

list of (build) dependencies

note: all versions are *fixed*!

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version = '3.8.0'

buildtype = 'dmpar'  # custom parameter for WRF
versionsuffix = '-' + buildtype  # part of module name

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]
```

Example easyconfig file

no easyblock specified, which implies using a software-specific easyblock (`EB_WRF`)

software name and version

build variant (specific to WRF)
('dmpar': distributed, MPI)

software metadata

toolchain name & version

sources & patches

list of (build) dependencies

note: all versions are *fixed*!

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```

5 (really) cool aspects of EasyBuild

- highly configurable and extendable
- integration with Lmod
- "extended dry run" mode
- integration with GitHub
- the EasyBuild community

Configuring and extending EasyBuild

- configuring can be done via config files, environment and/or command line options
  - *all* configuration options are supported on all 3 levels
  - CLI overrides environment which overrides config files (which override default settings)
  - http://easybuild.readthedocs.io/en/latest/Configuration.html
- easy to extend EasyBuild:
  - (also) use own easyconfigs repositories via `--robot-paths`
  - add additional easyblocks, toolchains, module naming schemes via --include-*
  - http://easybuild.readthedocs.io/en/latest/Including_additional_Python_modules.html

Inspecting current configuration

http://easybuild.readthedocs.io/en/latest/Configuration.html

Use '`eb --show-config`' to get an overview of the current configuration.

```
$ EASYBUILD_PREFIX=/tmp eb --buildpath /dev/shm --show-config
#
# Current EasyBuild configuration
# (C: command line argument, D: default value, E: environment variable, F: configuration file)
#
buildpath       (C) = /dev/shm
installpath     (E) = /tmp
packagepath     (E) = /tmp/packages
prefix          (E) = /tmp
repositorypath (E) = /tmp/ebfiles_repo
robot-paths     (D) = /home/example/easybuild-easyconfigs/easybuild/easyconfigs
sourcepath      (E) = /tmp/sources
```

Integration with Lmod

- support for using Lmod as modules tool was added in July 2013
- kind of out of necessity...
  - installing lots of modules was (too) easy using EasyBuild
  - traditional Tcl-based modules tool was too slow (no module cache, hierarchy support, ...)
- later also:
  - support for using a hierarchical module naming scheme (July 2014)
  - support for module files in Lua syntax (April 2015)
- Lmod (& Lua syntax) became the default in EasyBuild v3.0.0 (November 2016)

Integration with Lmod

- synergy between Lmod & EasyBuild has grown over time
  - communities engaging with each other
  - increased adoption for both tools thanks to integration
  - (significant) enhancements to both tools inspired by or thanks to other community
    - improved performance, Lmod's `update_lmod_system_cache_files` script, ...
  - joint papers on "Modern Scientific Software Management"
  - lead developers became good friends :)

Flat module naming scheme

- all modules are always available for loading
- long(er) module names, '`module avail`' may be overwhelming for users
- too easy to load incompatible modules together

legend

(not available)

(available)

(loaded)

GCC/5.3.0

GCC/6.1.0

OpenMPI/1.10.2-GCC-5.3.0

OpenMPI/2.1.0-GCC-5.3.0

OpenMPI/1.10.3-GCC-6.1.0

OpenMPI/2.1.0-GCC-6.1.0

FFTW/3.3.4-gompi-2016.04

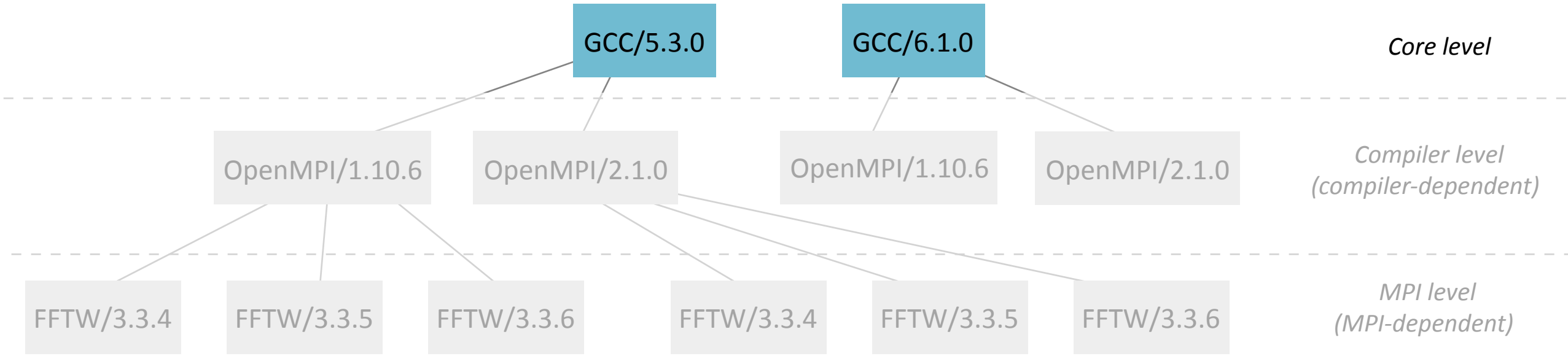
FFTW/3.3.6-gompi-2016.04

FFTW/3.3.4-gompi-2016.07

FFTW/3.3.6-gompi-2016.07

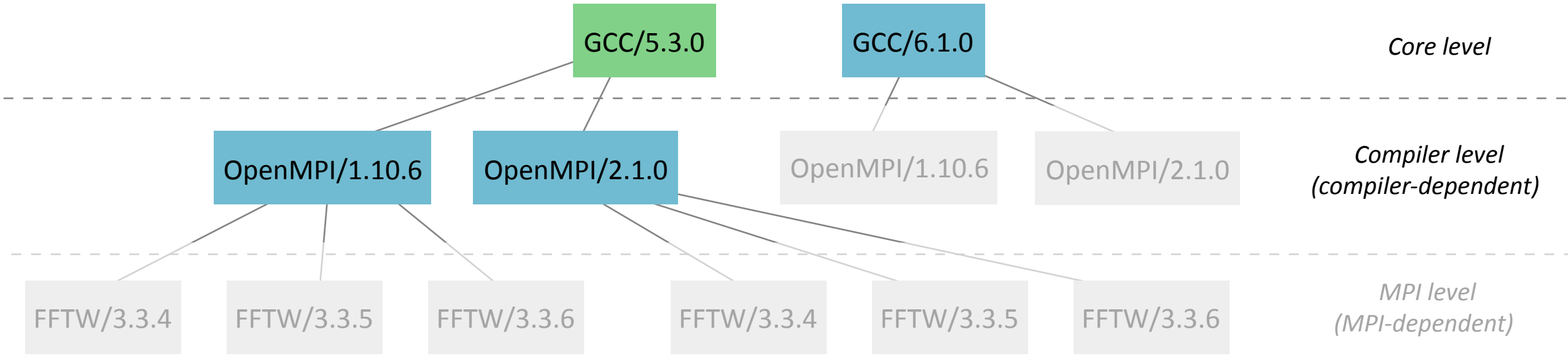
Hierarchical module naming scheme (1)

- modules are organised in a tree-like fashion
- initially, only 'core' modules are available for loading
  (typically: Core - Compiler - MPI)
- other modules are only visible via '`module spider`'



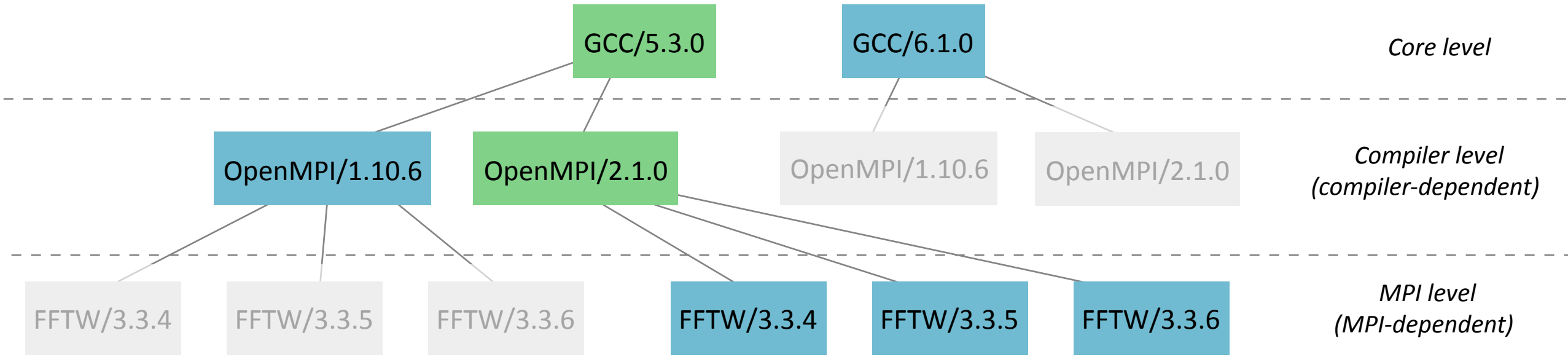
Hierarchical module naming scheme (2)

- Core modules may extend `$MODULEPATH` with an additional location
- loading a Core module may make more modules available
- in this example, loading a GCC module makes OpenMPI modules available



Hierarchical module naming scheme (3)

- even more modules may be made available by loading other modules
- for example, loading an OpenMPI modules reveals MPI-dependent modules
- EasyBuild can organise modules in hierarchy for you!



Transparency of performed install procedure

http://easybuild.readthedocs.io/en/latest/Extended_dry_run.html

- '`eb --extended-dry-run`' ('`eb -x`') reveals planned installation procedure
- runs in a matter of seconds
- shows commands that will be executed, build environment, generated module file, ...
- any errors that occur in used easyblock are ignored but clearly reported
- not 100% accurate since easyblock may require certain files to be present, etc.
- very useful when debugging easyblocks, instant feedback as a first pass
- implementation motivated by requests from the community
- helps to avoid impression that EasyBuild is a magic black box for installing software

Example output of --extended-dry-run (1)


```
$ eb WRF-3.8.0-intel-2016b-dmpar.eb -x

== temporary log file in case of crash /tmp/eb-Dh1wOp/easybuild-0bu9u9.log

== processing EasyBuild easyconfig /home/example/eb/easybuild-easyconfigs/easybuild/
easyconfigs/w/WRF/WRF-3.8.0-intel-2016b-dmpar.eb

...

*** DRY RUN using 'EB_WRF' easyblock (easybuild.easyblocks.wrf @ /home/example/eb/easybuild-
easyblocks/easybuild/easyblocks/w/wrf.py) ***

== building and installing WRF/3.8.0-intel-2016b-dmpar...
fetching files... [DRY RUN]

[fetch_step method]
Available download URLs for sources/patches:
  * http://www2.mmm.ucar.edu/wrf/src//$source
  * http://www.mmm.ucar.edu/wrf/src//$source

List of sources:
  * WRFV3.8.0.TAR.gz will be downloaded to /home/example/eb/sources/w/WRF/WRFV3.8.0.TAR.gz
```

Example output of `--extended-dry-run` (2)


```
$ eb WRF-3.8.0-intel-2016b-dmpar.eb -x
...

building... [DRY RUN]

[build_step method]
  running command "tcsh ./compile -j 4 wrf"
  (in /home/example/eb/software/WRF/3.8.0-intel-2016b-dmpar/WRF-3.8.0)
  running command "tcsh ./compile -j 4 em_real"
  (in /home/example/eb/software/WRF/3.8.0-intel-2016b-dmpar/WRF-3.8.0)
  running command "tcsh ./compile -j 4 em_b_wave"
  (in /home/example/eb/software/WRF/3.8.0-intel-2016b-dmpar/WRF-3.8.0)
...
[sanity_check_step method]
Sanity check paths - file ['files']
  * WRFV3/main/libwrflib.a
  * WRFV3/main/real.exe
  * WRFV3/main/wrf.exe
Sanity check paths - (non-empty) directory ['dirs']
  * WRFV3/main
  * WRFV3/run
Sanity check commands
  (none)
```

Example output of `--extended-dry-run` (3)


```
$ eb WRF-3.8.0-intel-2016b-dmpar.eb -x
...

[make_module_step method]
Generating module file /home/example/eb/modules/all/WRF/3.8.0-intel-2016b-dmpar,
with contents:

    #%Module
    proc ModulesHelp { } {
        puts stderr { The Weather Research and Forecasting (WRF) Model }
    }
    module-whatis {Description: WRF - Homepage: http://www.wrf-model.org}

    set root /home/example/eb/software/WRF/3.8.0-intel-2016b-dmpar

    conflict WRF

    if { ![ is-loaded intel/2016b ] } {
        module load intel/2016b
    }
    if { ![ is-loaded JasPer/1.900.1-intel-2016b ] } {
        module load JasPer/1.900.1-intel-2016b
    }
```

Integration with GitHub

http://easybuild.readthedocs.io/en/latest/Integration_with_GitHub.html

- contributing to EasyBuild required sufficient experience with Git
  - + following EasyBuild policy for pull requests: target `develop` branch, PR titles, ...
- this was a limiting factor, not all EasyBuilders are familiar enough with Git
- process can also be quite time-consuming when contributing frequently
- weekend project:
  - leverage `GitPython` and GitHub API to automate contributions
  - enhance '`eb`' command line interface with `--new-pr`, `--update-pr`

Integration with GitHub

http://easybuild.readthedocs.io/en/latest/Integration_with_GitHub.html

- contribution process (manual):
  - `git checkout develop`
  - `git checkout -b my_branch`
  - `git add <easyconfig files>`
  - `git commit -m "my awesome stuff"`
  - `git push origin my_branch`
  - visit `github.com/my_account`
  - issue pull request for `my_branch` to `hpcugent:develop`

Integration with GitHub

http://easybuild.readthedocs.io/en/latest/Integration_with_GitHub.html

- contribution process (fully automated):

```
eb --new-pr <easyconfig files>
```

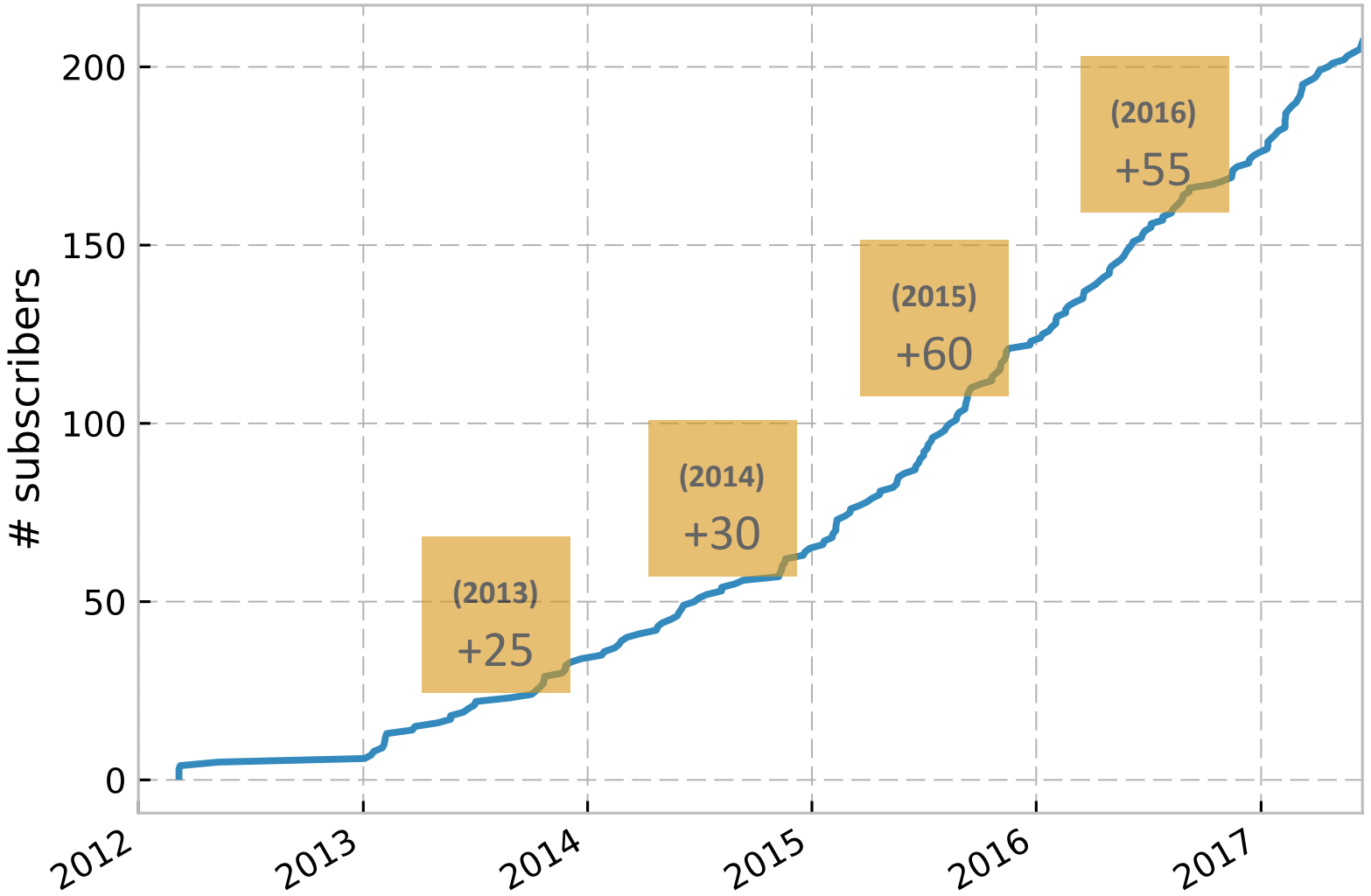
- 4-5 `git` commands + handful of mouse clicks reduced to a single `eb` command!
- to update an existing pull request: `eb --update-pr <PR#> ...`
- significantly lowers the hurdle for contributors: no Git or GitHub experience required
- huge time-saver even for experienced contributors (+ reduced local branches clutter)
- optional: submit test report with

```
eb --from-pr <PR#> --force --robot --upload-test-report
```

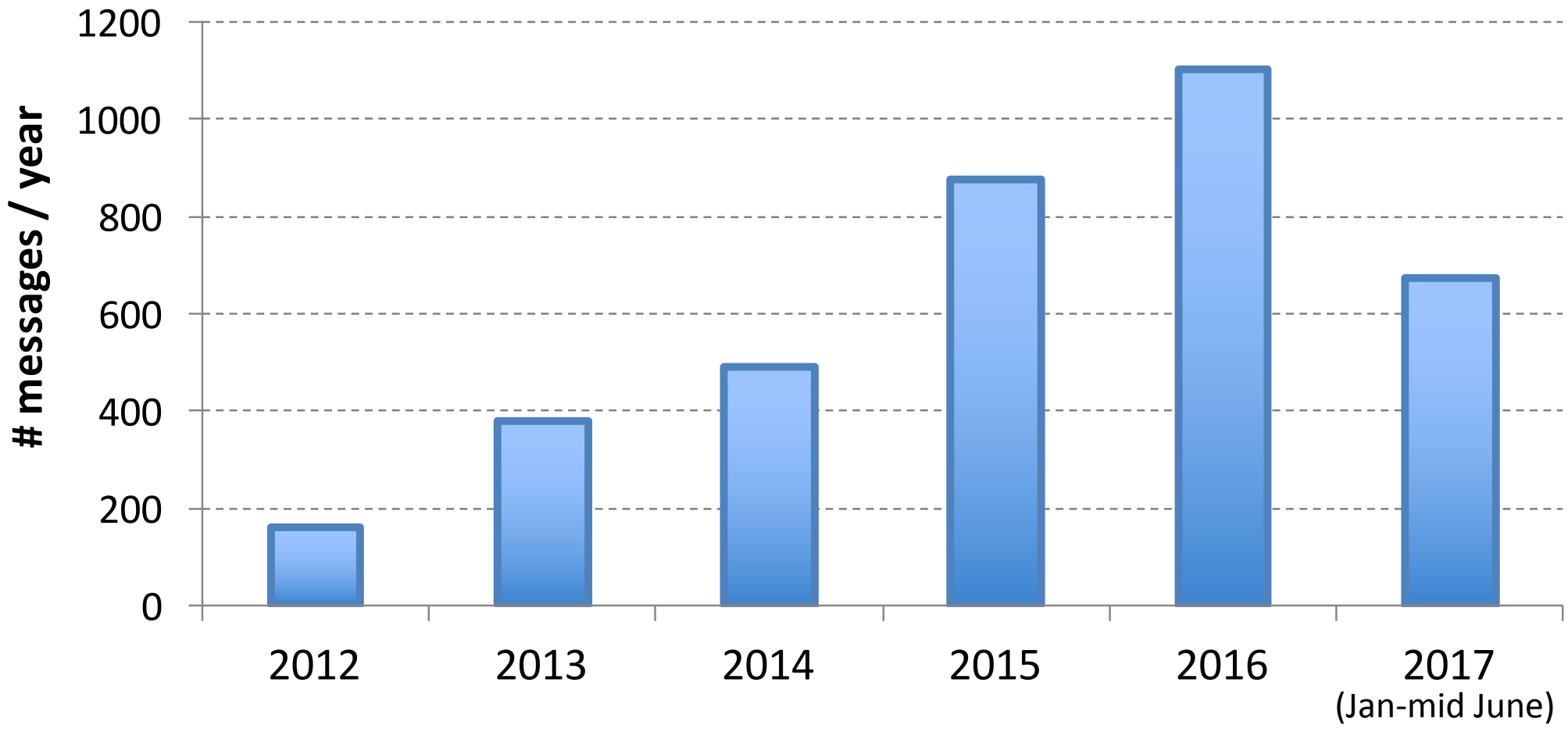
The EasyBuild community

- EasyBuild community has been growing rapidly the last couple of years
- **hundreds of HPC sites and companies worldwide, incl. JSC, CSCS, Pfizer, Bayer, ...**
- very welcoming & supportive to newcomers
- significant overlap between EasyBuild & Lmod communities
- active mailing list: https://lists.ugent.be/wws/info/easybuild
- active IRC (`#easybuild` on FreeNode) & Slack channel (`easybuild.slack.com`)
- users are also contributing: bug reports, feature requests, code contributions, ...

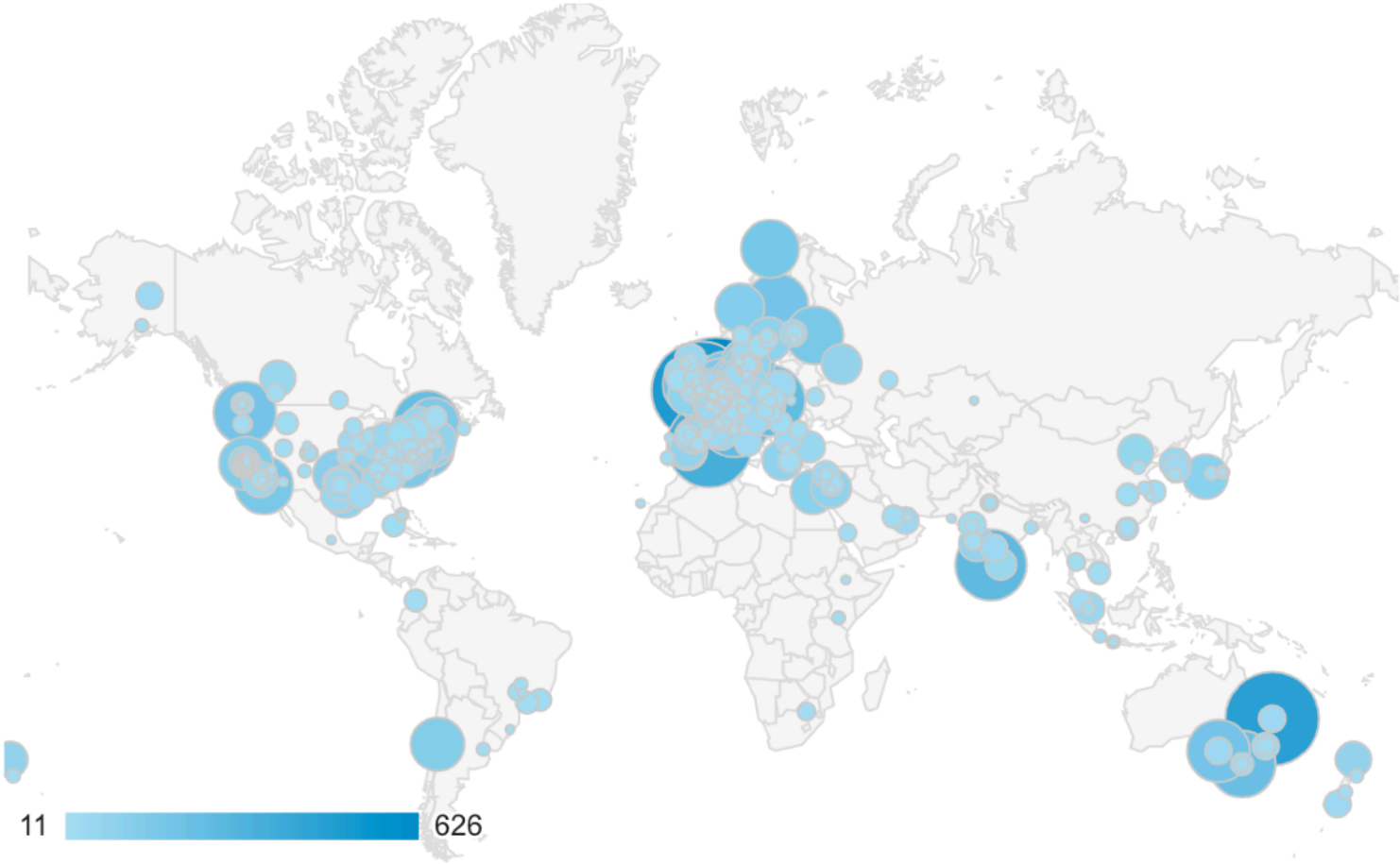
EasyBuild mailing list (subscribers)



EasyBuild mailing list (traffic)

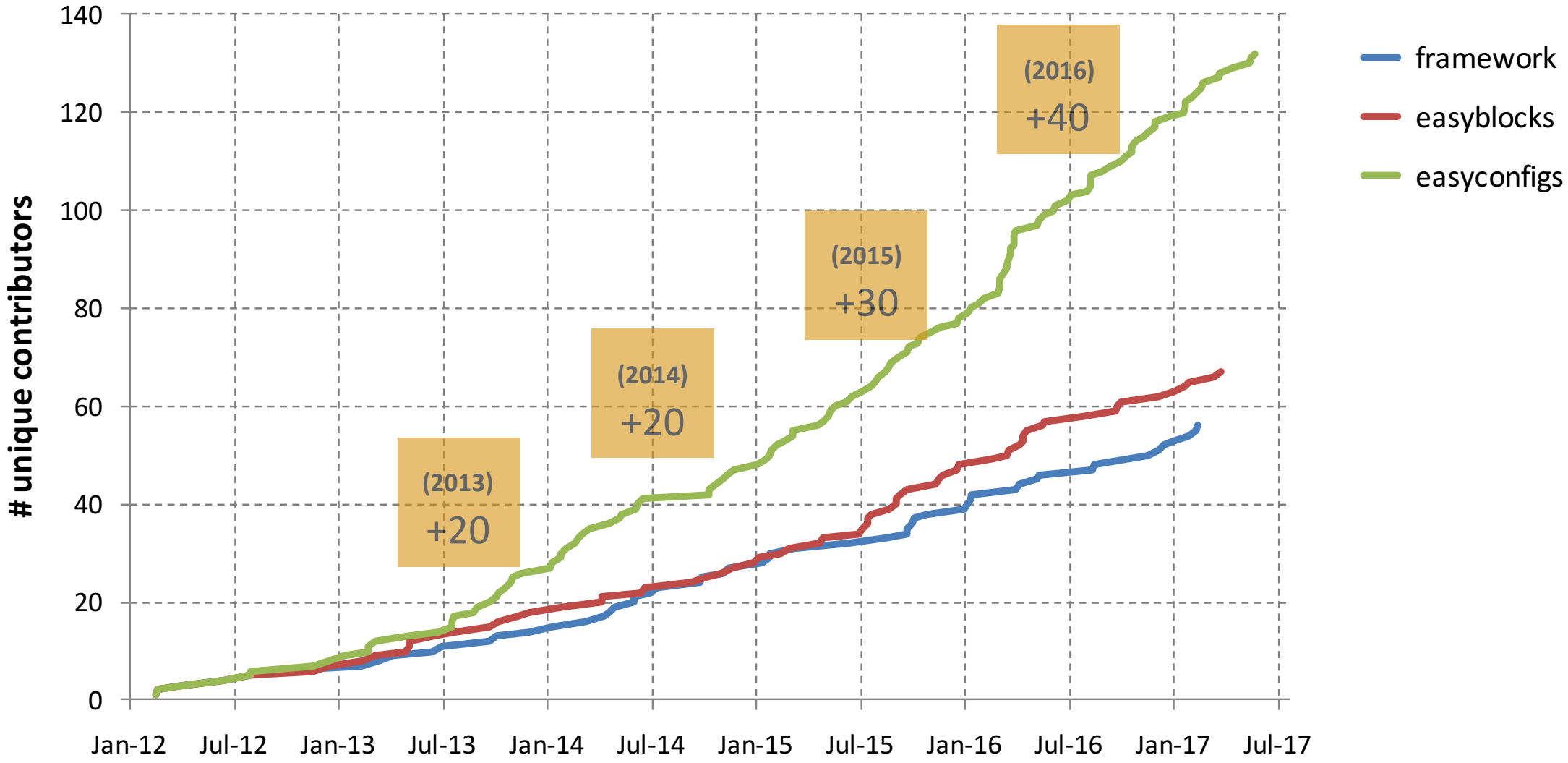


The sun never sets on EasyBuild...



cities from where EasyBuild documentation was visited at least 10 times during the last year
source: Google Analytics for easybuild.readthedocs.io

Contributors, contributors, contributors!



Community (common) toolchains

http://easybuild.readthedocs.io/en/latest/Common-toolchains.html

- `intel` and `foss`[1] toolchains are most commonly used in EasyBuild community
- helps to focus efforts of HPC sites using one or both of these toolchains
- updated twice a year, clear versioning scheme: `<year>{a,b}` (`2016b`, `2017a`, ...)
- latest version:
  - `foss/2017a`

    binutils 2.27, GCC 6.3.0, OpenMPI 2.0.2, OpenBLAS 0.2.19, LAPACK 3.7.0, FFTW 3.3.6
  - `intel/2017a`

    binutils 2.27 + GCC 6.3.0 as base

    version 2017.1.132 of Intel compilers, Intel MPI and Intel MKL

(1) FOSS: Free and Open Source Software

Other features that were not covered...

http://easybuild.readthedocs.io

- letting users manage their software stack on top of centrally provided modules
- installing hidden modules, hiding certain dependencies & toolchains
- support for using RPATH linking *(experimental)*
- partial installations: only (re)generate module file, install additional extensions
- submitting installations as jobs to an HPC cluster via `--job`
- creating packages (RPMs, ...) for software installations done with EasyBuild
- using EasyBuild on Cray systems, integration with Cray Programming Environment

Future work

- stable support for RPATH (95% done)
- SHA256 checksums for sources in all easyconfigs included in release
- automated style checking of (easyconfig) pull requests
- querying of latest available version of a particular software package (via `anitya`?)
- slightly more flexibility w.r.t. dependency versions
- getting rid of dependency on `setuptools` (too much of a PITA...)
- support for using EasyBuild on top of Python 3
- easyconfig files in YAML syntax (.yeb): work in progress...

Papers on EasyBuild (& Lmod)

Modern Scientific Software Management Using EasyBuild and Lmod

Markus Geimer (JSC), Kenneth Hoste (HPC-UGent), Robert McLay (TACC)

http://hpcugent.github.io/easybuild/files/hust14_paper.pdf

Making Scientific Software Installation Reproducible On Cray Systems Using EasyBuild

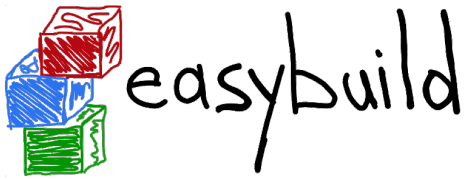
Petar Forai (IMP), Guilherme Peretti-Pezzi (CSCS), Kenneth Hoste (HPC-UGent)

https://cug.org/proceedings/cug2016_proceedings/includes/files/pap145.pdf

Scientific Software Management in Real Life: Deployment of EasyBuild on a Large Scale System

Damian Alvarez, Alan O'Cais, Markus Geimer (JSC), Kenneth Hoste (HPC-UGent)

http://hpcugent.github.io/easybuild/files/eb-jsc-hust16.pdf



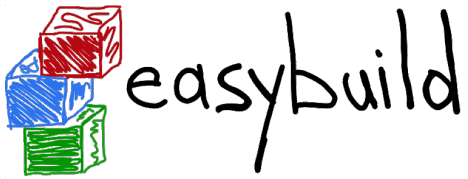
VS

http://spack.rtfd.io/

- requires Python 2(.6), GPLv2
- targeted to HPC user support teams
- stable releases since Nov'12
- supports >1.2k tools/apps/libs + ~1k extensions
- fixed dependency/toolchain versions
- *requires* a modules tool (Lmod/Tmod)
- framework + easyblocks (.py) + easyconfigs (.eb)
- can do both `$LD_LIBRARY_PATH` & `RPATH`
- supports Linux HPC systems (incl. Cray)

- Python 2 & Python 3 compatible, LGPL
- (mainly) for scientific software developers
- alpha software (no stable release yet)
- supports >1.5k software packages (incl. exts)
- very flexible dependency management
- compatible with Lmod/Tmod, dotkit
- core library + packages (.py)
- only does `RPATH`
- supports Linux, macOS, Cray, ...

Both are backed by an active & supportive community!



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- only does `RPATH`
- supports Linux, macOS, Cray, ...
- *no stickers (yet)*

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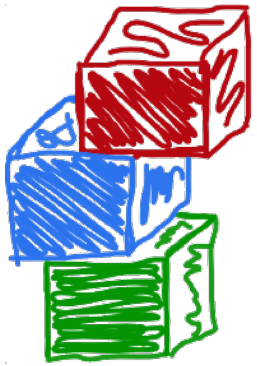

easybuild

Questions?

kenneth.hoste@ugent.be

http://hpcugent.github.io/easybuild
http://easybuild.readthedocs.io

GHENT UNIVERSITY http://www.ugent.be/hpc

https://www.vscentrum.be Vlaams Supercomputer Centrum

(disorganised set of)

EXTRA SLIDES

EasyBuild requirements

http://easybuild.readthedocs.io/en/latest/Installation.html#requirements

- focus is on Linux x86_64 HPC systems
  - RedHat-based (CentOS, SL, ...), also on Debian and SuSE derivatives
  - also (kind of) works on macOS, but not a target platform
  - Windows support only via new Windows Subsystem for Linux (WSL)
  - ongoing efforts to enhance support on AARCH64 (ARM) and PowerLinux
- Python 2.6 or more recent Python 2, incl. setuptools (no Python 3 support yet)
- system C/C++ compiler (GCC), used to kickstart installation of compiler toolchain
- an environment modules tool (Lmod is highly recommended!)

Installing EasyBuild

http://easybuild.readthedocs.io/en/latest/Installation.html

- installing Python packages can be messy, cfr. plethora of Python installation tools
- **bootstrap script** for EasyBuild was created out of frustration

```
# download bootstrap script from
# https://raw.github.com/hpcugent/easybuild-framework/develop/easybuild/scripts/bootstrap_eb.py

$ python bootstrap_eb.py $PREFIX
$ module use $PREFIX/modules/all
$ module load EasyBuild
```

- standard installation tools like `easy_install`, `pip`, etc. work too
- packaging efforts under way (see OpenHPC; WIP in Fedora)

Updating EasyBuild

http://easybuild.readthedocs.io/en/latest/Installation.html#updating-an-existing-easybuild-installation

- new releases are fully backwards-compatible (except for new major versions)
- to update EasyBuild:
  - re-bootstrap to obtain a module for latest EasyBuild release
  - or use '`eb --install-latest-eb-release`' to install module for latest release
  - install a specific EasyBuild version with EasyBuild using an easyconfig file

    https://github.com/hpcugent/easybuild-easyconfigs/tree/develop/easybuild/easyconfigs/e/EasyBuild

Configuring EasyBuild (1)

http://easybuild.readthedocs.io/en/latest/Configuration.html

You should configure EasyBuild to your preferences, via:

- configuration file(s): key-value lines, text files (e.g., `prefix=/tmp`)
- environment variables (e.g., `$EASYBUILD_PREFIX` set to `/tmp`)
- command line parameters (e.g., `--prefix=/tmp`)

Each configuration option can be set on each of these configuration levels.

Priority among different options: cmdline, env vars, config file. For example:

- `--prefix` overrules `$EASYBUILD_PREFIX`
- `$EASYBUILD_PREFIX` overrules `prefix` in configuration file

Configuring EasyBuild (2)

http://easybuild.readthedocs.io/en/latest/Configuration.html

By default, EasyBuild will (ab)use `$HOME/.local/easybuild`.

Use '`eb --show-config`' to get an overview of the current configuration.

```
$ EASYBUILD_PREFIX=/tmp eb --buildpath /dev/shm --show-config
#
# Current EasyBuild configuration
# (C: command line argument, D: default value, E: environment variable, F: configuration file)
#
buildpath       (C) = /dev/shm
installpath     (E) = /tmp
packagepath     (E) = /tmp/packages
prefix          (E) = /tmp
repositorypath (E) = /tmp/ebfiles_repo
robot-paths     (D) = /Users/kehoste/work/easybuild-easyconfigs/easybuild/easyconfigs
sourcepath      (E) = /tmp/sources
```

Contributing to EasyBuild

http://easybuild.readthedocs.io/en/latest/Contributing.html

EasyBuild has improved significantly thanks to the community.

You too can contribute back, by:

- sending feedback
- reporting bugs
- joining the discussion (mailing lists, EasyBuild conf calls)
- sharing suggestions and ideas for changes & additional features
- contributing easyconfigs, enhancing easyblocks, adding support for new software...
- extending & enhancing documentation

Adding support for additional software

- for each software installation, an **easyconfig file** is required
  - defines easyconfig parameters that specify to EasyBuild what to install, and how
  - existing easyconfig files can serve as examples
  - for version or toolchain updates, a tweaked easyconfig can be *generated* via `eb --try-*`
  - see http://easybuild.readthedocs.io/en/latest/Writing_easyconfig_files.html
- for 'standard' installation procedures, a **generic easyblock** can be used
  - generic installation can be controlled where needed via easyconfig parameters
- for custom installation procedures, a **software-specific easyblock** is must be implemented
  - see http://easybuild.readthedocs.io/en/latest/Implementing-easyblocks.html

Common generic easyblocks

http://easybuild.readthedocs.io/en/latest/version-specific/generic_easyblocks.html

- **`ConfigureMake`**
  standard '`./configure`' - '`make`' - '`make install`' installation procedure
- **`CMakeMake`**
  same as ConfigureMake, but using *CMake* for configuring
- **`PythonPackage`**
  installing Python packages ('`python setup.py install`', '`pip install`', ...)
- **`MakeCp`**
  no (standard) configuration step, build with '`make`', install by copying binaries/libraries
- **`Tarball`**: just unpack sources and copy everything to installation directory
- **`Binary`**: run binary installer (specified via '`install_cmd`' easyconfig parameter)

Easyconfig files vs easyblocks

http://easybuild.readthedocs.io/en/latest/Implementing-easyblocks.html

- thin line between using custom easyblock and 'fat' easyconfig with generic easyblock
- custom easyblocks are "do once and forget", **central solution to build peculiarities**
- reasons to consider implementing a software-specific easyblock include:
  - 'critical' values for easyconfig parameters required to make installation succeed
  - toolchain-specific aspects of the build and installation procedure (e.g., configure options)
  - interactive commands that need to be run
  - custom (configure) options for dependencies
  - having to create or adjust specific (configuration) files
  - 'hackish' usage of a generic easyblock

Log files

http://easybuild.readthedocs.io/en/latest/Logfiles.html

- **EasyBuild thoroughly logs executed installation procedure**
  - active EasyBuild configuration
  - easyconfig file that was used
  - modules that were loaded + resulting changes to environment
  - defined environment variables
  - output of executed commands
  - informative log messages produced by easyblock
- log is file is copied to software installation directory for future reference
- can be used to debug build problems or see how installation was performed exactly

Log files: example

```
== 2016-04-24 13:34:31,906 main.EB_HPL INFO This is EasyBuild 3.1.2 (framework:
3.1.2, easyblocks: 3.1.2) on host example.
...
== 2016-04-24 13:34:35,503 main.EB_HPL INFO configuring...
== 2016-04-24 13:34:48,817 main.EB_HPL INFO Starting configure step
...
== 2016-04-24 13:34:48,823 main.EB_HPL INFO Running method configure_step part of
step configure
...
== 2016-04-24 13:34:48,823 main.run DEBUG run_cmd: running cmd /bin/bash
make_generic (in /tmp/user/easybuild_build/HPL/2.0/goolf-1.4.10/hpl-2.0/setup)
== 2016-04-24 13:34:48,823 main.run DEBUG run_cmd: Command output will be logged
to /tmp/easybuild-W85p4r/easybuild-run_cmd-XoJwMY.log
== 2016-04-24 13:34:48,849 main.run INFO cmd "/bin/bash make_generic" exited with
exitcode 0 and output:
...
```

In numbers

included in EasyBuild v3.2.1:

- about 50k LoC of Python (incl. framework, easyblocks, and logging/option parsing support)
- about 15k LoC more for unit/integration test suites
- 1,228 supported software applications (excl. extensions, software versions)
- 25 different toolchain definitions (excl. toolchain versions)
- 185 software-specific easyblocks, 30 generic easyblocks
- 7,036 easyconfig files
  - different software versions, variants, using different toolchains, ...

Basic usage

http://easybuild.readthedocs.io/en/latest/Using_the_EasyBuild_command_line.html

http://easybuild.readthedocs.io/en/latest/Typical_workflow_example_with_WRF.html

- specify software name/version and toolchain to 'eb' command
- commonly via easyconfig filename(s):

```
eb GCC-4.9.2.eb Clang-3.6.0-GCC-4.9.2.eb
```

- check whether required toolchain & dependencies are available using `--dry-run/-D`:

```
eb Python-2.7.13-intel-2017a.eb -D
```

- enable dependency resolution via `--robot/-r`:

```
eb WRF-3.8.0-intel-2016b-dmpar.eb -dr
```

Using a custom module naming scheme

- a couple of different module naming schemes are included in EasyBuild
  - see `--avail-module-naming-schemes`
  - specify active module naming scheme via `--module-naming-scheme`
  - default: `EasyBuildMNS` (`<name>/<version>-<toolchain>-<versionsuffix>`)
- **you can implement your own module naming scheme relatively easily**
  - specify how to compose module name using provided metadata
  - via Python module that defines custom derivative class of `ModuleNamingScheme`
  - make EasyBuild aware of it via `--include-module-naming-schemes`
- decouple naming of install dirs vs modules via `--fixed-installdir-naming-scheme`