



## EasyBuild

Getting Scientific Software Installed With Ease

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[http://users.ugent.be/~kehoste/EasyBuild\\_conf-call-SE\\_20160615.pdf](http://users.ugent.be/~kehoste/EasyBuild_conf-call-SE_20160615.pdf)

Swedish Application Expert meeting – June 15th 2016 (via video link)

# whoami



- 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
  
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- IRC (Freenode): boegel
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# HPC-UGent in a nutshell



<http://www.ugent.be/hpc/en> – <http://www.vscentrum.be>

- HPC team at central IT dept. of Ghent University (Belgium)
- 8+1 team members: 1 manager, ~2 user support, ~6 sysadmin
- 4+1 Tier2 clusters + one Tier1 cluster (8.5k cores)
- ~1.8k 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



# “Please install <software> on the HPC?”

The most common type of support request from users is to install (scientific) software; this covers over 25% of support tickets at HPC-UGent.

Installing (lots of) *scientific* software is:

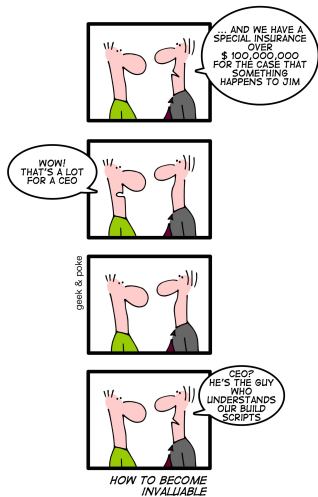
- error-prone, trial-and-error
- tedious, hard to get right
- repetitive & boring (well. . .)
- time-consuming (hours, days, even weeks)
- frustrating (e.g., dependency hell)
- sometimes simply not worth the effort. . .



# Houston, we have a problem

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

- huge burden on HPC user support teams
- hard to provide a consistent software stack
- researchers lose lots of time (waiting)
- sites typically resort to in-house scripting
- very little collaboration among HPC sites :(



# EasyBuild: building software with ease



<http://hpcugent.github.io/easybuild/>

- framework for installing (scientific) software on HPC systems
- collection of Python packages and modules
- in-house since 2009, open-source (GPLv2) since 2012
- now: thriving community; actively contributing, driving development
- new release every 6–8 weeks (latest: EasyBuild v2.8.1, May 30th 2016)
- supports over 940 different software packages
  - including CP2K, GAMESS-US, GROMACS, NAMD, NWChem, OpenFOAM, PETSc, QuantumESPRESSO, WRF, WPS, ...
- well documented: <http://easybuild.readthedocs.io>

# EasyBuild: feature highlights

- 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 build specifications ('*easyconfig files*')
- highly **configurable**, via config files/environment/command line
- **dynamically extendable** with additional *easyblocks*, *toolchains*, ...
- support for **custom module naming schemes** (incl. hierarchical)
- **transparency** via support for 'dry run' installations
- **comprehensively tested**: lots of unit tests, regression testing, ...
- actively developed, **collaboration** between various HPC sites
- worldwide **community**

# What EasyBuild is (not)

EasyBuild is **not**:

- YABT (Yet Another Build Tool); it does *not* replace make, CMake
- a replacement for your favorite package manager
- a magic solution to all your (installation) problems

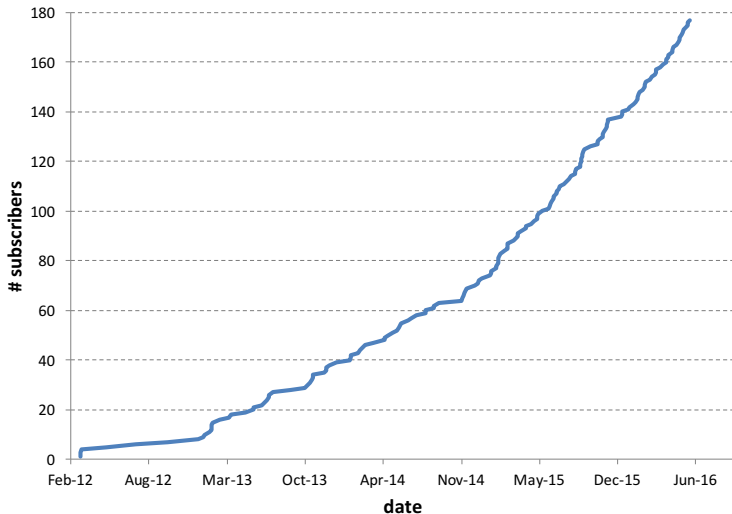
EasyBuild can be (and maybe already *is*) a:

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

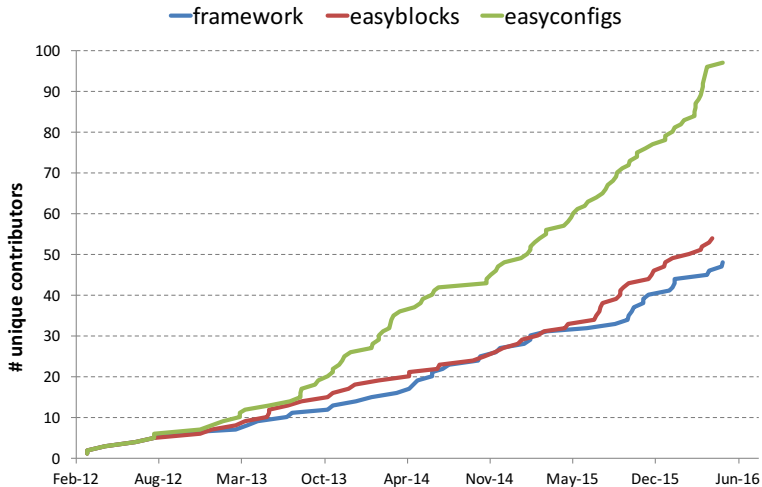
# EasyBuild community

- worldwide: Europe, US, New Zealand, Australia, Cuba, ...
  - incl. large sites like Jülich Supercomputer Centre, CSCS, CSC.fi, ...
- active mailing list & IRC channel
  - <https://lists.ugent.be/wws/info/easybuild> (recommended!)
  - #easybuild at [chat.freenode.net](http://chat.freenode.net)
- bi-weekly (short) conference calls via Google Hangouts
- meetings on a regular basis
  - sessions at ISC/SC
  - hackathons
  - EasyBuild User Meeting
- development is highly community driven
- rough estimate: about 100 HPC sites using EasyBuild

## EasyBuild mailing list



## EasyBuild contributors



# HUST'14 paper

## 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](http://hpcugent.github.io/easybuild/files/hust14_paper.pdf)

- paper at HPC User Support Tools workshop (HUST'14 @ SC14)
- explains basics of module tools, EasyBuild and Lmod
- highlights issues with current approaches in software installation
- advocates use of a hierarchical module naming scheme
- presents EasyBuild and Lmod as adequate tools for (automated) software/module management on HPC systems

# Recent developments

- better transparency via 'eb --extended-dry-run'  
[http://easybuild.readthedocs.io/en/latest/Extended\\_dry\\_run.html](http://easybuild.readthedocs.io/en/latest/Extended_dry_run.html)
- significant performance & responsiveness improvements of 'eb'
- support for PGI as a toolchain compiler
- better GitHub integration (but still experimental)
  - incl. support for submitting/updated pull requests using 'eb'!
- *stable* Cray support
  - proper integration of EasyBuild with the Cray PE
  - presented at Cray User Group 2016:  
*Making Scientific Software Installation Reproducible On Cray Systems Using EasyBuild*  
[https://cug.org/proceedings/cug2016\\_proceedings/includes/files/pap145.pdf](https://cug.org/proceedings/cug2016_proceedings/includes/files/pap145.pdf)

# Do you want to know more?

- EasyBuild website: <http://hpcugent.github.io/easybuild>
- EasyBuild documentation: <http://easybuild.readthedocs.io>
- stable EasyBuild releases: <http://pypi.python.org/pypi/easybuild>
  - EasyBuild framework: <http://pypi.python.org/pypi/easybuild-framework>
  - easyblocks: <http://pypi.python.org/pypi/easybuild-easyblocks>
  - easyconfigs <http://pypi.python.org/pypi/easybuild-easyconfigs>
- source repositories on GitHub
  - EasyBuild meta package + docs: <https://github.com/hpcugent/easybuild>
  - EasyBuild framework: <https://github.com/hpcugent/easybuild-framework>
  - easyblocks: <https://github.com/hpcugent/easybuild-easyblocks>
  - easyconfigs: <https://github.com/hpcugent/easybuild-easyconfigs>
- EasyBuild mailing list: [easybuild@lists.ugent.be](mailto:easybuild@lists.ugent.be)  
<https://lists.ugent.be/www/subscribe/easybuild>
- Twitter: @easy\_build
- IRC: #easybuild on [chat.freenode.net](http://chat.freenode.net)