easybuild

building software with ease

6th EasyBuild hackathon @ Vienna, Austria

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HPC-UGent: in a nutshell

- HPC team at central IT dept. of Ghent University (Belgium)
  - 9 team members: 1 manager, ~3 user support, ~5 sysadmin
  - 6 Tier2 clusters + one Tier1 (8.5k cores), ~1k servers in total
  - ~1.2k user accounts, all research domains
  - tasks incl. hardware, system administration, user support/training, …
- member of Flemish Supercomputer Centre (VSC)
  - virtual centre, collaboration between Flemish university associations

AUTOMATE

- Quattor (system configuration)
- Django + Python scripting (user administration)
- **EasyBuild (end-user software installation)**

where possible & sensible:

- Free and Open Source Software (FOSS)
- share our efforts with the HPC community

“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- poor/outdated documentation
- …

Existing tools are not what we need

Standard packaging solutions (RPM, .deb) are not a good fit.

- building *from source* is preferred in an HPC context
- packaging scientific software requires huge amounts of effort
- packaging formats (e.g. `.spec`) don't fit peculiarities well
- collection of build scripts is hard to maintain (alone)

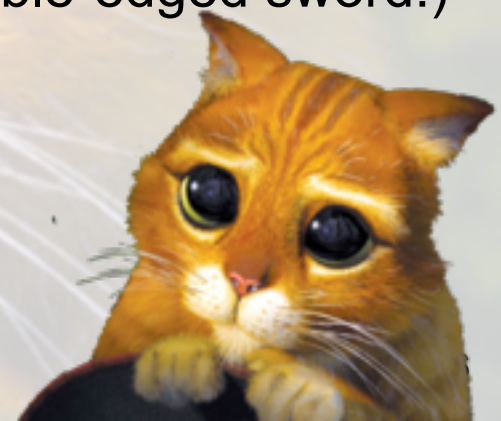
Lots of duplication of work across HPC sites!

Some solutions are (too) OS-dependent:
Portage (Gentoo), Homebrew, …

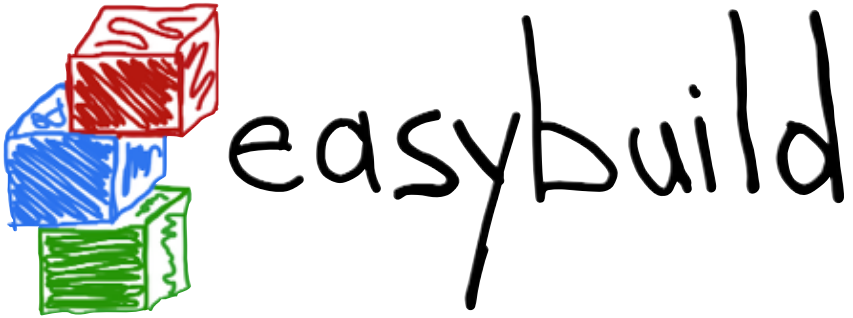
Others are software-specific:
Dorsal (DOLFIN), gmkpack (ALADIN), …

Our build tool wish list

- a **flexible framework** for building/installing (scientific) software
- fully **automates** software builds
- allows for **reproducible** builds
- supports **co-existence** of versions/builds
- enables **sharing** with the HPC community (double-edged sword!)
- **automagic dependency** resolution



EasyBuild: building software with ease



http://hpcugent.github.io/easybuild

EasyBuild is a *software build and installation framework*.

- written in **Python**
- started in 2009, in-house for ~2.5 years, **GPLv2** since 2012
- **stable API** since EasyBuild v1.0 (Nov'12), latest is v1.13.0
- continuously enhanced and extended, thoroughly tested
- *release early, release often strategy* (major version every 4-6 weeks)
- development is highly **community-driven**

Requirements

- **Linux** / OS X
- used daily on Scientific Linux 5.x/6.x (Red Hat-based)
- also tested on Fedora, Debian, Ubuntu, CentOS, SLES, ...
- some known issues on OS X, *focus is on Linux (HPC)*
- no Windows support (and none planned for now)
- **Python** v2.4 or more recent v2.x (no Python 3 support yet)
- modules tool: **Tcl(/C) environment modules** or **Lmod**
- (system C/C++ compiler to bootstrap a GCC toolchain)

Key features

- execute software build procedures **fully autonomously**

  also interactive installers, code patching, generating module file, ...

- thorough **logging** and archiving

  entire build process is logged thoroughly, logs stored in install dir;

  easyconfig file used for build is archived (file/svn/git repo)

- automatic **dependency resolution**

  build entire software stack with a single command, using `--robot`

- building software in **parallel**

  e.g., on a (PBS) cluster, using `--job`

- comprehensive **testing**: unit tests, regression testing

- thriving, growing **community**

‘Quick’ demo for the impatient

```
eb HPL-2.0-goolf-1.4.10-no-OFED.eb --robot
```

- **downloads** all required sources (best effort)
- **builds/installs** *goolf* toolchain (be patient) + HPL with it

  goolf: GCC, OpenMPI, LAPACK, OpenBLAS, FFTW, ScaLAPACK
- **generates module file** for each software package
- default: source/build/install dir in `$HOME/.local/easybuild`

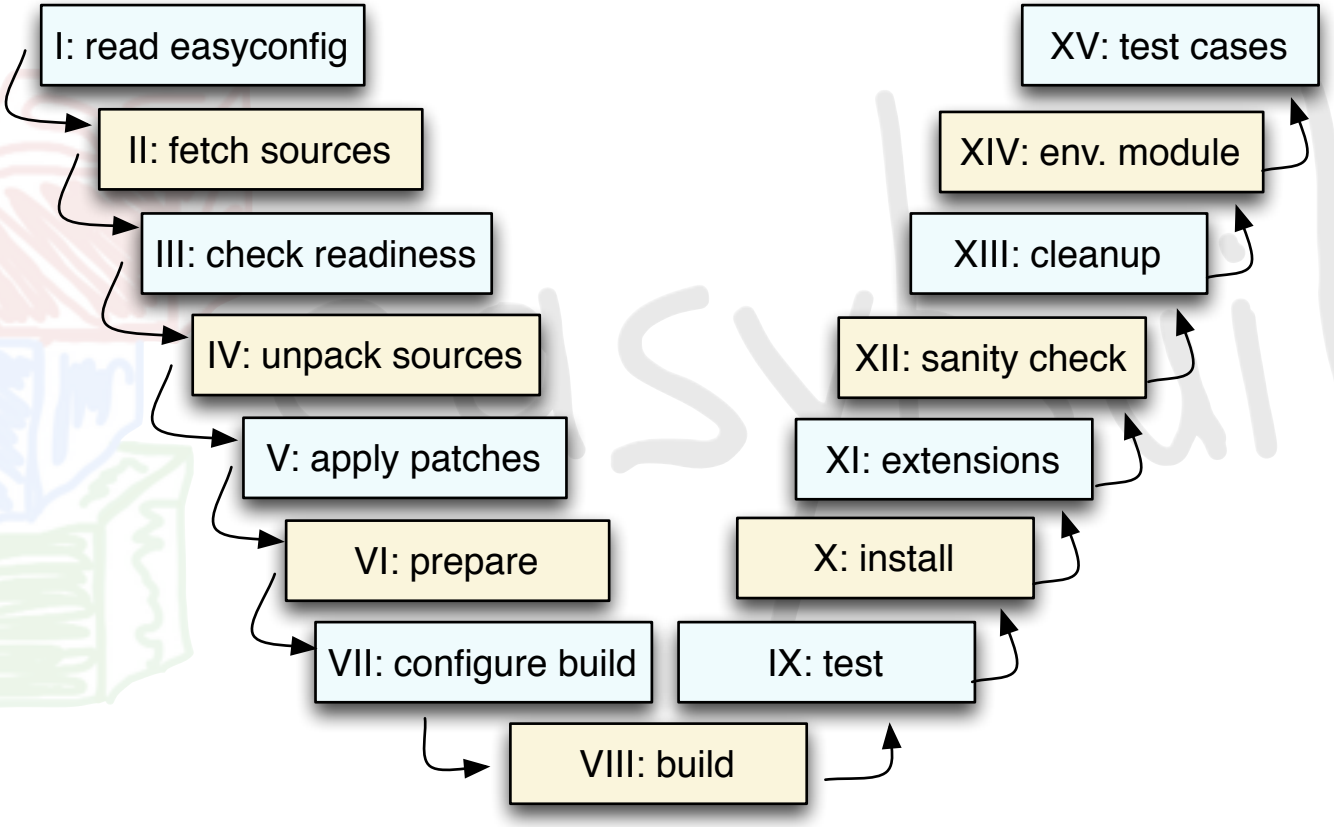
  can be changed by configuring EasyBuild differently

Some terminology

- **framework**
  - core of EasyBuild: Python packages & modules, *eb* wrapper script
  - provides (lots of) supporting functionality
- **easyblock**
  - a Python module implementing a particular build procedure
  - can be generic (e.g., make & cp) or software-specific (e.g., WRF)
  - talks to framework API, can be viewed as a ‘plugin’
- **easyconfig (file)**
  - text file with build specifications
  - supplied to EasyBuild, either directly or via ‘robot’ (for dependencies)
  - new easyconfigs with slightly different specs can be *generated*
- **compiler toolchain**
  - collection of compilers & libraries for building software with
  - usually C/C++/Fortran compilers + libs for MPI, BLAS, LAPACK, FFT
  - EasyBuild will define build environment for used toolchain ($CC, …)

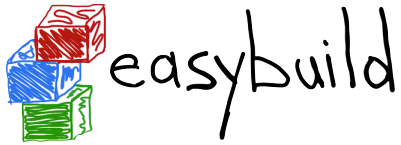
Step-wise install procedure

build and install procedure as implemented by EasyBuild



most of these steps can be customised if required,

via *easyconfig parameters* or a *custom easyblock*



List of supported software (v1.13.0)

483 different software packages (2,501 example easyconfigs)

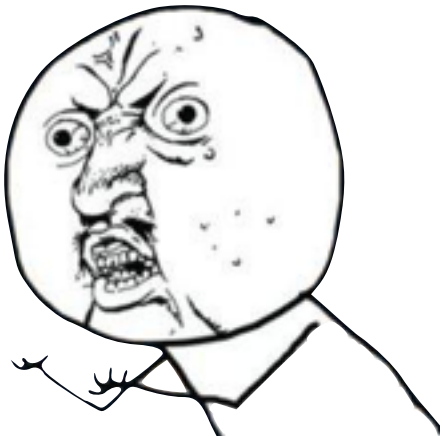
a2ps ABAQUS ABINIT ABySS ACML **ALADIN** Allinea ALLPATHS-LG AMOS AnalyzeFMRI ant APBS ARB argtable aria2 Armadillo arpack-ng ASE ATLAS Autoconf Automake bam2fastq BamTools Bash BayesTraits bbcp bbFTP bbftpPRO bc beagle-lib BEDTools BFAST binutils BioPerl Biopython BiSearch Bison BitSeq BLACS BLAST BLAT BOINC Bonnie++ Boost Bowtie Bowtie2 BWA byacc bzip2 cairo CAP3 CBLAS ccache CCfits CD-HIT CDO CEM CFITSIO cflow CGAL cgdb Chapel CHARMM Clang CLHEP CLooG Clustal-Omega ClustalW2 CMake Coreutils Corkscrew **CP2K** CPLEX CRF++ Cube CUDA Cufflinks cURL cutadapt CVS CVXOPT Cython DB Diffutils DL_POLY_Classic Docutils **DOLFIN** Doxygen **EasyBuild** ECore ed Eigen ELinks ELPA EMBOSS EPD ErlangOTP ESMF ESPResSo expat eXpress FASTA fastahack FASTX-Toolkit FCM FDTD_Solutions Ferret FFC FFTW FIAT file findutils fixesproto flex FLTK FLUENT fmri FoldX fontconfig FRC_align freeglut FreeSurfer freetype FSL g2clib g2lib GATE GATK gawk GCC gcccuda GDAL GDB Geant4 GEMSTAT GenomeAnalysisTK GEOS gettext GHC Ghostscript GIMPS git GLib GLIMMER GLPK glproto GMAP GMP GMT gnuplot gnutls Go google-sparsehash GPAW gperf gperftools Greenlet grep grib_api GROMACS GSL GTI guile gzip h4toh5 h5py h5utils Harminv HDF HDF5 HH-suite HMMER horton HPL HTSeq hwloc Hypre icc ifort imake imkl impi Infernal inputproto Inspector Instant Iperf ipp IPython IsoInfer ispc itac Jansson JasPer Java Jellyfish Jinja2 JUnit kbproto LAPACK less lftp libcircle libctl libdrm libffi libgtextutils libharu libibmad libibumad libibverbs libICE libidn Libint libint2 libjpeg-turbo libmatheval libpciaccess libpng libpthread-stubs libreadline libSM libsmm LIBSVM LibTIFF libtool libungif libunistring libunwind libX11 libXau libXaw libxc libxcb libXext libXfixes libXi libxml2 libXmu libXp libXpm libxslt libXt libyaml likwid Lmod Lua LWM2 lxml lynx LZO M4 MAFFT make makedepend Maple MariaDB Mathematica MATLAB matplotlib mc MCL mcpp MDP Meep MEME Mercurial Mesa Mesquite MetaVelvet METIS MMSEQ Molden Molekel molmod Mothur motif MPFR mpi4py mpiBLAST MPICH MPICH2 MrBayes MTL4 MUMmer MUMPS MUSCLE MUST MUSTANG MVAPICH2 nano NASM NCBI-Toolkit ncdf4 **NCL** ncurses NEdit netaddr netCDF netCDF-C++ netCDF-Fortran netcdf4-python netifaces netloc nettle **NEURON** nodejs ns numactl numexpr numpy NWChem O2scl Oases OCaml Oger OPARI2 OpenBabel OpenBLAS **OpenFOAM OpenFOAM-Extend** OpenIFS OpenMPI OpenPGM OpenSSL ORCA orthomcl otcl OTF OTF2 packmol PAML pandas PANDAseq PAPI parallel Paraview ParFlow ParMETIS ParMGridGen Pasha patch paycheck PCC PCRE PDT Perl PETSc petsc4py phonopy PhyML picard pixman pkg-config PLINK PnMPI popt PP PRACE Primer3 printproto problog protobuf pscom PSI psmpi2 PyQuante pysqlite pyTables **Python** python-dateutil python-meep PyYAML PyZMQ QLogicMPI Qt qtop QuadProg++ **QuantumESPRESSO** R RAxML RCS RNAz ROOT Rosetta rSeq RSEQtools Ruby Sablotron SAMtools ScaLAPACK Scalasca ScientificPython scikit-learn scipy SCons SCOOP Score-P SCOTCH SDCC sed segemehl setuptools Shapely SHRiMP sickle Silo slalib-c SLEPc SOAPdenovo SOAPdenovo2 SOAPec Sphinx SQLite SRA-Tookit Stacks Stow Stride SuiteSparse SURF SWIG sympy Szip TAMkin Tar tbb TCC Tcl tclcl tcsh Tesla-Deployment-Kit texinfo Theano TiCCutils TiMBL TinySVM Tk TopHat Tornado TotalView TREE-PUZZLE **Trilinos** Trinity UDUNITS UFC UFL util-linux Valgrind VCFtools Velvet ViennaRNA Vim Viper vsc-base vsc-mympirun vsc-mympirun-scoop vsc-processcontrol VSC-tools VTK VTune **WIEN2k** wiki2beamer **WPS WRF** xbitmaps xcb-proto XCrySDen xextproto XML XML-LibXML XML-Simple xorg-macros xproto xtrans XZ yaff YamCha YAML-Syck Yasm ZeroMQ zlib zsh zsync

Installing EasyBuild

https://github.com/hpcugent/easybuild/wiki/Installing-EasyBuild

Using Python install tools (there be dragons here!):

```
mkdir -p /tmp/lib/python/2.7/site-packages

export PYTHONPATH=/tmp/lib/python/2.7/site-packages:$PYTHONPATH

easy_install --prefix=/tmp easybuild  # don't use --user, it's
   evil

export PATH=/tmp/bin
```



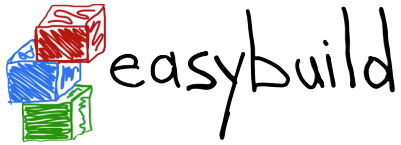
Installing EasyBuild

https://github.com/hpcugent/easybuild/wiki/Installing-EasyBuild

By cloning the EasyBuild repositories (development setup):

```
cd /tmp

git clone https://github.com/hpcugent/easybuild-framework.git

git clone https://github.com/hpcugent/easybuild-easyblocks.git

git clone https://github.com/hpcugent/easybuild-easyconfigs.git

export PYTHONPATH=/tmp/easybuild-easyconfigs:/tmp/easybuild-
  easyblocks:/tmp/easybuild-framework:$PYTHONPATH

export PATH=/tmp/bin:$PATH
```

This avoids Python trickery, but shouldn't be a production setup.



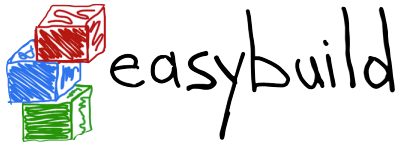
Installing EasyBuild

https://github.com/hpcugent/easybuild/wiki/Bootstrapping-EasyBuild

Using the bootstrap script (highly recommended):

```
wget https://raw.github.com/hpcugent/easybuild-framework/develop/
   easybuild/scripts/bootstrap_eb.py

python bootstrap_eb.py /tmp  # specify your install prefix

export MODULEPATH=/tmp/modules/all:$MODULEPATH

module load EasyBuild
```

If this doesn't work, let us know!



Configuring EasyBuild

https://github.com/hpcugent/easybuild/wiki/Configuration

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

You *should* configure EasyBuild to your preferences, using:

- **configuration files** (key-value lines, text files)
- **environment variables** (e.g. `$EASYBUILD_BUILDPATH`)
- **command line parameters** (e.g. `--buildpath`)

Consistency across these options is *guaranteed (see `eb --help | tail`)*

Different options in order of preference: cmdline, env vars, config file

`eb –buildpath` overrules `$EASYBUILD_BUILDPATH`,

`$EASYBUILD_BUILDPATH` overrules `buildpath` in configuration file

First steps with *eb*

installing EasyBuild with EasyBuild:

```
eb EasyBuild-1.5.0.eb
module load EasyBuild/1.5.0
```

Building & installing bzip2 with dummy toolchain (system compiler):

```
eb --software-name=bzip2 --toolchain-name=dummy
```

Install *goolf* compiler toolchain (be patient):

```
eb goolf-1.4.10-no-OFED.eb --robot # no-OFED indicates no IB support
```

Install gzip v1.6 with goolf toolchain, log with debug info to stdout:

```
eb gzip-1.6-goolf-1.4.10-no-OFED.eb -ld
```

EasyBuild command line

eb --help

eb -a

eb bzip2-1.0.6.eb -ldr

eb --dry-run

eb --list-toolchains

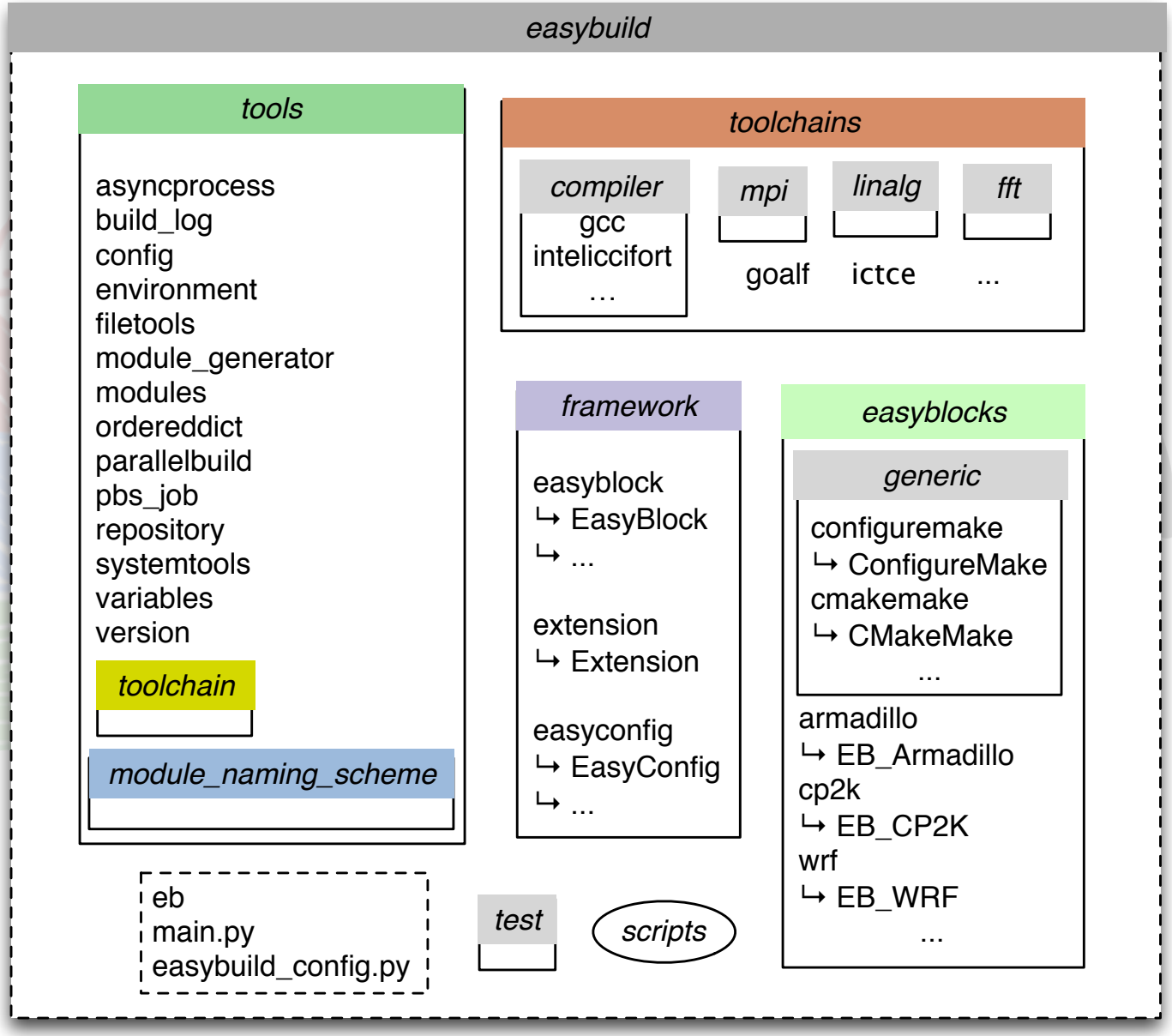
eb bzip2-1.0.6.eb --try-toolchain=ictce,6.2.5 --robot

eb -S, eb --search

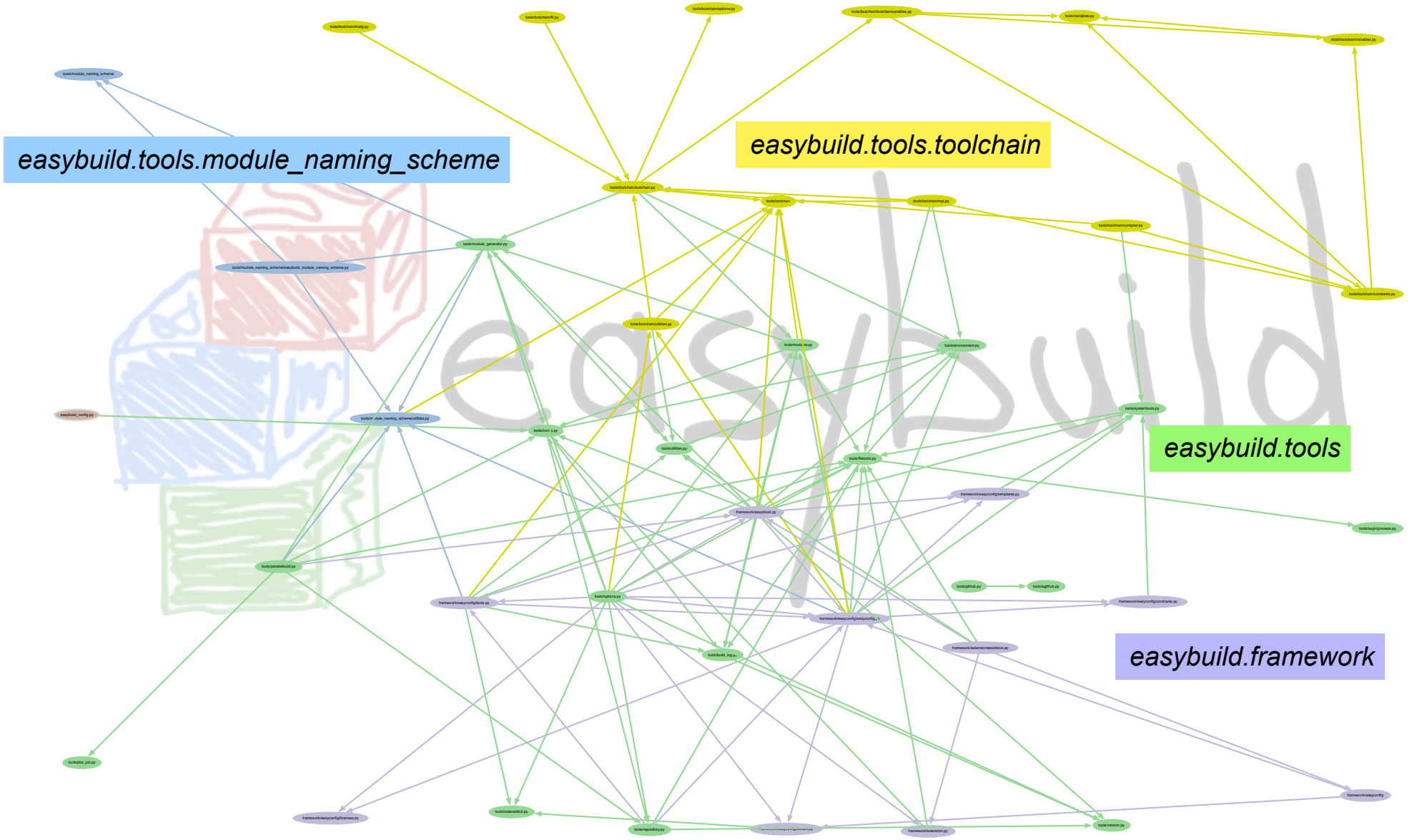
eb --from-pr

eb --from-pr --upload-test-report —github-user=boegel

High-level design (framework)



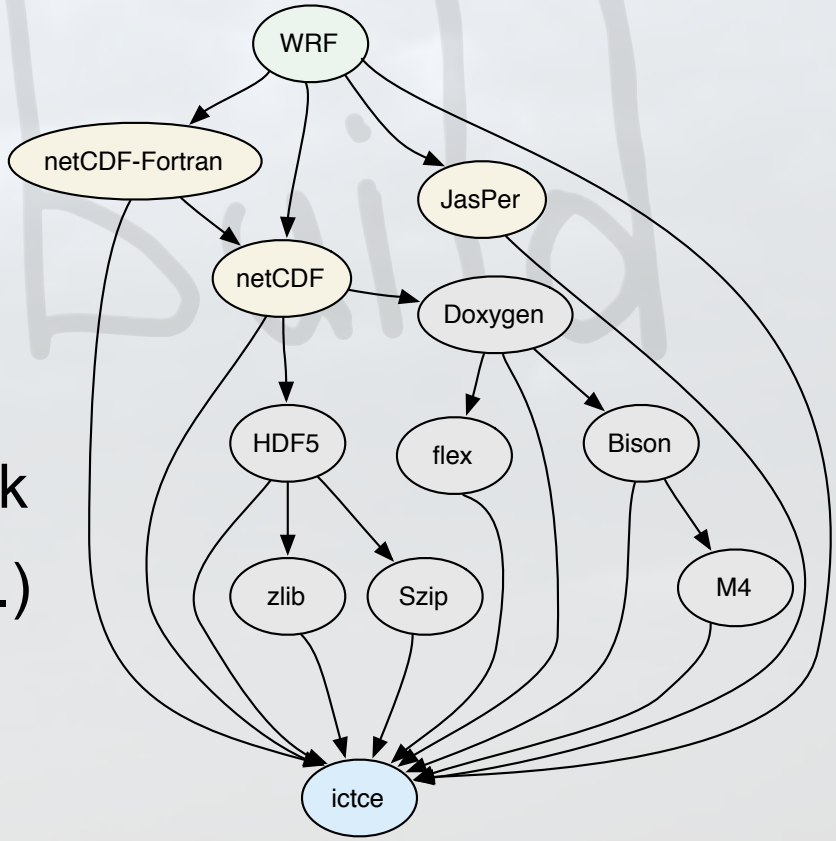
High-level design (framework)



Use case: building WRF

*building and installing **WRF** (Weather Research and Forecasting Model)*

- *http://www.wrf-model.org*
- complex(ish) **dependency graph**
- *very* **non-standard build procedure**
  - interactive `configure` script (!)
  - resulting `configure.wrf` needs work
    (hardcoding, tweaking of options, ...)
  - `compile` script (wraps around `make`)
  - no actual installation step



Use case: building WRF with *eb*

*building and installing **WRF** (Weather Research and Forecasting Model)*

- easyblock that comes with EasyBuild implements build procedure
  - running interactive `configure` script **autonomously**
  - **patching** configure.wrf
  - **building** with `compile` script
  - **testing** build with standard included tests/benchmarks
- easyconfig files for different versions, toolchains, build options, ...
- building and installing WRF becomes child's play, for example:

```
eb --software=WRF,3.4 --toolchain-name=ictce --robot
```

Use case: easyblock for WRF

part I: imports, class constructor, custom easyconfig parameter

```
1  import fileinput, os, re, sys
2
3  import easybuild.tools.environment as env
4  from easybuild.easyblocks.netcdf import set_netcdf_env_vars
5  from easybuild.framework.easyblock import EasyBlock
6  from easybuild.framework.easyconfig import MANDATORY
7  from easybuild.tools.filetools import patch_perl_script_autoflush, run_cmd, run_cmd_qa
8  from easybuild.tools.modules import get_software_root
9
10 class EB_WRF(EasyBlock):
11
12   def __init__(self, *args, **kwargs):
13     super(EB_WRF, self).__init__(*args, **kwargs)
14     self.build_in_installdir = True
15
16   @staticmethod
17   def extra_options():
18     extra_vars = [('buildtype', [None, "Type of build (e.g., dmpar, dm+sm).", MANDATORY])]
19     return EasyBlock.extra_options(extra_vars)
20
21   def configure_step(self):
22     # prepare to configure
23     set_netcdf_env_vars(self.log)
24
```

import required functionality

class definition

class constructor, specify building in installation dir

define custom easyconfig parameters

Use case: easyblock for WRF

part II: configuration (1/2)

```
21  def configure_step(self):
22    # prepare to configure
23    set_netcdf_env_vars(self.log)
24
25    jasper = get_software_root('JasPer')
26    if jasper:
27      jasperlibdir = os.path.join(jasper, "lib")
28      env.setvar('JASPERINC', os.path.join(jasper, "include"))
29      env.setvar('JASPERLIB', jasperlibdir)
30
31    env.setvar('WRFIO_NCD_LARGE_FILE_SUPPORT', '1')
32
33    patch_perl_script_autoflush(os.path.join("arch", "Config_new.pl"))
34
35    known_build_types = ['serial', 'smpar', 'dmpar', 'dm+sm']
36    self.parallel_build_types = ["dmpar", "smpar", "dm+sm"]
37    bt = self.cfg['buildtype']
38
39    if not bt in known_build_types:
40      self.log.error("Unknown build type: '%s' (supported: %s)" % (bt, known_build_types))
41
```

configuration step function

set environment variables for dependencies

set WRF-specific env var for build options

patch configure script to run it autonomously

check whether specified build type makes sense

Use case: easyblock for WRF

part II: configuration (2/2)

```
42      # run configure script
43      bt_option = "Linux x86_64 i486 i586 i686, ifort compiler with icc"
44      bt_question = "\s*(?P<nr>[0-9]+).\s*%s\s*\(%s\)" % (bt_option, bt)
45
46      cmd = "./configure"
47      qa = {"(1=basic, 2=preset moves, 3=vortex following) [default 1]:": "1",
48            "(0=no nesting, 1=basic, 2=preset moves, 3=vortex following) [default 0]:": "0"}
49      std_qa = {r"%s.*\n(.*\n)*Enter selection\s*\[[0-9]+-[0-9]+\]\s*:" % bt_question: "%(nr)s"}
50
51      run_cmd_qa(cmd, qa, no_qa=[], std_qa=std_qa, log_all=True, simple=True)
52
53      # patch configure.wrf
54      cfgfile = 'configure.wrf'
55
56      comps = {
57               'SCC': os.getenv('CC'), 'SFC': os.getenv('F90'),
58               'CCOMP': os.getenv('CC'), 'DM_FC': os.getenv('MPIF90'),
59               'DM_CC': "%s -DMPI2_SUPPORT" % os.getenv('MPICC'),
60              }
61
62      for line in fileinput.input(cfgfile, inplace=1, backup='.orig.comps'):
63          for (k, v) in comps.items():
64              line = re.sub(r"^(%s\s*=\s*).*$" % k, r"\1 %s" % v, line)
65          sys.stdout.write(line)
66
```

prepare Q&A for configuring

run configure script autonomously

patch generated configuration file

Use case: easyblock for WRF

part III: build step & skip install step (since there is none)

build step function

```
67  def build_step(self):
68    # build WRF using the compile script
69    par = self.cfg['parallel']
70    cmd = "./compile -j %d wrf" % par
71    run_cmd(cmd, log_all=True, simple=True, log_output=True)
72
73    # build two test cases to produce ideal.exe and real.exe
74    for test in ["em_real", "em_b_wave"]:
75        cmd = "./compile -j %d %s" % (par, test)
76        run_cmd(cmd, log_all=True, simple=True, log_output=True)
77
78  def install_step(self):
79    pass
80
```

build WRF (in parallel)

build WRF utilities as well

no actual installation step (build in installation dir)

Use case: installing WRF

specify build details in easyconfig file (.eb)

software name and version

compiler toolchain specification and options

custom parameter for WRF

```
1  name = 'WRF'
2  version = '3.4'
3
4  homepage = 'http://www.wrf-model.org'
5  description = 'Weather Research and Forecasting'
6
7  toolchain = {'name': 'ictce','version': '5.3.0'}
8  toolchainopts = {'opt': False}  # no -O2
9
10 sources = ['%sV%s.TAR.gz' % (name, version)]
11 patches = ['WRF_parallel_build_fix.patch',
12            'WRF-%(version)s_known_problems.patch',
13            'WRF_tests_limit-runtimes.patch',
14            'WRF_netCDF-Fortran_separate_path.patch']
15
16 dependencies = [('JasPer', '1.900.1'),
17                 ('netCDF', '4.2.1.1'),
18                 ('netCDF-Fortran', '4.2')]
19
20 buildtype = 'dmpar'
```

software website and description (informative)

list of source files

list of patches for sources

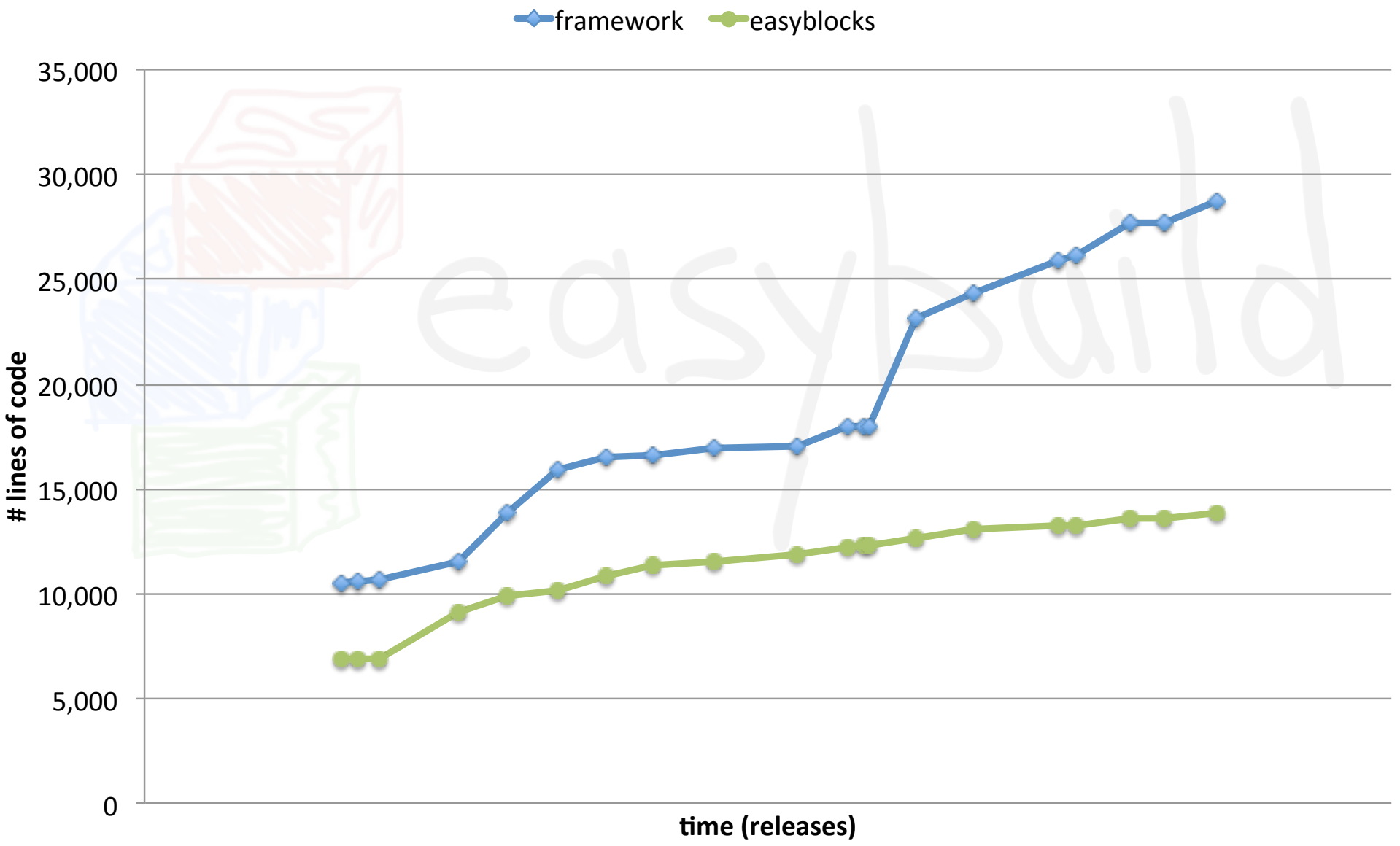
list of dependencies

```
eb WRF-3.4-ictce-5.3.0-dmpar.eb --robot
```

Growth: codebase

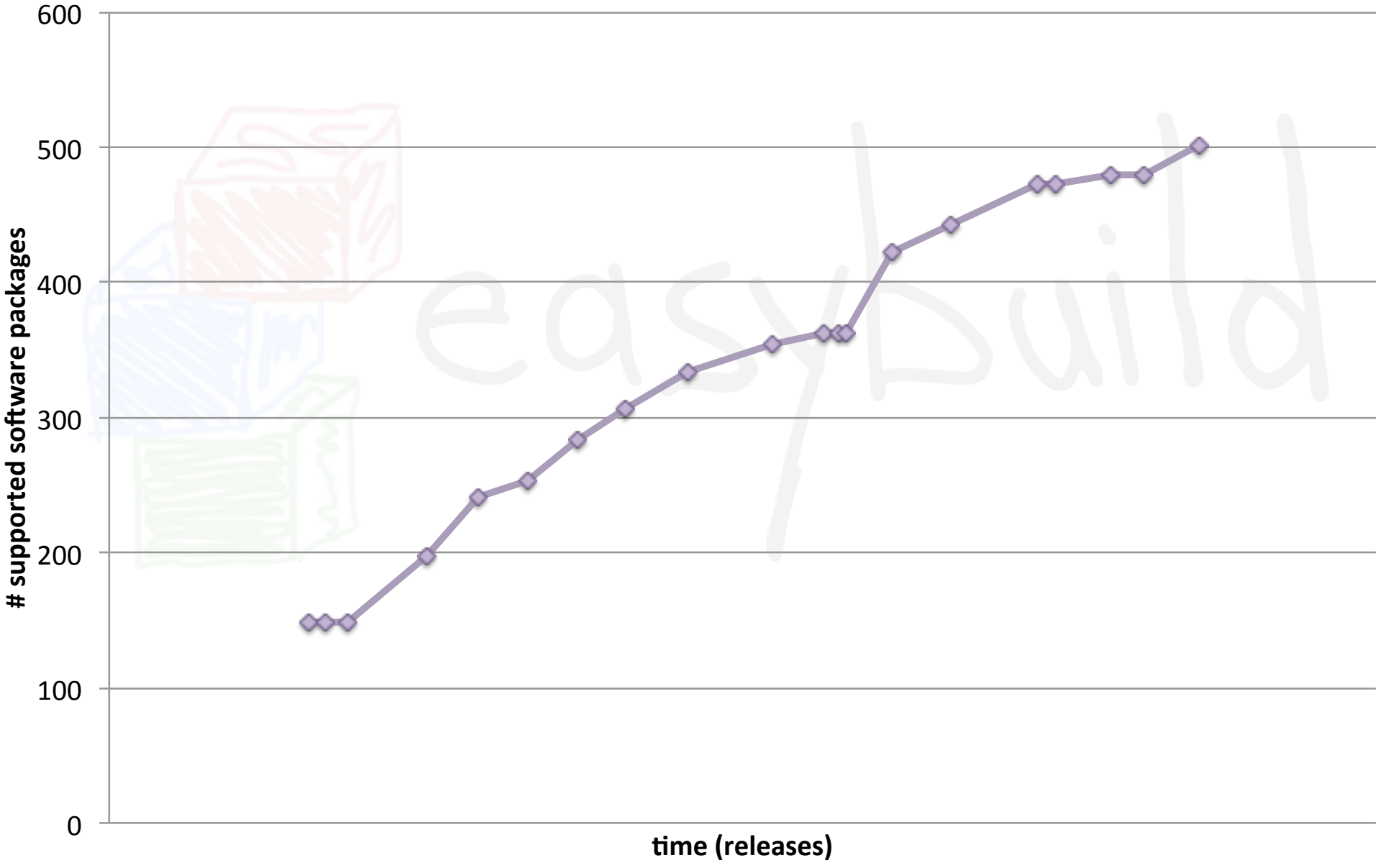
 # lines of code

```
find . -name '*.py' | xargs cat | egrep -v '^#|^[ ]*$' | wc -l
```



Growth: supported software

 # supported software packages (incl. toolchains)



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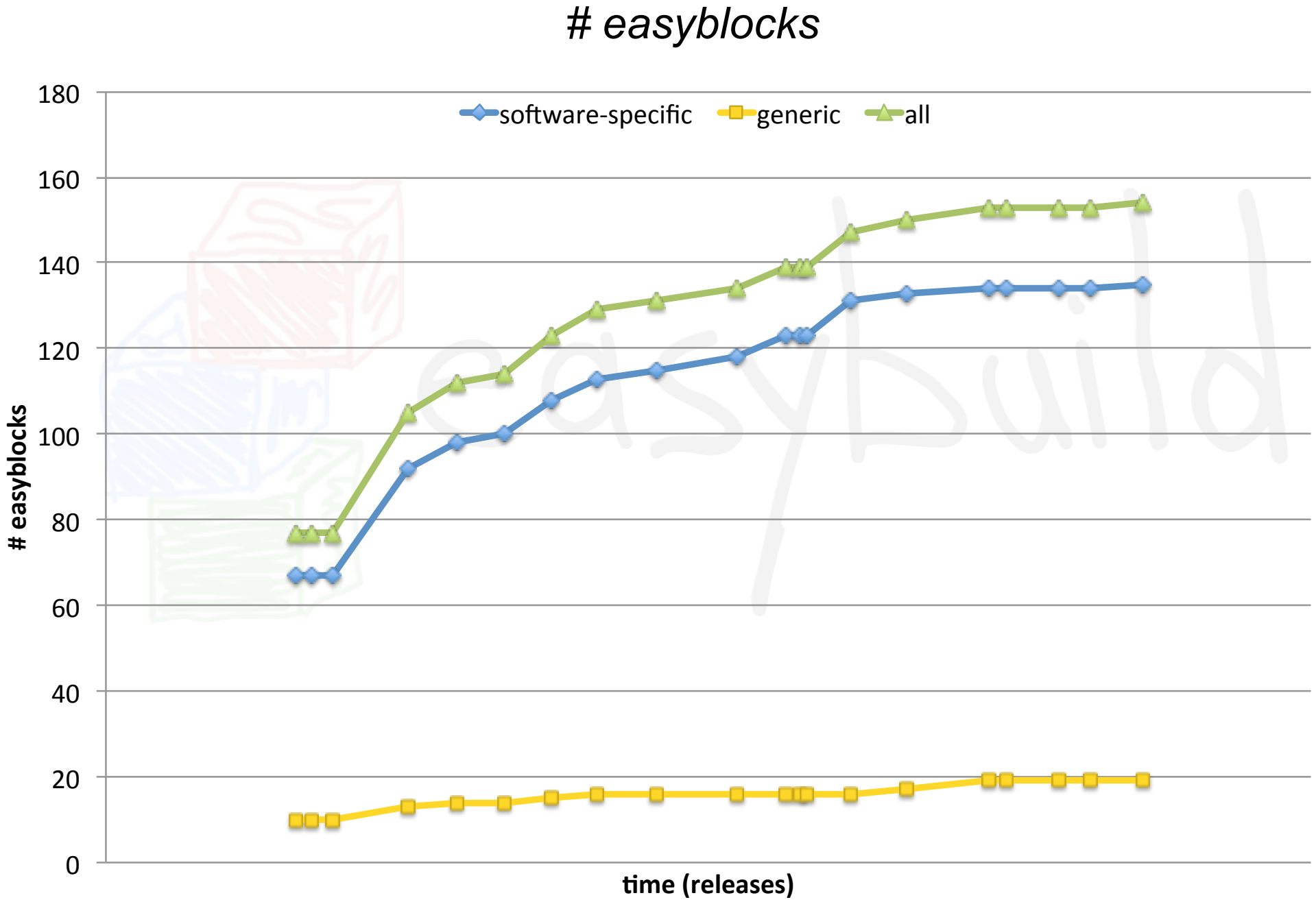
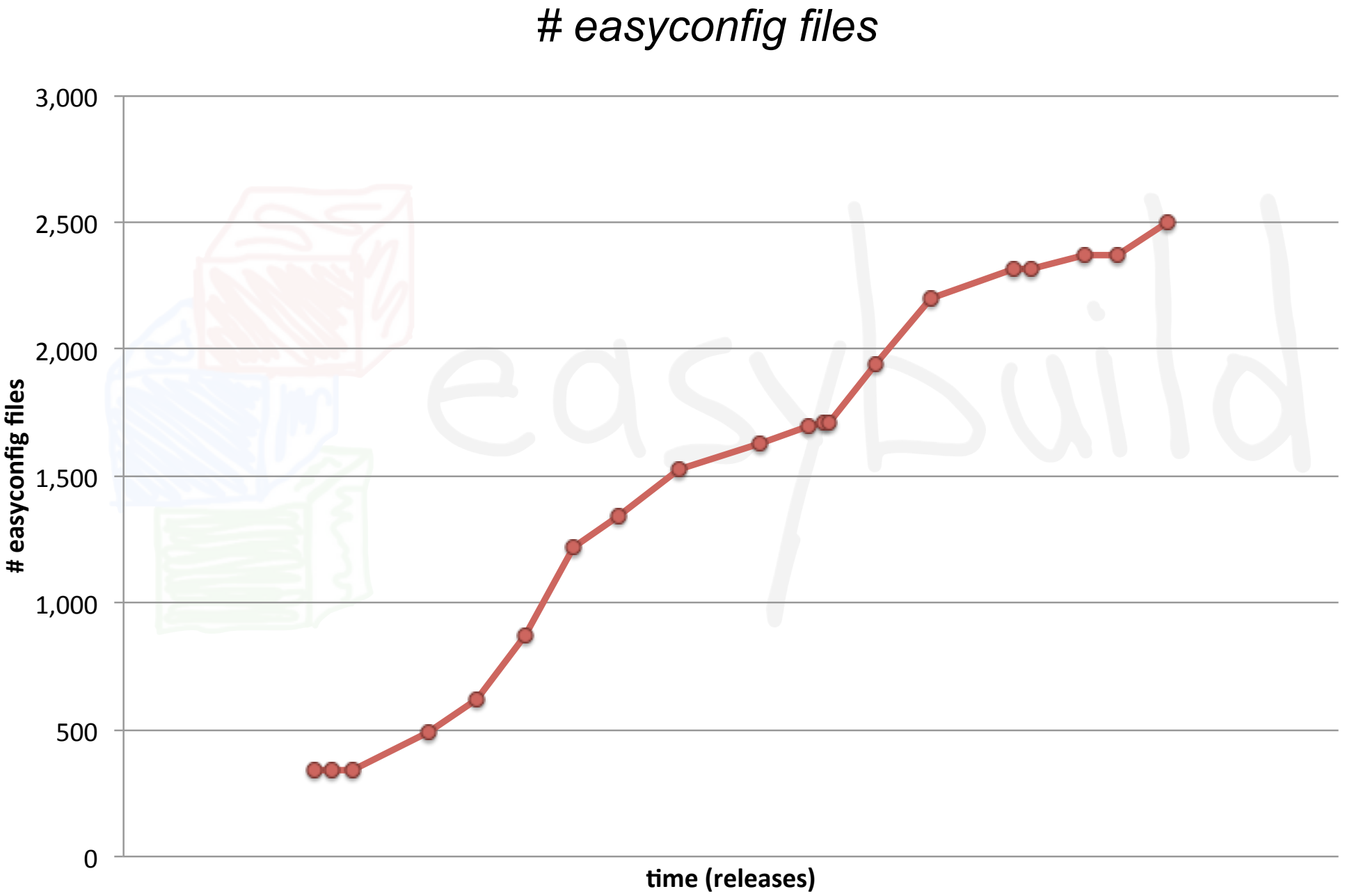
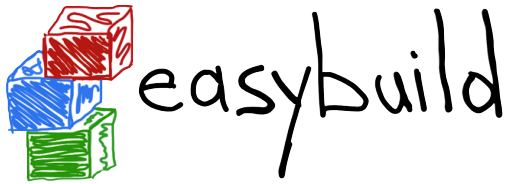


Growth: supported software





Growth: community

EasyBuild community is growing slowly but steadily:

- Ghent University (HPC-UGent & users)
- K.U. Leuven, Antwerp Univ., Hasselt Univ. (VSC members)
- University of Luxembourg
- Gregor Mendel Institute (Austria)
- The Cyprus Institute
- University of Basel (Switzerland)
- Jülich Supercomputer Centre (Germany)
- Bayer (Germany)
- University of Auckland (New Zealand)
- NVIDIA Corp.
- Kiev Polytechnic Institute (NTTU, Ukraine)
- Idaho National Lab (US)
- Pacific Northwest National Lab (US)
- UC Davis (US)
- ...

easybuild

building software with ease

Do you want to know more?

website: *http://hpcugent.github.com/easybuild*

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

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

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

Twitter: *@easy_build*

IRC: *#easybuild on freenode.net*

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6th EasyBuild hackathon @ Vienna, Austria

June 18th 2014

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