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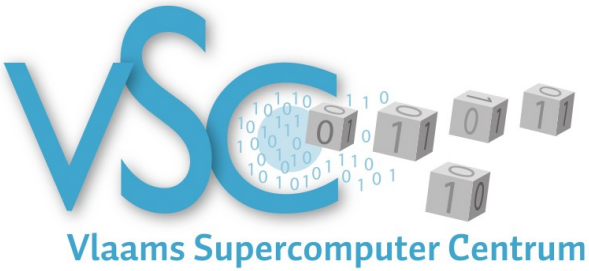

Getting Scientific Software Installed
HPC Knowledge Meeting '14 @ Barcelona, Spain
Jan 14th 2014

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HPC-UGent @ Ghent University, Belgium

- central contact for High Performance Computing at university
- established in 2008, part of central IT department (DICT)
- member of Flemish Supercomputer Centre (VSC)
  - collaboration between Flemish university associations

Vlaams Supercomputer Centrum

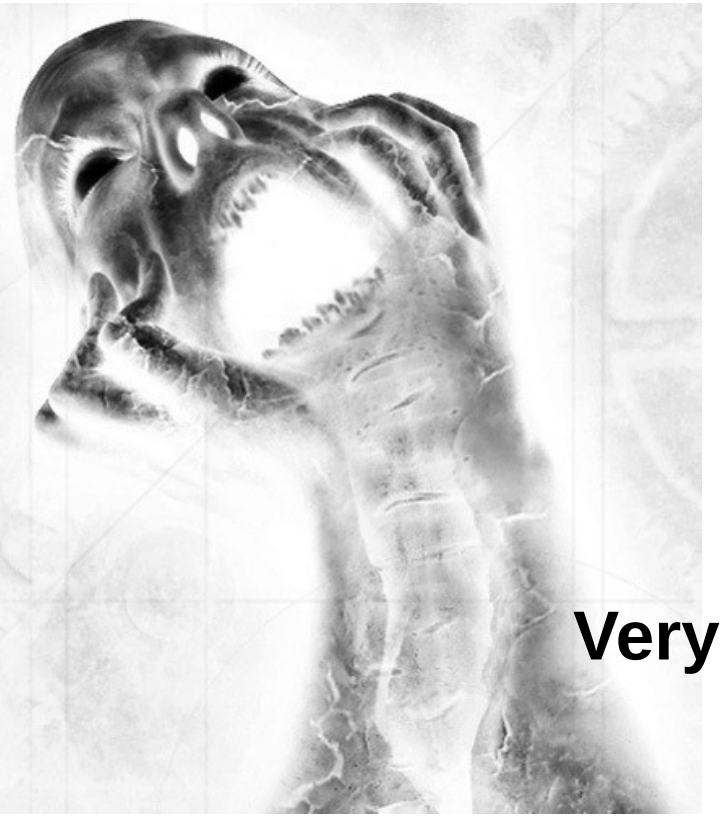
- our computing infrastructure:
  - seven Tier 2 systems (capacity computing)
  - one Tier 1 system

    #119 in Top500 (June'12), currently at #306
- HPC-UGent team currently consists of 8 FTEs
  - system administration of HPC infrastructure
    - top-down for Tier2 systems: hardware, configuration, user support
    - Tier1: owned by UGent, setup together with HP, user support
  - user support and training
    - EasyBuild grew out of need from this
  - convincing groups to switch to central infrastructure

Building scientific software is... fun!

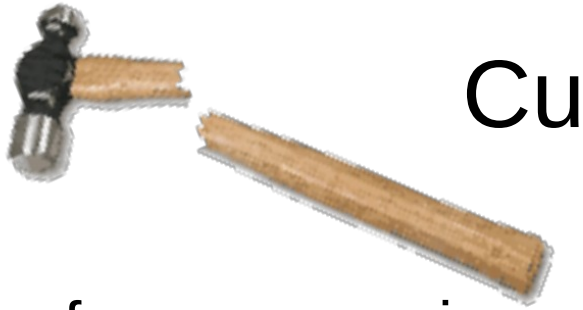
Scientists focus on the *functionality* of their software,
not on portability, build system, ...

Common **issues** with build procedures of scientific software:



- **incomplete**, e.g. no install step
- requiring human **interaction**
- heavily **customised** and **non-standard**
- uses **hard-coded** settings
- poor and/or outdated **documentation**

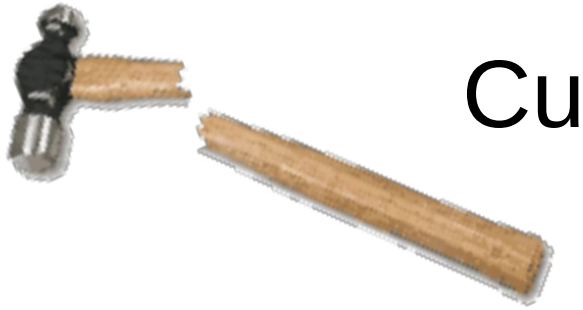
Very time-consuming for user support teams!



Current tools are lacking

- building from **source** is preferred in an HPC environment
  - **performance** is critical, instruction selection is key (e.g. AVX)
- existing build tools are
  - hard to **maintain** (e.g., bash scripts)
  - stand-alone, **no reuse** of previous efforts
  - **OS-dependent** (HomeBrew, *Ports, ...)
  - **custom** to (groups of) software packages

    e.g., Dorsal (DOLFIN), gmkpack (ALADIN)

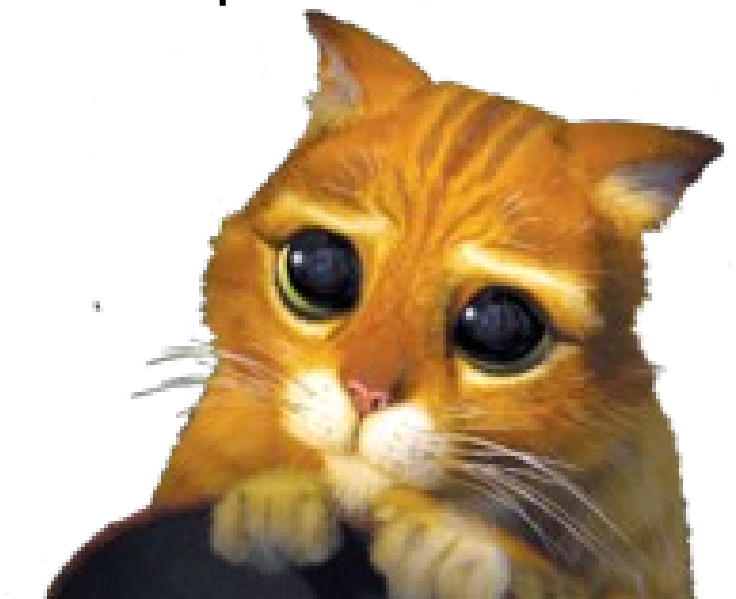


Current tools are lacking

- not a lot of packaged scientific software available (RPMs, ...)
  - requires **huge effort,** which is duplicated across distros
- Hard to install multiple versions of a program
  - version
  - Compiler (intel / gcc / clang)
  - Mpi stack (openmpi, intel mpi, mpich)
  - Math kernel (Atlas, Openblas, Gotoblas, IMKL)

Our build tool wish list

- **flexible** framework
- allows for **reproducible** builds
- supports **co-existence** of versions/builds
- enables **sharing** of build procedure implementations
- fully **automates** builds
- **dependency** resolution



Building software with ease

a software build and installation framework

- written in **Python**
- developed in-house for 2.5 years before public release
- **open-source (GPLv2)** since April 2012
- EasyBuild v1.0: **stable API** (November 2012)
- **monthly releases** (latest: v1.10, Dec 24th 2013)
- continuously enhanced and extended
- *http://hpcugent.github.io/easybuild*

‘Quick’ demo for the impatient

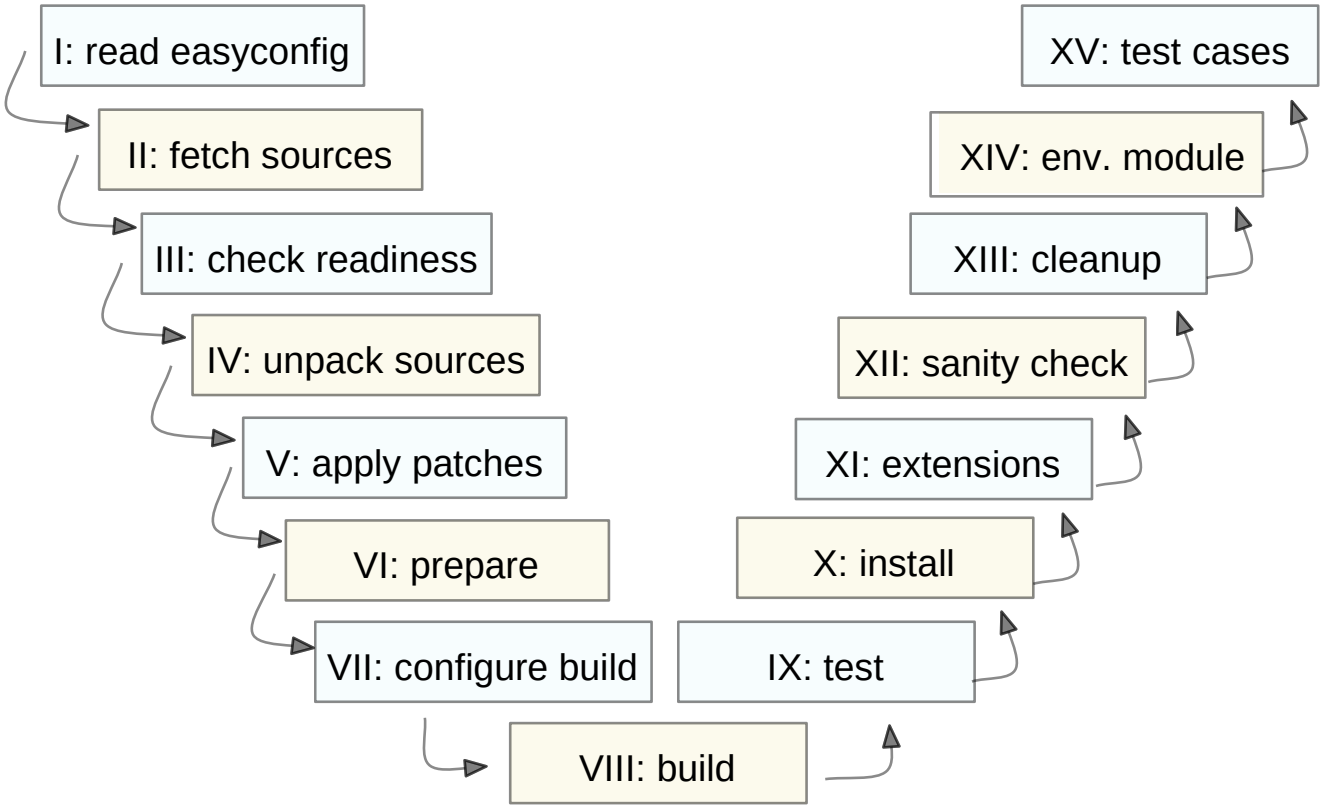
```
eb HPL-2.0-goolf-1.4.10.eb -r
```

- downloads all required sources (best effort)
- builds *goolf* toolchain (be patient), and builds HPL with it

  goolf: GCC, OpenMPI, OpenBlas, ScaLAPACK, FFTW
- Generates a module file
- default: source/build/install dir in `$HOME/.local/easybuild`

Step-wise install procedure

build and install procedure as implemented by EasyBuild



most of these steps can be customized if required

Features

- **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 stack of software with a single command, using `--robot`
- running **interactive** installers **autonomously**
  - by passing a Q&A Python dictionary to the `run_cmd_qa` function
- building software in **parallel**
  - e.g., on a (PBS) cluster, by using `--job`
- comprehensive **testing**: unit tests, regression testing

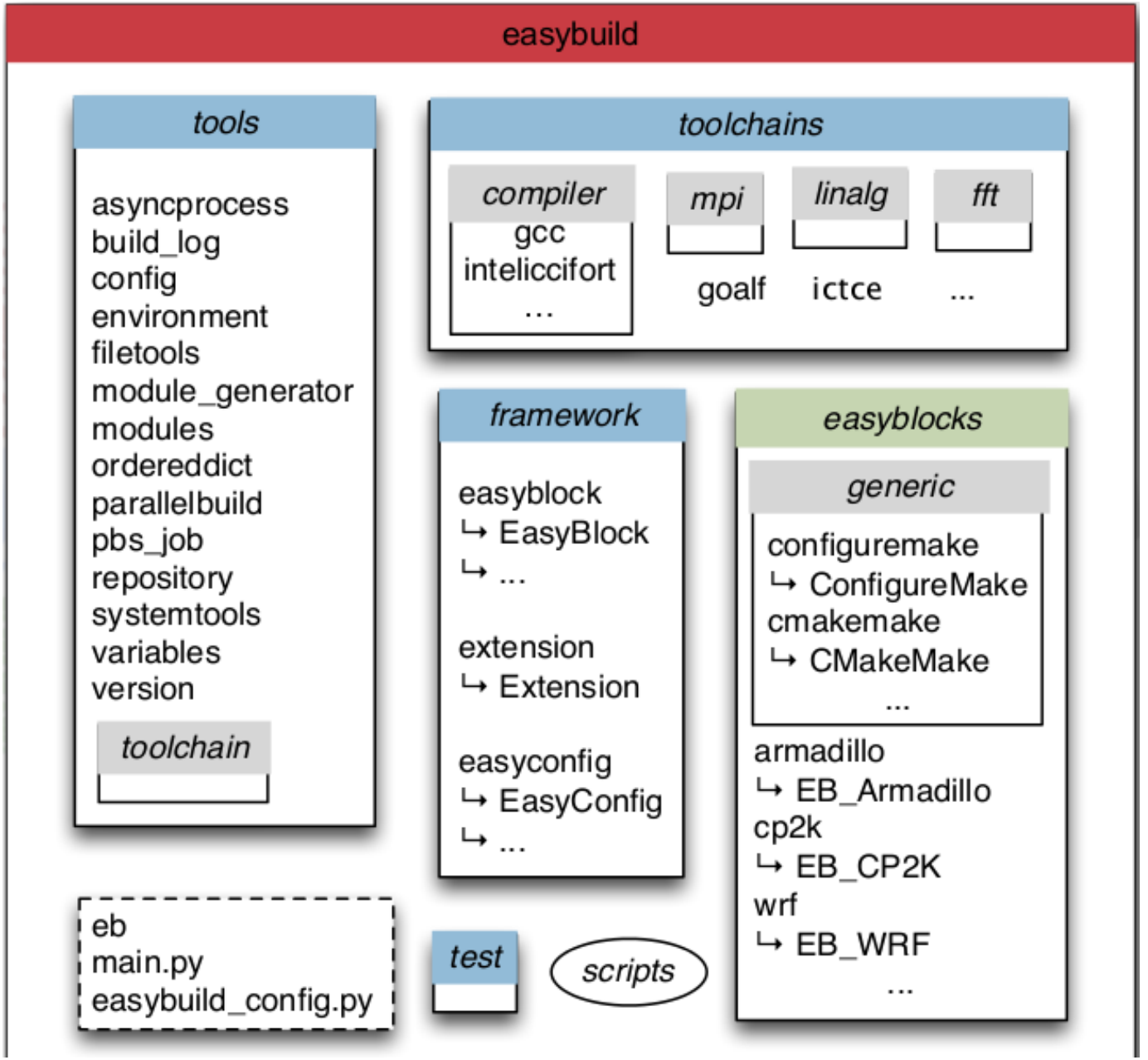
Supported Packages

- 443 packages build out of the box
- Over 3000 example (tested!) easyconfigs
- Including
  - ALADIN, CP2K, DOLFIN, OpenFOAM, NEURON, WPS, WRF

    QuantumESPRESSO, MWChem

a2ps ABAQUS ABINIT ABySS ACML ALADIN Allinea ALLPATHS-LG AMOS AnalyzeFMRI ant ARB aria2 Armadillo arpack-ng ASE ATLAS Autoconf Automake bam2fastq BamTools Bash bbcp bbFTP bbftpPRO beagle-lib BEDTools BFAST binutils biodeps BioPerl Biopython BiSearch Bison BLACS BLAST BLAT BOINC Bonnie++ Boost Bowtie Bowtie2 BWA byacc bzip2 cairo CAP3 CBLAS ccache CCfits CD-HIT CDO CFITSIO cflow CGAL cgdb cgmpich cgmpolf cgmvapich2 cgmvolf cgompi cgoolf Chapel CHARMM Clang ClangGCC CLHEP ClustalW2 CMake Corkscrew CP2K CPLEX CRF++ Cube CUDA Cufflinks cURL cutadapt CVXOPT Cython DB Diffutils DL_POLY_Classic Docutils DOLFIN Doxygen EasyBuild ECore ed Eigen ELinks EMBOSS EPD ErlangOTP ESMF ESPResSo expat FASTA fastahack FASTX-Toolkit FCM FDTD_Solutions Ferret FFC FFTW FIAT findutils fixesproto flex FLTK FLUENT fmri FoldX fontconfig FRC_align freeglut FreeSurfer freetype FSL g2clib g2lib GATE GATK gawk GCC gcccuda GDAL GDB Geant4 GenomeAnalysisTk GEOS gettext GHC Ghostscript GIMPS git GLib GLIMMER GLPK glproto gmacml GMP gmpich2 gmpolf gmvapich2 gmvolf gnuplot gnutls goalf gompi gompic google-sparsehash goolf goolfc GPAW gperf Greenlet grib_api GROMACS GSL GTI guile gzip h5py h5utils Harminv HDF HDF5 HH-suite HMMER horton HPCBIOS_Bioinfo HPCBIOS_Debuggers HPCBIOS_LifeSciences HPCBIOS_Math HPCBIOS_Profiler s HPL HTSeq hwloc Hypre icc iccifort ictce ifort iiqmpi imake imkl impi Infernal inputproto Inspector Instant iomkl Iperf ipp IPython iqacml itac Jansson JasPer Java Jinja2 JUnit kbproto LAPACK lftp likwid LWM2 lxml lynx LZO M4 make makedepend Maple MariaDB Mathematica MATLAB matplotlib mc MCL MDP Meep MEME Mercurial Mesa Mesquite MetaVelvet METIS Molden molmod Mothur motif MPFR mpi4py mpiBLAST MPICH MPICH2 MrBayes MTL4 MUMmer MUMPS MUSCLE MUST MVAPICH2 nano NASM NCBI-Toolkit ncdf4 NCL ncurses netCDF netCDF-C++ netCDF-Fortran netloc nettle NEURON ns numactl numexpr numpy NWChem O2scl Oases Oger OPARI2 OpenBabel OpenBLAS OpenFOAM OpenIFS OpenMPI OpenPGM OpenSSL ORCA orthomcl otcl OTF OTF2 packmol PAML pandas PANDAseq PAPI parallel Paraview ParFlow ParMETIS ParMGridGen Pasha paycheck PCC PCRE PDT Perl PETSc petsc4py phonopy picard pixman pkg-config PLINK PnMPI PP Primer3 printproto problog PSI PyQuante pysqlite pyTables Python python-meep PyYAML PyZMQ QLogicMPI Qt qtop QuantumESPRESSO R RAxML RCS RNAz ROOT Rosetta Sablotron SAMtools ScaLAPACK Scalasca ScientificPython scikit-learn scipy SCons SCOOP Score-P SCOTCH SDCC setuptools Shapely SHRiMP Silo SLEPc SOAPdenovo Sphinx SQLite Stacks Stow Stride SuiteSparse SURF SWIG sympy Szip TAMkin Tar tbb TCC Tcl tclcl tcsh Theano TiCCutils TiMBL TinySVM Tk TopHat Tornado TotalView Trilinos Trinity UDUNITS UFC UFL util-linux Valgrind Velvet ViennaRNA Viper VTK VTune WIEN2k wiki2beamer WPS WRF xbitmaps xcb-proto XCrySDen xextproto XML XML-LibXML XML-Simple xorg-macros xproto xtrans yaff YamCha YAML-Syck Yasm ZeroMQ zlib zsh zsync

EasyBuild: high-level design



Terminology

- **framework**
  - Python packages and modules forming *the core of EasyBuild*
  - provides (loads of) supporting functionality
  - very modular and dynamic design w.r.t. easyblocks, toolchains, ...
- **easyblock**
  - a Python module providing *implementation of a build procedure*
  - can be generic or software-specific
- **easyconfig file (.eb)**
  - *build specification*:

    software name/version, toolchain, build options, ...
  - simple text files, Python syntax

High-level design: easyblocks

- **build procedure implementations**
- modular design, dynamically extensible
  - add your easyblock in the Python search path
  - EasyBuild will pick it up
- object-oriented scheme
  - subclass from existing easyblocks or abstract class *EasyBlock*

High-level design: easyblocks

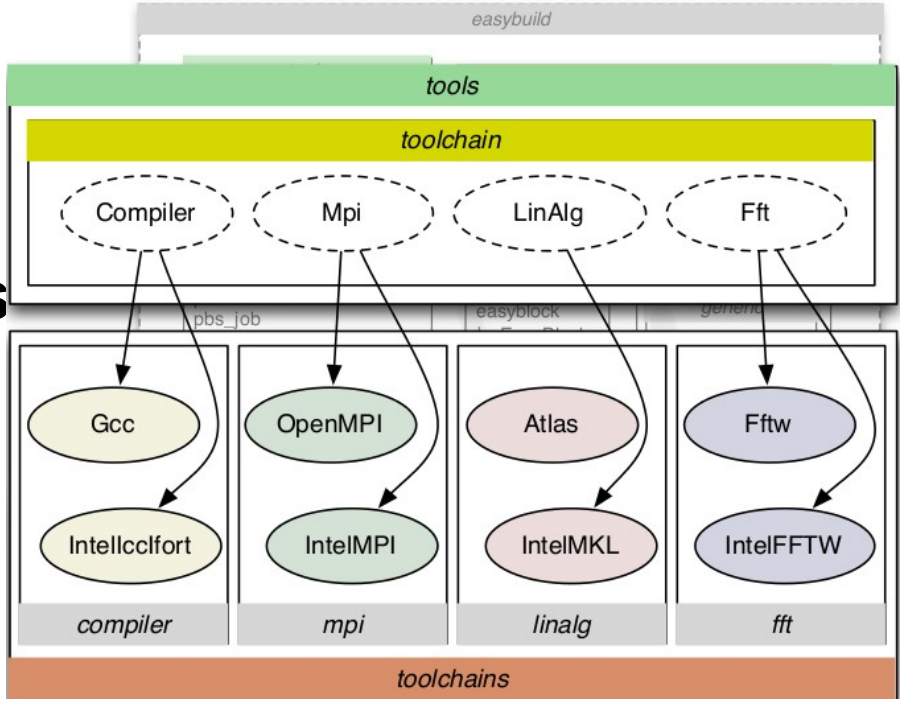
- **build procedure implementations**
- *easyblocks.generic*: **generic easyblocks**
  - custom support for groups of applications
  - e.g., *ConfigureMake*, *CMakeMake*, ...
- *easyblocks*: **application-specific easyblocks**

High-level design: framework

tools package

- **supporting functionality**, e.g.:
  - `run_cmd` for shell commands
  - `run_cmd_qa` for interactive commands
  - `extract_file` for unpacking
  - `apply_patch` for patching
- *tools.toolchain* package for compiler toolchains
- *tools.module_naming_scheme* for module naming schemes

High-level design: framework



toolchains package

- support for **compiler toolchains**
- relies on *tools.toolchain*
- toolchains are defined in here
- organized in subpackages:
  - *toolchains.compiler*
  - *toolchains.mpi*
  - *toolchains.linalg* (BLAS, LAPACK, ...)
  - *toolchains.fft*
- very modular design for allowing extensibility
- plug in a Python module for compiler/library to extend it

High-level design: framework

module_naming_scheme package

- support for **custom module naming schemes**
- Flat vs tree
  - e.g.: always prefix compiler/toolchain
- define your module naming scheme
  - EasyBuild picks up any scheme following the specifications
  - see *“Using a custom module naming scheme”* wiki page
- our naming scheme: *EasyBuildModuleNamingScheme*
- available since EasyBuild v1.8.0, with limited capabilities
  - only *name*, *version*, *versionsuffix* and *toolchain* available

High-level design: framework

test package

- unit testing of EasyBuild

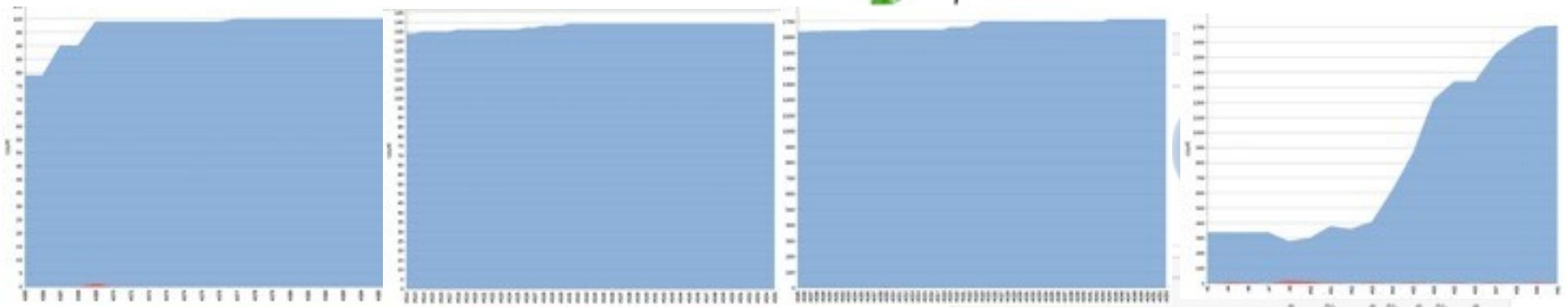
```
python -m test.framework.suite
```

mainly for EasyBuild developers

- New features must have tests
- New bugfixes must have a failing and working test

Comprehensive testing

- **unit tests** are run automagically by Jenkins
- **regression test** results are pulled in on request
- publicly accessible: *https://jenkins1.ugent.be/view/EasyBuild*



unit tests (framework) unit tests (easyblocks) unit tests (easyconfigs) full regression test

Known problems

- Beter tests
  - Validate installations
  - Benchmarks
  - Require domain specific knowledge
- -rpath vs $LD_LIBRARY_PATH
- Sources being removed from the web
- Others?

EasyBuild dependencies

- **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
  - no Windows support (and none planned for now)
- **Python v2.4** or more recent version (2.x, no Python 3 support yet)
- **environment modules** (or Lmod)
- system C/C++ compiler to bootstrap a GCC toolchain

Installing EasyBuild :(

EasyBuild suffers from the mess that is Python packaging...

```
$ easy_install --user easybuild
```

error: option --user not recognized (only for recent versions of easy_install / setuptools)

"You should be using pip!"

```
$ pip install --user easybuild
```

```
pip: No such file or directory
```
(pip not installed)

"Just use --prefix with easy_install!"

```
$ easy_install --prefix=$HOME easybuild
$ export PATH=$HOME/bin:$PATH
$ eb --version
ERROR: Failed to locate EasyBuild's main script
```
($PYTHONPATH is not set correctly)

Bootstrapping EasyBuild

The easiest way to install EasyBuild is by **bootstrapping** it.

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

```
$ wget http://hpcugent.github.com/easybuild/bootstrap_eb.py
$ python bootstrap_eb.py $HOME
```

This will install EasyBuild using EasyBuild, and produce a module:

```
$ export MODULEPATH=$HOME/modules/all:$MODULEPATH
$ module load EasyBuild
$ eb --version
This is EasyBuild 1.8.2 (framework: 1.8.2, easyblocks: 1.8.2)
```

We’re also looking into a packaged release (RPM, .deb, ...).

Configuring EasyBuild

By default, EasyBuild will install software to

`$HOME/.local/easybuild/software`

and produce modules files in

`$HOME/.local/easybuild/modules/all`

You can instruct EasyBuild otherwise by **configuring** it, using:

- a **configuration file**, e.g., `$HOME/.easybuild/config.cfg`
- **environment variables**, e.g., `$EASYBUILD_INSTALLPATH`
- **command line,** e.g. `--installpath`

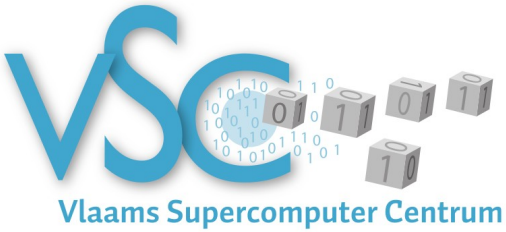
https://github.com/hpcugent/easybuild/wiki/Configuration

(note: documentation needs work)

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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building software with ease

Introduction to EasyBuild
EasyBuild hackathon @ Nicosia, Cyprus
Oct 22th 2013

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