easybuild

building software with ease

FOSS for Scientists devroom @ FOSDEM’13
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Who are we?

- primary contact for High Performance Computing at Ghent University
- part of central IT department (DICT)
- member of Flemish Supercomputer Centre (VSC)

- HPC-UGent team consists of 7 FTEs
- 6 Tier2 systems, one Tier1 system (#163 in Top500)
  - 528 workernodes, 8448 cores, 33TB memory, 152.3 TFlops
- system administration, user support & training, ...
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** build procedure
- requiring human **interaction**
- heavily **customized**
- use **hard-coded** settings
- poor and/or outdated **documentation**

Very **time-consuming** for user support teams!
NEW VERSIONS NWCHEM, WRF AND OPENFOAM REQUESTED

GOT NWCHEM TO BUILD IN JUST 4 DAYS THIS TIME
building from **source** is preferred in an HPC environment

**performance** is critical, instruction selection is key (e.g. AVX)

not a lot of packaged scientific software available (RPMs, ...)

requires **huge effort**, which is duplicated across distros

existing build tools are

hard to **maintain** (e.g., bash scripts)

stand-alone, **no reuse** of previous effort

**OS-dependent** (HomeBrew, *Ports, ...)

**custom** to (groups of) software packages

e.g., Dorsal (DOLFIN), gmkpack (ALADIN)
Our build tool wish list

› flexible framework

› allows for reproducible builds

› supports co-existence of versions/builds

› automated builds and dependency resolution

› enables sharing of build procedure implementations
Building software with ease

easybuild

a software build and installation framework

- written in **Python**
- developed in-house (HPC-UGent) for 2.5 years
- open-source (GPLv2) since April 2012
- stable API since Nov. 2012 (v1.0.0)
- continuously enhanced and extended

http://hpcugent.github.com/easybuild
What does EasyBuild need?

- **Linux / OS X**
  - used daily on Scientific Linux 5.x/6.x (Red Hat-based)
  - also tested on Fedora, Debian, Ubuntu, CentOS, SLES, ...
  - a couple of known issues on OS X
  - no Windows support (and none planned for now)

- **Python 2.4** or more recent 2.x

- **environment modules** (lmod support planned)

- system C/C++ compiler to bootstrap a GCC toolchain
$ easy_install --user easybuild

$ eb HPL-2.0-goalf-1.1.0-no-OFED.eb --robot

downloads all required sources (best effort)

constructs goalf toolchain, and builds HPL with it

goalf: GCC, OpenMPI, ATLAS, LAPACK, FFTW, ScaLAPACK, BLACS

default: source/build/install dir in $HOME/.local/easybuild

note: we need a better quick demo
Terminology

framework
- Python packages forming the heart of EasyBuild
- provides (loads of) supporting functionality
- very modular design w.r.t. toolchains and easyblocks

easyblock
- Python module providing an implementation of a build procedure
- generic or software-specific

easyconfig file (.eb)
- build specification: name, version, toolchain, build options, ...
- simple text files, Python syntax
High-level design

easybuild

tools
asyncprocess
build_log
cfg
environment
filetools
module_generator
modules
ordereddict
parallelbuild
pbs_job
repository
systemtools
variables
version

toolchain
easyblock
EasyBlock
... extension
Extension
easyconfig
EasyConfig
...

framework

toolchains

framework
generic

easyblocks

armadillo

configuremake
ConfigureMake
cmakemake
CMakeMake
...

cp2k

EB_Armadillo

EB_CP2K

EB_WRF

gcc
intellicifort
...
golaf
ictce
...

fft

mpif77

...
Step-wise install procedure

build and install procedure as implemented by EasyBuild

most of these steps can be customized if required
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
Example use case (2/2)

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

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

  eb --software=WRF,3.4 --toolchain-name=ictce --robot
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
  - software stack be built 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
Our build tool wish list

- **flexible** framework
  => additional support plugs in easily
- allows for **reproducible** builds
  => easyblocks + robust framework = reproducibility
- supports **co-existence** of versions/builds
  => installs in custom prefix, generates env. modules
- **automated** builds and **dependency** resolution
  => ‘robot’ feature for handling dependency hells
- enables **sharing** of build procedure implementations
  => easyblocks can be shared or contributed back
List of supported software (v1.1.0)

198 different software packages (488 example easyconfigs)

ABINIT ABySS ACML ALADIN AMOS ant Armadillo ASE ATLAS Autoconf BEAGLE BFAST BiSearch Bison BLACS BLAST Boost Bowtie2 BWA byacc bzip2 CGAL Chapel CLHEP ClustalW2 CMake CP2K CPLEX Cufflinks cURL CVXOPT Cython Docutils DOLFIN Doxygen ECore Eigen ESPResSo expat FASTX-Toolkit FFC FFTW FIAT flex freetype FSL g2clib g2lib GATE GCC Geant4 GEOS GHC git glproto gmacml GMP gmvapich2 goalf gompi google-sparsehash GPAW Greenlet grib_api GSL guile h5py h5utils Harminv HDF HDF5 HMMER HPL hwloc Hypre icc iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifort iccifot
Current status

EasyBuild v1.1.0 released January 27 2013
  planned monthly releases (v1.x.0), bugfix releases as needed
  various features pending:
    more flexibility, e.g., module naming scheme, lmod support
    bring documentation wiki up-to-date
    generate packages for supported software (RPMs, .deb, ...)
    support for more software and additional compiler toolchains
  small community, growing steadily
    UGent + VSC partners
    University of Luxembourg
    Gregor Mendel Institute (Austria)
    ...
Call for contributions

- **feedback**
  - give it a spin, let us know how it turns out
  - what features do you require that are missing?

- **report problems**
  - via mail, GitHub issue tracker, IRC, ...

- **help verify the correctness of easyblocks/easyconfigs**

- **contribute back**
  - features in framework, support for additional compilers/libraries
  - easyblocks and/or easyconfig files (new software, updates, ...)

Let's build a community to tackle this problem together!
easybuild
building software with ease

**website:** [http://hpcugent.github.com/easybuild](http://hpcugent.github.com/easybuild)

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

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

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