easybuild

building software with ease

Supercomputing'13 BoF lightning talk

Getting Scientific Software Installed: Tools & Best Practices

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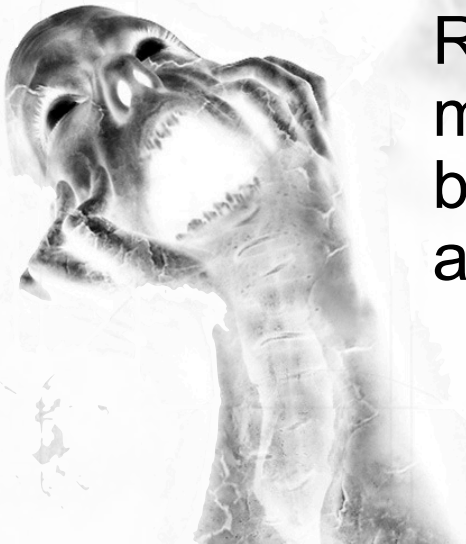
Building scientific software is... fun!

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

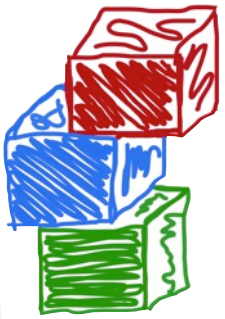
Build procedures are: incomplete, interactive, non-standard,
use hard-coded settings, poorly documented, unstable, ...

Very time-consuming for user support teams!



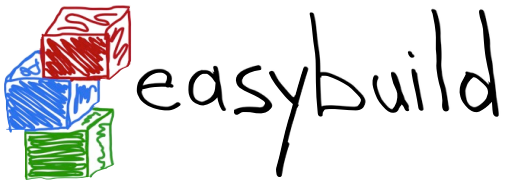
Requirements for HPC systems: build from source, multiple builds per application, reproducibility of builds, automated builds, consistency (e.g, modules, across sites, ...), *reuse of efforts* (across the globe), ...

Building software with ease



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** with v1.0.0 since Nov. 2012 (SC'12)
- continuously enhanced and extended (monthly releases)
- *http://hpcugent.github.com/easybuild*



Quick start

1) Easily install EasyBuild by bootstrapping it:

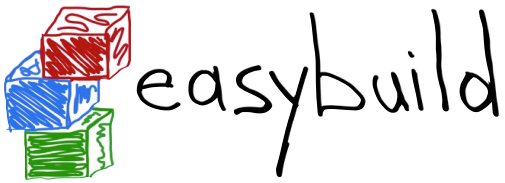
```
$ wget http://hpcugent.github.com/easybuild/bootstrap_eb.py
$ python bootstrap_eb.py <install path>
```

2) Set module path, load EasyBuild module, basic configuration:

```
$ export MODULEPATH=<install path>/modules/all:$MODULEPATH
$ module load EasyBuild
$ export EASYBUILD_INSTALLPATH=<install path>
```

3) Example: build WRF & all deps (!) with GCC-based toolchain:

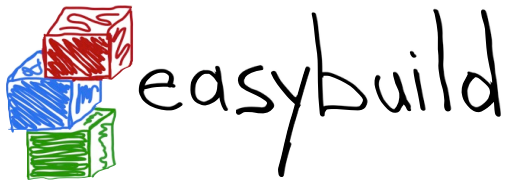
```
$ eb WRF-3.4-goolf-1.4.10-dmpar.eb --robot
$ module av WRF
  WRF/3.4-goolf-1.4.10-dmpar
```



List of supported software (v1.9.0)

396 different software packages (1,939 'example' builds)

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 BFAST binutils BioPerl Biopython BiSearch Bison BLACS BLAST BLAT BOINC Bonnie++ Boost Bowtie Bowtie2 BWA byacc bzip2 cairo CBLAS ccache CCfits CD-HIT CDO CFITSIO cflow CGAL cgdb Chapel Clang CLHEP ClustalW2 CMake Corkscrew **CP2K** CPLEX CRF++ Cube CUDA Cufflinks cURL CVXOPT Cython DB Diffutils DL_POLY_Classic Docutils **DOLFIN** Doxygen **EasyBuild** ECore ed Eigen ELinks EMBOSS EPD 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** GDAL GDB Geant4 GenomeAnalysisTK GEOS gettext GHC GIMPS git GLib GLIMMER GLPK glproto GMP gnuplot gnutls google-sparsehash GPAW gperf Greenlet grib_api GROMACS GSL GTI guile gzip h5py h5utils Harminv HDF HDF5 HH-suite HMMER horton HPL hwloc Hypre icc ifort imake imkl impi Infernal inputproto Inspector Instant Iperf ipp IPython itac JasPer Java Jinja2 JUnit kbproto LAPACK lftp libctl libdrm libffi libgtextutils libharu libibmad libibumad libibverbs libICE libidn Libint libint2 libmatheval libpciaccess libpng libpthread-stubs libreadline libSM libsmm LibTIFF libtool libungif libunistring libX11 libXau libXaw libxc libxcb libXext libXfixes libXi libxml2 libXmu libXp libXpm libxslt libXt libyaml likwid LWM2 lxml lynx LZO M4 make makedepend Maple MariaDB Mathematica MATLAB matplotlib mc MCL MDP Meep MEME Mercurial Mesa Mesquite MetaVelvet METIS 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 nettle **NEURON** ns numactl numexpr numpy **NWChem** Oases Oger OPARI2 OpenBabel OpenBLAS **OpenFOAM** OpenIFS OpenMPI OpenPGM OpenSSL ORCA orthomcl otcl OTF OTF2 PAML pandas PANDAseq PAPI parallel Paraview ParFlow ParMETIS ParMGridGen Pasha paycheck PCC PCRE PDT Perl **PETSc** petsc4py phonopy picard pixman pkg-config PLINK PnMPI Primer3 printproto problog PSI PyQuante pysqlite pyTables Python python-meep PyYAML PyZMQ QLogicMPI Qt **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 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 VSC-tools 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



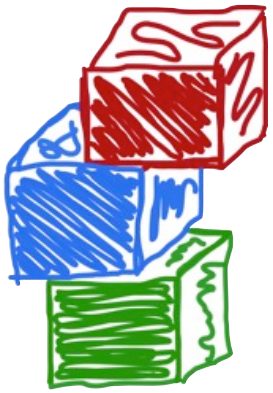
Current features, future directions

currently (EasyBuild v1.9.0):

- support for GCC and Intel compilers (adding more should be fairly easy)
- support for Intel MPI, MPICH, MPICH2, MVAPICH2, OpenMPI libraries
- robust *framework* providing supporting functionality
- very *dynamic* design: plugin support for new compiler/MPI/application/...
- *generates* Tcl module files, supports using C/Tcl env mod & Lmod tools
- using a *custom module naming scheme* you can easily define yourself
- *fully autonomous* builds, build logging, automagic dependency resolution, ...

future directions:

- new build spec format (easyconfig files, .eb) to handle explosion
- better support for site customization (e.g. OpenMPI configure options, ...)
- support for more software applications and platforms
- better error reporting
- **community drives most new features, *get involved!***



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Do you want to know more?

website: *http://hpcugent.github.io/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*

YouTube: *search for "EasyBuild intro", "EasyBuild WRF"*

IRC: *#easybuild on freenode.net*