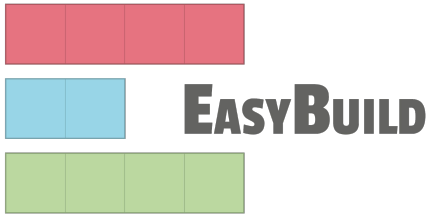


EasyBuild + EESSI UK workshop

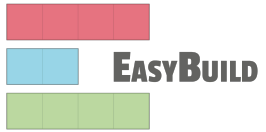
27-28 April 2023, London (UK)

https://easybuild.io/eb-eessi-uk-workshop-2023-04

https://tutorial.easybuild.io/2023-eb-eessi-uk-workshop

Agenda - day 1

(all times are BST)



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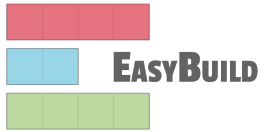
Practical information



- Tutorial website: https://tutorial.easybuild.io/2023-eb-eessi-uk-workshop
- If you need help, consider asking questions in the EasyBuild Slack
- Prepared environment for hands-on demos & exercises

Prepared environment

- Small Rocky 8 cluster (in the cloud)

- **You need to create an account!**
  - Signup: https://mokey.eum23.learnhpc.eu/auth/signup
  - Accounts will only be approved for access on 26-27-28 April 2023, so **please record your username/password !**
    - "Reset password" link does **not** work, instead raise any login problem in Slack

- Access via `ssh` or web browser **(pick one and stick to it!)**
  - Shell access: `ssh eum23.learnhpc.eu`
    - Use login node, or start interactive shell on workernode: `srun --time 600 -c 1 --pty /bin/bash -l`
  - Via browser: https://eum23.learnhpc.eu

- System will be up until the end of the tutorial (~18:00 BST on Fri 28 April 2023)

Agenda - day 1

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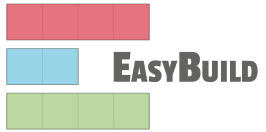

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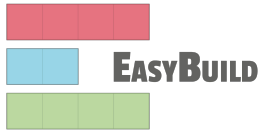
What is EasyBuild?



- **EasyBuild is a software build and installation framework**
- Strong focus on scientific software, performance, and HPC systems
- Open source (GPLv2), implemented in Python (2.7, 3.5+)
- Brief history:
  - Created in-house at HPC-UGent in 2008
  - First released publicly in Apr'12 (version 0.5)
  - EasyBuild 1.0.0 released in Nov'12 (during SC12)
  - Worldwide community has grown around it since then!

https://easybuild.io

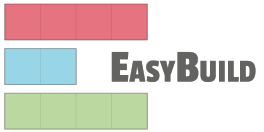
https://docs.easybuild.io

https://github.com/easybuilders

https://easybuild.io/join-slack

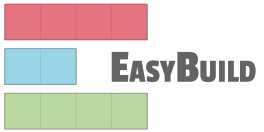
Twitter: @easy_build

EasyBuild in a nutshell



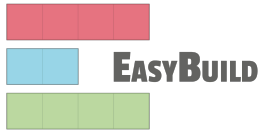
- **Tool to provide a *consistent and well performing* scientific software stack**
- Uniform interface for installing scientific software on HPC systems
- Saves time by *automating* tedious, boring and repetitive tasks
- Can empower scientific researchers to self-manage their software stack
- **A platform for collaboration among HPC sites worldwide**
- Has become an “expert system” for installing scientific software

Key features of EasyBuild (1/2)



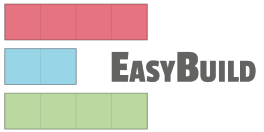
- Supports fully **autonomously** installing (scientific) software,
  including dependencies, generating environment module files, ...
- **No admin privileges are required** (only write permission to installation prefix)
- Highly configurable, easy to extend, support for hooks, easy customisation
- Detailed logging, fully transparent via support for “dry runs” and trace mode
- Support for using custom module naming schemes (incl. hierarchical)

Key features of EasyBuild (2/2)



- Integrates with various other tools (Lmod, Singularity, FPM, Slurm, GC3Pie, ...)
- **Actively developed and supported by worldwide community**
- **Frequent stable releases** since 2012 (every 6 - 8 weeks)
- **Comprehensive testing**: unit tests, testing contributions, regression testing
- **Various support channels** (mailing list, Slack, conf calls) + yearly user meetings

Focus points in EasyBuild



Performance

- Strong preference for building software from source
- Software is optimized for the processor architecture of build host (by default)

Reproducibility

- Compiler, libraries, and required dependencies are mostly controlled by EasyBuild
- Fixed software versions for compiler, libraries, (build) dependencies, ...

Community effort

- Development is highly driven by EasyBuild community
- Lots of active contributors, integration with GitHub to facilitate contributions

What EasyBuild is *not*

- EasyBuild is **not YABT (Yet Another Build Tool)**
  - It does not try to replace `CMake`, `make`, `pip`, etc.
  - It wraps around those tools and automates installation procedures
- EasyBuild does **not replace traditional Linux package managers** (`yum`, `dnf`, `apt`, ...)
  - You should still install some software via OS package manager: OpenSSL, Slurm, etc.
- EasyBuild is **not a magic solution** to all your (software installation) problems
  - You may still run into compiler errors (unless somebody worked around it already)

Agenda - day 1

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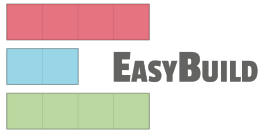

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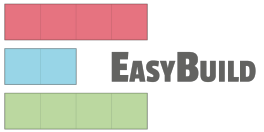
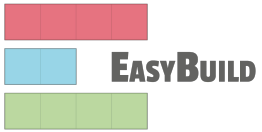
https://tutorial.easybuild.io/2023-eb-eessi-uk-workshop

EasyBuild terminology



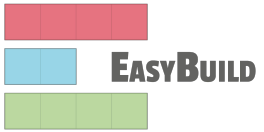
- It is important to briefly explain some terminology often used in EasyBuild
- Some concepts are specific to EasyBuild: easyblocks, easyconfigs, …
- Overloaded terms are clarified: modules, extensions, toolchains, …

EasyBuild terminology: framework



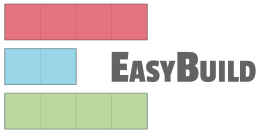
- The EasyBuild framework is the **core of EasyBuild**
- **Collection of Python modules**, organised in packages
- Implements **common functionality** for building and installing software
- Support for applying patches, running commands, generating module files, ...
- Examples: `easybuild.toolchains`, `easybuild.tools`, ...
- Provides `eb` command, but can also be leveraged as a Python library
- GitHub repository: https://github.com/easybuilders/easybuild-framework

EasyBuild terminology: easyblock



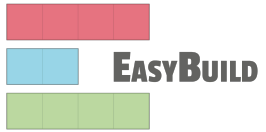
- A **Python module** that implements a specific software installation procedure
  - Can be viewed as a “plugin” to the EasyBuild framework
- **Generic easyblocks** for “standard” stuff: `cmake` + `make` + `make install`, Python packages, etc.
- **Software-specific easyblocks** for complex software (OpenFOAM, TensorFlow, WRF, …)
- Installation procedure can be controlled via easyconfig parameters
  - Additional configure options, commands to run before/after build or install command, …
  - Generic easyblock + handful of defined easyconfig parameters is sufficient to install a lot of software
- GitHub repository: https://github.com/easybuilders/easybuild-easyblocks
- Easyblocks do not need to be part of the EasyBuild installation (see `--include-easyblocks`)

EasyBuild terminology: easyconfig file



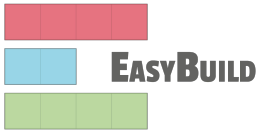
- Text file that specifies what EasyBuild should install (in Python syntax)
- **Collection of values for easyconfig parameters** (key-value definitions)
- Filename typically ends in '`.eb`'
- Specific filename is expected in some contexts (when resolving dependencies)
  - Should match with values for `name`, `version`, `toolchain`, `versionsuffix`
  - `<name>-<version>-<toolchain><versionsuffix>.eb`
- GitHub repository: https://github.com/easybuilders/easybuild-easyconfigs

EasyBuild terminology: easystack file



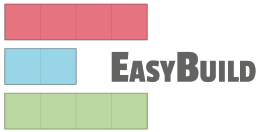
- New concept since EasyBuild v4.3.2 (Dec'20), **experimental feature**
- Concise description for software stack to be installed (in YAML syntax)
- Basically **specifies a set of easyconfig files** (+ associated info)
- Still a work-in-progress, only basic functionality implemented currently
- More info: https://docs.easybuild.io/en/latest/Easystack-files.html

EasyBuild terminology: extensions



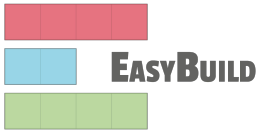
- **Additional software that can be installed *on top* of other software**
- Common examples: Python packages, Perl modules, R libraries, …
- *Extensions* is the general term we use for this type of software packages
- Can be installed in different ways:
  - As a stand-alone software packages (separate module)
  - In a bundle together with other extensions
  - As an actual extension, to provide a “batteries included” installation

EasyBuild terminology: dependencies



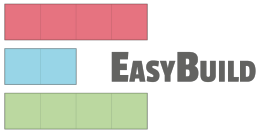
- Software that is **required to build/install or run other software**
- **Build dependencies**: only required when building/installing software (not to use it)
  - Examples: CMake, pip, pkg-config, …
- **Run-time dependencies**: (also) required to use the installed software
  - Examples: Python, Perl, R, …
- **Link-time dependencies**: libraries that are required by software to link to
  - Examples: glibc, OpenBLAS, FFTW, …
- Currently in EasyBuild: no distinction between link-time and run-time dependencies

EasyBuild terminology: toolchains



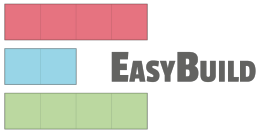
- **Compiler toolchain: set of compilers + libraries for MPI, BLAS/LAPACK, FFT, …**
- Toolchain component: a part of a toolchain (compiler component, etc.)
- **Full toolchain**: C/C++/Fortran compilers + libraries for MPI, BLAS/LAPACK, FFT
- **Subtoolchain** (partial toolchain): compiler-only, only compiler + MPI, etc.
- **System toolchain**: use compilers (+ libraries) provided by the operating system
- **Common toolchains**: widely used toolchains in EasyBuild community:
  - `foss`: GCC + OpenMPI + (FlexiBLAS +) OpenBLAS + FFTW
  - `intel`: Intel compilers + Intel MPI + Intel MKL

EasyBuild terminology: modules



- Very overloaded term: kernel modules, Python modules, Perl modules …
- In EasyBuild context: "*module*" usually refers to an **environment module file**
  - **Shell-agnostic specification of how to "activate" a software installation**
  - Expressed in Tcl or Lua syntax (scripting languages)
  - Consumed by a modules tool (**Lmod**, Environment Modules, …)
- Other types of modules will be qualified explicitly (Python modules, etc.)
- EasyBuild automatically generates a module file for each installation

Bringing all EasyBuild terminology together



The EasyBuild **framework** leverages **easyblocks** to automatically build and install (scientific) software, potentially including additional **extensions**, using a particular compiler **toolchain**, as specified in **easyconfig files** which each define a set of **easyconfig parameters**.

EasyBuild ensures that the specified **(build) dependencies** are in place, and automatically generates a set of (environment) **modules** that facilitate access to the installed software.

An **easystack** file can be used to specify a collection of software to install with EasyBuild.

Agenda - day 1

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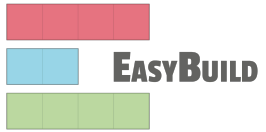

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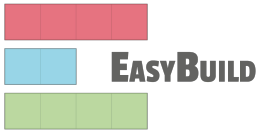
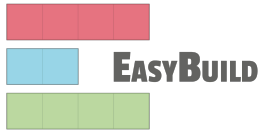
Installing EasyBuild: requirements



- **Linux** as operating system (CentOS, RHEL, Ubuntu, Debian, SLES, ...)
  - EasyBuild also works on macOS, but support is very basic
- **Python** 2.7 or 3.5+
  - Only Python standard library is required for core functionality of EasyBuild
  - Using Python 3.6+ is highly recommended!
- An **environment modules tool** (`module` command)
  - Default is Lua-based Lmod implementation, highly recommended!
  - Tcl-based implementations are also supported

Installing EasyBuild: different options



- Installing EasyBuild using a standard Python installation tool
  - `pip install easybuild`
  - … or a variant thereof (`pip3 install --user`, using `virtualenv`, etc.)
  - May require additional commands, for example to update environment
- **Installing EasyBuild as a module, with EasyBuild *(recommended!)***
  - 3-step “bootstrap” procedure, via temporary EasyBuild installation using `pip`
- Development setup
  - Clone GitHub repositories:

    `easybuilders/easybuild-{framework,easyblocks,easyconfigs}`
  - Update `$PATH` and `$PYTHONPATH` environment variables

Installing EasyBuild as a module (recommended)

3-step bootstrap procedure

- **Step 1: Use `pip` to obtain a temporary installation of EasyBuild**

```
export TMPDIR=/tmp/$USER/easybuild
pip3 install --prefix $TMPDIR easybuild
# update environment to use this temporary EasyBuild installation
export PATH=$TMPDIR/bin:$PATH
export PYTHONPATH=$TMPDIR/lib/python3.9/site-packages:$PYTHONPATH
# instruct EasyBuild to use python3 command
export EB_PYTHON=python3
```

Installing EasyBuild as a module (recommended)

3-step bootstrap procedure

- **Step 2: Use EasyBuild to install EasyBuild (as a module) in home directory**

```
eb --install-latest-eb-release --prefix $HOME/easybuild
# and then clean up the temporary EasyBuild installation
rm -r $TMPDIR
```

- **Step 3: Load EasyBuild module to use final installation**

```
module use $HOME/easybuild/modules/all
module load EasyBuild
```

Verifying the EasyBuild installation

- Check EasyBuild version:

```
eb --version
```

- Show help output (incl. long list of supported configuration settings)

```
eb --help
```

- Show the current (default) EasyBuild configuration:

```
eb --show-config
```

- Show system information:

```
eb --show-system-info
```

Updating EasyBuild

- Updating EasyBuild (in-place) that was installed with pip:

```
pip install --upgrade easybuild
```

  (+ additional options like `--user`, or using `pip3`, depending on your setup)

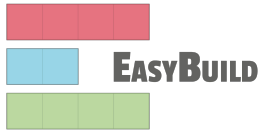
- Use current EasyBuild to install latest EasyBuild release as a module:

```
eb --install-latest-eb-release
```

  - This is *not* an in-place update, but a new EasyBuild installation!
  - You need to load (or swap to) the corresponding module afterwards:

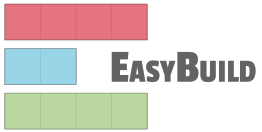
```
module load EasyBuild/4.5.4
```

Configuring EasyBuild



- EasyBuild should work fine out-of-the-box if you are using Lmod as modules tool
- ... but it will (ab)use `$HOME/.local/easybuild` to install software into, etc.
- It is ***strongly*** recommended to configure EasyBuild properly!
- Main questions you should ask yourself:
  - Where should EasyBuild install software (incl. module files)?
  - Where should auto-downloaded sources be stored?
  - Which filesystem is best suited for software build directories (I/O-intensive)?

Primary configuration settings



- Most important configuration settings: (strongly recommended to specify the ones in **bold**!)
  - Modules tool + syntax (`modules-tool` + `module-syntax`)
  - **Software + modules installation path** (`installpath`)*
  - **Location of software sources "cache"** (`sourcepath`)*
  - **Parent directory for software build directories** (`buildpath`)*
  - Location of easyconfig files archive (`repositorypath`)*
  - Search path for easyconfig files (`robot-paths` + `robot`)
  - Module naming scheme (`module-naming-scheme`)
- Several locations* (+ others) can be controlled at once via `prefix` configuration setting
- *Full* list of EasyBuild configuration settings (~270) is available via `eb --help`

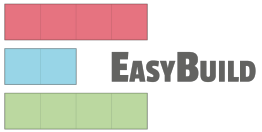
Configuration levels

- There are 3 different configuration levels in EasyBuild:
  - **Configuration files**
  - **Environment variables**
  - **Command line options to the `eb` command**

- Each configuration setting can be specified via each “level” (no exceptions!)

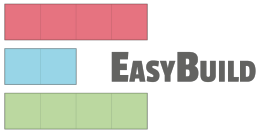
- Hierarchical configuration:
  - Configuration files override default settings
  - Environment variables override configuration files
  - eb command line options override environment variables

EasyBuild configuration files



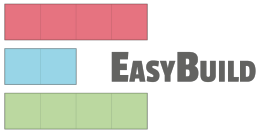
- EasyBuild configuration files are in standard INI format (`key=value`)
- EasyBuild considers multiple locations for configuration files:
  - User-level: `$HOME/.config/easybuild/config.cfg` (or via `$XDG_CONFIG_HOME`)
  - System-level: `/etc/easybuild.d/*.cfg` (or via `$XDG_CONFIG_DIRS`)
  - See output of `eb --show-default-configfiles`
- Output produced by `eb --confighelp` is a good starting point
- Typically for “do once and forget” static configuration (like modules tool to use, ...)
- **EasyBuild configuration files and easyconfig files are very different things!**

$EASYBUILD_* environment variables



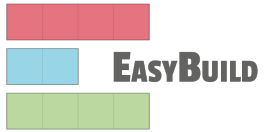
- Very convenient way to configure EasyBuild
- **There is an `$EASYBUILD_*` environment variable for each configuration setting**
  - Use all capital letters
  - Replace every dash (–) character with an underscore (_)
  - Prefix with `EASYBUILD_`
  - Example: `module-syntax` → `$EASYBUILD_MODULE_SYNTAX`
- Common approach: using a shell script or module file to (dynamically) configure EasyBuild

Command line options for `eb` command



- **Configuration settings specified as command line option always "win"**
- Use double-dash + name of configuration setting, like `--module-syntax`
- Some options have a corresponding shorthand (`eb --robot` == `eb -r`)
- In some cases, only command line option really makes sense (like `eb --version`)
- Typically used to control configuration settings for current EasyBuild session;
  for example: `eb --installpath /tmp/$USER`

Inspecting the current configuration



- It can be difficult to remember how EasyBuild was configured
- Output produced by **`eb --show-config`** is useful to remind you
- Shows configuration settings that are different from default
- Always shows a couple of key configuration settings
- Also shows on which level each configuration setting was specified
- Full current configuration: `eb --show-full-config`

Inspecting the current configuration: example

```
$ cat $HOME/.config/easybuild/config.cfg
[config]
prefix=/apps

$ export EASYBUILD_BUILDPATH=/tmp/$USER/build

$ eb --installpath=/tmp/$USER --show-config
# Current EasyBuild configuration
# (C: command line argument, D: default value,
#  E: environment variable, F: configuration file)
buildpath       (E) = /tmp/example/build
containerpath   (F) = /apps/containers
installpath     (C) = /tmp/example
packagepath     (F) = /apps/packages
prefix          (F) = /apps
repositorypath  (F) = /apps/ebfiles_repo
robot-paths     (D) = /home/example/.local/easybuild/easyconfigs
sourcepath      (F) = /apps/sources
```

Minimal EasyBuild configuration for hands-on

- **Use home directory as main prefix directory**

  (location for installed software, downloaded sources, ...)

  ```
  export EASYBUILD_PREFIX=$HOME/easybuild
  ```

- **Use *local* temporary directory for build directories** (important!)

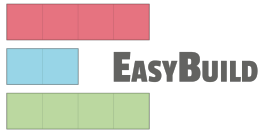
  ```
  export EASYBUILD_BUILDPATH=/tmp/$USER
  ```

- **Ensure prepared software stack is visible** via "`module avail`"

  ```
  module use /easybuild/modules/all
  ```

Agenda - day 1

(all times are BST)



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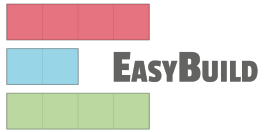
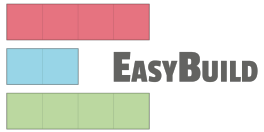
Basic usage of EasyBuild



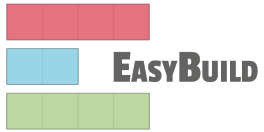
- **Use `eb` command to run EasyBuild**
- Software to install is usually specified via name(s) of easyconfig file(s), or easystack file
- `--robot` (`-r`) option is required to also install missing dependencies (and toolchain)
- Typical workflow:
  - Find or create easyconfig files to install desired software
  - Inspect easyconfigs, check missing dependencies + planned installation procedure
  - Double check current EasyBuild configuration
  - Instruct EasyBuild to install software (while you enjoy a coffee... or two)

Specifying easyconfigs to use



- There a different ways to specify to the `eb` command which easyconfigs to use
  - Specific relative/absolute paths to (directory with) easyconfig files
  - Names of easyconfig files (triggers EasyBuild to search for them)
  - Easystack file to specify a whole stack of software to install (via `eb --easystack`)
- Easyconfig filenames only matter when missing dependencies need to be installed
  - "Robot" mechanism searches based on dependency specs + easyconfig filename
- `eb --search` can be used to quickly search through available easyconfig files

Inspecting easyconfigs via `eb --show-ec`



- To see the contents of an easyconfig file, you can use `eb --show-ec`
- No need to know where it is located, EasyBuild will do that for you!

```
$ eb --show-ec TensorFlow-2.6.0-foss-2021a.eb
easyblock = 'PythonBundle'

name = 'TensorFlow'
version = '2.6.0'

homepage = 'https://www.tensorflow.org/'
description = "An open-source software library for Machine Intelligence"

toolchain = {'name': 'foss', 'version': '2021a'}
toolchainopts = {'pic': True}
…
```

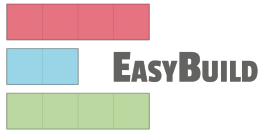
Checking dependencies via `eb --dry-run`

To check which dependencies are required, you can use `eb --dry-run` (or `eb -D`):

- Provides overview of all dependencies (both installed and missing)
- Including compiler toolchain and build dependencies

```
$ eb SAMtools-1.14-GCC-11.2.0.eb -D
 ...
 * [x] $CFGS/n/ncurses/ncurses-6.2-GCCcore-11.2.0.eb (module: ncurses/6.2-GCCcore-11.2.0)
 * [x] $CFGS/p/pkg-config/pkg-config-0.29.2.eb (module: pkg-config/0.29.2)
 * [x] $CFGS/o/OpenSSL/OpenSSL-1.1.eb (module: OpenSSL/1.1)
 * [x] $CFGS/c/cURL/cURL-7.78.0-GCCcore-11.2.0.eb (module: cURL/7.78.0-GCCcore-11.2.0)
 * [ ] $CFGS/s/SAMtools/SAMtools-1.14-GCC-11.2.0.eb (module: SAMtools/1.14-GCC-11.2.0)
```

Checking *missing* dependencies via `eb --missing`

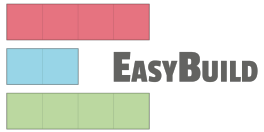


To check which dependencies are still *missing*, use `eb --missing` (or `eb -M`):

- Takes into account available modules, only shows what is still missing

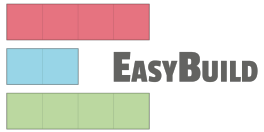
```
$ eb PyTables-3.6.1-foss-2021b.eb -M
3 out of 69 required modules missing:
* LZO/2.10-GCCcore-11.2.0 (LZO-2.10-GCCcore-11.2.0.eb)
* Blosc/1.21.1-GCCcore-11.2.0 (Blosc-1.21.1-GCCcore-11.2.0.eb)
* PyTables/3.6.1-foss-2021b (PyTables-3.6.1-foss-2021b.eb)
```

Inspecting software install procedures



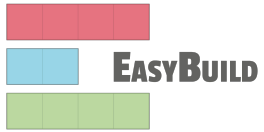
- EasyBuild can quickly unveil how exactly it *would* install an easyconfig file
- Via `eb --extended-dry-run` (or `eb -x`)
- Produces detailed output in a matter of seconds
- Software is not actually installed, all shell commands and file operations are skipped!
- Some guesses and assumptions are made, so it may not be 100% accurate…
- Any errors produced by the easyblock are reported as being ignored
- Very useful to evaluate changes to an easyconfig file or easyblock!

Inspecting software install procedures: example



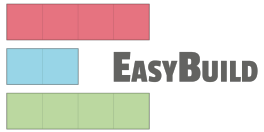

```
$ eb Boost-1.77.0-GCC-11.2.0.eb -x
...

preparing... [DRY RUN]

[prepare_step method]
Defining build environment, based on toolchain (options) and specified dependencies...

Loading toolchain module...

module load GCC/11.2.0

Loading modules for dependencies...

module load bzip2/1.0.8-GCCcore-11.2.0
module load zlib/1.2.11-GCCcore-11.2.0
module load XZ/5.2.5-GCCcore-11.2.0
```

Inspecting software install procedures: example




```
$ eb Boost-1.77.0-GCC-11.2.0.eb -x
...
Defining build environment...
  ...
  export CXX='g++'
  export CXXFLAGS='-O2 -ftree-vectorize -march=native -fno-math-errno -fPIC'
  ...

configuring... [DRY RUN]

[configure_step method]
  running command "./bootstrap.sh --with-toolset=gcc
  --prefix=/tmp/example/Boost/1.77.0-GCC-11.2.0 --without-libraries=python,mpi"
  (in /tmp/example/build/Boost/1.77.0/GCC-11.2.0/Boost-1.77.0)
```

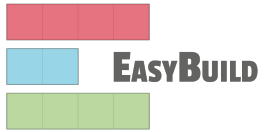
Inspecting software install procedures: example




```
$ eb Boost-1.77.0-GCC-11.2.0.eb -x
...

[sanity_check_step method]
Sanity check paths - file ['files']
  * lib/libboost_system-mt-x64.so
  * lib/libboost_system.so
  * lib/libboost_thread-mt-x64.so
Sanity check paths - (non-empty) directory ['dirs']
  * include/boost
Sanity check commands
  (none)

...
```

Agenda - day 1

(all times are BST)



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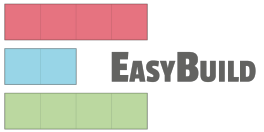
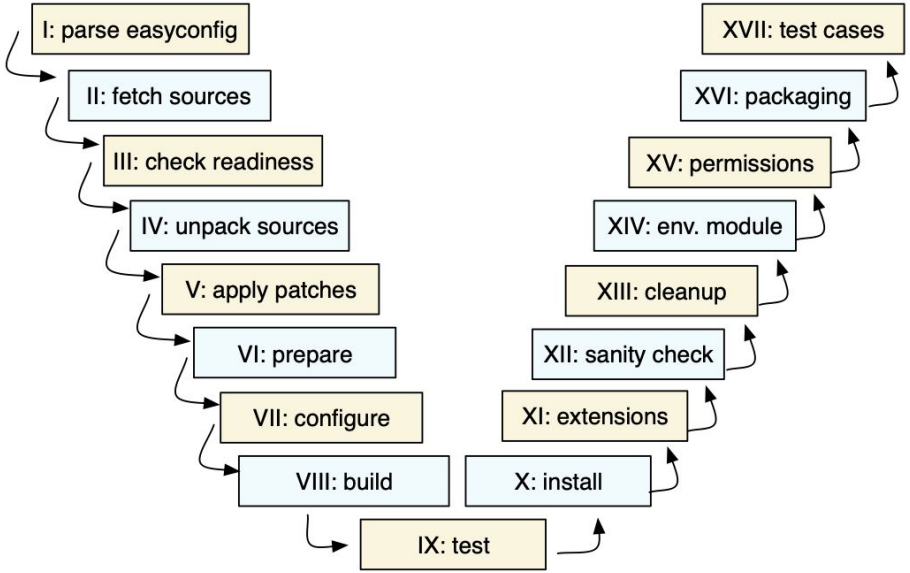
Installing software with EasyBuild



- To install software with EasyBuild, just run the `eb` command:
  - `eb SAMtools-1.14-GCC-11.2.0.eb`
- If any dependencies are still missing, you will need to also use `--robot`:
  - `eb BCFtools-1.14-GCC-11.2.0.eb --robot`
- To see more details while the installation is running, enable trace mode:
  - `eb BCFtools-1.14-GCC-11.2.0.eb --robot --trace`
- To reinstall software, use `eb --rebuild` (or `eb --force`)

Step-wise installation procedure



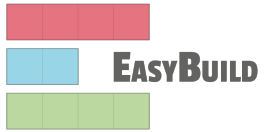
- EasyBuild framework defines step-wise installation procedure, leaves some unimplemented
- Easyblock completes the implementation, override or extends installation steps where needed

Using software installed with EasyBuild

To use the software you installed with EasyBuild, load the corresponding module:

```
# inform modules tool about modules installed with EasyBuild
module use $HOME/easybuild/modules/all
# check for available modules for BCFtools
module avail BCFtools
# load BCFtools module to "activate" the installation
module load BCFtools/1.14-GCC-11.2.0
```

Stacking software installations



- It's easy to "stack" software installed in different locations
- EasyBuild doesn't care much where software is installed
- As long as the required modules are available to load, it can pick them up
- End users can easily manage a software stack on top of what's installed centrally!

```
module use /easybuild/modules/all

eb --installpath $HOME/easybuild my-software.eb
```

Agenda - day 1

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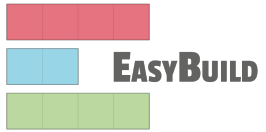

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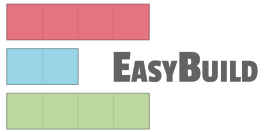
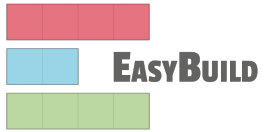
Troubleshooting failing installations



- Sometimes stuff still goes wrong…
- Being able to troubleshoot a failing installation is a useful/necessary skill
- Problems that occur include (but are not limited to):
  - Missing source files
  - Missing dependencies (perhaps overlooked required dependencies)
  - Failing shell commands (non-zero exit status)
  - Running out of memory or storage space
  - Compiler errors (or crashes)
- EasyBuild keeps a thorough log for each installation which is very helpful

Troubleshooting: error messages

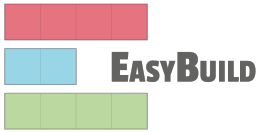


- When EasyBuild detects that something went wrong, it produces an error
- Very often due to a shell command that produced a non-zero exit code...
- Sometimes the problem is clear directly from the error message:

```
== building...
== FAILED: Installation ended unsuccessfully (build directory:
/tmp/example/example/1.0/GCC-11.2.0):
build failed (first 300 chars): cmd "make" exited with exit code 2 and output:
/usr/bin/g++ -O2 -ftree-vectorize -march=native -std=c++14 -c -o core.o core.cpp
g++: error: unrecognized command line option '-std=c++14' (took 1 sec)
```

- In some cases, the error message itself does not reveal the problem...

Troubleshooting: log files

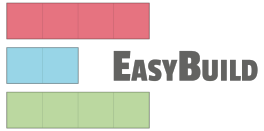


- EasyBuild keeps track of the installation in a detailed log file
- During the installation, it is stored in a temporary directory:

```
$ eb example.eb
== Temporary log file in case of crash /tmp/eb-r503td0j/easybuild-17flov9v.log
...
```

- Includes executed shell commands and output, build environment, etc.
- More detailed log file when debug mode is enabled (`debug` configuration setting)
- There is a log file per EasyBuild session, and one per performed installation
- **When an installation completes successfully,**
  the log file is copied to a subdirectory of the software installation directory

Troubleshooting: navigating log files



- **EasyBuild log files are well structured, and fairly easy to search through**
- Example log message, showing prefix ("== "), timestamp, source location, log level:

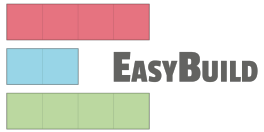
```
== 2022-05-25 13:11:19,968 run.py:222 INFO running cmd:  make -j 9
```

- Different steps of installation procedure are clearly marked:

```
== 2022-05-25 13:11:48,817 example INFO Starting sanity check step
```

- To find actual problem for a failing shell command, look for patterns like:
  - ERROR
  - Error 1
  - error:
  - failure
  - not found
  - No such file or directory
  - Segmentation fault

Troubleshooting: inspecting the build directory

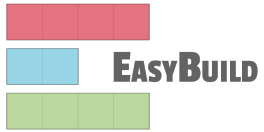


- EasyBuild leaves the build directory in place when the installation failed

```
== FAILED: Installation ended unsuccessfully (build directory:
/tmp/build/example/1.0/GCC-11.2.0): build failed ...
```

- Can be useful to inspect the contents of the build directory for debugging
- For example:
  - Check `config.log` when `configure` command failed
  - Check `CMakeFiles/CMakeError.log` when `cmake` command failed (good luck...)

Troubleshooting: hands-on exercise

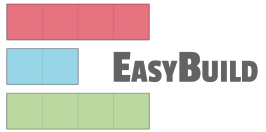


- **Highly recommended to try the exercise on tutorial website!**
- Try to fix the problems you encounter with the “broken” easyconfig file…

```
$ eb subread.eb
...
== FAILED: Installation ended unsuccessfully (build directory:
/tmp/example/Subread/2.0.3/GCC-8.5.0): build failed (first 300 chars):
Couldn't find file subread-2.0.3-source.tar.gz anywhere, and downloading
it didn't work either...
Paths attempted (in order): ...
```

Agenda - day 1

(all times are BST)



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- [15:00-15:30] (coffee break)
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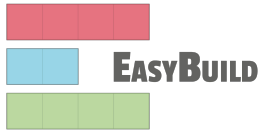
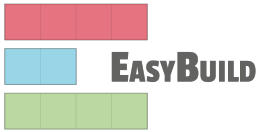
Adding support for additional software



- Every installation performed by EasyBuild requires an easyconfig file
- Easyconfig files can be:
  - Included with EasyBuild itself (or obtained elsewhere)
  - Derived from an existing easyconfig (manually or automatic)
  - Created from scratch
- Most easyconfigs leverage a generic easyblock
- Sometimes using a custom software-specific easyblock makes sense...

Easyblocks vs easyconfigs



- When can you get away with using an easyconfig leveraging a generic easyblock?
- When is a software-specific easyblock really required?
- Easyblocks are “implement once and forget”
- Easyconfig files leveraging a generic easyblock can become too involved (subjective)
- Reasons to consider implementing a custom easyblock:
  - 'critical' values for easyconfig parameters required to make installation succeed
  - custom (configure) options related to toolchain or included dependencies
  - interactive commands that need to be run
  - having to create or adjust specific (configuration) files
  - 'hackish' usage of a generic easyblock
  - complex or very non-standard installation procedure

Writing easyconfig files

- Collection of easyconfig parameter definitions (Python syntax), collectively specify what to install
- Some easyconfig parameters are mandatory, and **must** always be defined:
  `name`, `version`, `homepage`, `description`, `toolchain`
- Commonly used easyconfig parameters (but strictly speaking not required):
  - `easyblock` (by default derived from software name)
  - `versionsuffix`
  - `source_urls`, `sources`, `patches`, `checksums`
  - `dependencies`, `builddependencies`
  - `preconfigopts`, `configopts`, `prebuildopts`, `buildopts`, `preinstallopts`, `installopts`
  - `sanity_check_paths`, `sanity_check_commands`

Generating tweaked easyconfig files

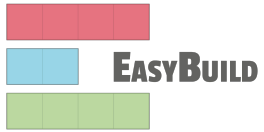
- Trivial changes to existing easyconfig files can be done automatically
- Bumping software version: `eb example-1.0.eb --try-software-version 1.1`
- Changing toolchain (version): `eb example.eb --try-toolchain GCC,11.2.0`
- Changing specific easyconfig parameters (limited): `eb --try-amend ...`
- Note the “try” aspect: additional changes may be required to make installation work
- EasyBuild does save the so generated easyconfig files in the `easybuild` subdirectory of the software installation directory and in the easyconfig archive.

Copying easyconfig files

- Small but useful feature: copy specified easyconfig file via `eb --copy-ec`
- Avoids the need to locate the file first via `eb --search`
- Typically used to create a new easyconfig using existing one as starting point
- Example:

```
$ eb --copy-ec SAMtools-1.14-GCC-11.2.0.eb SAMtools.eb
...
SAMtools-1.14-GCC-11.2.0.eb copied to SAMtools.eb
```

Hands-on: creating easyconfig files



- Step-wise example + exercise of creating an easyconfig file from scratch
- For fictitious software packages: `eb-tutorial` + `py-eb-tutorial`
- **Great exercise to work through these yourself!**

```
name = 'eb-tutorial'

version = '1.0.1'

homepage = 'https://easybuilders.github.io/easybuild-tutorial'

description = "EasyBuild tutorial example"
```

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Agenda - day 1

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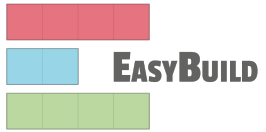

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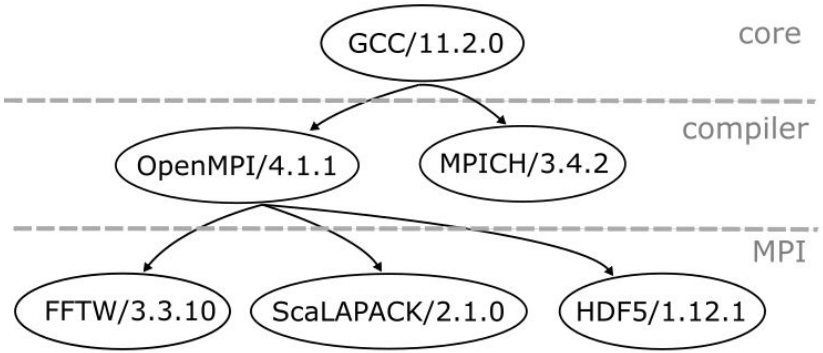
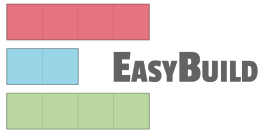
Flat vs hierarchical module naming schemes

- Handful of supported module naming schemes (MNS), `EasyBuildMNS` is the default
- Flat module naming scheme (like `EasyBuildMNS`)
  - Clear mapping of easyconfig filename to name of generated module file
  - All modules immediately available for loading
- Hierarchical scheme typically has 3 levels
  - **core** level for things like compilers
  - **compiler** level
  - **MPI** level
  - Use “gateway modules” to access different levels

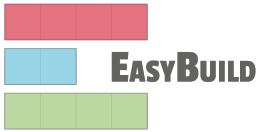


Pros and cons of using a flat vs hierarchical MNS



- Flat MNS
  - ± all modules visible (can be overwhelming)
  - \+ guaranteed unique
  - − long module names that can be confusing
  - − potential compatibility issues unless you are careful
- Hierarchical MNS
  - \+ short/clean module names (and no visible toolchains)
  - ± less visible modules (need to use `module spider` + `module avail`)
  - ± automatic swapping with Lmod when changing compiler/mpi
  - \+ modules that can be loaded are compatible with each other
  - − requires gateway modules which might have little meaning for users

Custom module naming schemes with EasyBuild



- You can also create your own module naming scheme (e.g., lower-case only)
  - Implement Python class that derives from the general `ModuleNamingScheme` class
  - Best to start from one of the existing schemes
  - There are (a lot) more things to tweak with hierarchical module naming schemes

- To configure EasyBuild to use your custom module naming scheme:

```
export EASYBUILD_INCLUDE_MODULE_NAMING_SCHEMES=$HOME/easybuild/example_mns.py
export EASYBUILD_MODULE_NAMING_SCHEME=ExampleMNS
```

- Use dry-run mode to test it, e.g.,

```
eb SciPy-bundle-2021.10-foss-2021b.eb -D
```

Hands-on example: installing HDF5 in an HMNS

- **We must avoid mixing modules from a flat and hierarchical MNS**!

```
module unuse $MODULEPATH
```

- Configure our setup to reuse the existing software installations

```
export EASYBUILD_INSTALLPATH_SOFTWARE=/easybuild/software

export EASYBUILD_MODULE_NAMING_SCHEME=HierarchicalMNS

export EASYBUILD_INSTALLPATH_MODULES=$HOME/hmns/modules
```

- Re-generate all modules for HDF5 using the new scheme (42 modules)

```
eb HDF5-1.12.1-gompi-2021b.eb --robot --module-only
```

- Explore the new hierarchy

```
module use $HOME/hmns/modules/all/Core
```