easybuild

ISC High Performance

The HPC Event.

EasyBuild tutorial
CSC'22

Kurt Lust (Univ. of Antwerp)

9-11 May 2022

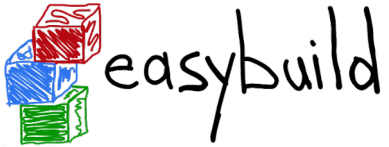
https://klust.github.io/easybuild-tutorial/2022-CSC_and_LO

Introduction to EasyBuild

What is EasyBuild?

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_01_what_is_easybuild/

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 as a tool for the interuniversity VSC project
  - First released publicly in Apr'11
  - EasyBuild 1.0 released in Nov'11 (during SC11)
  - Worldwide community has grown around it since then!

https://easybuild.io

https://docs.easybuild.io

https://github.com/easybuilders

https://easybuild.slack.com
(https://easybuild.io/join-slack)

Twitter: @easy_build

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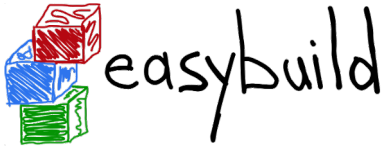
EasyBuild in a nutshell



- **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

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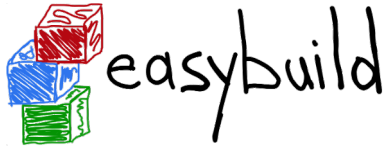
Key features of EasyBuild (1/2)



- Supports fully **autonomously** installing (scientific) software, including dependencies, generating environment module files, …
- **No admin privileges are required** (only write permission to install path)
- 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)

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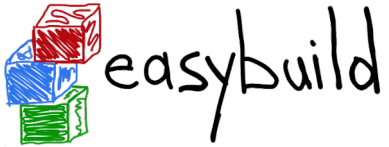
Key features of EasyBuild (2/2)



- Integrates with various other tools (Lmod, Singularity, Slurm, …)
- **Actively developed and supported by worldwide community**
- **Frequent stable releases** since 2011 (every 6 - 8 weeks)
- **Comprehensive testing**: unit tests, testing contributions, regression testing
  - But no Cray test systems
- **Various support channels** (mailing list, Slack, conf calls) + yearly user meetings

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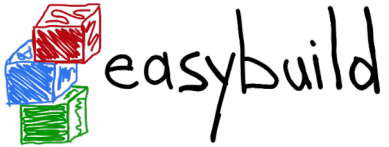
Focus points in EasyBuild



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
  - Cray systems are an exception as EasyBuild interfaces with the Cray PE modules
- 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

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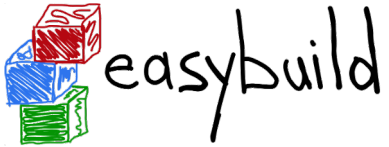
What EasyBuild is *not*



- 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 will still run into compiler errors (unless somebody worked around it already)

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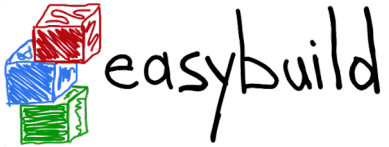
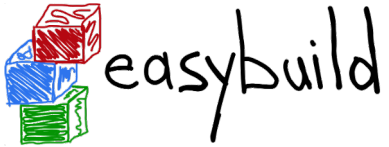


Introduction to EasyBuild

The Lmod module system

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_02_Lmod/

Lmod: LUA environment modules

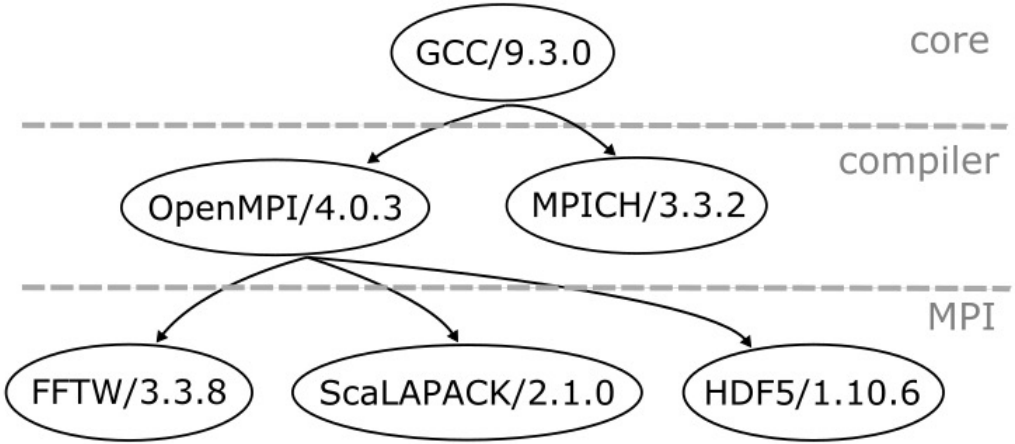


- Choices
  - Environment modules 3: C implementation, Tcl modules, supported by Cray
  - Environment modules 4 or 5: Tcl implementation + modules, NOT supported by Cray
  - Lmod: LUA implementation + modules, supported by Cray (with some delay)
- Hierarchical module scheme
  - Unconventional hierarchy used in the Cray PE
  - Partly used to organise the software stacks on LUMI (versions and specific hardware)

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_02_Lmod/

Lmod hierarchy

- Model hierarchy: 3 levels
  - Core level: compilers
  - Compiler level: provides libraries that only need the compiler, and MPI modules
  - MPI level: Software that is compiled with MPI support



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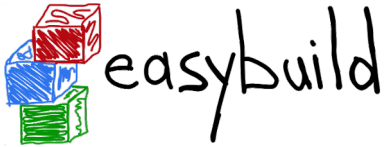
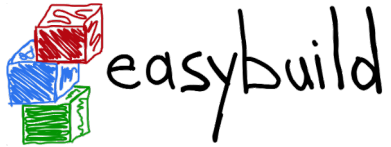
Lmod hierarchy



- Distinction between
  - Installed modules: All modules that can be loaded one way or another, sometimes by first loading other modules
    => module spider and module keyword
  - Available modules: The modules that can be loaded right away
    => module avail
- Examples in the HPE Cray PE:
  - cray-mpich can only be loaded if a compiler module and network target module are loaded
  - Many of the performance monitoring tools only become available after loading perftools-base
  - cray-fftw only becomes avialable when a processor target module is loaded

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_02_Lmod/

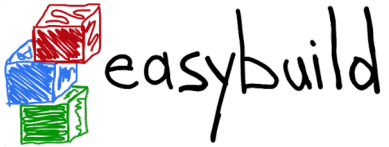
Lmod hierarchy: Building blocks



- MODULEPATH determines which modules are available
  - Some modules change the MODULEPATH to add a new level of available modules
- “One name rule”
- “Family” concept: extension of the “one name rule”
  - No two modules of the same family can be loaded
  - Example on LUMI: The PrgEnv modules belong to the “PrgEnv” family
  - Example on mahti: Compiler modules aocc/3.2.0, gcc/9.4.0, gcc/11.2.0 belong to the “compiler” family
- Be careful with module naming to exploit this!

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_02_Lmod/

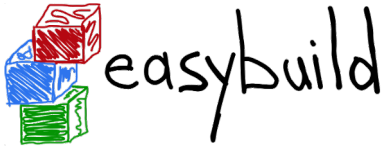
module spider



- module spider : Long list of all installed software with short description
  - Will also look into modules for “extensions” and show those also, marked with an “E”
- module spider gnuplot : Shows all versions of gnuplot on the system
  module spider CMake
- module spider gnuplot/5.4.3-cpeGNU-21.12 : Shows help information for the specific module, including what should be done to make the module available
  - But this does not completely work with the Cray PE modules
- module spider CMake/3.22.2 : Will tell you which module contains CMake and how to load it

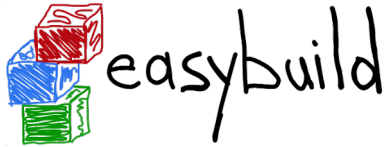
https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_02_Lmod/

module keyword



- Currently not yet very useful due to a bug in Cray Lmod
- It searches in the module short description and help for the keyword.
  - E.g., try
    module keyword https
- We do try to put enough information in the modules to make this a suitable additional way to discover software that is already installed on the system
  - Thinking of proposing an extension to EasyBuild to make this a bit easier without getting ugly looking module help and whatis information

Sticky modules and module purge



- On some systems, you will be taught to avoid module purge (which unloads all modules)
- Sticky modules are modules that are not unloaded by module purge, but reloaded.
  - They can be force-unloaded with module –-force purge and module –-force unload
- Used on LUMI for the software stacks and modules that set the display style of the modules
  - But keep in mind that the modules are reloaded, which implies that the target modules and partition module will be switched (back) to those for the current node.

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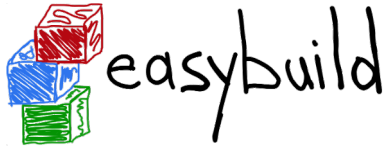
Changing how the module list is displayed



- You may have noticed that you don’t see directories in the module view but descriptive texts
- This can be changed by loading a module
  - ModuleLabel/label : The default view
  - ModuleLabel/PEhierarchy : Descriptive texts, but the PE hierarchy is unfolded
  - ModuleLabel/system : Module directories
- Turn colour on or off using ModuleColour/on or ModuleColour/off
- Show some hidden modules with ModulePowerUser/LUMI
  - This will also show undocumented/unsupported modules!

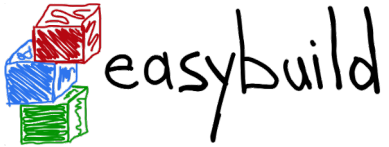
https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_02_Lmod/

Introduction to EasyBuild

The HPE Cray PE

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_03_CPE/

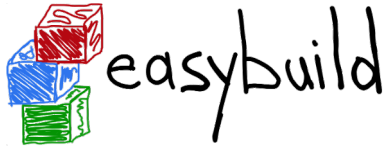
HPE Cray PE components



- Cray compiler environments
  - Compilers preferably used through universal compiler wrappers
  - cc, CC, ftn commands
  - Behaviour depends on the loaded compiler module and target modules
- On LUMI:
  - Cray Compiling Environment (CCE): Clang/LLVM C/C++ and Cray Fortran front-end with LLVM-based backend
  - 3rd party: GNU
  - 3rd party: AMD Optimizing C/C++ and Fortran Compilers (AOCC)
  - 3rd party: AMD ROCm compilers

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_03_CPE/

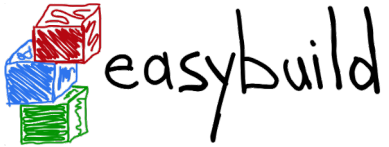
HPE Cray PE components (2)



- Cray Scientific and Math Library
  - LibSci with BLAS, LAPACK, ScaLAPACK, IRT
  - FFTW
  - HDF5 and NetCDF
  - Wrappers take care of adding the right compiler/linker flags based on loaded modules
- Cray Message Passing Toolkit
  - Libfabric-based with Cassini provider for SlingShot 11
  - UCX will no longer work after the late May LUMI upgrade
- DSMML, Cray Performance Analysis Tools, Cray Debugging Support Tools

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_03_CPE/

Programming Environment Modules

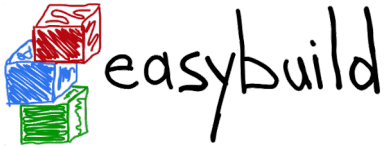


- What they do is determined by a single configuration file
- When interfacing with EasyBuild replaced by an EasyBuild-controlled module

HPE Cray PE	Compiler module	LUMI stack
PrgEnv-cray	cce	cpeCray
PrgEnv-gnu	gcc	cpeGNU
PrgEnv-aocc	aocc	cpeAOCC
PrgEnv-amd	rocm	cpeAMD

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_03_CPE/

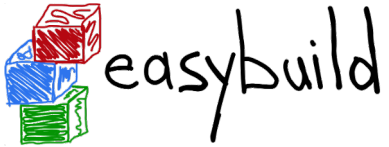
Choosing versions through the cpe module



- Loading cpe/yy.mm
  - Sets the default versions of the Cray PE modules to the versions that come with the particular HPE Cray PE release
  - Reloads already loaded PE modules to switch to the default version
- But buggy due to Cray bugs and Lmod limitations
  - Never load with other modules in a single module command
  - May need to load twice to switch all modules to the new version
- In the LUMI software stacks, the LUMI module takes part of this role over
  - needs to be improved
  - cpeCray/cpeGNU etc. modules always (re)load the right versions

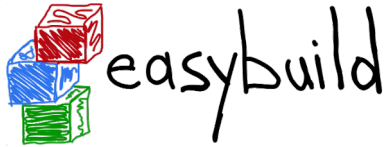
https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_03_CPE/

Target modules



- craype-x86-* set the target architecture for CPU optimisation
- craype-accel-* set the target architecture for OpenMP offload
  - And dummy craype-accel-host
- craype-network-* set the communication library to be used by Cray MPICH.
- craype-hugepages* modules for Cray Huge Pages support (cce and gcc only)
- EasyBuild currently also uses the target modules rather than command line switches to set optimisation target architectures

Unexpected behaviour



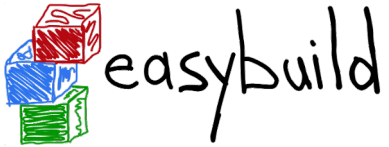
- Dynamic linking needed for system libraries and Cray PE libraries.
- But not all modules set LD_LIBRARY_PATH. Some set CRAY_LD_LIBRARY_PATH instead and will use by default fallback libraries in /opt/cray/pe/lib64
  - And these correspond to the default version of the Cray PE as set in the system
  - So the behaviour of a program may change after a change of default version of the PE

Introduction to EasyBuild

LUMI software stacks

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_04_LUMI_software_stack/

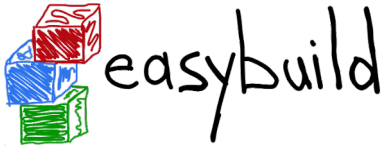
Software stacks: LUMI solution



- Software organised in extensible software stacks based on a particular release of the PE
  - Many base libraries and some packages already pre-installed
  - Easy way to install additional packages in project space
- Modules managed by Lmod
  - More powerful than the (old) Modules Environment which is also supported by HPE Cray
  - Powerful features to search for modules
- EasyBuild is our primary tool for software installations
  - But uses HPE Cray specific toolchains
  - Offer a library of installation recipes
  - User installations integrate seamlessly with the central stack
  - We can help you with setting up Spack also, but this is not yet automated

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_04_LUMI_software_stack/

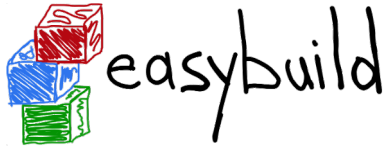
LUMI software stacks



- CrayEnv: Cray environment with some additional tools pushed in through EasyBuild
- LUMI stacks, each one corresponding to a particular release of the PE
  - Work with the Cray PE modules, but accessed through a replacement for the PrgEnv-* modules
  - Tuned versions for the 4 types of hardware: zen2 (login, large memory nodes), zen3 (LUMI-C compute nodes), zen2 + NVIDIA GPU (visualisation partition), zen3 + MI250X (LUMI-G GPU partition)
  - Some software may be installed outside those stacks
- Far future: Stack based on common EB toolchains as-is
  - MPI may be the problem

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_04_LUMI_software_stack/

3 ways to access the Cray PE on LUMI



- Very bare environment available directly after login
  - What you can expect on a typical Cray system
  - Few tools as only the base OS image is available
  - User fully responsible for managing the target modules
- CrayEnv
  - “Enriched” Cray PE environment
  - Takes care of managing the target modules: (re)loading CrayEnv will reload an optimal set for the node you’re on
  - Some additional tools, e.g., newer build tools (offered here and not in the bare environment as we need to avoid conflicts with other software stacks)
  - Otherwise used in the way discussed in this course

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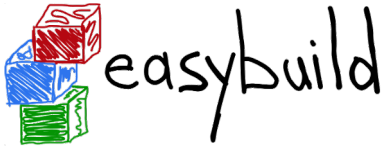
3 ways to access the Cray PE on LUMI



- LUMI software stack
  - Each stack based on a particular release of the HPE Cray PE
  - Other modules are accessible but hidden from the default view
  - Better not to use the PrgEnv modules but the LUMI toolchains

HPE Cray PE	LUMI toolchain	What?
PrgEnv-cray	cpeCray	Cray Compiling Environment
PrgEnv-gnu	cpeGNU	GNU C/C++ and Fortran
PrgEnv-aocc	cpeAOCC	AMD CPU compilers
PrgEnv-amd	cpeAMD	AMD ROCm GPU compilers (LUMI-G only)

  - cpeXXX modules also load the MPI libraries and LibSci just as the PrgEnv-* modules
  - Environment in which we install most software

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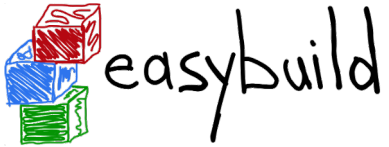
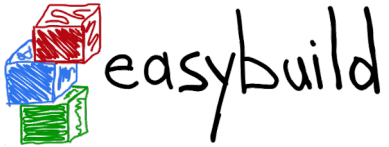
3 ways to access the Cray PE on LUMI



- The LUMI software stack uses two levels of modules
  - LUMI/21.08, LUMI/21.12: Versions of the LUMI stack
  - partition/L, partition/C, partition/EAP (and future partition/D, partition/G): To select software optimised for the respective LUMI partition
    - partition/L is for both the login nodes and the large memory nodes (4TB)
    - partition/EAP doesn't really have any software preinstalled (except for tools that we have everywhere)
  - Hidden partition/common for software that is available everywhere, but be careful using it for your own installs
  - When (re)loaded, the LUMI module will load the best matching partition module.
  - Hence be careful in job scripts: When your job starts, the environment will be that of the login nodes, but if you trigger a reload of the LUMI module it will be that of the compute node!

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_04_LUMI_software_stack/

Partition module



- Targets for the partition modules:

Partition	CPU target	GPU target
partition/L	craype-x86-rome	craype-accel-host
partition/C	craype-x86-milan	craype-accel-host
partition/G	craype-x86-trento	craype-accel-amd-gfx90a
partition/D	craype-x86-rome	craype-accel-nvidia80
partition/EAP	craype-x86-rome	craype-accel-amd-gfx908

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_04_LUMI_software_stack/

Introduction to EasyBuild

Terminology

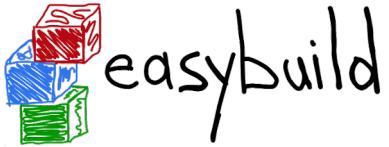
https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_05_terminology/

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, …

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_05_terminology/

EasyBuild terminology: toolchains

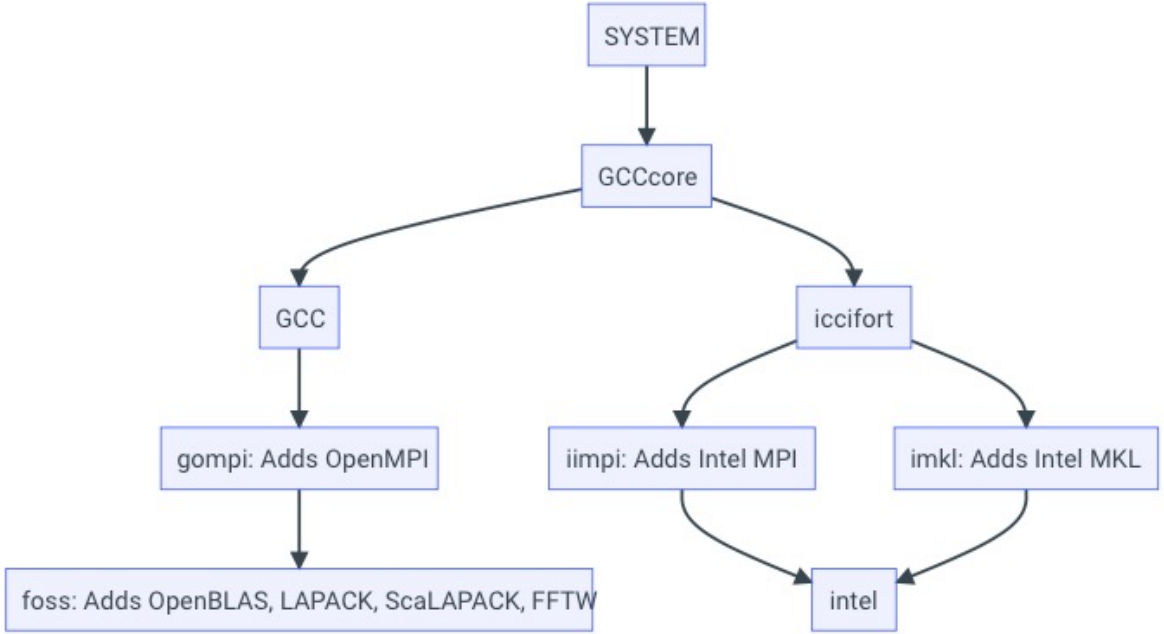


- Compiler toolchain: set of compilers + libraries for MPI, BLAS/LAPACK, FFT, …
- Toolchain component: a part of a toolchain (compiler component, etc.)
- Full toolchain: C/C++/Fortran compilers + libraries for MPI, BLAS/LAPACK, FFT
- Subtoolchain (partial toolchain): compiler-only, only compiler + MPI,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

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_05_terminology/

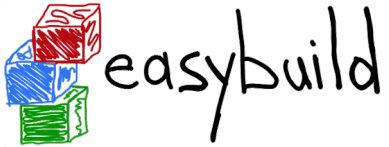
EasyBuild terminology: toolchains

- Organised in a hierarchy



https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_05_terminology/

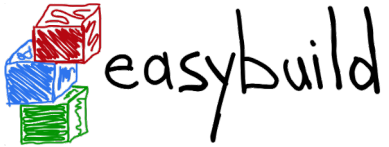
EasyBuild terminology: framework



- 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

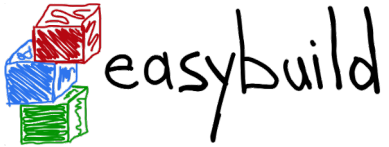
https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_05_terminology/

EasyBuild terminology: easyblock



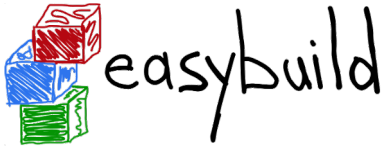
- A Python module that implements a specific software installation procedure
  - Can be viewed as a “plugin” to the EasyBuild framework
- Generic easyblocks for “standard” stuff: cmake + make + make install, Python packages, etc.
- Software-specific easyblocks for complex software (OpenFOAM, TensorFlow, 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



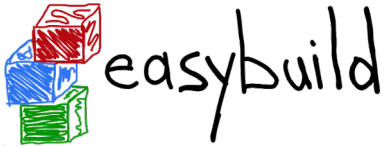
- Text file that specifies what EasyBuild should install (in Python syntax)
- **Collection of values for easyconfig parameters** (key-value definitions)
- Filename typically ends in '`.eb`'
- Specific filename is expected in some contexts (when resolving dependencies)
  - Should match with values for `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 currently
- More Info: https://docs.easybuild.io/en/latest/Easystack-files.html
- My personal experience: Still a bit buggy, but a promising way to organise (re-)installation of a software stack

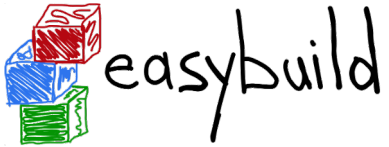
EasyBuild terminology: extensions



- **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
- Feature can work together with Lmod to be able to find extensions included in a module easily but turned off at the moment because of problems with Cray Lmod 8.3.1

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_05_terminology/

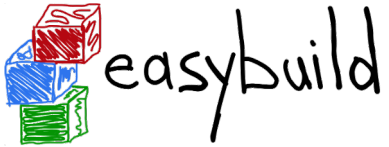
EasyBuild terminology: dependencies



- 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, when linked statically or using RPATH
  - Examples: glibc, OpenBLAS, FFTW, ...
- Currently in EasyBuild: no distinction between link-time and run-time dependencies

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_05_terminology/

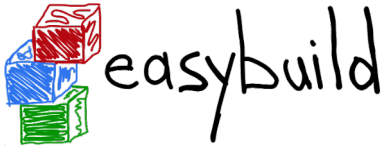
EasyBuild terminology: modules



- 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

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_05_terminology/

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.

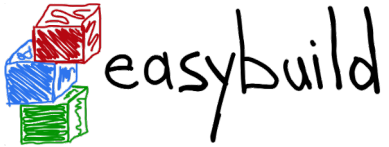
https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_05_terminology/

Introduction to EasyBuild

Installation

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_06_installation/

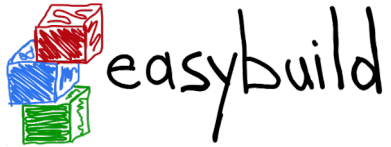
Installing EasyBuild: requirements



- **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 is highly recommended!
- An **environment modules tool** (module command)
  - Default is Lua-based Lmod implementation, highly recommended!
  - Tcl-based implementations are also supported

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_06_installation/

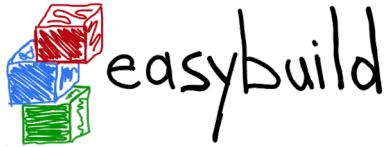
Installing EasyBuild: different options



- 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

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_06_installation/

Installing EasyBuild as a module (recommended)



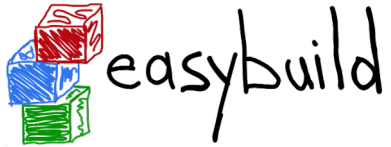
3-step bootstrap procedure

- **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/python3.6/site-packages:$PYTHONPATH
# instruct EasyBuild to use python3 command
export EB_PYTHON=python3
```

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_06_installation/

Installing EasyBuild as a module (recommended)



3-step bootstrap procedure

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

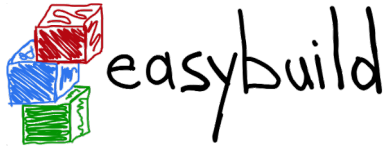
```
eb --install-latest-eb-release --prefix $HOME/easybuild
# and then clean up the temporary EasyBuild installation
rm -r $TMPDIR
```

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

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

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_06_installation/

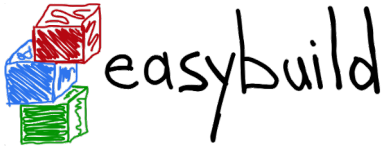
Approach on LUMI



- Each version of the LUMI software stack is bootstrapped to ensure that it can be rebuild on an “empty” system
- Tend to fix the version of EasyBuild for each LUMI stack to ensure that a rebuild of the already installed software is possible
- Use the bootstrapping process
  - There is no `pip` in the system Python so we call the `setup.py` script through Python
  - Then use that version to do a proper install in `partition/common`, using the configuration modules

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_06_installation/

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:

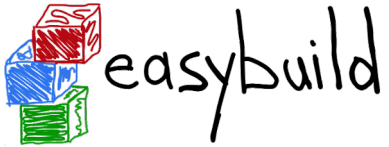
```
eb --show-config
```

- Show system information:

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

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_06_installation/

Updating EasyBuild



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

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

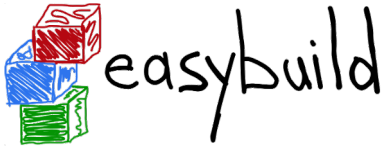
  (+ additional options like `--user`, or using `pip3`, depending on your setup)

- 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:

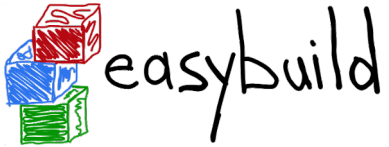
```
module load EasyBuild/4.5.4
```



Introduction to EasyBuild

Configuring EasyBuild

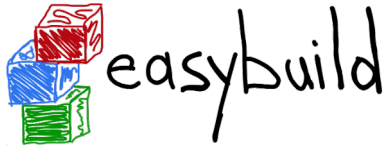
Configuring EasyBuild



- 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)?

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_07_configuration/

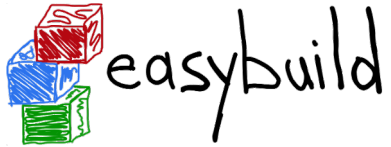
Primary configuration settings



- 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 (work) 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
  - Defaults are as if `--prefix=$HOME/.local/easybuild`
- *Full* list of EasyBuild configuration settings (~250) is available via `eb --help`

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_07_configuration/

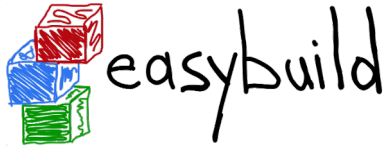
Configuration levels



- 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

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_07_configuration/

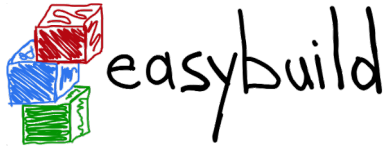
EasyBuild configuration files



- 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!**

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_07_configuration/

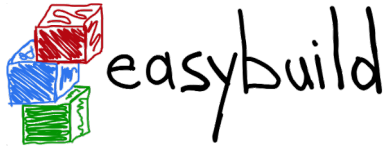
$EASYBUILD_* environment variables



- 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
  - Which is what we do on LUMI with `EasyBuild-user`, `EasyBuild-production` and `EasyBuild-infrastructure`

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_07_configuration/

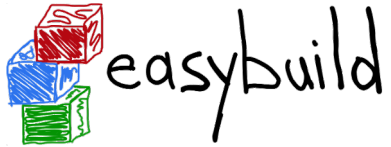
Command line options for `eb` command



- **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`

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_07_configuration/

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`

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_07_configuration/

Inspecting the current configuration: fictitious 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
```

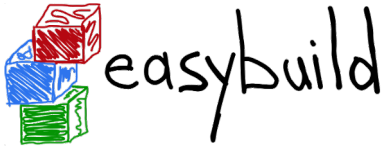
https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_07_configuration/

Introduction to EasyBuild

Basic usage

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_08_basic_usage/

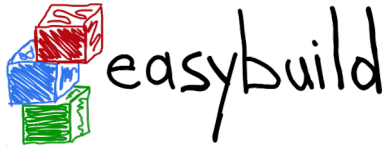
Basic usage of EasyBuild



- **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)

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_08_basic_usage/

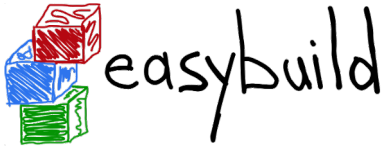
Specifying easyconfigs to use



- 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

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_08_basic_usage/

Searching for easyconfigs

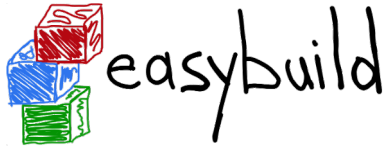


- EasyBuild has 2 options to search for an easyconfig
  - `eb --search` : Output with full paths
  - `eb -S` : Output grouped per repository, common part of the path replaced with a variable

```
$ eb --search openfoam-9
 * /appl/lumi/LUMI-EasyBuild-contrib/easybuild/easyconfigs/o/OpenFOAM/OpenFOAM-9-cpeGNU-21.08.eb
 * /appl/lumi/LUMI-EasyBuild-contrib/easybuild/easyconfigs/o/OpenFOAM/OpenFOAM-9-cpeGNU-21.12.eb
$ eb -S openfoam-9
CFGS1=/appl/lumi/LUMI-EasyBuild-contrib/easybuild/easyconfigs/o/OpenFOAM
 * $CFGS1/OpenFOAM-9-cpeGNU-21.08.eb
 * $CFGS1/OpenFOAM-9-cpeGNU-21.12.eb
```

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_08_basic_usage/

Searching for easyconfigs

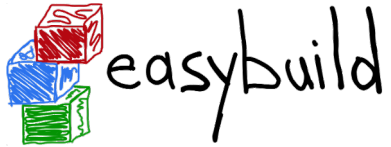


- Search can also use regular expressions
  - But be careful that bash does not expand special characters!

```
$ eb -S '^gromacs-2021.*cpeGNU.*'
CFGS1=/appl/lumi/LUMI-EasyBuild-contrib/easybuild/easyconfigs/g/GROMACS
 * $CFGS1/GROMACS-2021-cpeGNU-21.08-PLUMED-2.7.2-CPU.eb
 * $CFGS1/GROMACS-2021.3-cpeGNU-21.08-CPU.eb
 * $CFGS1/GROMACS-2021.4-cpeGNU-21.12-PLUMED-2.7.4-CPU.eb
 * $CFGS1/GROMACS-2021.4-cpeGNU-21.12-PLUMED-2.8.0-CPU.eb
 * $CFGS1/GROMACS-2021.5-cpeGNU-21.12-CPU.eb
```

- Note that the easyconfigs that come with EasyBuild are not included in the path used for search and dependency resolution.

Inspecting easyconfigs via `eb --show-ec`

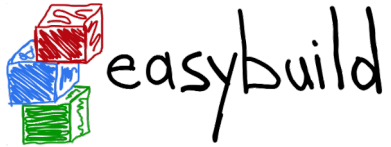


- To see the contents of an easyconfig file, you can use eb --show-ec
- No need to know where it is located, EasyBuild will do that for you!

```
$ eb --show-ec bzip2-1.0.8-cpeCray-21.12.e
…
name =    'bzip2'
version = ‘1.0.8’

homepage = 'https://www.sourceware.org/bzip2/’
…
toolchain = {'name': 'cpeCray', 'version': '21.12'}
toolchainopts = {'pic': True}

source_urls = ['https://sourceware.org/pub/%(name)s/']
sources =     [SOURCE_TAR_GZ]
patches =     ['bzip2-%(version)s-pkgconfig-manpath.patch']
…
```

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_08_basic_usage/

Checking dependencies via `eb --dry-run`



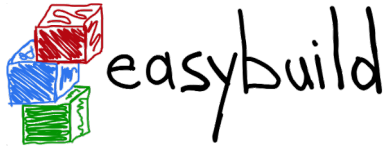
To check which dependencies are required, you can use `eb --dry-run` (or `eb -D`):

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

```
$ eb SAMtools-1.14-cpeGNU-21.12.eb -D
…
CFGS=/appl/lumi
 * [x] $CFGS/mgmt/ebrepo_files/LUMI-21.12/LUMI-common/buildtools/buildtools-21.12.eb (module: buildtools/21.12)
 * [x] $CFGS/mgmt/ebrepo_files/LUMI-21.12/LUMI-L/cpeGNU/cpeGNU-21.12.eb (module: cpeGNU/21.12)
 * [x] $CFGS/mgmt/ebrepo_files/LUMI-21.12/LUMI-L/ncurses/ncurses-6.2-cpeGNU-21.12.eb (module: ncurses/6.2-cpeGNU-21.12)
…
 * [x] $CFGS/mgmt/ebrepo_files/LUMI-21.12/LUMI-L/Brotli/Brotli-1.0.9-cpeGNU-21.12.eb (module: Brotli/1.0.9-cpeGNU-21.12)
 * [x] $CFGS/mgmt/ebrepo_files/LUMI-21.12/LUMI-L/cURL/cURL-7.78.0-cpeGNU-21.12.eb (module: cURL/7.78.0-cpeGNU-21.12)
 * [ ] $CFGS/LUMI-EasyBuild-contrib/easybuild/easyconfigs/h/HTSlib/HTSlib-1.14-cpeGNU-21.12.eb (module: HTSlib/1.14-
cpeGNU-21.12)
 * [ ] $CFGS/LUMI-EasyBuild-contrib/easybuild/easyconfigs/s/SAMtools/SAMtools-1.14-cpeGNU-21.12.eb (module:
SAMtools/1.14-cpeGNU-21.12)
```

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_08_basic_usage/

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

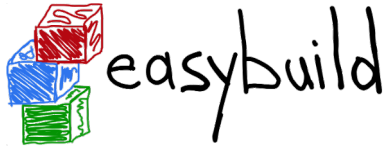


To check which dependencies are still *missing*, use `eb --missing` (or `eb -M`):

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

```
$ eb SAMtools-1.14-cpeGNU-21.12.eb -M
2 out of 11 required modules missing:

* HTSlib/1.14-cpeGNU-21.12 (HTSlib-1.14-cpeGNU-21.12.eb)
* SAMtools/1.14-cpeGNU-21.12 (SAMtools-1.14-cpeGNU-21.12.eb)
```

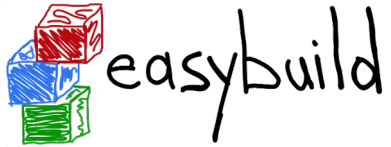
Inspecting software install procedures



- 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!

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_08_basic_usage/

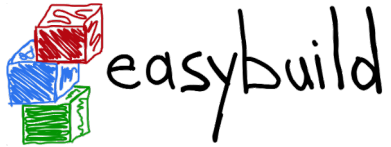
Inspecting software install procedures: example




```
$ eb HTSlib-1.14-cpeGNU-21.12.eb -x
...
[prepare_step method]
Defining build environment, based on toolchain (options) and specified dependencies...

Loading toolchain module...

module load cpeGNU/21.12

Loading modules for dependencies...

module load buildtools/21.12
module load zlib/1.2.11-cpeGNU-21.12
module load bzip2/1.0.8-cpeGNU-21.12
...
```

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_08_basic_usage/

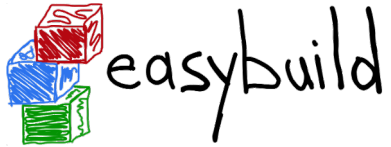
Inspecting software install procedures: example




```
$ eb HTSlib-1.14-cpeGNU-21.12.eb -x
...
Defining build environment...
...
  export CC='cc'
  export CFLAGS='-O2 -ftree-vectorize -fno-math-errno’
...
configuring... [DRY RUN]
[configure_step method]
 running command "./configure --prefix=/users/kurtlust/LUMI-user-appl/SW/LUMI-
21.12/L/HTSlib/1.14-cpeGNU-21.12"
  (in /run/user/10012026/easybuild/build/HTSlib/1.14/cpeGNU-21.12/HTSlib-1.14)
```

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_08_basic_usage/

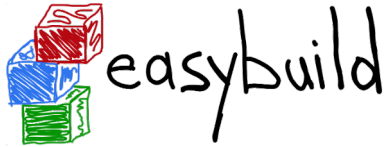
Inspecting software install procedures: example




```
$ eb HTSlib-1.14-cpeGNU-21.12.eb -x
...
building... [DRY RUN]
[build_step method]
  running command "make  -j 256"
  (in /run/user/10012026/easybuild/build/HTSlib/1.14/cpeGNU-21.12/HTSlib-1.14)
testing... [DRY RUN]
[test_step method]
installing... [DRY RUN]
...
```

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_08_basic_usage/

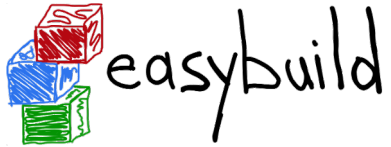
Inspecting software install procedures: example




```
$ eb HTSlib-1.14-cpeGNU-21.12.eb -x
...
Sanity check paths - file ['files']
  * bin/bgzip
  * bin/tabix
  * lib/libhts.so
Sanity check paths - (non-empty) directory ['dirs']
  * include
Sanity check commands
  * bgzip --version
  * htsfile --version
  * tabix --version...
```

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_08_basic_usage/

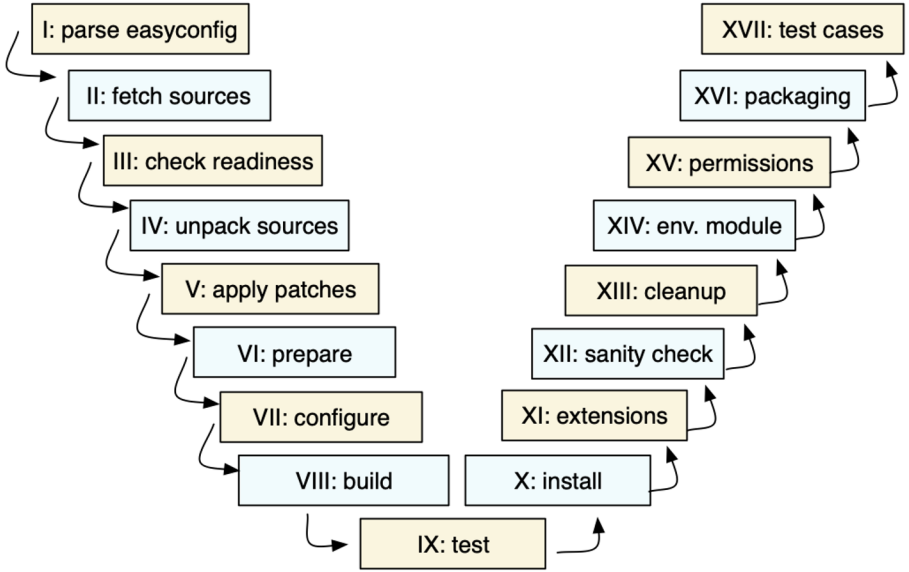
Installing software with EasyBuild



- 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`)

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_08_basic_usage/

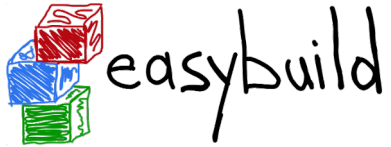
Step-wise installation procedure



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

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_08_basic_usage/

Using software installed with EasyBuild



- On LUMI modules are readily available (at least if the Lmod cache doesn't cause problems)
- Regular EasyBuild installation:

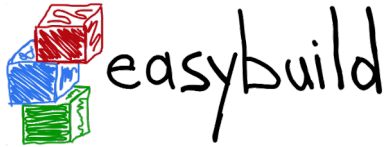
```
# inform modules tool about modules installed with EasyBuild
module use $HOME/easybuild/modules/all
```

- Then in both cases:

```
# 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
```

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_08_basic_usage/

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
```

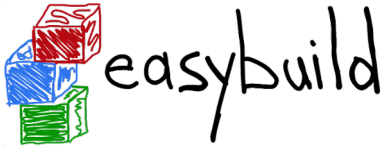
https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/1_Intro/1_08_basic_usage/

Using Easybuild

Troubleshooting

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/2_Using/2_01_troubleshooting/

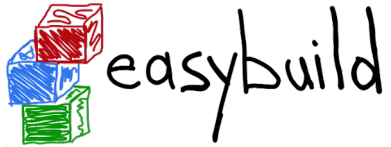
Troubleshooting failing installations



- 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 or patch files
  - Checksum errors
  - 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

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/2_Using/2_01_troubleshooting/

Troubleshooting: error messages



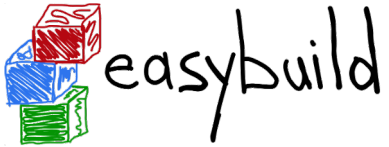
- When EasyBuild detects that something went wrong, it produces an error
- Very often due to a shell command that produced a non-zero exit code...
- Sometimes the problem is clear directly from the error message:

```
== 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...

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/2_Using/2_01_troubleshooting/

Troubleshooting: log files



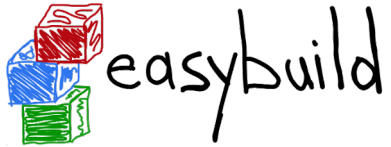
- EasyBuild keeps track of the installation in a detailed log file
- During the installation, it is stored in a temporary directory:

```
$ 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

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/2_Using/2_01_troubleshooting/

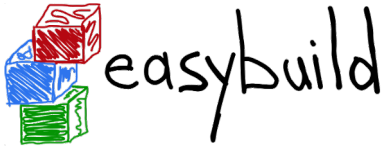
Troubleshooting: last log file



- EasyBuild has a nice trick to access the log file after a failed installation
  - `eb --last-log` returns the file name (including path) of that log file
  - So

```
vim $(eb --last-log)
```

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:

```
== 2021-06-25 13:11:19,968 run.py:222 INFO running cmd:  make -j 9
```

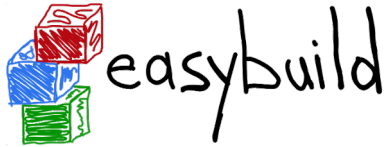
- Different steps of installation procedure are clearly marked:

```
== 2021-06-25 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

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/2_Using/2_01_troubleshooting/

Troubleshooting: inspecting the build directory

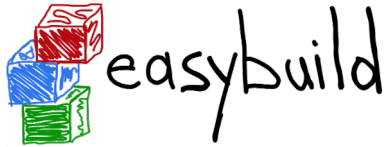


- EasyBuild leaves the build directory in place when the installation failed

  `== 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
  - Rooted at `$EASYBUILD_BUILDPATH`
- For example:
  - Check `config.log` when `configure` command failed
  - Check `CMakeFiles/CMakeError.log` when `cmake` command failed

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/2_Using/2_01_troubleshooting/

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…

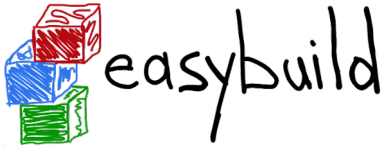
```
$ eb subread.eb
...
== FAILED: Installation ended unsuccessfully (build directory:
/tmp/example/Subread/2.0.1/GCC-8.5.0): build failed (first 300 chars):
Couldn't find file subread-2.0.1-source.tar.gz anywhere, and downloading
it didn't work either...
Paths attempted (in order): ...
```

https://easybuilders.github.io/easybuild-tutorial/2022-CSC_and_LO/2_Using/2_01_troubleshooting/

Using Easybuild

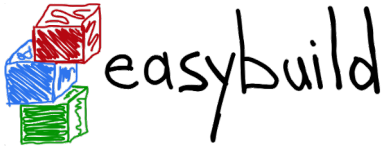
Creating easyconfig files

Adding support for additional software



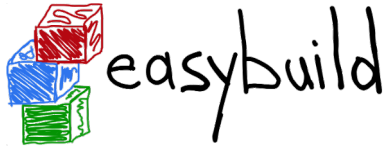
- Every installation performed by EasyBuild requires an easyconfig file
- Easyconfig files can be:
  - Included with EasyBuild itself (or obtained elsewhere)
  - Derived from an existing easyconfig (manually or automatic)
  - Created from scratch
- Most easyconfigs leverage a generic easyblock
- Sometimes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

Easyblocks vs easyconfigs



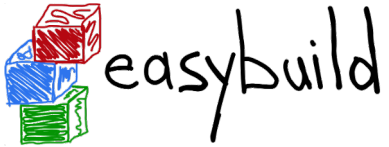
- When can you get away with using an easyconfig leveraging a generic easyblock?
- When is a software-specific easyblock really required?
- Easyblocks are “implement once and forget”
- Easyconfig files leveraging a generic easyblock can become too involved (subjective)
- Reasons to consider implementing 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



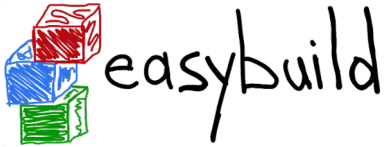
- Collection of easyconfig parameter definitions (Python syntax),
  collectively specify what to install
- Some easyconfig parameters are mandatory, and **must** always be defined:
  `name, version, homepage, description, toolchain`
- Commonly used easyconfig parameters (but strictly speaking not required):
  - `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,9.4.0`
- 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-1.11-GCC-10.2.0.eb SAMtools.eb
...
SAMtools-1.10-GCC-10.2.0.eb copied to SAMtools.eb
```

Hands-on: creating easyconfig files

- Step-wise example + exercise of creating an easyconfig file from scratch
- For a fictive 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"
```

Using Easybuild

Using external modules from the Cray PE

External modules

- Modules not installed through EasyBuild
- Lack:
  - The metadata provided in modules generated by EasyBuild through the EBROOT and EBVERSION environment variables
  - A corresponding easyconfig file to tell EasyBuild about further dependencies
- Use:

```
dependencies = [('cray-fftw', EXTERNAL_MODULE)]
```

```
dependencies = [('cray-fftw/3.3.8.12', EXTERNAL_MODULE)]
```

- But metadata can be added through various mechanisms
  - Default metadata definition file included with EasyBuild (outdated)
  - Own metadata definition files
  - Discovery mechanism: EasyBuild recognises certain environment variables used by Cray modules

Using Easybuild

Implementing easyblocks

- Text-only

Advanced topics

Using EasyBuild as a library

- Text-only

Advanced topics

Using hooks to customise EasyBuild

- Text-only

Advanced topics

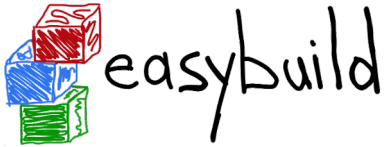
Submitting installations as Slurm jobs

- Text-only

Advanced topics

Module naming schemes

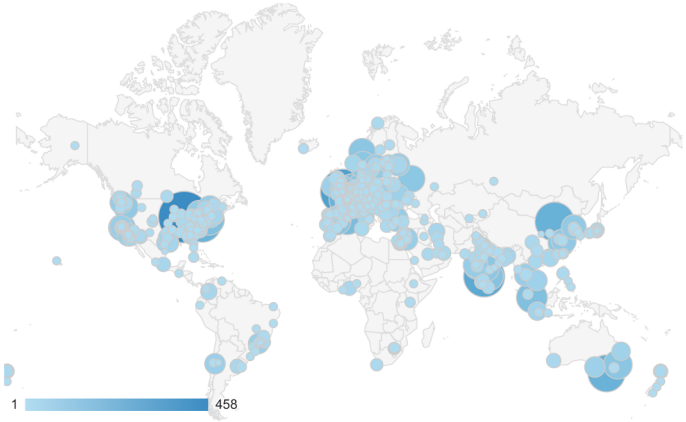
- Text-only



Advanced topics

GitHub integration

The EasyBuild community

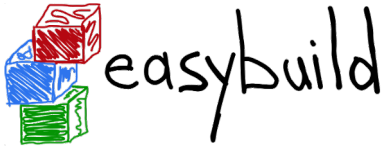


easybuild

- Documentation read all over the world
- HPC sites, consortia, and companies
- Slack: >450 members, ~100 active members per week, 226K messages
- Regular online conf calls...and we even meet in person sometimes!

https://easybuilders.github.io/easybuild-tutorial/2021-isc21/community

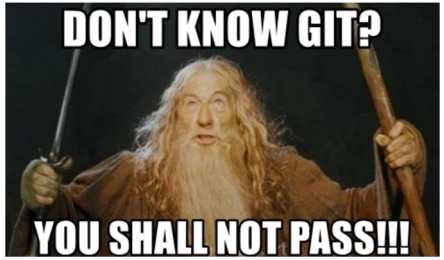
Contributing to EasyBuild



There are several ways to contribute to EasyBuild, including:

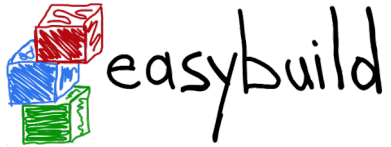
- providing feedback
- reporting bugs
- joining the discussions (mailing list, Slack, conf calls)
- sharing suggestions/ideas for enhancements & additional features
- contributing easyconfigs, enhancing easyblocks,
  adding support for new software, implementing additional features, ...
- extending & enhancing documentation

GitHub integration features



- EasyBuild has strong integration with GitHub, which facilitates contributions
- Some additional Python packages required for this: GitPython, keyring
- Also required some additional configuration, incl. providing a GitHub token
- **Enables creating, updating, reviewing pull requests using eb command!**
- Makes testing contributions very easy (~2,000 easyconfig pull requests per year!)
- Extensively documented:
  https://docs.easybuild.io/en/latest/Integration_with_GitHub.html

Opening a pull request in 1, ~~2, 3~~




```
$ mv sklearn.eb scikit-learn-0.19.1-intel-2017b-Python-3.6.3.eb
$ mv scikit-learn*.eb easybuild/easyconfigs/s/scikit-learn
$ git checkout develop && git pull upstream develop
$ git checkout -b scikit_learn_0191_intel_2017b
$ git add easybuild/easyconfigs/s/scikit-learn
$ git commit -m "{data}[intel/2017b] scikit-learn v0.19.1"
$ git push origin scikit_learn_0191_intel_2017b
```

+ log into GitHub to actually open the pull request (clickety, clickety...)

one single `eb` command

no git commands

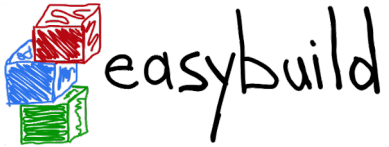
no GitHub interaction

metadata is automatically derived from easyconfig

saves a lot of time!

```
eb --new-pr sklearn.eb
```

Topics we didn't cover...



- Using RPATH linking
- Building Docker/Singularity container images with EasyBuild (experimental)

https://docs.easybuild.io - https://easybuild.io/tutorial

- **EasyBuild: GPLv2 license - Spack: MIT/Apache 2.0 license**
- no stable releases yet for Spack (< 1.0), EasyBuild is stable since 2012
- roughly on par w.r.t. amount of supported software (but differences w.r.t. which software)
- **targeted to different use cases: HPC support teams (EasyBuild) vs developers (Spack)**
- **fixed dependency/toolchain versions in EasyBuild vs flexible CLI in Spack**
- both support running on top of Python 2.7 and 3.5+
- macOS support in EasyBuild is limited (no toolchains/testing for macOS)
- **both projects are backed by an active & supportive community!**
- For a more detailed (but very outdated) comparison, see https://archive.fosdem.org/2018/schedule/event/installing_software_for_scientists

Just one more thing...

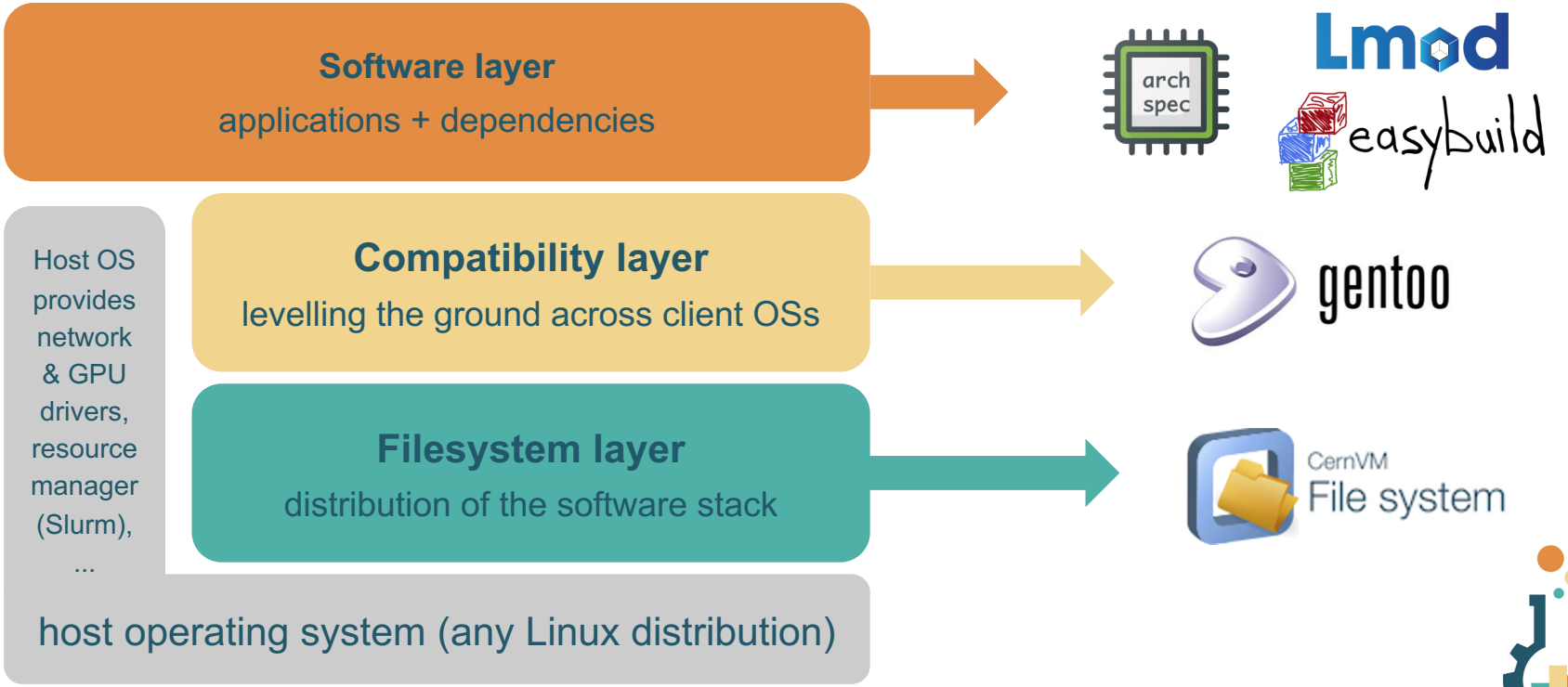
https://www.eessi-hpc.org *https://eessi.github.io/docs*

- **European Environment for Scientific Software Installations (EESSI)**
- Collaboration between different European partners in HPC community
- Goal: building a **common** scientific software stack,
  for HPC systems & beyond (personal workstations, cloud instances, …)
- Heavily inspired by Compute Canada software stack
- Focus on performance, automation, testing, collaboration, ...

High-level overview of the EESSI project

https://www.eessi-hpc.org

https://eessi.github.io/docs



- EESSI is based on EasyBuild while E4S is based on Spack
- Different distribution mechanisms
  - EESSI strictly via CernVM FS
    - Can use CernVM FS from a container, but performance may be slow without close enough cache
  - E4S via build caches with binaries for multiple platforms, or rebuild otherwise + containers for Docker, singularity, Shifter and CharlieCloud