EASYBUILD

EESSI

EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS

Introduction to EasyBuild & EESSI

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https://carlaconference.org/devops-school-for-hpc

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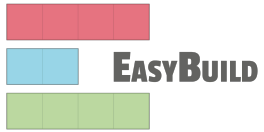
- Masters & PhD in Computer Science from Ghent University (Belgium)
- Joined HPC-UGent team in October 2010
- Main tasks: user support & training, software installations
- Slowly also became EasyBuild lead developer & release manager
- Now also involved with EESSI and MultiXscale EuroHPC Centre-of-Excellence
- Likes family, beer, loud music, FOSS, helping people, dad jokes, stickers, ...
- Doesn't like C++, CMake, SCons, Bazel, TensorFlow, OpenFOAM, ...

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
- 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! (>1,000 members on EasyBuild Slack)

https://easybuild.io

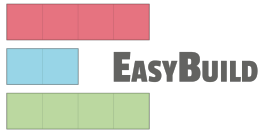
https://docs.easybuild.io

https://blog.easybuild.io

https://github.com/easybuilders

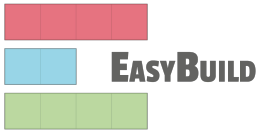
https://easybuild.io/join-slack

EasyBuild in a nutshell



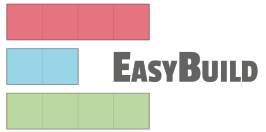
- **Tool** to provide a ***consistent and well performing*** scientific software stack
- Uniform interface for installing scientific software on HPC systems
- Saves time by ***automating*** tedious, boring and repetitive tasks
- Can empower scientific researchers to self-manage their software stack
-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

Key features of EasyBuild (1/2)



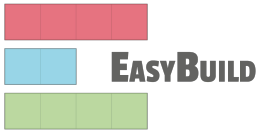
- Supports fully **autonomously** installing (scientific) software, including dependencies, generating environment module files, ...
- **No admin privileges are required** (only write permission to installation prefix)
- **Highly configurable**, easy to extend, support for hooks, easy customisation
- 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, …

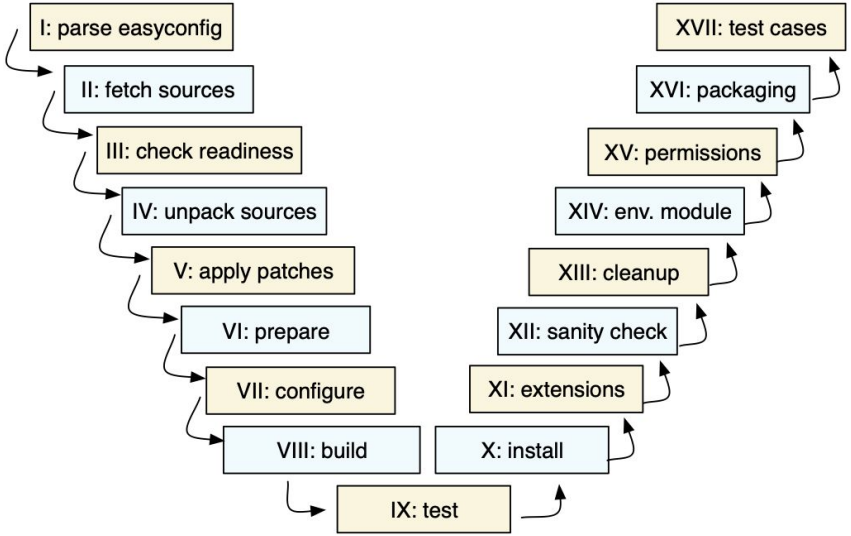
Community effort

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

What EasyBuild is *not*

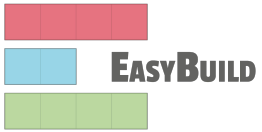
- EasyBuild is **not YABT (Yet Another Build Tool)**
  - It does not try to replace `CMake`, `make`, `pip`, etc.
  - It wraps around those tools and automates installation procedures
- EasyBuild does **not replace traditional Linux package managers** (`yum`, `dnf`, `apt`, ...)
  - You should still install some software via OS package manager
  - Anything that is run with admin privileges and should be updated in-place (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)

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
- Easyconfig file provides the details (software version, dependencies, toolchain, ...)

EasyBuild terminology in a nutshell



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.

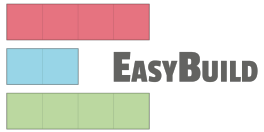
EasyBuild v5.0

- **Released on 18 March 2025**
- Concludes a development effort that was started in March 2023 (103 weeks)
- 1,364 merged pull requests
  (framework: 245, easyblocks: 345, easyconfigs: 804)
- **There will be no more EasyBuild 4.x releases,**
  so you must migrate to EasyBuild v5.x!
- Including backwards-incompatible changes, changes in default configuration, …
- Overview of changes in EasyBuild v5.0: https://docs.easybuild.io/easybuild-v5

Installing EasyBuild: requirements

- **Linux** as operating system (CentOS, RHEL, Ubuntu, Debian, SLES, ...)
  - EasyBuild also works on macOS, but support is very basic
- **Python** 3.6+ (Python 3.9+ recommended)
  - Only Python standard library is required for core functionality of EasyBuild
- An **environment modules tool** (`module` command)
  - Default is Lua-based **Lmod** implementation, highly recommended!
    - On RHEL-based Linux: easy to install Lmod via EPEL
  - Tcl-based implementation (Environment Modules) is 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
  - 2-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: pip install in Python venv

```
$ python3 -m venv eb-env
$ source eb-env/bin/activate

(eb-env) $ pip install easybuild archspec rich
Collecting easybuild
…
Installing collected packages: easybuild-framework, easybuild-easyconfigs,
easybuild-easyblocks, easybuild, archspec, rich, …
Successfully installed archspec-0.2.5 easybuild-5.0.0
easybuild-easyblocks-5.0.0 easybuild-easyconfigs-5.0.0
easybuild-framework-5.0.0 rich-14.0.0 …
…
(eb-env) $ eb --version
This is EasyBuild 5.1.1 (framework: 5.1.1, easyblocks: 5.1.1) on host …
```

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
```

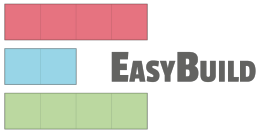
- Show system information:

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

- Check required (and optional) dependencies:

```
eb --check-eb-deps
```

Updating EasyBuild (with pip or 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:

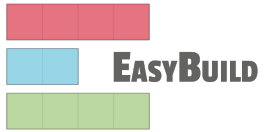
```
eb --install-latest-eb-release
```

  (you may need to install wheel first: `pip install wheel`)

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

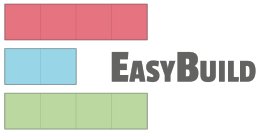
```
module load EasyBuild/5.1.1
```

Configuring EasyBuild



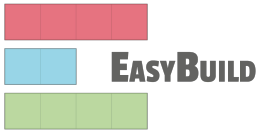
- EasyBuild should work fine out-of-the-box if you are using Lmod as modules tool
- ... but it will (ab)use `$HOME/.local/easybuild` to install software into, etc.
- **It is *strongly* recommended to configure EasyBuild properly!**
- Main questions you should ask yourself:
  - Where should EasyBuild 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 (~280) is available via `eb --help`

Configuration levels

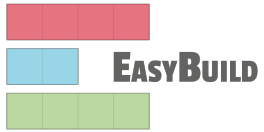


- There are 3 different configuration levels in EasyBuild:
  - **Configuration files** (see `eb --show-default-configfiles`)
  - **Environment variables** (`$EASYBUILD_XYZ`)
  - **Command line options to the `eb` command**

- 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

Inspecting the current configuration

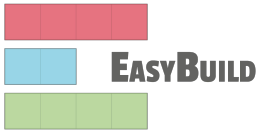


- It can be difficult to remember how EasyBuild was configured
- Output produced by **`eb --show-config`** is useful to remind you
- Shows configuration settings that are different from default
- Always shows a couple of key configuration settings
- Also shows on which level each configuration setting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

Inspecting the current configuration: example

```
$ cat $HOME/config.cfg
[config]
prefix=$HOME/easybuild
buildpath=/tmp/$USER

$ export EASYBUILD_CONFIGFILES=$HOME/config.cfg

$ eb --installpath=/tmp/$USER --show-config
# Current EasyBuild configuration
# (C: command line argument, D: default value,
#  E: environment variable, F: configuration file)
buildpath       (F) = /tmp/ec2-user
configfiles     (E) = /home/ec2-user/config.cfg
containerpath   (F) = /home/ec2-user/easybuild/containers
installpath     (C) = /tmp/ec2-user
packagepath     (F) = /home/ec2-user/easybuild/packages
prefix          (F) = /home/ec2-user/easybuild
repositorypath  (F) = /home/ec2-user/easybuild/ebfiles_repo
robot-paths     (D) = /home/ec2-user/eb-env/easybuild/easyconfigs
rpath           (D) = True
sourcepath      (F) = /home/ec2-user/easybuild/sources
```

Basic usage of EasyBuild



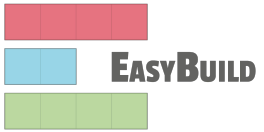
- **Use `eb` command to run EasyBuild**
- Software to install is usually specified via name(s) of easyconfig file(s), or easystack file
- `--robot` (`-r`) option is required to also install missing dependencies (and toolchain)
- Typical workflow:
  - Find or create easyconfig files to install desired 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)

Search for easyconfigs via `eb --search`

To search for easyconfig files to install (case-insensitive), use `eb --search`

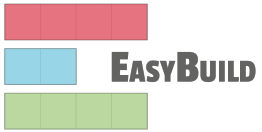
```
$ eb --search bcftools
== found valid index for /home/ec2-user/eb-env/easybuild/easyconfigs, so using it...
 * /home/example/eb-env/easybuild/easyconfigs/b/BCFtools/BCFtools-1.12-GCC-10.3.0.eb
 * /home/example/eb-env/easybuild/easyconfigs/b/BCFtools/BCFtools-1.14-GCC-11.2.0.eb
 * /home/example/eb-env/easybuild/easyconfigs/b/BCFtools/BCFtools-1.15.1-GCC-11.3.0.eb
 * /home/example/eb-env/easybuild/easyconfigs/b/BCFtools/BCFtools-1.17-GCC-12.2.0.eb
 * /home/example/eb-env/easybuild/easyconfigs/b/BCFtools/BCFtools-1.18-GCC-12.3.0.eb
 * /home/example/eb-env/easybuild/easyconfigs/b/BCFtools/BCFtools-1.19-GCC-13.2.0.eb
 * /home/example/eb-env/easybuild/easyconfigs/b/BCFtools/BCFtools-1.21-GCC-13.3.0.eb
```

Installing software with EasyBuild



- To install software with EasyBuild, just run the `eb` command:
  - `eb BCFtools-1.18-GCC-12.3.0.eb`
- If any dependencies are still missing, you will need to also use `--robot`:
  - `eb SAMtools-1.18-GCC-12.3.0.eb --robot`
- More details while the installation is running via trace output (default in EasyBuild v5.x)
  - `eb BCFtools-1.18-GCC-12.3.0.eb --robot --trace`
- To reinstall software, use `eb --rebuild` (or `eb --force`)

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/1.18-GCC-12.3.0
```

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 BCFtools-1.18-GCC-12.3.0.eb
easyblock = 'ConfigureMake'

name = 'BCFtools'
version = '1.18'

homepage = 'https://www.htslib.org/'
description = """Samtools is a suite of programs for interacting with high-throughput
sequencing data.
 BCFtools - Reading/writing BCF2/VCF/gVCF files and calling/filtering/summarising SNP and
short indel sequence
 variants"""

toolchain = {'name': 'GCC', 'version': '12.3.0'}
toolchainopts = {'pic': True}
…
```

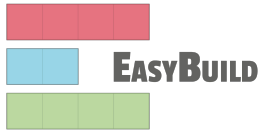
Checking dependencies via `eb --dry-run`

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

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

```
$ eb BCFtools-1.18-GCC-12.3.0.eb -Dr
 ...
 * [x] $CFGS/x/XZ/XZ-5.4.2-GCCcore-12.3.0.eb (module: XZ/5.4.2-GCCcore-12.3.0)
 * [x] $CFGS/g/GSL/GSL-2.7-GCC-12.3.0.eb (module: GSL/2.7-GCC-12.3.0)
 * [x] $CFGS/h/HTSlib/HTSlib-1.18-GCC-12.3.0.eb (module: HTSlib/1.18-GCC-12.3.0)
 * [ ] $CFGS/b/BCFtools/BCFtools-1.18-GCC-12.3.0.eb (module:
BCFtools/1.18-GCC-12.3.0)
```

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

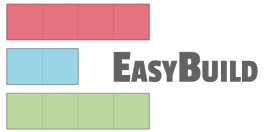


To check which dependencies are still *missing*, use `eb --missing` (or `eb -M`):

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

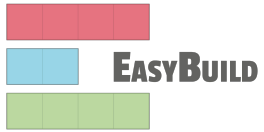
```
$ eb BCFtools-1.18-GCC-12.3.0.eb --missing

1 out of 23 required modules missing:

* BCFtools/1.18-GCC-12.3.0 (BCFtools-1.18-GCC-12.3.0.eb)
```

Inspecting software install procedures



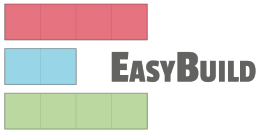
- EasyBuild can quickly unveil how exactly it *would* install an easyconfig file
- Via `eb --extended-dry-run` (or `eb -x`)
- Produces detailed output in a matter of seconds
- **Software is not actually installed, shell commands + file operations are skipped!**
- Some guesses and assumptions are made, 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



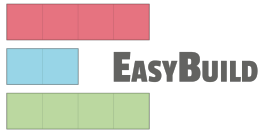

```
$ eb Boost-1.82.0-GCC-12.3.0.eb -x
...
Defining build environment...
  ...
  export CXX='g++'
  export CXXFLAGS='-O2 -ftree-vectorize -march=native -fno-math-errno -fPIC'
  ...

configuring... [DRY RUN]

[configure_step method]
  running shell command "./bootstrap.sh --with-toolset=gcc
--prefix=/home/example/software/Boost/1.82.0-GCC-12.3.0 --without-libraries=python,mpi"
  (in /tmp/example/build/Boost/1.82.0/GCC-12.3.0)
  ...
```

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: log files

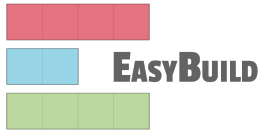


- EasyBuild keeps track of the installation in a detailed log file
- During the installation, it is stored in a temporary directory:

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

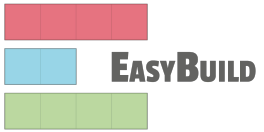
- Includes executed shell commands and output, build environment, etc.
- More detailed log file when debug mode is enabled (`debug` configuration setting)
- There is a log file per EasyBuild session, and one per performed installation
- **When an installation completes successfully,**
  the log file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

Troubleshooting: inspecting the build directory



- EasyBuild leaves the build directory in place when the installation 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 with EasyBuild v5.x



- **EasyBuild v5.x makes troubleshooting failing installations significantly easier**
- When a shell command run by EasyBuild fails:
  - The problem will be reported in a more user-friendly way
  - You can quickly inspect (only) the output of that command
  - A script is generated to start an **interactive shell session** to debug “in context”: in the correct working directory + prepared build environment
- Made possible by switching to new `run_shell_cmd` function

https://docs.easybuild.io/interactive-debugging-failing-shell-commands

Improved error reporting in EasyBuild v5.x

EasyBuild 5.x produces clearer error messages when a shell command failed:

```
ERROR: Shell command failed!
      full command              ->  make  -j 8 LDFLAGS='-lfast'
      exit code                 ->  2
      called from               ->  'build_step' function in /.../easyblocks/generic/configuremake.py (line 357)
      working directory         ->  /tmp/ec2-user/kenneth/easybuild/build/BCFtools/1.18/GCC-12.3.0/bcftools-1.18
      output (stdout + stderr)  ->  /tmp/eb-i61vle8x/run-shell-cmd-output/make-1ynysa6f/out.txt
      interactive shell script  ->  /tmp/eb-i61vle8x/run-shell-cmd-output/make-1ynysa6f/cmd.sh
```

- Colors to draw attention to the most important parts of the error message
- File with (only) command output + path to build directory are easy to find
- **Auto-generated `cmd.sh` script starts interactive subshell in correct build environment!**

https://docs.easybuild.io/interactive-debugging-failing-shell-commands

Adding support for additional software

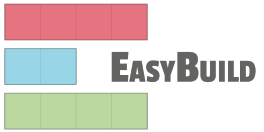
- **Every installation performed by EasyBuild requires an easyconfig file**
- Easyconfig files can be:
  - Included with EasyBuild itself (or obtained elsewhere)
  - Derived from an existing easyconfig (manually or automatic)
  - Created from scratch
- Most easyconfigs leverage a generic easyblock
-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

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`

https://docs.easybuild.io/writing-easyconfig-files

Easyblocks vs easyconfigs



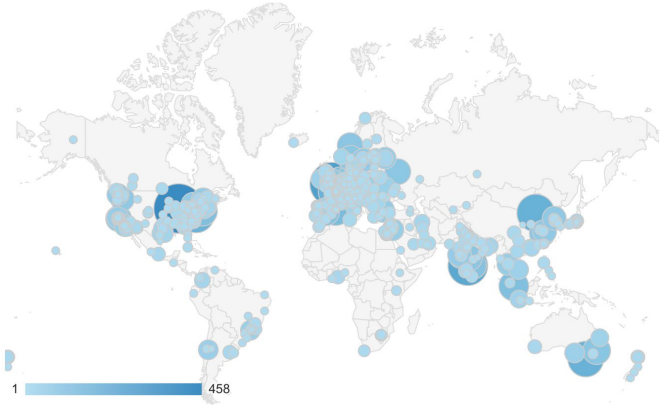
- When can you get away with using an easyconfig leveraging a generic easyblock?
- When is a software-specific easyblock really required?
- Easyblocks are *“implement once and forget”*
- Easyconfig files leveraging a generic easyblock can become too complicated (subjective)
- Reasons to consider implementing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

Exercise on creating easyconfig file from scratch

- Step-wise example + exercise of creating an easyconfig file from scratch
- For fictitious software packages: `eb-tutorial` + `py-eb-tutorial`
- Sources available at https://github.com/easybuilders/easybuild-tutorial/tree/main/docs/files
- **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"
```

The EasyBuild community

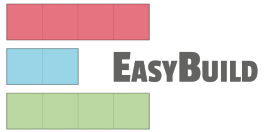


EASYBUILD

- Documentation is read all over the world
- HPC sites, consortia, and companies
- Slack: >1000 members,

  ~180 active members per week
- Bi-weekly online conf calls + yearly user meeting

Contributing to EasyBuild



There are several ways to contribute to EasyBuild, including:

- Providing feedback (positive or negative)
- 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 requires some additional configuration, incl. providing a GitHub token
- **Enables creating, updating, reviewing pull requests using `eb` command!**
- Makes testing contributions very easy: ~2,500 easyconfig pull requests per year!
- Extensively documented:
  docs.easybuild.io/integration-with-github

Opening a pull request in 1, 2, 3

```
$ mv sklearn.eb scikit-learn-1.4.2-gfbf-2023a.eb
$ mv scikit-learn*.eb easybuild/easyconfigs/s/scikit-learn
$ git checkout develop && git pull upstream develop
$ git checkout -b scikit_learn_142_gfbf_2023a
$ git add easybuild/easyconfigs/s/scikit-learn
$ git commit -m "{data}[gfbf/2023a] scikit-learn v1.4.2"
$ git push origin scikit_learn_142_gfbf_2023a
```

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

one single `eb` command

no git commands

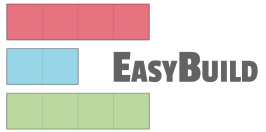
no GitHub interaction

metadata is automatically derived from easyconfig

saves a lot of time!

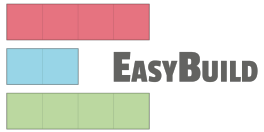
`eb --new-pr sklearn.eb`

Customizing EasyBuild via Hooks



- Hooks allow you to customize EasyBuild easily and consistently
- Set of Python functions that are automatically picked up by EasyBuild
- Can be used to ”hook” custom code into specific installation steps
- Make EasyBuild use your hooks via `hooks` configuration option
- Examples:
  - Inject or tweak configuration options
  - Change toolchain definitions
  - Custom checks to ensure that site policies are taken into account
- Extensively documented: docs.easybuild.io/hooks

Hooks: examples



- EUM'22 talk by Alex: Building a heterogeneous MPI stack with EasyBuild

  https://easybuild.io/eum22/#eb-mpi

- `contrib/hooks` subdirectory in easybuild-framework GitHub repository:

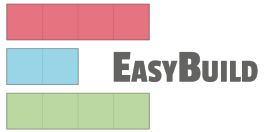
  https://github.com/easybuilders/easybuild-framework/tree/develop/contrib/hooks

Hooks: examples

Ensure that software is installed with a specific license group:

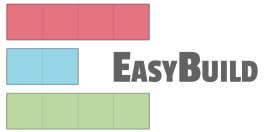
```
def parse_hook(self, *args, **kwargs):
    if self.name == 'example':
        # use correct license group for software ‘example’
        self['group'] = 'licensed_users_example'
```

Implementing Easyblocks



- An easyblock may be required for more complex software installations
- This requires some Python skills, and familiarity with EasyBuild framework
- A software-specific easyblock can derived from a generic easyblock
- Focus is usually on configure/build/installs steps of installation procedure
- See also https://docs.easybuild.io/implementing-easyblocks

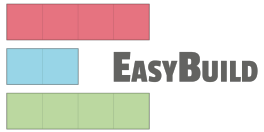
Submitting Installations as Slurm Jobs



- EasyBuild can *distribute* the installation of a software stack as jobs on a cluster
- Slurm is the default job backend in EasyBuild v5.x
- Use "`eb ... --job --robot`" to submit software installations

  to be performed with EasyBuild as Slurm jobs
- See also https://docs.easybuild.io/submitting-jobs

Questions?

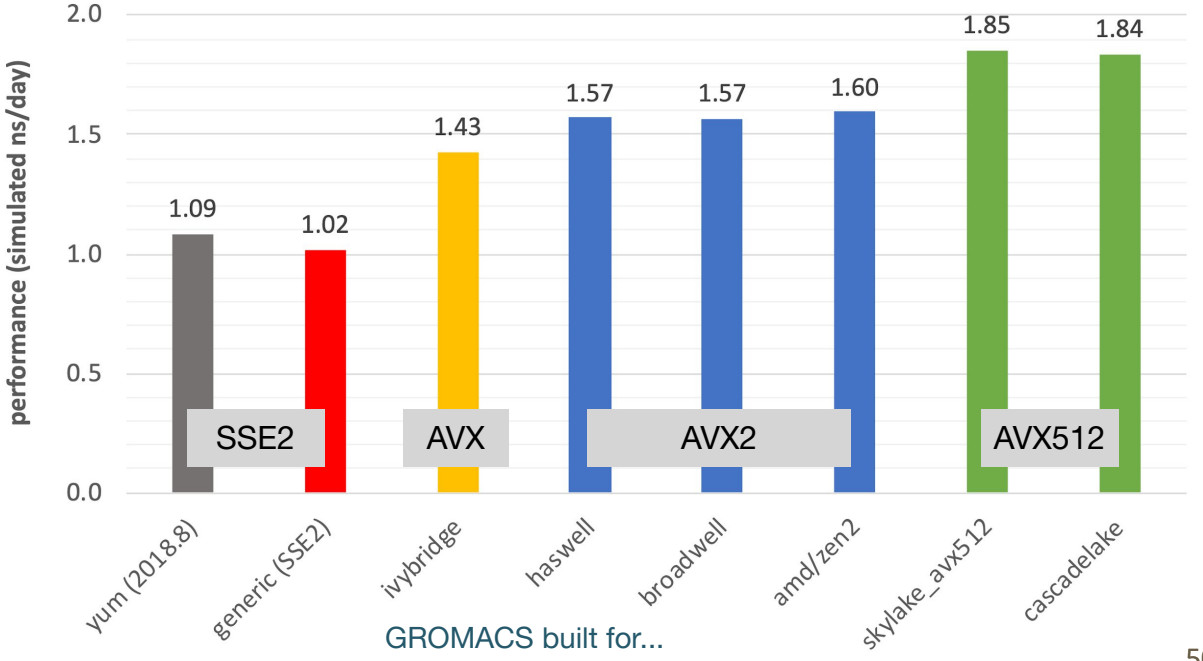


- Website: https://easybuild.io
- Documentation: https://docs.easybuild.io
- Tutorials: https://tutorial.easybuild.io
- EasyBuild User Meeting: https://easybuild.io/eum (slides+recording of *all* talks available!)
- Getting help:
  - Mailing list: https://lists.ugent.be/wws/subscribe/easybuild
  - **Slack: https://easybuild.slack.com - https://easybuild.io/join-slack**
  - Bi-weekly conference calls: https://github.com/easybuilders/easybuild/wiki/Conference-calls

Optimized scientific software installations

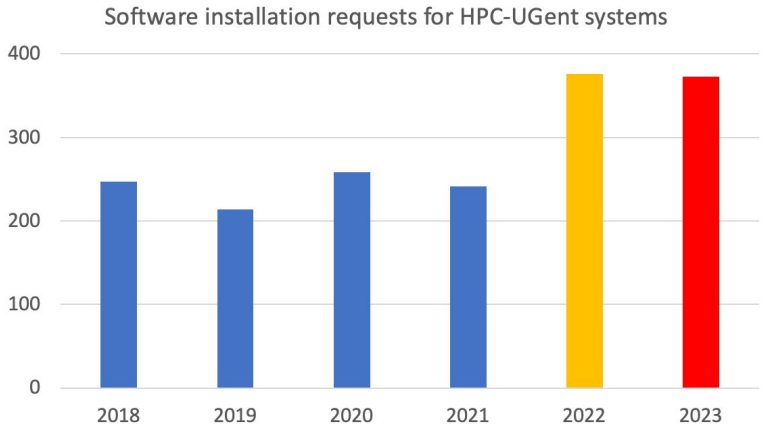
- Software should be optimized for the system it will run on (keep the P in HPC!)
- Impact on performance is often significant for scientific software!

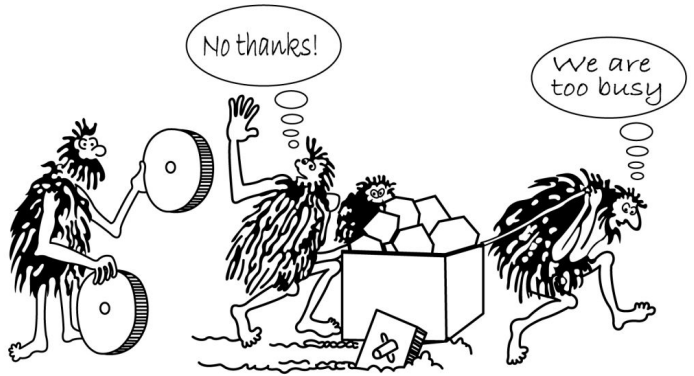
- Example: GROMACS 2020.1 (PRACE benchmark, Test Case B)
- Metric: (simulated) ns/day, higher is better
- Test system: dual-socket Intel Xeon Gold 6420 (Cascade Lake, 2x18 cores)
- **Performance of different GROMACS binaries, on exact same hardware/OS**



The changing landscape of scientific computing

- **Explosion of available scientific software** applications (bioinformatics, AI boom, …)
- Increasing interest in **cloud** for scientific computing (flexibility!)
- **Increasing variety in processor (micro)architectures** beyond Intel & AMD:
  Arm is ~~coming~~ already here (see Fugaku, JUPITER, …), RISC-V is coming (soon?)
- In strong contrast: available (wo)manpower **in HPC support teams is (still) limited**…





What if you no longer have to install

*a **broad range of scientific software***

from scratch on every laptop, HPC cluster,

or cloud instance you use or maintain,

without compromising on performance?

EESSI in a nutshell

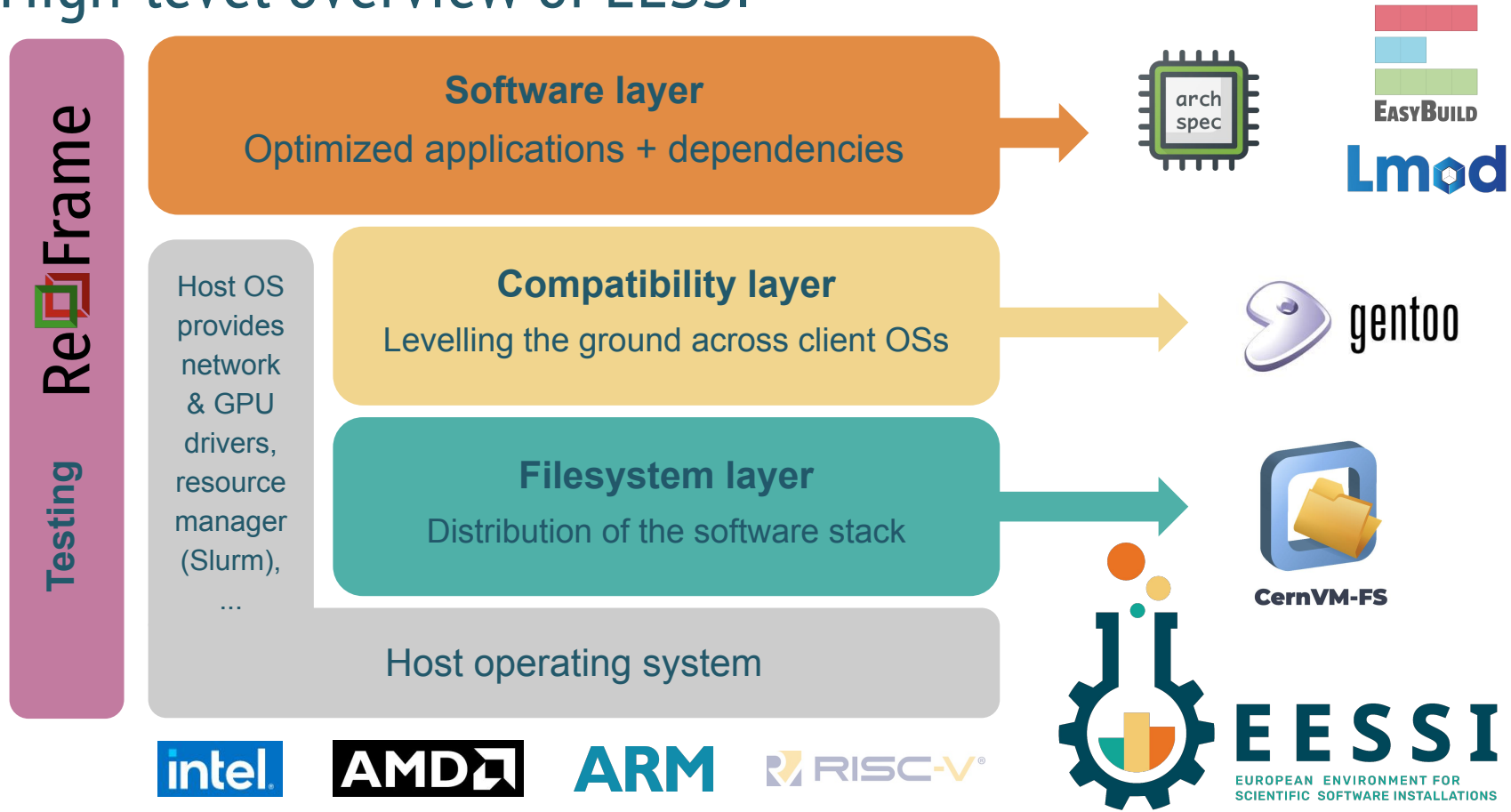
- *European Environment for Scientific Software Installations (EESSI)*
- **Shared repository of (optimized!) scientific software *installations***
- Avoid duplicate work across (HPC) sites by collaborating on a shared software stack
- Uniform way of providing software to users, regardless of the system they use!
- Should work on any Linux OS and system architecture
  - From laptops and personal workstations to HPC clusters and cloud
  - Support for different CPUs, interconnects, GPUs, etc.
- **Focus on performance, automation, testing, collaboration**

https://www.eessi.io/docs/

Major goals of EESSI

- Providing a truly **uniform software stack**
  - Use the (exact) same software environment everywhere
  - **Without sacrificing performance** for “mobility of compute”
    (like is typically done with containers/conda)
- **Avoid duplicate work** (for researchers, HPC support teams, sysadmins, …)
  - Tools that automate software installation process
    (EasyBuild, Spack) are not sufficient anymore
  - Go beyond sharing build recipes => work towards a shared software stack
- Facilitate HPC training, development of (scientific) software, …

High-level overview of EESSI



EESSI ingredients

Compatibility layer

Abstraction from the host operating system

Filesystem Layer

Global distribution of software installations via CernVM-FS

EESSI

EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS

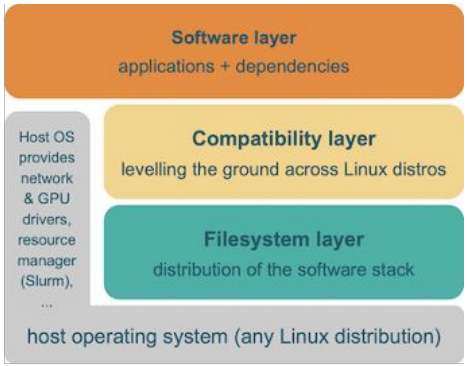
Software Layer

Optimized software installations for specific CPU microarchitectures

Intuitive user interface: module avail, module load, …

Automatic selection of best suited part of software stack for CPU microarchitectures

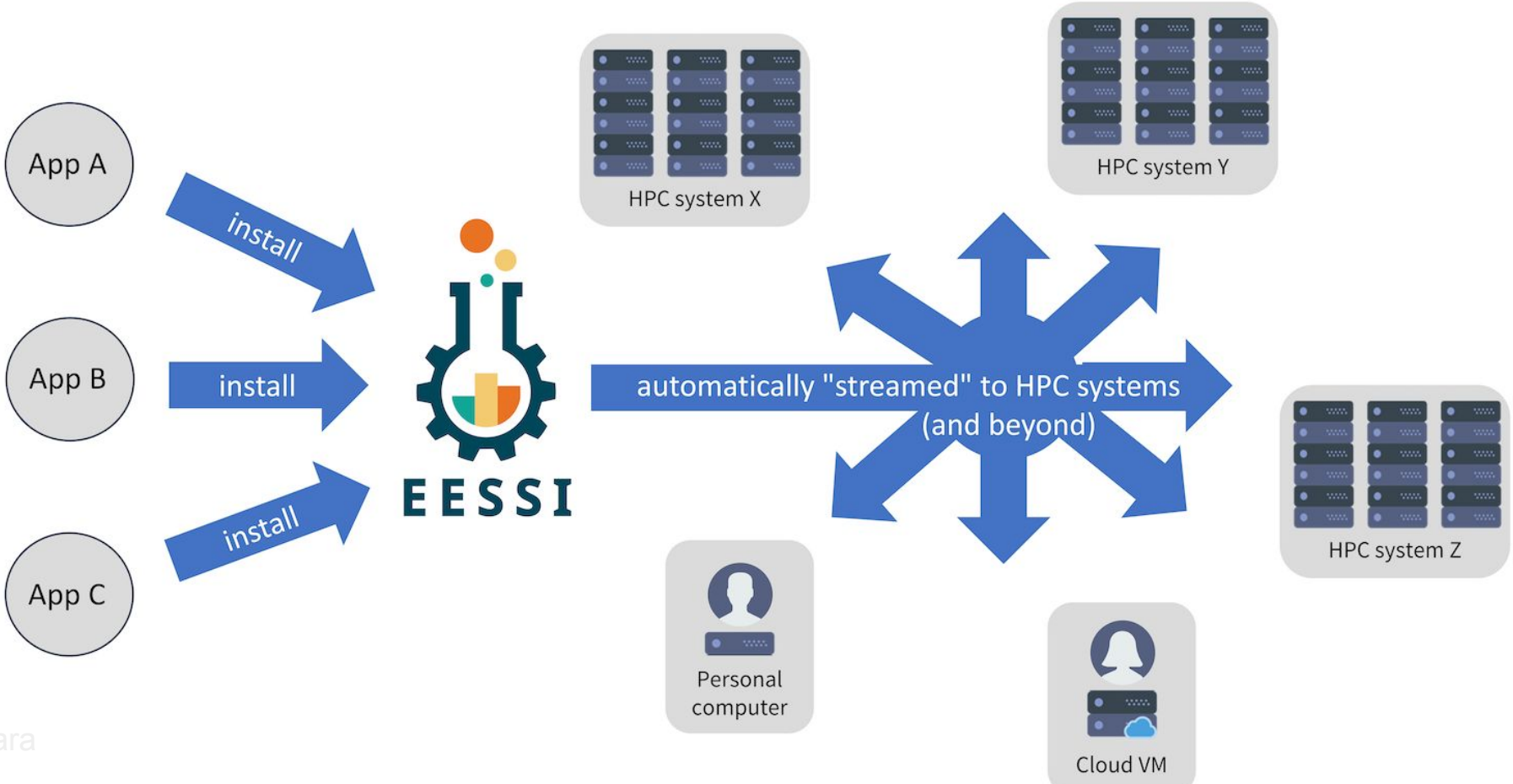
How does EESSI work?



- Software installations included in EESSI are:
  - Automatically **“streamed in” on demand** (via CernVM-FS)
  - Built to be **independent of the host operating system**

    “Containers without the containing”
  - **Optimized** for specific CPU generations + specific GPU types
- Initialization script **auto-detects** CPU + GPU of the system

EESSI as a shared software stack

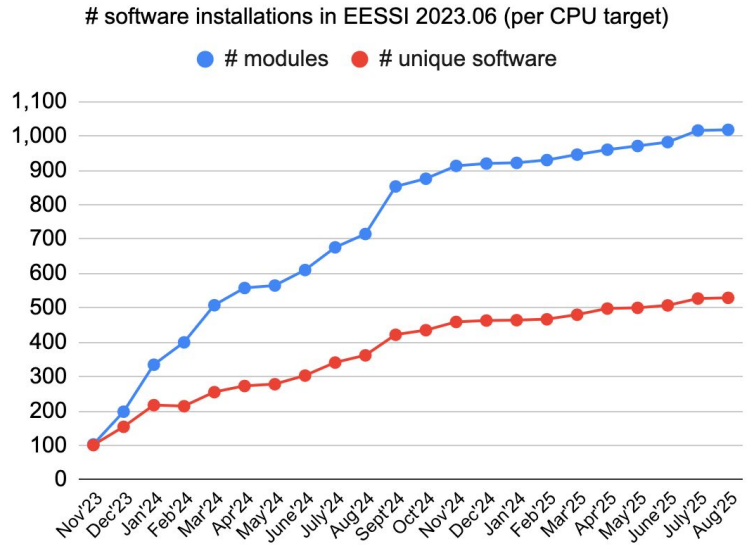


Overview of available software in EESSI

Currently > 1,000 software installations available per supported CPU target

via `software.eessi.io` CernVM-FS repository; increasing every week

- **13** (+1) **supported CPU targets** (x86_64 + Arm), see https://eessi.io/docs/software_layer/cpu_targets
- **Over 500 different software packages**, excl. extensions: Python packages, R libraries
- **Over 15,000 software installations in total**
- Including ESPResSo, GROMACS, LAMMPS, OpenFOAM, PyTorch, R, QuantumESPRESSO, TensorFlow, waLBerla, WRF, ...
- eessi.io/docs/available_software/overview



- Using `foss/2023a` and `foss/2023b` toolchains in EESSI 2023.06
- Using `foss/2024a` and `foss/2025a` toolchains in EESSI 2025.06

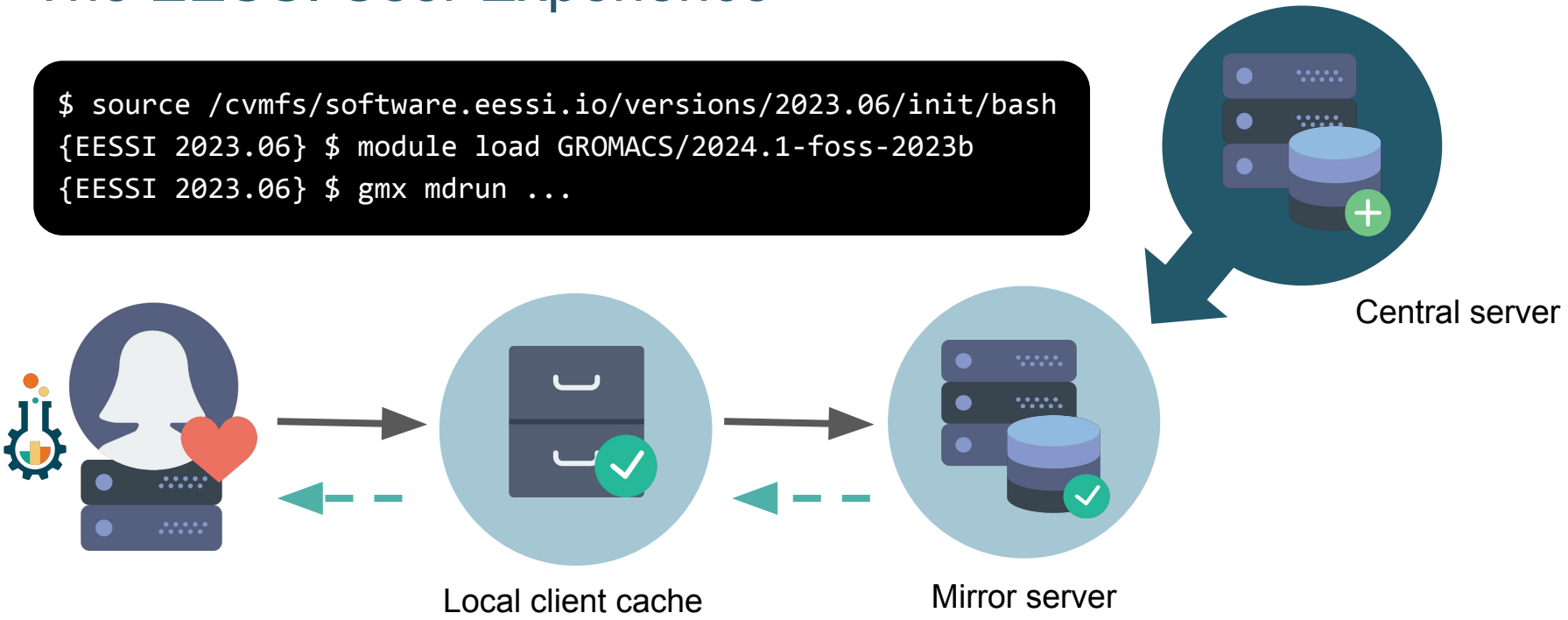
Getting access EESSI via CernVM-FS (demo)

```
# Native installation
# Installation commands for RHEL-based distros
# like CentOS, Rocky Linux, Almalinux, Fedora, …

# install CernVM-FS
sudo yum install -y
https://ecsft.cern.ch/dist/cvmfs/cvmfs-release/cvmfs-release-latest.noarch.rpm
sudo yum install -y cvmfs

# create client configuration file for CernVM-FS
# (no proxy, 10GB local CernVM-FS client cache)
sudo bash -c "echo 'CVMFS_CLIENT_PROFILE="single"' > /etc/cvmfs/default.local"
sudo bash -c "echo 'CVMFS_QUOTA_LIMIT=10000' >> /etc/cvmfs/default.local"

# Make sure that EESSI CernVM-FS repository is accessible
sudo cvmfs_config setup
```

Alternative ways of accessing EESSI are available, via a container image, via cvmfsexec, …
eessi.io/docs/getting_access/native_installation - eessi.io/docs/getting_access/eessi_container

The EESSI User Experience

```
$ source /cvmfs/software.eessi.io/versions/2023.06/init/bash
{EESSI 2023.06} $ module load GROMACS/2024.1-foss-2023b
{EESSI 2023.06} $ gmx mdrun ...
```



EESSI provides **on-demand streaming**

of (scientific) software (like music, TV-series, …)

Using EESSI (demo)

eessi.io/docs/using_eessi/eessi_demos

```
/cvmfs/software.eessi.io/versions/2023.06/software
`-- linux
    |-- aarch64
    |   |-- a64fx
    |   |-- generic
    |   |-- neoverse_n1
    |   |-- neoverse_v1
    |   `-- nvidia/grace
    `-- x86_64
        |-- amd
        |   |-- zen2
        |   |-- zen3
        |   `-- zen4
        |-- generic
        `-- intel
            |-- cascadelake
            |-- haswell
            |-- icelake
            |-- haswell
            `-- sapphirerapids
                |-- modules
                `-- software
```

```
$ source /cvmfs/software.eessi.io/versions/2023.06/init/bash
Found EESSI pilot repo @
/cvmfs/software.eessi.io/versions/2023.06!
archdetect says x86_64/amd/zen3
Using x86_64/amd/zen3 as software subdirectory
...
Environment set up to use EESSI pilot software stack, have fun!

{EESSI 2023.06} $ module load R/4.3.2-gfbf-2023a

{EESSI 2023.06} $ which R
/cvmfs/software.eessi.io/versions/2023.06/software/linux/x86_64/
amd/zen3/software/R/4.3.2-gfbf-2023a/bin/R

{EESSI 2023.06} $ R --version
R version 4.3.2
```

Automatically detects CPU microarchitecture

Website: https://eessi.io

Join our Slack channel (see join link on website)

Documentation: https://eessi.io/docs

Blog: https://eessi.io/docs/blog

GitHub: https://github.com/EESSI

Paper (open access): https://doi.org/10.1002/spe.3075

EESSI YouTube channel

Bi-monthly online meetings

(first Thursday, odd months, 2pm CEST)

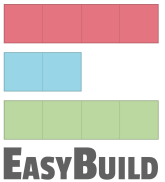
Webinar series: Different aspects of EESSI

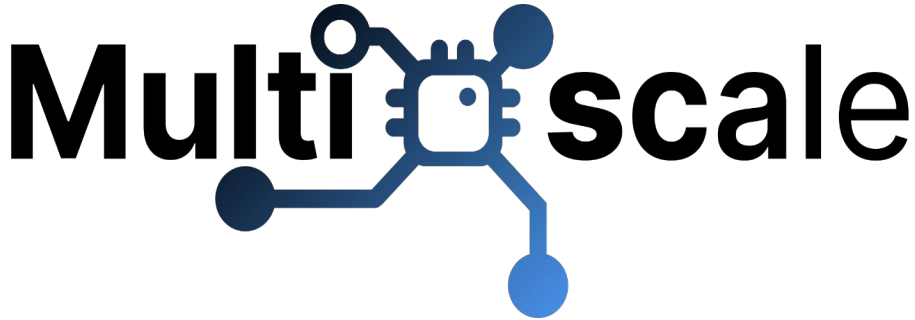
5 Mondays in a row May-June 2025

https://eessi.io/docs/training/2025/webinar-series-2025Q2

- Introduction to EESSI
- Introduction to CernVM-FS
- Introduction to EasyBuild
- EESSI for CI/CD *(26 May)*
- Using EESSI as the base for a system stack *(2 June)*

Slides + recordings available





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