EasyBuild tutorial
ISC'22

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29 May 2022

https://easybuild.io/tutorial/isc22

Agenda

(all times are CEST)

ISC High Performance
The HPC Event.

easybuild

- [14:00-14:10] **Practical information w.r.t. prepared environment for hands-on**
- [14:10-14:30] Introduction to EasyBuild: scope & terminology
- [14:30-14:50] Installing & configuring EasyBuild + basic usage
- [14:50-15:30] Installing software with EasyBuild + troubleshooting
- [15:30-16:00] Adding support for additional software
- [16:00-16:30] *(coffee break)*
- [16:30-16:50] Module naming schemes (incl. hierarchical)
- [16:50-17:30] Integration of EasyBuild in JSC, EESSI, and LUMI
- [17:30-17:45] The EasyBuild community + contributing to EasyBuild
- [17:45-18:00] Q&A + closing remarks (incl. quick comparison with other tools)

Practical information

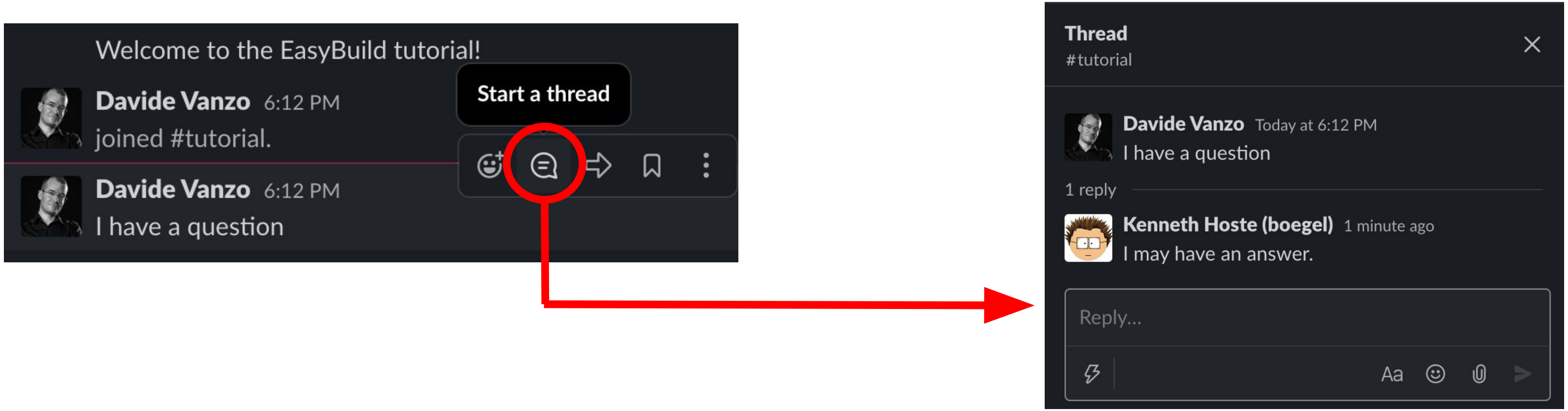
- **Sunday 29th of May 2022, 14:00 - 18:00 CEST**
- Tutorial website: https://easybuild.io/tutorial/isc22
- Please join the `#tutorial-isc22` channel in the EasyBuild Slack to ask questions!
- Prepared environment for hands-on demos & exercises

Q&A via dedicated channel in EasyBuild Slack

- Questions or problems?
  Speak up in #tutorial-isc22 on EasyBuild Slack!

- **Join via** https://easybuild.io/join-slack

- **Use threads to avoid overflowing the channel!**



Welcome to the EasyBuild tutorial!

Davide Vanzo 6:12 PM
joined #tutorial.

Davide Vanzo 6:12 PM
I have a question

Thread
#tutorial

Davide Vanzo Today at 6:12 PM
I have a question

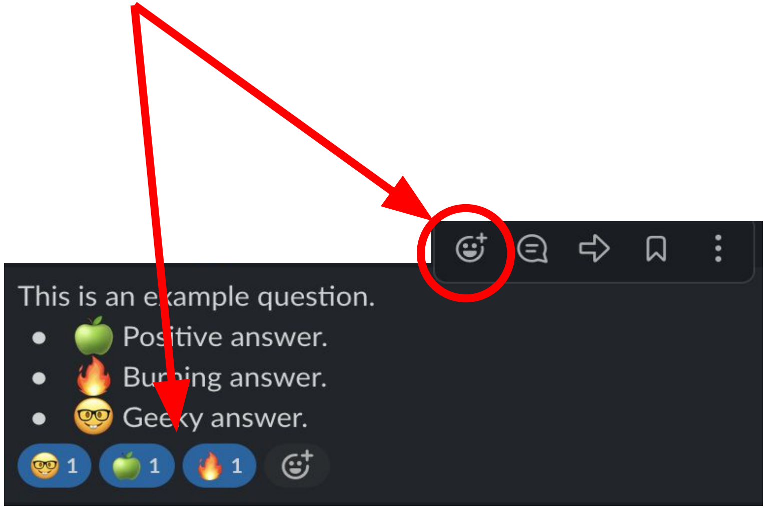
1 reply

Kenneth Hoste (boegel) 1 minute ago
I may have an answer.

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/practical_info

Emoji polls in Slack

- Small polls will be posted in the `#tutorial-isc22` Slack channel.
- **Vote** for one (or more) answers using the corresponding emoji !



This is an example question.

- 🍏 Positive answer.
- 🔥 Burning answer.
- 🤓 Geeky answer.

Prepared environment

- Small Rocky 8 cluster (in the cloud)

- **You need to create an account!**
    - Signup: https://mokey.isc22.learnhpc.eu/auth/signup
    - Accounts will only be approved for access on 29 May 2022, so **please record your username/password !**
        - Reset Password link does **not** work, instead raise any login problem in Slack

- Access via `ssh` or web browser **(pick one and stick to it!)**
    - Shell access: `ssh isc22.learnhpc.eu`
    - Via browser: https://isc22.learnhpc.eu

- System will be up until the end of the conference (18:15 CEST, Thursday 2 June 2022)

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What is EasyBuild?

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

https://easybuild.io

https://docs.easybuild.io

https://github.com/easybuilders

https://easybuild.io/join-slack

Twitter: @easy_build

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/introduction

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)

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/introduction

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

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/introduction

Focus points in EasyBuild

Performance

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

Reproducibility

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

Community effort

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

What EasyBuild is ***not***

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

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/introduction

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-isc22/introduction

EasyBuild terminology: framework

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

EasyBuild terminology: easyblock

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

EasyBuild terminology: easyconfig file

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

EasyBuild terminology: easystack file

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

EasyBuild terminology: extensions

easybuild

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

EasyBuild terminology: dependencies

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

EasyBuild terminology: toolchains

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

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/introduction

EasyBuild terminology: modules

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

Bringing all EasyBuild terminology together

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

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

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

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Installing EasyBuild: requirements

- **Linux** as operating system (CentOS, RHEL, Ubuntu, Debian, SLES, ...)
  - EasyBuild also works on macOS, but support is very basic

- **Python** 2.7 or 3.5+
  - Only Python standard library is required for core functionality of EasyBuild
  - Using Python 3 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-isc22/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-isc22/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/python3.9/site-packages:$PYTHONPATH
# instruct EasyBuild to use python3 command
export EB_PYTHON=python3
```

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/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-isc22/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-isc22/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
    ```

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/installation

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-isc22/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 directories** (`buildpath`)*
  - Location of easyconfig files archive (`repositorypath`)*
  - Search path for easyconfig files (`robot-paths` + `robot`)
  - Module naming scheme (`module-naming-scheme`)
- Several locations* (+ others) can be controlled at once via `prefix` configuration setting
- *Full* list of EasyBuild configuration settings (~270) is available via `eb --help`

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/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-isc22/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-isc22/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

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/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-isc22/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-isc22/configuration

Inspecting the current configuration: example

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

$ export EASYBUILD_BUILDPATH=/tmp/$USER/build

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

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/configuration

Minimal EasyBuild configuration for hands-on

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

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

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

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

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

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

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

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/configuration

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-isc22/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-isc22/basic_usage

Inspecting easyconfigs via `eb --show-ec`

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

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

name = 'TensorFlow'
version = '2.6.0'

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

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

Checking dependencies via `eb --dry-run`

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

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

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

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

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

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

```
$ eb PyTables-3.6.1-foss-2021b.eb -M

3 out of 69 required modules missing:

* LZO/2.10-GCCcore-11.2.0 (LZO-2.10-GCCcore-11.2.0.eb)

* Blosc/1.21.1-GCCcore-11.2.0 (Blosc-1.21.1-GCCcore-11.2.0.eb)

* PyTables/3.6.1-foss-2021b (PyTables-3.6.1-foss-2021b.eb)
```

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/basic_usage

Inspecting software install procedures

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

Inspecting software install procedures: example

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

preparing... [DRY RUN]

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

Loading toolchain module...

module load GCC/11.2.0

Loading modules for dependencies...

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

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/basic_usage

Inspecting software install procedures: example

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

configuring... [DRY RUN]

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

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/basic_usage

Inspecting software install procedures: example

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

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


...
```

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/basic_usage

Agenda

(all times are CEST)

- [14:00-14:10] Practical information w.r.t. prepared environment for hands-on
- [14:10-14:30] Introduction to EasyBuild: scope & terminology
- [14:30-14:50] Installing & configuring EasyBuild + basic usage
- [14:50-15:30] **Installing software with EasyBuild + troubleshooting**
- [15:30-16:00] Adding support for additional software
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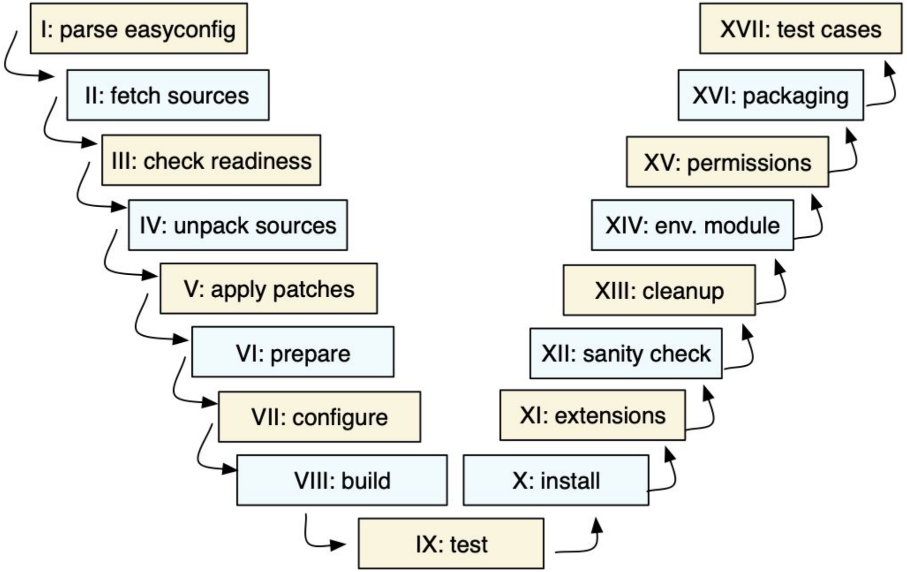
- [17:45-18:00] Q&A + closing remarks (incl. quick comparison with other tools)

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-isc22/installing_software

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-isc22/installing_software

Using software installed with EasyBuild

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

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

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/installing_software

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-isc22/installing_software

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

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/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-isc22/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-isc22/troubleshooting

Troubleshooting: navigating log files

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

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

- Different steps of installation procedure are clearly marked:

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

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

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/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
- For example:
  - Check `config.log` when `configure` command failed
  - Check `CMakeFiles/CMakeError.log` when `cmake` command failed (good luck...)

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/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/2.0.3/GCC-8.5.0): build failed (first 300 chars):
Couldn't find file subread-2.0.3-source.tar.gz anywhere, and downloading
it didn't work either...
Paths attempted (in order): ...
```

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/troubleshooting

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Adding support for additional software

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

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/adding_support_additional_software

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

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/adding_support_additional_software

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://easybuilders.github.io/easybuild-tutorial/2022-isc22/adding_support_additional_software

Generating tweaked easyconfig files

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

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/adding_support_additional_software

Copying easyconfig files

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

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

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/adding_support_additional_software

Hands-on: creating easyconfig files

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

```
name = 'eb-tutorial'

version = '1.0.1'

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

description = "EasyBuild tutorial example"
```

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/adding_support_additional_software

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The HPC Event.

easybuild

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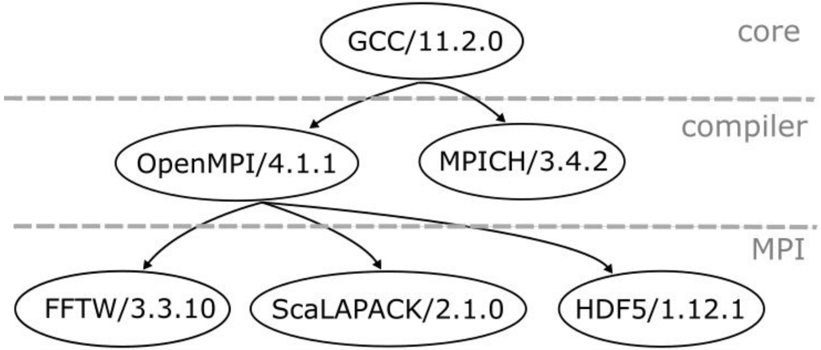
Flat vs hierarchical module naming schemes

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



https://easybuilders.github.io/easybuild-tutorial/2022-isc22/module_naming_schemes

Pros and cons of using a flat vs hierarchical MNS

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

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/module_naming_schemes

Custom module naming schemes with EasyBuild

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

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

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

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

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/module_naming_schemes

Hands-on example: installing HDF5 in an HMNS

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

```
module unuse $MODULEPATH
```

- Configure our setup to reuse the existing software installations

```
export EASYBUILD_INSTALLPATH_SOFTWARE=/easybuild/software

export EASYBUILD_MODULE_NAMING_SCHEME=HierarchicalMNS

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

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

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

- Explore the new hierarchy

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

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/module_naming_schemes

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https://easybuild.io/tutorial/isc22

EasyBuild at Jülich Supercomputing Centre

by Sebastian Achilles

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/integration_jsc

Jülich Supercomputing Centre

- JSC is a German supercomputing centre since 1987
  - About 250 experts for all aspects of supercomputing and simulation sciences

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/integration_jsc

Jülich Supercomputing Centre

- JSC is a German supercomputing centre since 1987
  - About 250 experts for all aspects of supercomputing and simulation sciences
- Currently 3 primary systems:
  - JUWELS - 70 Petaflops, #8 in Top500 (modular supercomputing)
  - JURECA-DC - 3.54 (CPU) + 14.98 (GPU) + 5 (KNL) Petaflops
  - JUSUF - AMD, V100 GPU. Interactive workflows and community services

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/integration_jsc

EasyBuild at JSC

- Used for production software stack at JSC since 2014

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/integration_jsc

EasyBuild at JSC

- Used for production software stack at JSC since 2014
- Geared towards average user experience
  - Hide lots of indirect software
  - Lots of toolchains => Module hierarchy
  - Renaming some modules, Lmod tweaks

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/integration_jsc

EasyBuild at JSC

- Used for production software stack at JSC since 2014
- Geared towards average user experience
  - Hide lots of indirect software
  - Lots of toolchains => Module hierarchy
  - Renaming some modules, Lmod tweaks
- Custom MNS, toolchains, easyconfigs, easyblocks
  - Maintenance and contribution issue
  - Working hard to minimise this

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/integration_jsc

Upgrading and retiring software

- Provide latest software to new projects by default
  - ***Stages*** concept
  - Updates once per year
  - Encourages users to adopt latest software & dependencies (performance, bug fixes,...)

Upgrading and retiring software

- Provide latest software to new projects by default
  - ***Stages*** concept
  - Updates once per year
  - Encourages users to adopt latest software & dependencies (performance, bug fixes,...)
- Give indirect access to "retired" software

Leveraging hooks for users & maintainers

- Very powerful alternative to customisations
  - Much more automated and flexible
  - Easier to maintain (particularly for easyconfigs)

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/integration_jsc

Leveraging hooks for users & maintainers

- Very powerful alternative to customisations
  - Much more automated and flexible
  - Easier to maintain (particularly for easyconfigs)

- Hooks to enable user space installations
  - Guide people on how to do this “properly”
  - Installation hierarchy: system → group → user

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/integration_jsc

Integration of EasyBuild in EESSI

EESSI

EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS

Presented by Sebastian Achilles

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/integration_eessi

Optimised scientific software everywhere without building or tuning: that's EESSI!

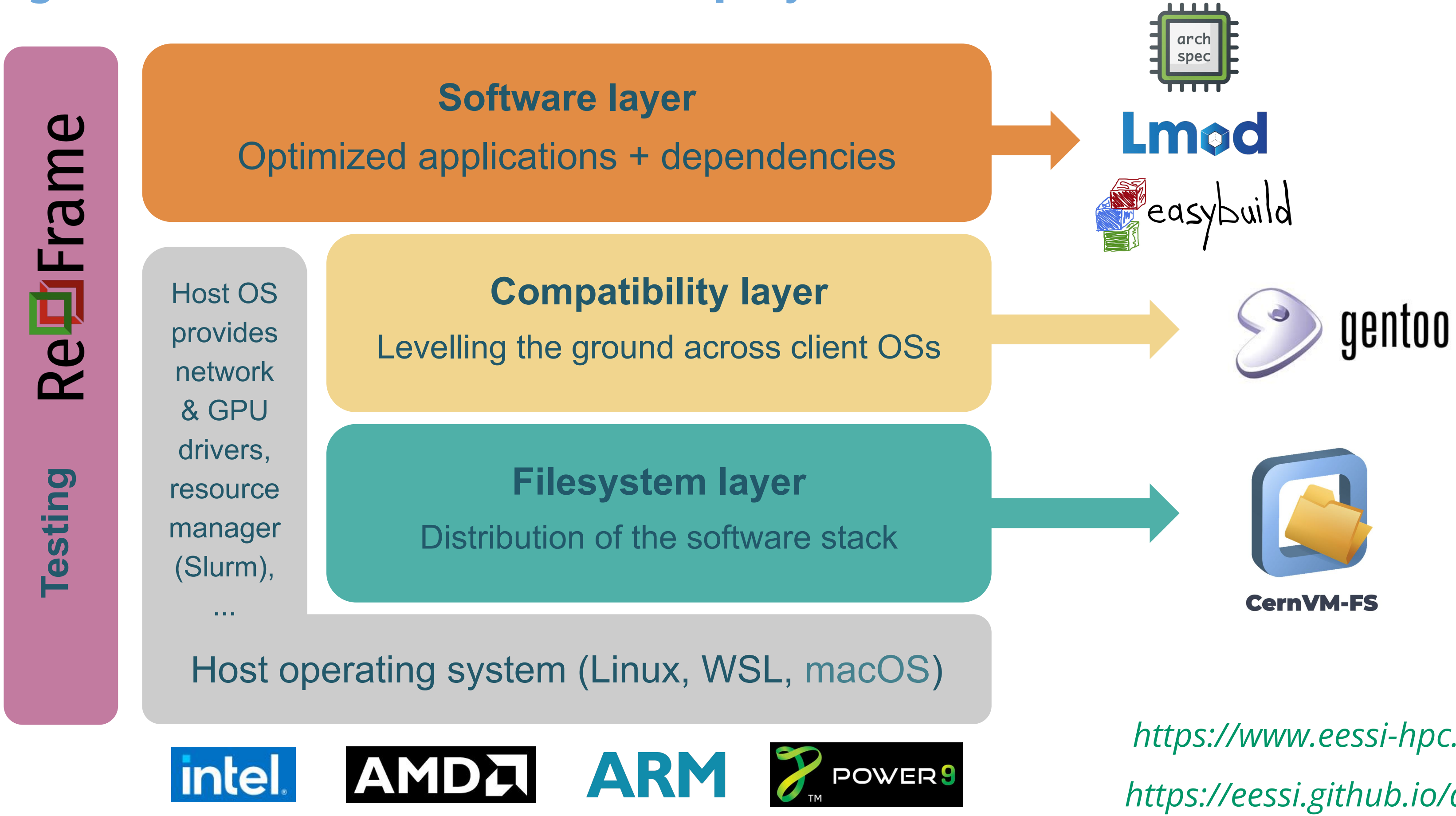
EESSI

- The challenge:
  - Same software everywhere (HPC, Cloud, servers, laptops)
  - Optimized for specific CPUs, well tested, works on different OSs
  - Plug ‘n play, limited setup
- The solution: EESSI - European Environment for Scientific Software Installations
  - “Streams” (scientific) software installations on-demand
  - Any machine, anywhere, nearly instantly available

https://www.eessi-hpc.org

https://eessi.github.io/docs

High-level overview of the EESSI project



ReFrame

Testing

Software layer

Optimized applications + dependencies

Compatibility layer

Levelling the ground across client OSs

Filesystem layer

Distribution of the software stack

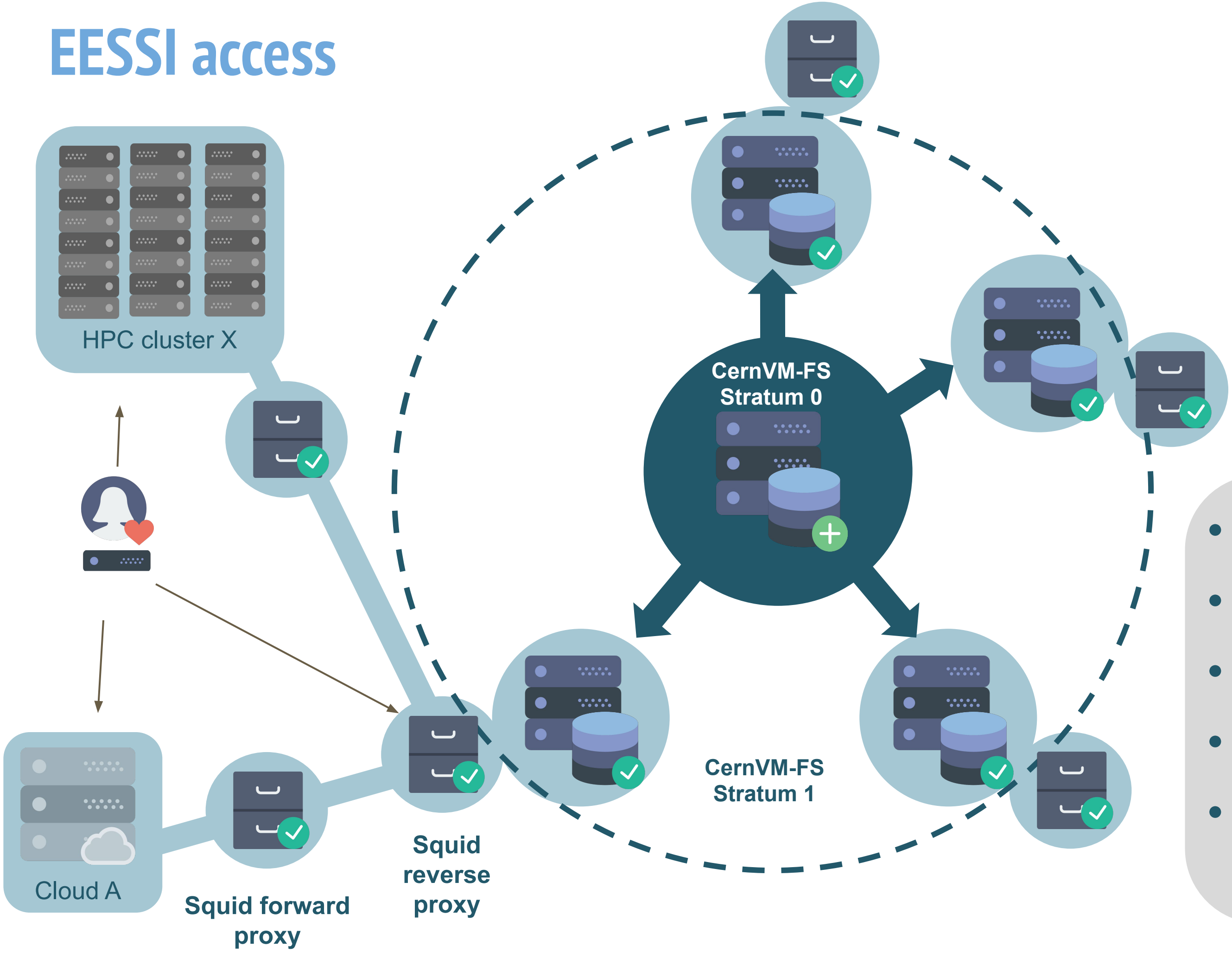
Host OS provides network & GPU drivers, resource manager (Slurm), ...

Host operating system (Linux, WSL, macOS)

https://www.eessi-hpc.org

https://eessi.github.io/docs

EESSI access



EESSI

CernVM-FS

https://cvmfs.readthedocs.io

- Global distribution of software installations
- Centrally managed software stack
- Redundant network of “mirrors”
- Multiple levels of caching
- **Same software stack everywhere**: laptops, HPC clusters, cloud VMs, …

(icons via https://www.flaticon.com/authors/smashicons)

Leveraging EESSI in different scenarios

- If EESSI is already available: just set up your environment by sourcing a script
- As a **system administrator**, to make EESSI available:
    - Only need to install CernVM-FS + EESSI configuration package
    - Should also consider setting up squid proxy and maybe own Stratum-1 server
- As an **end user on an HPC system**, to access EESSI without having admin rights:
    - Run a container image via Singularity that includes CernVM-FS to access EESSI
    - See instructions at https://eessi.github.io/docs/pilot
- As a **software developer** in a CI environment like GitHub Actions
    - Use EESSI action in your workflow to leverage the available software in your tests

- EESSI ***not ready for production yet***, but testing + feedback is welcome!
- Website: https://www.eessi-hpc.org
- Documentation: https://eessi.github.io/docs
- Introduction to EESSI (EUM'21): https://www.youtube.com/watch?v=1CXwzIW_MsU
- **Join the EESSI mailing list and Slack: https://www.eessi-hpc.org/join**
- Monthly update meetings, open to join for anyone interested

  https://github.com/EESSI/meetings/wiki
- EESSI hackathons (Dec'21 + Jan'22, plans for more):

  https://github.com/EESSI/hackathons

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/integration_eessi

Integration of EasyBuild in LUMI

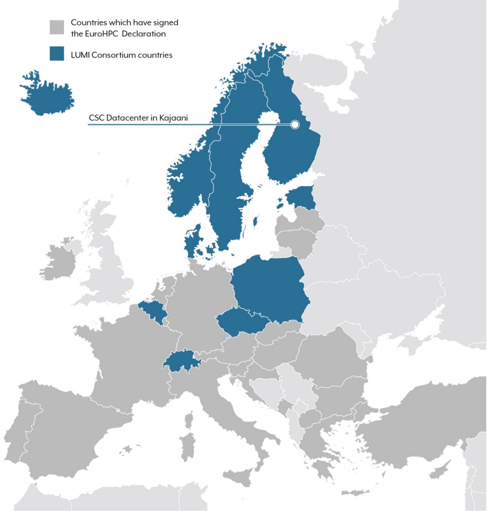
by Kurt Lust

LUMI User Support Team (LUST) & University of Antwerp

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/integration_lumi

What is LUMI?

- LUMI is one of the EuroHPC JU pre-exascale systems
- Located in the CSC Kajaani data centre, hosted by a consortium of 10 countries who shared the investment with EuroHPC JU.
- HPE Cray EX system using SUSE Linux/COS and the HPE Cray Programming Environment (PE)
- Compute resources:
  - GPU partition: 2560 nodes with 1 AMD Trento CPU and 4 AMD MI250X GPUs
    - GPU-first node, SlingShot 11 interconnect attached to the GPUs
    - Cache-coherent unified memory
  - CPU partition: 1536 nodes with 2 64-core AMD Zen3 CPUs
  - Small interactive data analysis and visualisation partition (8 CPU-only nodes and 8 nodes with NVIDIA GPU)
  - OpenShift/Kubernetes partition
  - Lustre storage + Ceph object storage


Countries which have signed the EuroHPC Declaration
LUMI Consortium countries
CSC Datacenter in Kajaani

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/integration_lumi

Challenges

- Integrate with the HPE Cray PE, which is installed with the OS and not with the user applications stack.
  - EasyBuild common toolchains pose problems and have little support for AMD GPUs
- Heterogeneous environment and fast evolving software
  - Software stack updates measured in updates/year rather than years/update
- Distributed support effort
  - Central LUMI User Support Team only 9 FTE, and they are employees of institutions in the consortium countries and not of CSC
  - Consortium countries should also provide support
- Combining distributed user management with a small central support team with little access to user data creates a software license management nightmare
- Need for customisation

Building block 1: Lmod to organise software stacks

- Versatile and well supported in EasyBuild (and Spack), and by the HPE Cray PE.
- Used Lmod hierarchy to implement software stacks
  - CrayEnv: "enriched" Cray Programming Environment
    - Management of Cray PE target modules
    - Some additional tools on top of the OS
  - LUMI software stack: 2-level hierarchy
    - Versions aligned with the versions of the Cray PE (21.08, 21.12)
    - Second level: partition module loads stack for a particular architecture
    - Automatic selection of the partition module, but can be overwritten, e.g., for cross-compiling
    - Meta-partitions for special needs, e.g., software installed once for all architectures

Building block 2: EasyBuild

- EasyBuild gives a very precise description of the installation process
  - Hence a good way of passing installation instructions to someone
- Configuration of each individual installation fully described by easyconfig file, not by command line arguments
- Configuration module integrates EasyBuild with the LUMI software stack
  - Environment variable points to the user installation
  - User installation in the module search path
  - 3 EasyBuild configuration modules configure EasyBuild to install software in the right location:
    - EasyBuild-production, EasyBuild-infrastructure : system stack
    - EasyBuild-user for the user configuration
- Fix the version of EasyBuild for each software stack

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/integration_lumi

Custom toolchains

- Common toolchains not fit for use on LUMI
  - Have support for the Cray and AMD compilers
  - Open MPI (foss) difficult to configure for LUMI, and no AMD GPU support anyway
  - Intel compilers have become a problem on AMD hardware
- Implement custom toolchains on top of Cray PE compilers
  - Build on CSCS implementation and an older implementation included in EasyBuild, but made several refinements
  - Compilers etc. not installed through EasyBuild
  - Replace the top level Cray PE module (PrgEnv-*) with one generated and managed through EasyBuild but otherwise use modules on the system

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

Software-specific easyblocks

- Probably the major nuisance when using EasyBuild on Cray systems
    - Several easyblocks contain code that only recognises certain compiler toolchains and abort for others
    - Some easyblocks detect dependencies through module names rather than EBROOT/EBVERSION variables and hence may fail for external modules
- Maintenance is an issue
    - Contributing back no guarantee that the support is maintained as testing is impossible in the EasyBuild test environment
    - But then you have to track changes yourself
- Tend to follow the CSCS approach and use generic easyblocks wherever possible, and "fatter" easyconfig files.

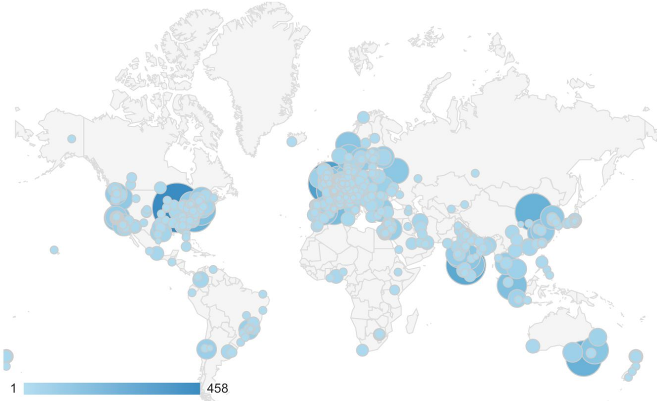
Agenda

(all times are CEST)

- [14:00-14:10] Practical information w.r.t. prepared environment for hands-on
- [14:10-14:30] Introduction to EasyBuild: scope & terminology
- [14:30-14:50] Installing & configuring EasyBuild + basic usage
- [14:50-15:30] Installing software with EasyBuild + troubleshooting
- [15:30-16:00] Adding support for additional software
- [16:00-16:30] *(coffee break)*
- [16:30-16:50] Module naming schemes (incl. hierarchical)
- [16:50-17:30] Integration of EasyBuild in JSC, EESSI, and LUMI
- [17:30-17:45] **The EasyBuild community + contributing to EasyBuild**
- [17:45-18:00] Q&A + closing remarks (incl. quick comparison with other tools)

The EasyBuild community

EasyBuild User Meeting 2020 (Barcelona)



- Documentation is read all over the world
- HPC sites, consortia, and companies
- Slack: >600 members, ~110 active members per week, 277K messages
- Regular online conf calls... and we even meet in person sometimes!

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/community

Contributing to EasyBuild

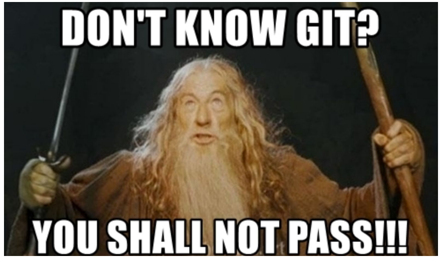
There are several ways to contribute to EasyBuild, including:

- 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

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/contributing

GitHub integration features



easybuild

- 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:

  https://docs.easybuild.io/en/latest/Integration_with_GitHub.html

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/contributing

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`

https://easybuilders.github.io/easybuild-tutorial/2022-isc22/contributing

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Topics we didn't cover...

- Implementing easyblocks
- Using easystacks to install a whole stack at once
- Using RPATH linking
- Using EasyBuild as a library
- Implementing hooks to customize EasyBuild
- Submitting installations as jobs on a cluster
- Building Docker/Singularity container images with EasyBuild (experimental)

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

easybuild vs Spack

- **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)**
- 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!**

easybuild vs Spack

- Some differences:
    - Spack will install some packages from a **binary cache**.
    - **Fixed dependency/toolchain versions in EasyBuild vs flexible CLI and the concretiser in Spack**
    - EasyBuild uses modules, in Spack this is only one of the mechanisms to activate software
- **The naughty one:** As Spack makes it so easy to create 100s of different configurations of a package, it is the ideal tool to quickly fill up your file system.
- For a more detailed (but somewhat outdated) comparison, see https://archive.fosdem.org/2018/schedule/event/installing_software_for_scientists

Questions?

- Website: https://easybuild.io
- Documentation: https://docs.easybuild.io
- Tutorials: https://easybuild.io/tutorial
- Yearly EasyBuild User Meeting: https://easybuild.io/eum
- 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