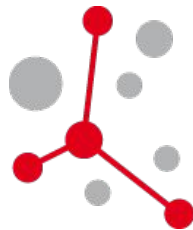


easybuild



ISC

High Performance

The HPC Event.

EasyBuild tutorial

ISC'21

Kenneth Hoste (HPC-UGent) - Alan O'Cais (ISC) - Bart Oldeman (Compute Canada)

June 25th 2021

<https://easybuild.io/tutorial/isc21>

- [12:00-12:10] **Practical information w.r.t. prepared environment for hands-on examples**
- [12:10-12:30] Introduction to EasyBuild: scope & terminology
- [12:30-13:00] Installing & configuring EasyBuild + basic usage
- [13:00-13:45] Installing software with EasyBuild + troubleshooting
- [13:45-14:15] *(coffee break)*
- [14:15-14:45] Module naming schemes (incl. hierarchical)
- [14:45-15:10] Adding support for additional software
- [15:10-15:30] Use of EasyBuild in large scale production systems at JSC and Compute Canada
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- [15:45-16:00] Q&A + closing remarks (incl. quick comparison with other tools)

Practical information

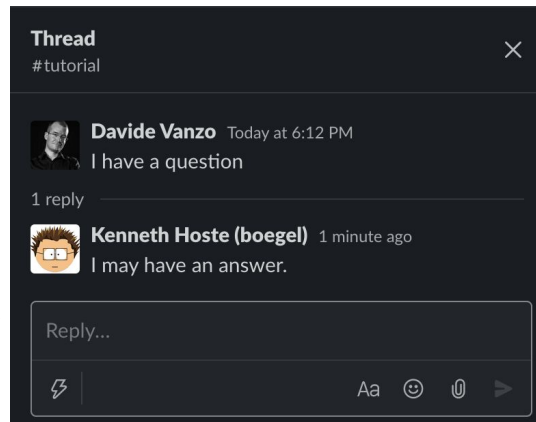
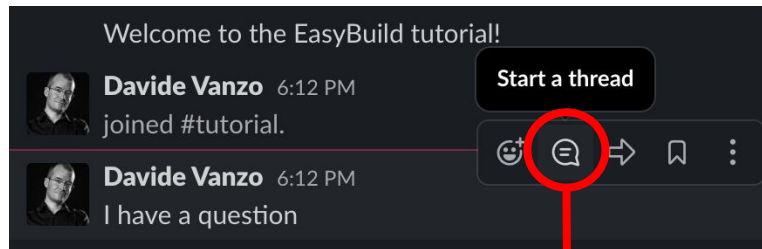


- **Friday June 25th 2021, 12:00 - 16:00 UTC**
- Tutorial website: <https://easybuild.io/tutorial/isc21>
- Please join the `#tutorial-isc21` channel in the EasyBuild Slack to ask questions!
- Prepared environment for hands-on demos & exercises

Q&A via dedicated channel in EasyBuild Slack



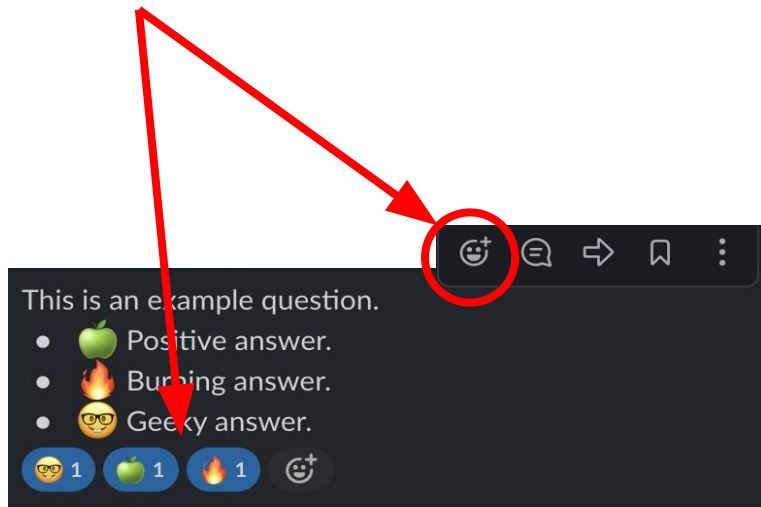
- Questions or problems?
Speak up in #tutorial-isc21 on EasyBuild Slack!
- Join via <https://easybuild.io/join-slack>
- Use threads to avoid overflowing the channel!



Emoji polls in Slack



- Small polls will be posted in the #tutorial-isc21 Slack channel.
- **Vote** for one (or more) answers using the corresponding emoji !



Prepared environment



- Small CentOS 7 cluster (in the cloud)
- **You need to create an account!**
 - Signup: <https://mokey.isc21.learnhpc.eu/auth/signup>
 - Accounts will only be approved for access on 24/25 June 2021, so **please record your username/password !**
- Access via ssh or web browser:
 - Shell access: `ssh isc21.learnhpc.eu`
 - Via browser: <https://isc21.learnhpc.eu>
- System will be up until the end of the conference (18:15 CEST, Friday 2 July 2021)

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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'11
 - EasyBuild 1.0 released in Nov'11 (during SC11)
 - Worldwide community has grown around it since then!

<https://easybuild.io>

<https://docs.easybuild.io>

<https://github.com/easybuilders>

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

Twitter: [@easy_build](#)

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 install path)
- Highly configurable, easy to extend, support for hooks, easy customisation
- Detailed logging, fully transparent via support for “dry runs” and trace mode
- Support for using custom module naming schemes (incl. hierarchical)

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 2011 (every 6 - 8 weeks)
- **Comprehensive testing:** unit tests, testing contributions, regression testing
- **Various support channels** (mailing list, Slack, conf calls) + yearly user meetings

Focus points in EasyBuild



Performance

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

Reproducibility

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

Community effort

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

What EasyBuild is not



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

EasyBuild terminology



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

EasyBuild terminology: framework



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

EasyBuild terminology: easyblock



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

EasyBuild terminology: easyconfig file



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

EasyBuild terminology: easystack file



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

EasyBuild terminology: extensions



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

EasyBuild terminology: dependencies



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

EasyBuild terminology: toolchains



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

EasyBuild terminology: modules



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

Bringing all EasyBuild terminology together



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

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

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

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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

Installing EasyBuild: different options



- Installing EasyBuild using a standard Python installation tool
 - `pip install easybuild`
 - ... or a variant thereof (`pip3 install --user`, using `virtualenv`, etc.)
 - May require additional commands, for example to update environment
- **Installing EasyBuild as a module, with EasyBuild (*recommended!*)**
 - 3-step “bootstrap” procedure, via temporary EasyBuild installation using `pip`
- Development setup
 - Clone GitHub repositories:
`easybuilders/easybuild-{framework,easyblocks,easyconfigs}`
 - Update `$PATH` and `$PYTHONPATH` environment variables

Installing EasyBuild as a module (recommended)



3-step bootstrap procedure

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

```
export TMPDIR=/tmp/$USER/easybuild  
  
pip3 install --prefix $TMPDIR easybuild  
  
# update environment to use this temporary EasyBuild installation  
  
export PATH=$TMPDIR/bin:$PATH  
  
export PYTHONPATH=$TMPDIR/lib/python3.6/site-packages:$PYTHONPATH  
  
# instruct EasyBuild to use python3 command  
  
export EB_PYTHON=python3
```

Installing EasyBuild as a module (recommended)



3-step bootstrap procedure

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

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

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

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

Verifying the EasyBuild installation



- Check EasyBuild version:

```
eb --version
```

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

```
eb --help
```

- Show the current (default) EasyBuild configuration:

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

- Show system information:

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

Updating EasyBuild



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

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

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

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

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

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

```
module load EasyBuild/4.4.0
```

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 (~250) is available via `eb --help`

Configuration levels



- There are 3 different configuration levels in EasyBuild:
 - **Configuration files**
 - **Environment variables**
 - **Command line options to the `eb` command**
- Each configuration setting can be specified via each “level” (no exceptions!)
- Hierarchical configuration:
 - Configuration files override default settings
 - Environment variables override configuration files
 - `eb` command line options override environment variables

EasyBuild configuration files



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

\$EASYBUILD_* environment variables



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

Command line options for `eb` command



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

Inspecting the current configuration



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

Inspecting the current configuration: example



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

$ export EASYBUILD_BUILDPATH=/tmp/$USER/build

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

Minimal EasyBuild configuration for hands-on



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

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

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

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

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

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

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

Basic usage of EasyBuild



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

Specifying easyconfigs to use



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

Inspecting easyconfigs via `eb --show-ec`



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

```
$ eb --show-ec TensorFlow-2.4.1-foss-2020b.eb
```

```
easyblock = 'PythonBundle'
```

```
name = 'TensorFlow'
```

```
version = '2.4.1'
```

```
homepage = 'https://www.tensorflow.org/'
```

```
description = "An open-source software library for Machine Intelligence"
```

```
toolchain = {'name': 'foss', 'version': '2020b'}
```

```
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-1.11-GCC-10.2.0.eb -D
```

```
...
* [ ] $CFGS/x/XZ/XZ-5.2.5-GCCcore-10.2.0.eb (module: XZ/5.2.5-GCCcore-10.2.0)
* [ ] $CFGS/c/cURL/cURL-7.72.0-GCCcore-10.2.0.eb (module: cURL/7.72.0-GCCcore-10.2.0)
* [x] $CFGS/g/GCC/GCC-10.2.0.eb (module: GCC/10.2.0)
* [x] $CFGS/n/ncurses/ncurses-6.2-GCCcore-10.2.0.eb (module: ncurses/6.2-GCCcore-10.2.0)
* [ ] $CFGS/s/SAMtools/SAMtools-1.11-GCC-10.2.0.eb (module: SAMtools/1.11-GCC-10.2.0)
```

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 h5py-3.1.0-foss-2020b.eb -M
```

```
2 out of 61 required modules missing:
```

```
* pkg-config/0.29.2-GCCcore-10.2.0 (pkg-config-0.29.2-GCCcore-10.2.0.eb)
```

```
* h5py/3.1.0-foss-2020b (h5py-3.1.0-foss-2020b.eb)
```

Inspecting software install procedures



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

Inspecting software install procedures: example



```
$ eb Boost-1.74.0-GCC-10.2.0.eb -x
```

```
...
```

```
preparing... [DRY RUN]
```

```
[prepare_step method]
```

```
Defining build environment, based on toolchain (options) and specified dependencies...
```

```
Loading toolchain module...
```

```
module load GCC/10.2.0
```

```
Loading modules for dependencies...
```

```
module load bzip2/1.0.8-GCCcore-10.2.0
```

```
module load zlib/1.2.11-GCCcore-10.2.0
```

```
module load XZ/5.2.5-GCCcore-10.2.0
```

Inspecting software install procedures: example



```
$ eb Boost-1.74.0-GCC-10.2.0.eb -x
```

```
...
```

```
Defining build environment...
```

```
...
```

```
export CXX='mpicxx'
```

```
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/1.74.0/GCC-10.2.0/obj --without-libraries=python,mpi"
```

```
(in /tmp/example/build/Boost/1.74.0/GCC-10.2.0/Boost-1.74.0)
```

Inspecting software install procedures: example



```
$ eb Boost-1.74.0-GCC-10.2.0.eb -x
```

```
...
```

```
[sanity_check_step method]
```

```
Sanity check paths - file ['files']
```

```
  * lib/libboost_system.so
```

```
  * lib/libboost_thread-mt-x64.so
```

```
Sanity check paths - (non-empty) directory ['dirs']
```

```
  * include/boost
```

```
Sanity check commands
```

```
  (none)
```

```
...
```

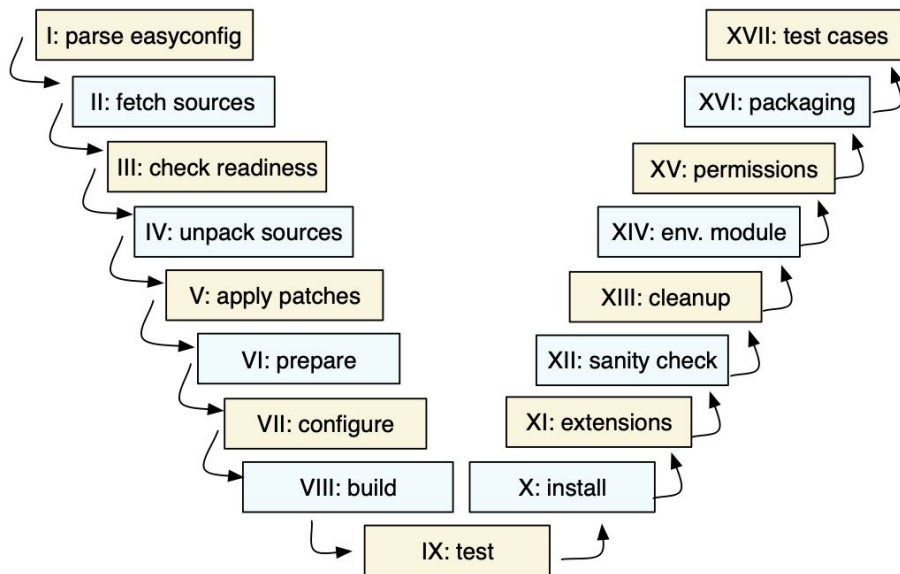

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Installing software with EasyBuild



- To install software with EasyBuild, just run the `eb` command:
 - `eb SAMtools-1.11-GCC-10.2.0.eb`
- If any dependencies are still missing, you will need to also use `--robot`:
 - `eb BCFtools-1.11-GCC-10.2.0.eb --robot`
- To see more details while the installation is running, enable trace mode:
 - `eb BCFtools-1.11-GCC-10.2.0.eb --robot --trace`
- To reinstall software, use `eb --rebuild` (or `eb --force`)

Step-wise installation procedure



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

Using software installed with EasyBuild



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

```
# inform modules tool about modules installed with EasyBuild

module use $HOME/easybuild/modules/all

# check for available modules for BCFtools

module avail BCFtools

# load BCFtools module to "activate" the installation

module load BCFtools/1.11-GCC-10.2.0
```

Stacking software installations



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

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

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

Troubleshooting failing installations



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

Troubleshooting: error messages



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

```
== building...
```

```
== FAILED: Installation ended unsuccessfully (build directory:
```

```
/tmp/example/example/1.0/GCC-10.2.0):
```

```
build failed (first 300 chars): cmd "make" exited with exit code 2 and output:
```

```
/usr/bin/g++ -O2 -ftree-vectorize -march=native -std=c++14 -c -o core.o core.cpp
```

```
g++: error: unrecognized command line option '-std=c++14' (took 1 sec)
```

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

Troubleshooting: log files



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

```
$ eb example.eb
```



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



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

Troubleshooting: navigating log files



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

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

- Different steps of installation procedure are clearly marked:

```
== 2021-06-25 13:11:48,817 example INFO Starting sanity check step
```

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

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-10.2.0): build failed ...
```
- Can be useful to inspect the contents of the build directory for debugging
- For example:
 - Check `config.log` when `configure` command failed
 - Check `CMakeFiles/CMakeError.log` when `cmake` command failed (good luck...)

Troubleshooting: hands-on exercise



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

```
$ eb subread.eb
```

```
...
```

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

```
Paths attempted (in order): ...
```

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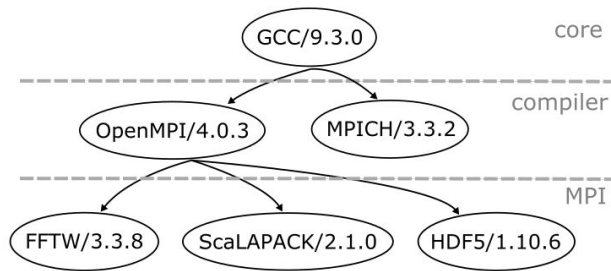


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Flat vs hierarchical module naming schemes



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



Pros and cons of using a flat vs hierarchical MNS



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

Custom module naming schemes with EasyBuild



- You can also create your own module naming scheme (e.g., lower-case only)
 - Implement Python class that derives from the general `ModuleNamingScheme` class
 - Best to start from one of the existing schemes
 - There are (a lot) more things to tweak with a 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-2020.11-foss-2020b-Python-2.7.18.eb -D
```


Hands-on example: installing HDF5 in an HMNS



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

```
module unuse $MODULEPATH
```

- Configure our setup to reuse the existing software installations

```
export EASYBUILD_INSTALLPATH_SOFTWARE=/easybuild/software
```

```
export EASYBUILD_MODULE_NAMING_SCHEME=HierarchicalMNS
```

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

- Re-generate all modules for HDF5 using the new scheme (41 modules)

```
eb HDF5-1.10.7-gompi-2020b.eb --robot --module-only
```

- Explore the new hierarchy

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

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Adding support for additional software



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

Easyblocks vs easyconfigs



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

Writing easyconfig files



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

Generating tweaked easyconfig files



- Trivial changes to existing easyconfig files can be done automatically
- Bumping software version: `eb example-1.0.eb --try-software-version 1.1`
- Changing toolchain (version): `eb example.eb --try-toolchain GCC,9.4.0`
- Changing specific easyconfig parameters (limited): `eb --try-amend ...`
- Note the “try” aspect: additional changes may be required to make installation work

Copying easyconfig files



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

```
$ eb --copy-ec SAMtools-1.11-GCC-10.2.0.eb SAMtools.eb
```

```
...
```

```
SAMtools-1.10-GCC-10.2.0.eb copied to SAMtools.eb
```

Hands-on: creating easyconfig files



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

```
name = 'eb-tutorial'
```

```
version = '1.0.1'
```

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

```
description = "EasyBuild tutorial example"
```


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JÜLICH
Forschungszentrum

by Alan O'Cais



- JSC is a German supercomputing centre since 1987
 - About 200 experts for all aspects of supercomputing and simulation sciences



- JSC is a German supercomputing centre since 1987
 - About 200 experts for all aspects of supercomputing and simulation sciences
- Currently 3 primary systems:
 - JUWELS - 73 Petaflops, #7 in Top500 ([modular supercomputing](#))
 - JURECA-DC - 3.54 (CPU) + 14.98 (GPU) + 5 (KNL) Petaflops
 - JUSUF - AMD, V100 GPU. Interactive workflows and community services



EasyBuild at JSC



- Used for production software stack at JSC since 2014



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



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



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)



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



EasyBuild at Compute Canada



- by Bart Oldeman



Compute Canada : the people

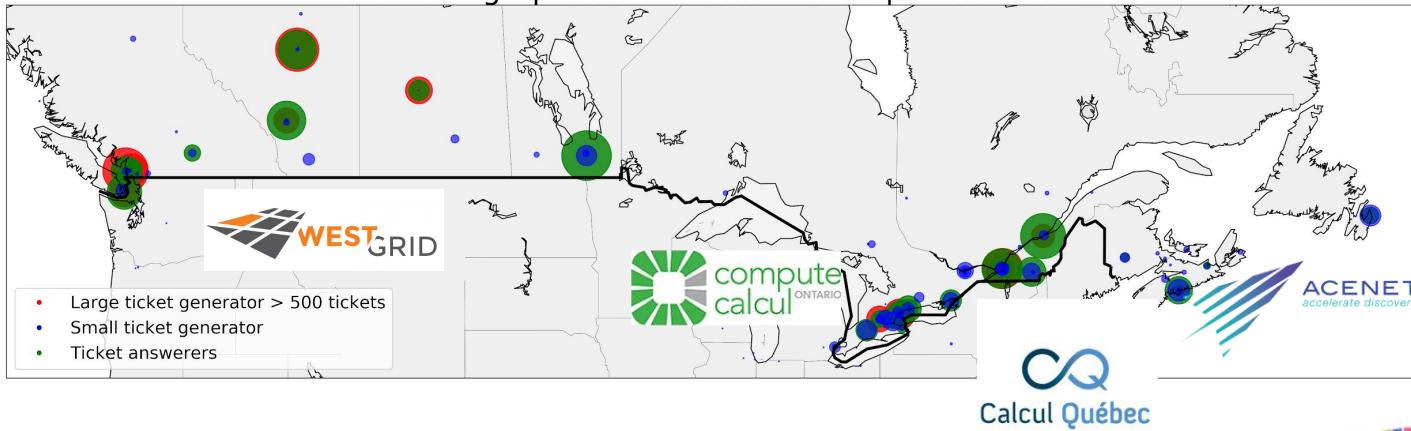


compute
canada



easybuild

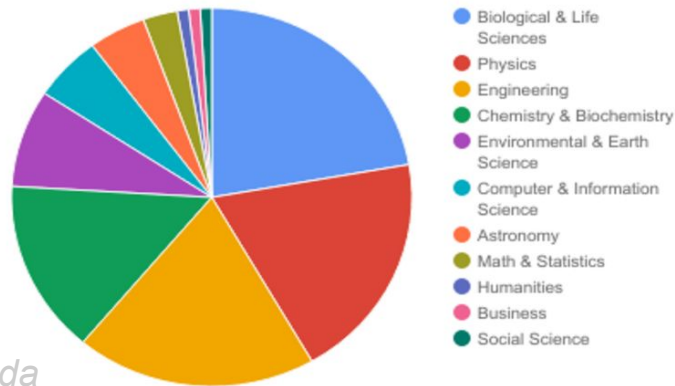
Network graph of ticket routes Compute Canada



All research
disciplines
supported

Free access for any
researcher at a
Canadian institution

- 4 regional consortia
- 35 member institutions
- ~200 technical staff
- ~15,000 user accounts
 - 20% growth per year



Compute Canada : the hardware



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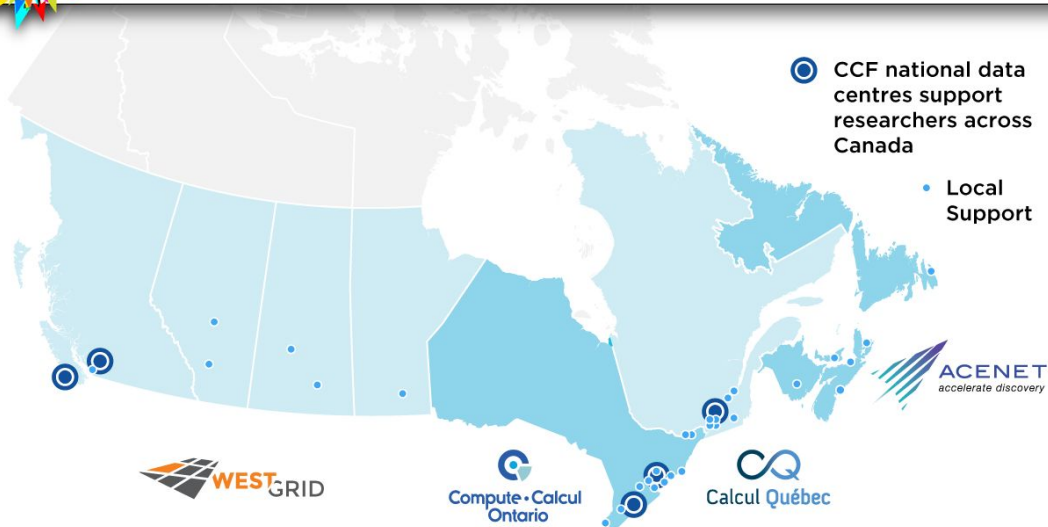
easybuild

5 major national systems
~15 legacy systems
270K cores, 2500 GPUs,
70 PB disk, 180 PB tape



compute
canada | calcul
canada

Canada's National ARC Platform



| System | Type | Network | Production |
|----------------|-----------|---------|------------|
| Arbutus | Cloud | 10 GbE | 2016 H2 |
| Cedar | General | OPA | 2017 H1 |
| Graham | General | EDR IB | 2017 H1 |
| Niagara | Large MPI | EDR IB | 2018 H1 |
| Béluga | General | EDR IB | 2019 H1 |

Goal



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easybuild

Users should be presented with an interface that is as consistent and easy to use as possible across all sites. It should also offer optimal performance.

- Accessible on every site, reliably and performantly: need a distribution mechanism
 - CernVM-FS : CERN Virtual Machine File System
- Independent of the OS (Ubuntu, CentOS, Fedora, etc.)
 - Gentoo Prefix (used to be Nix)
- Automated, tracked, reproducible installation (humans are not so consistent)
 - **EasyBuild**
- Needs a module interface that scales well
 - Lmod with a hierarchical structure

CernVM-FS content delivery



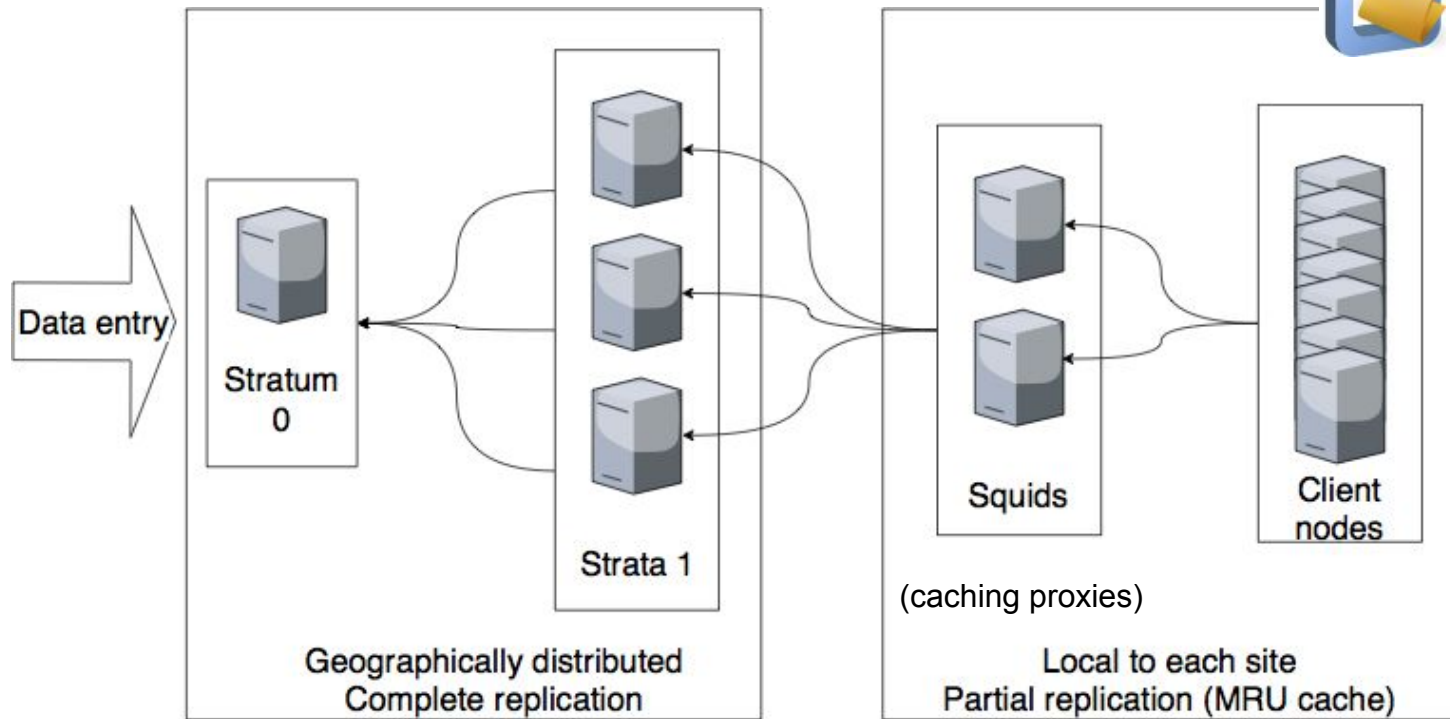
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easybuild



CernVM
File system



Software: design overview



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easybuild

Easybuild layer: modules for Intel, NVHPC, OpenMPI, CUDA, MKL, high-level applications. Multiple architectures (sse3, avx, avx2, avx512)

`/cvmfs/soft.computeCanada.ca/easybuild/{modules,software}/ 2017-2020`

Easybuild-generated modules around Nix profiles (GONE):

~~GCC, Eclipse, Qt+Perl+Python no longer~~

~~`/cvmfs/soft.computeCanada.ca/nix/var/nix/profiles/[a-z]*`~~

Compatibility: ~~Nix~~ Gentoo Prefix layer: GNU libc, autotools, make, bash, cat, ls, awk, grep, etc.

`module gentoo/2020 =>`

`$EPREFIX=/cvmfs/soft.computeCanada.ca/gentoo/2020, $EBROOTGENTOO=$EPREFIX/usr`

Gray area: ~~Slurm~~, Lustre client libraries, IB/OmniPath/InfiniPath client libraries (all dependencies of OpenMPI). In Gentoo layer, but can be overridden using PATH & LD_LIBRARY_PATH.

OS kernel, daemons, drivers, libcuda, anything privileged (e.g. the sudo command): always local. Some legally restricted software too (VASP)

Compute Canada Software Stack



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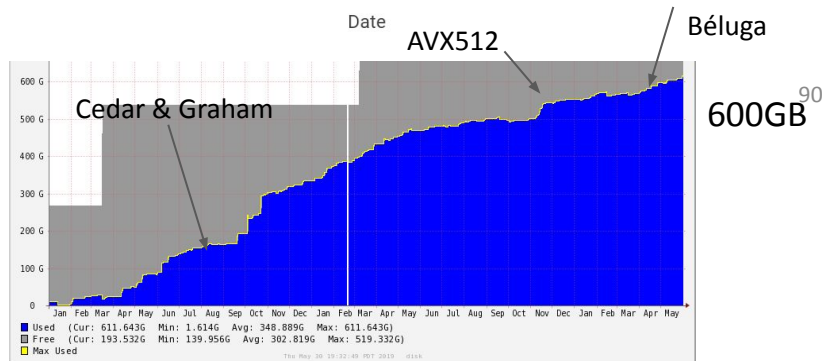
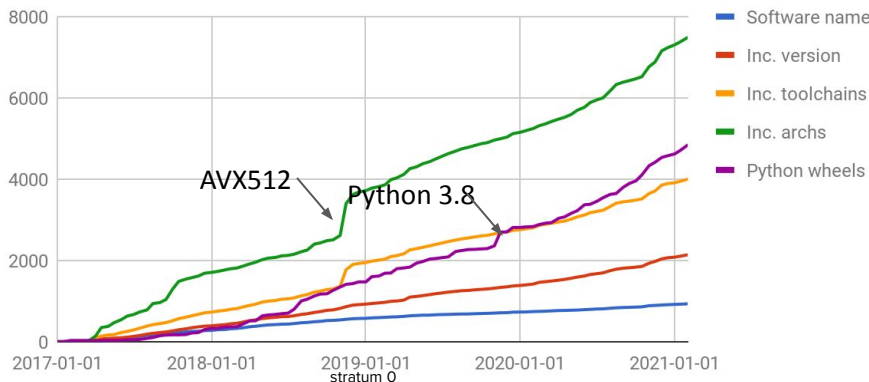
Available software

800+ scientific
applications

6,000+ permutations of
version/arch/toolchain

| Type | Modules |
|----------------|---------|
| AI | 5 |
| Bioinformatics | 239 |
| Chemistry | 63 |
| Data | 19 |
| Geo/Earth | 23 |
| Mathematics | 82 |
| MPI libraries | 7 |
| Physics | 48 |
| Various tools | 176 |
| Visualisation | 28 |
| Misc | 38 |

Number of software packages available through modules and python wheels



- Two major new clusters with Skylake CPUs
- Built new modules with AVX512 for most packages
- High deduplication
- [Further details](https://easybuilders.github.io/easybuild-tutorial/2021-isc21/computecanada)

Design choices / EasyBuild features



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easybuild

- Compatibility layer => filtering of a lot of dependencies (M4, cmake, etc.)
- Toolchains based combinations of
 - Intel/GCC, OpenMPI, MKL, Cuda
 - => gomkl(c)/ iomkl(c) toolchains
 - => We are (ab)using the --try-toolchain, --try-software-version, --try-update-deps
- Custom module naming scheme:
 - Hierarchical, lower case
 - No versionsuffix at all
 - Toolchains are hidden
- No \$LD_LIBRARY_PATH, instead RPATH using wrapper for linker (ld).

- Injecting custom configuration options for OpenMPI
- Injecting footer code in compiler and MPI modules to support installation in user's home directories
- Splitting the installation of Intel into redistributable and non-redistributable parts
- Stripping down Python modules (dropping extensions)

- Installing Python wrappers and side packages (PyQt5 with Qt5, OpenCV-python with OpenCV, etc.) whenever possible
- Using `multi_deps` so that modules are compatible with all versions of Python
- Not installing most Python packages as modules, but by providing Python wheels to users they can install using `pip` in virtual environments
- [Not supporting Anaconda](https://easybuilders.github.io/easybuild-tutorial/2021-isc21/computecanada)

You can use this too!

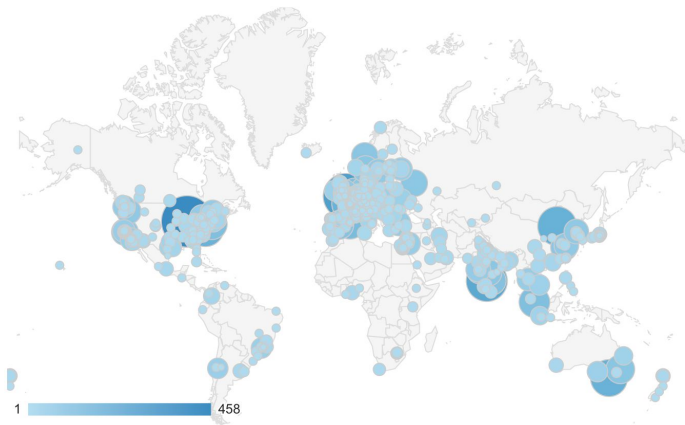


Mounting our software stack:

https://docs.compute canada.ca/wiki/Accessing_CVMFS

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The EasyBuild community



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

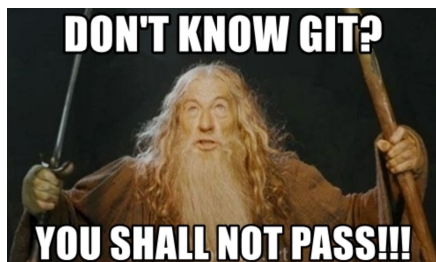
Contributing to EasyBuild



There are several ways to contribute to EasyBuild, including:

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

GitHub integration features



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

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

Opening a pull request in 1, 2, 3



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

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

one single `eb` command
no git commands
no GitHub interaction



metadata is automatically
derived from easyconfig
saves a lot of time!

`eb --new-pr sklearn.eb`

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Topics we didn't cover...



- Implementing easyblocks
- Using RPATH linking
- Using EasyBuild as a library
- Implementing hooks to customize EasyBuild
- Submitting installations as jobs on a cluster
- Integration with the Cray Programming Environment
- Building Docker/Singularity container images with EasyBuild (experimental)

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



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

Just one more thing...

<https://www.eessi-hpc.org>

<https://eessi.github.io/docs>

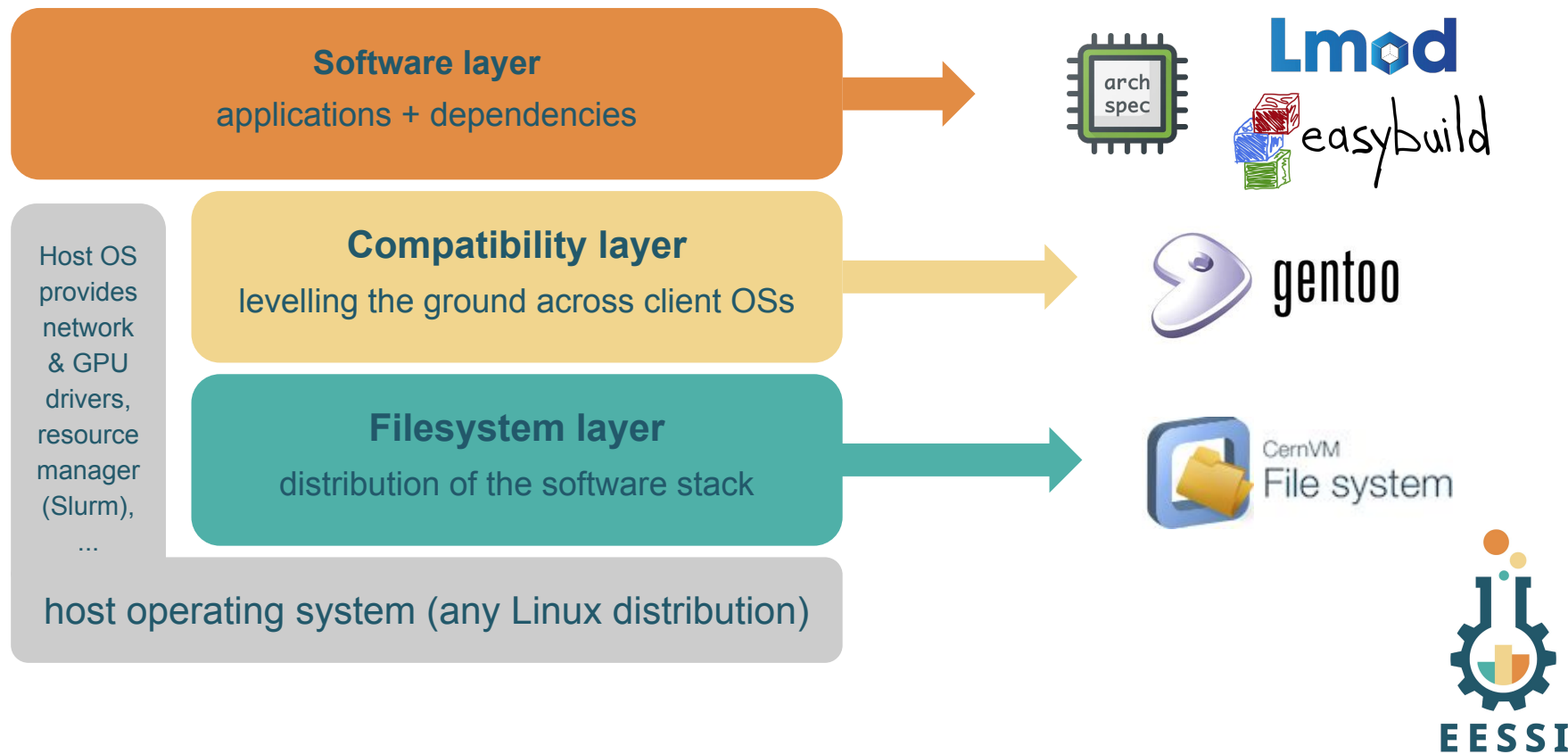


- **European Environment for Scientific Software Installations (EESSI)**
- Collaboration between different European partners in HPC community
- Goal: building a **common** scientific software stack,
for HPC systems & beyond (personal workstations, cloud instances, ...)
- Heavily inspired by Compute Canada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

High-level overview of the EESSI project

<https://www.eessi-hpc.org>

<https://eessi.github.io/docs>



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/www/subscribe/easybuild>
 - Slack: <https://easybuild.slack.com> - <https://easybuild.io/join-slack>
 - Bi-weekly conference calls: <https://github.com/easybuilders/easybuild/wiki/Conference-calls>