

Online introductory tutorial

Tue June 23rd 2020

<https://github.com/easybuilders/easybuild/wiki/EasyBuild-tutorial>



Acknowledgements



Tutorial organisers:

- Maxime Boissonneault (Compute Canada)
- Markus Geimer (Jülich Supercomputing Centre, Germany)
- Kenneth Hoste (HPC-UGent, Belgium)
- Christian Kniep (AWS)
- Alan O'Cais (Jülich Supercomputing Centre, Germany)
- Åke Sandgren (Umeå University, Sweden)

Acknowledgements



Reviewers & helping hands:

- Michael Kelsey (Texas A&M University, US)
- Terje Kvernes (University of Oslo, Norway)
- Miguel Dias Costa (National University of Singapore)

Background



- EasyBuild tutorial proposal accepted for ISC'20
- Accepted ISC'20 tutorials have been postponed to ISC'21
- We figured to seize the opportunity and host it online in 2020 as well...

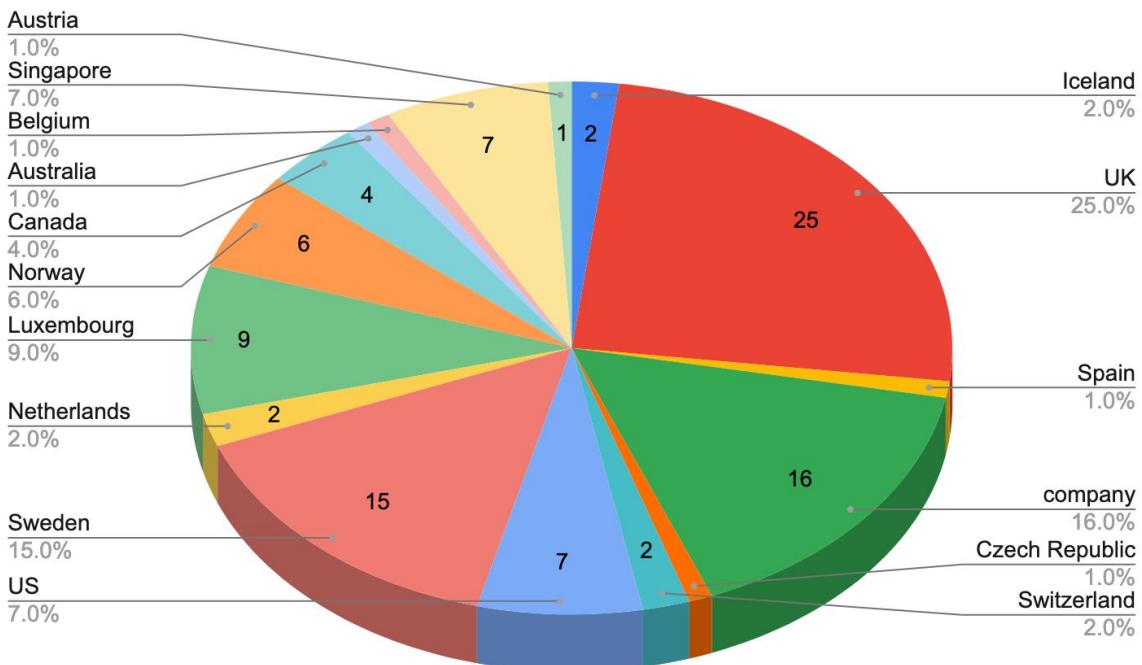


Attendance



- 101 registrations
- 7 companies
- 15 countries

Registration for EasyBuild tutorial, by country



Agenda (1/3)

(times are in UTC)



[11:00 - 11:10] Welcome & practical info

[11:10 - 11:25] General introduction to EasyBuild

[11:25 - 11:50] Installation and configuration of EasyBuild (hands-on)

[11:50 - 12:30] Basic usage of EasyBuild + installing software (hands-on)

[12:30 - 12:40] (*short break*)

Agenda (2/3)

(times are in UTC)



[12:40 - 13:00] Troubleshooting (hands-on)

[13:00 - 13:20] Hierarchical module naming schemes

[13:20 - 14:00] Adding support for additional software (hands-on)

[14:00 - 14:10] (*short break*)

Agenda (3/3)

(times are in UTC)



[14:10 - 15:25] EasyBuild at the Jülich Supercomputing Centre

[14:25 - 15:40] EasyBuild at Compute Canada

[14:40 - 15:55] Contributing back to EasyBuild

[14:55 - 16:10] Comparison with other tools

[15:10 - 16:15] Getting help

[15:15 - 16:00] Q&A

Practical information



- Event page: <https://github.com/easybuilders/easybuild/wiki/EasyBuild-Tutorial>
- These slides:
https://github.com/easybuilders/easybuild-tutorial/raw/master/docs/files/easybuild_tutorial_slides_isc20.pdf
- Tutorial site: <https://easybuilders.github.io/easybuild-tutorial>
- Streaming via YouTube: <https://www.youtube.com/c/easybuilders>
- Recordings will be available shortly after the live tutorial

Practical information: Slack



- Questions or problems?

Speak up in #tutorial on EasyBuild Slack!

Practical information: Slack



- Questions or problems?

Speak up in #tutorial on EasyBuild 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

Start a thread

A red circle highlights the 'Start a thread' button, and a red arrow points from it to the expanded thread view on the right.

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.

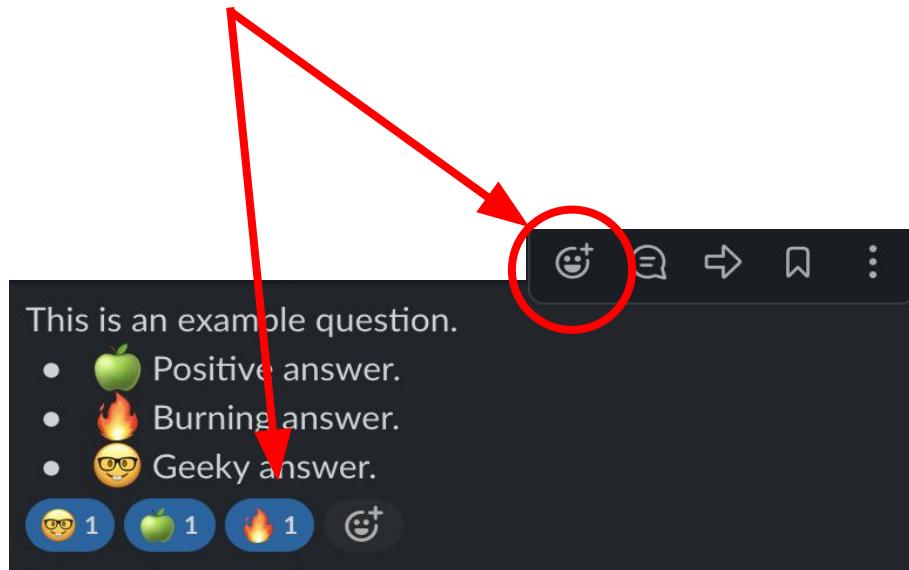
Reply...

Aa Aa U U 11

Emoji polls in Slack



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



Prepared environment



- Docker container image (also usable via Singularity)
 - also usable via Singularity (*with some limitations*)
 - CentOS 7.8 + Lmod 8
 - Pre-installed software stack in /easybuild
 - Use `python3` to run EasyBuild
- Resources available in AWS Cloud9





AWS Cloud9 login procedure

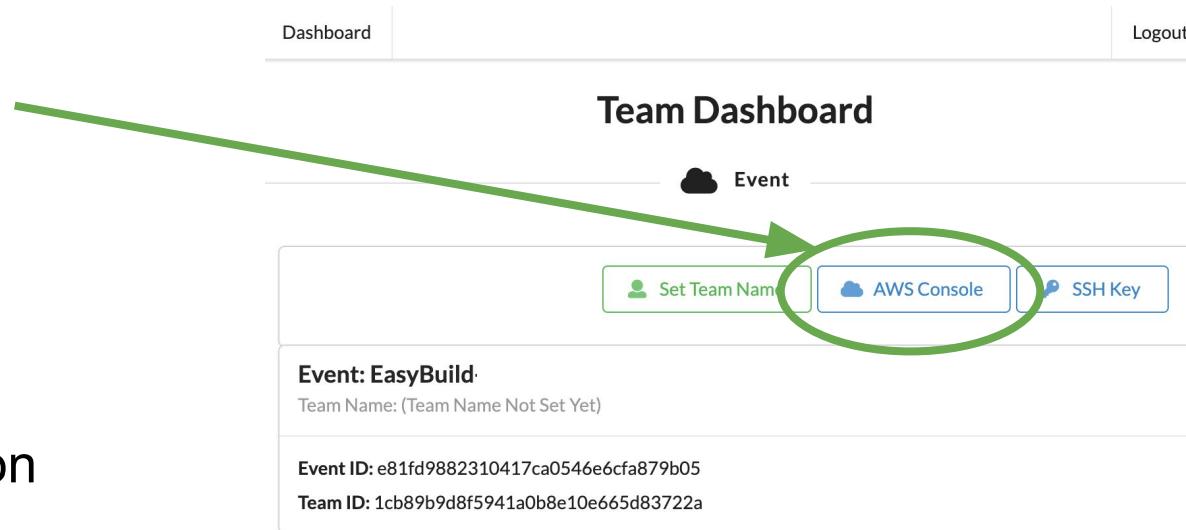
- **Use the login URL you received via email**
- Open AWS console
- Open IDE
- Search for Cloud 9
- Start a Terminal session

aws Cloud9 login procedure

- Use the login URL you received via email

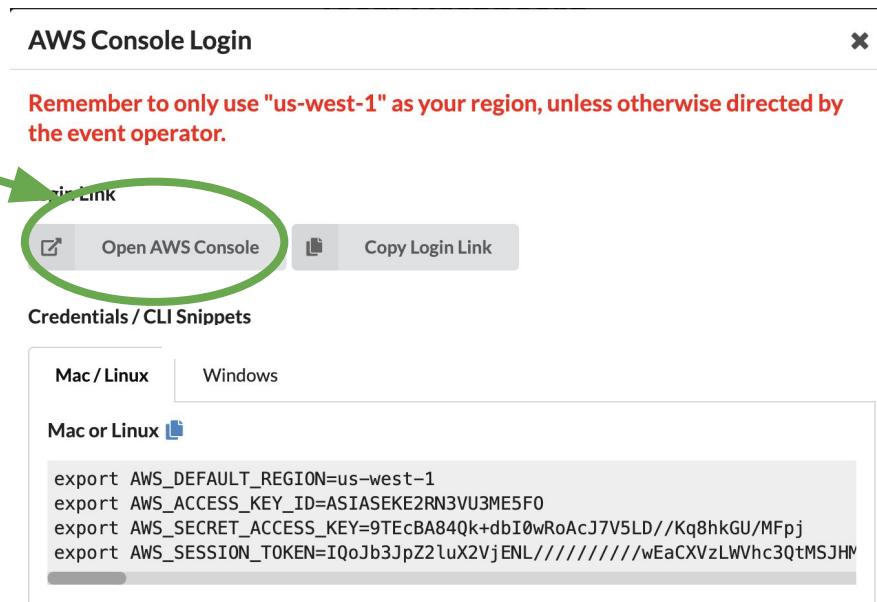
- Click “AWS console”

- Open IDE
- Search for Cloud 9
- Start a Terminal session



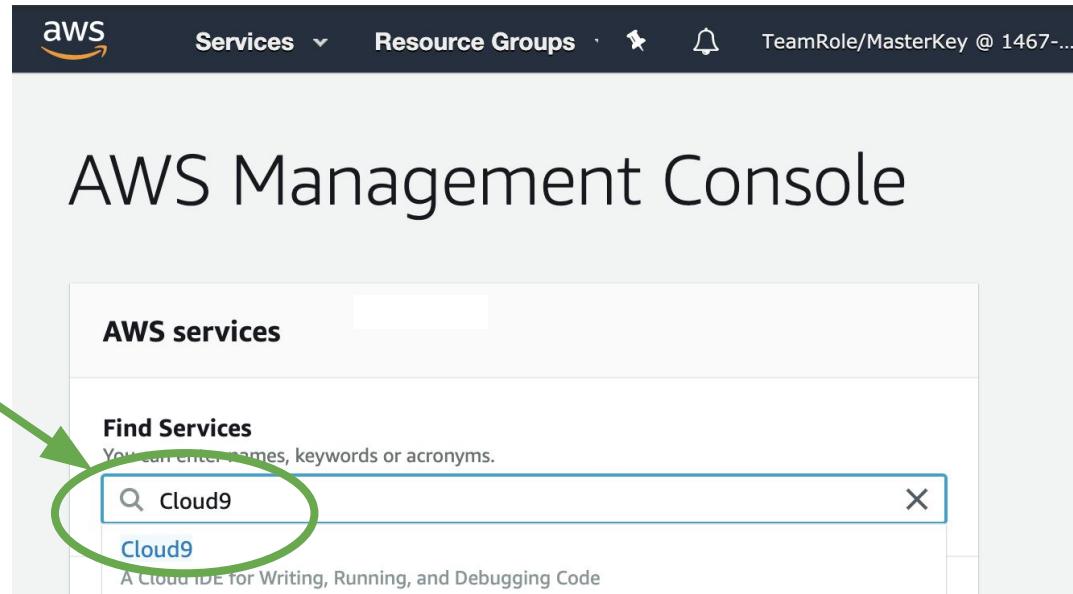
aws Cloud9 login procedure

- Use the login URL you received via email
- Click “Open AWS console”
- Open IDE
- Search for Cloud 9
- Start a Terminal session



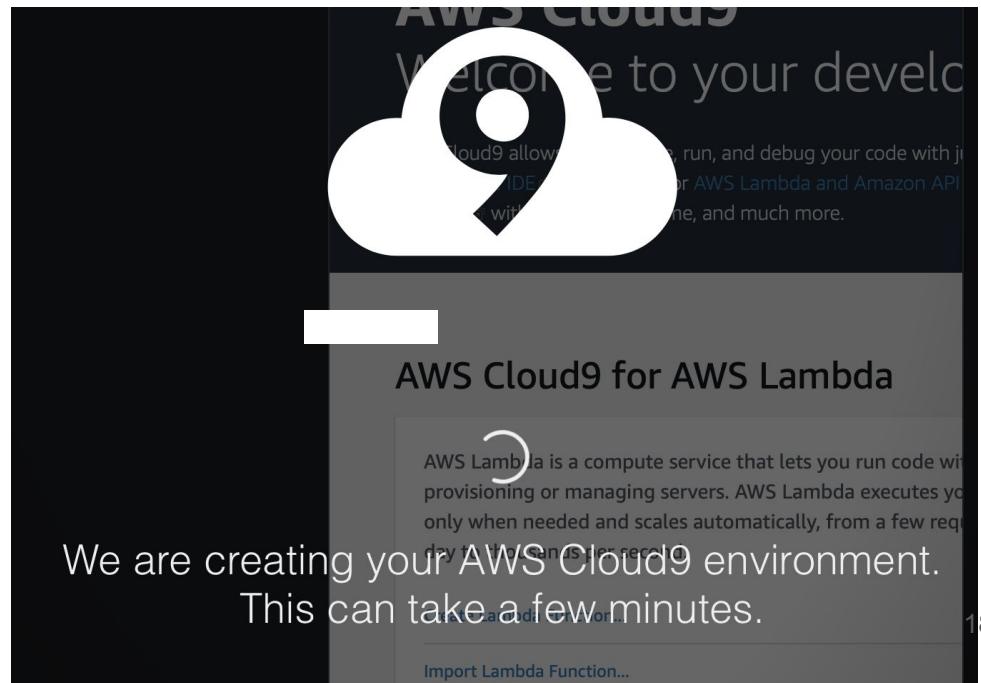
aws Cloud9 login procedure

- Use the login URL you received via email
- Open AWS console
- Open IDE
- Search for Cloud 9
- Start a Terminal session



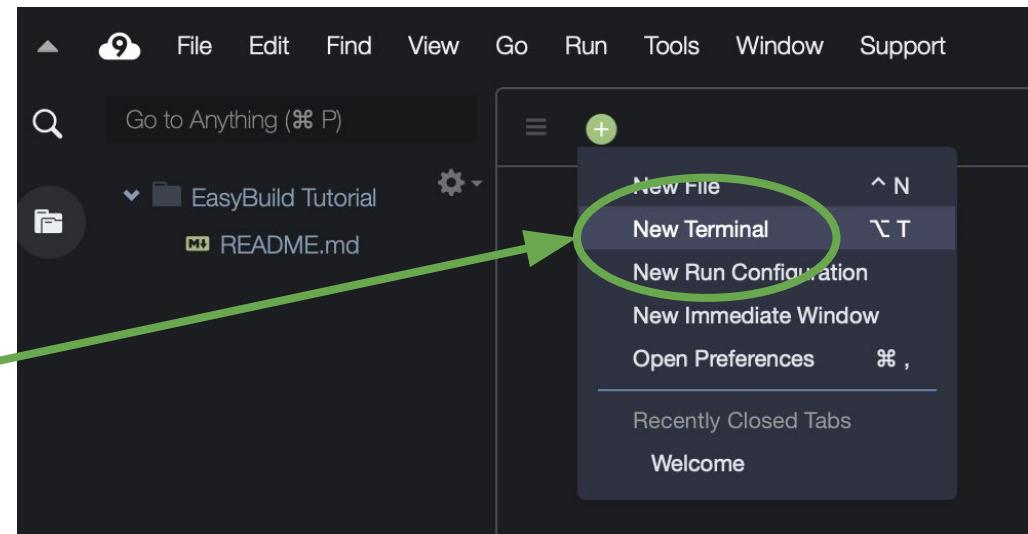
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aws Cloud9 login procedure

- Use the login URL you received via email
- Open AWS console
- Open IDE
- Search for Cloud 9
- Start a Terminal session



Running the container image with Docker



https://easybuilders.github.io/easybuild-tutorial/practical_information



Copy paste this command from the tutorial page!

```
mkdir -p isc20_easybuild_tutorial  
  
docker run -ti --rm --mount  
type=bind,source=$PWD/isc20_easybuild_tutorial,target=  
/home/easybuild --hostname tutorial easybuilders/tutorial:isc20
```

Running the container image with **Singularity**



https://easybuilders.github.io/easybuild-tutorial/practical_information



Copy paste this command from the tutorial page!

```
mkdir -p isc20_easybuild_tutorial
```

```
singularity run --cleanenv --home $PWD/isc20_easybuild_tutorial  
docker://easybuilders/tutorial:isc20
```

There are some limitations when using Singularity!

Recommended screen setup

Left:
Welcome to the official EasyBuild tutorial!

This is an introductory tutorial to EasyBuild, a command line tool for installing (scientific) software on High Performance Computing (HPC) systems.

tutorial site

It aims to explain what EasyBuild is, how to build software with it, make you familiar with some of the features it provides, and show how it is used by large HPC sites to maintain their central software stacks.

Through hands-on exercises and demos, you will learn how EasyBuild can help you to get scientific software installed in an efficient way.

Intended audience

This tutorial is primarily intended for people new to EasyBuild, but even if you're already familiar with the project it could be interesting to step through it.

Our main target audience includes:

Top right:
YouTube live stream

The tutorial materials are available at <https://easybuilders.github.io/easybuild-tutorial>.

terminal (in AWS)

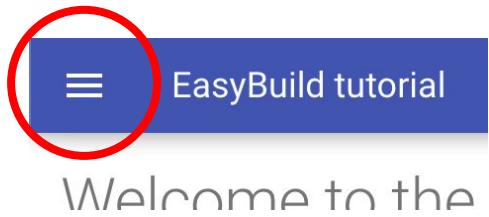
To access the pre-installed software run 'module use /easybuild/modules/all', and then check which modules are installed using 'module avail'.

In case of questions or problems contact the tutorial organisers via the #tutorial channel in the EasyBuild Slack, join via <https://easybuild-slack.herokuapp.com>.

```
[easybuild@tutorial ~]$
```

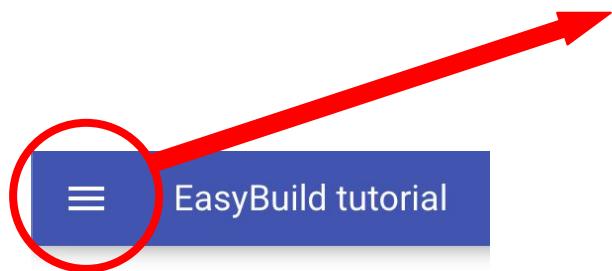
Tutorial site

Hamburger button to
access tutorial overview



Tutorial site

Hamburger button to
access tutorial overview



A screenshot of the "EasyBuild tutorial" website. The sidebar on the left contains the following navigation links:

- Home
- Practical information
- Introduction
- Installation
- Configuration
- Basic usage

The "Basic usage" link is currently highlighted with a blue background. To the right of the sidebar, the main content area shows some introductory text about configuration and installation.

Tutorial site

Hamburger button to
access tutorial overview



Welcome to the

A screenshot of a website page showing the "Workflow" section of the "EasyBuild tutorial". The page has a dark header with the title "EasyBuild tutorial" and a GitHub link. On the left is a sidebar with a blue header containing a three-line hamburger menu icon and the text "EasyBuild tutorial". Below the sidebar, there is a list of topics: Home, Practical information, Introduction, Installation, Configuration, and Basic usage. To the right of the sidebar, the main content area displays the first few lines of the "Workflow" section. A red arrow points from the text "Mini hamburger button to access tutorial section contents" to the mini-hamburger icon in the sidebar. Another red arrow points from the text "Table of contents" to the top right corner of the page, where a "Table of contents" icon is located.

Table of contents

Workflow

Specifying easyconfigs

Example command

Easyconfig filenames

Searching for easyconfigs

Search index

Inspecting easyconfigs

Mini hamburger button to
access tutorial section contents

Tutorial site

Hamburger button to
access tutorial overview



Welcome to the

**Use copy button
In code snippets!**

A screenshot of a mobile-style website. At the top, there's a header with a logo and the text "EasyBuild tutorial". Below it is a GitHub link "EasyBuild @ GitHub". The main content area has a sidebar on the left with a "Home" link and a "≡" icon (mini hamburger button) circled in red. A red arrow points from the "≡" icon on the homepage to this one. The main content area lists several sections: "Practical information", "Introduction", "Installation", "Configuration", and "Basic usage". To the right of the sidebar, there's a list of links: "Workflow", "Specifying easyconfigs", "Example command", "Easyconfig filenames", "Searching for easyconfigs", "Search index", and "Inspecting easyconfigs". A green arrow points from the "copy" icon on the homepage to the "≡" icon here.

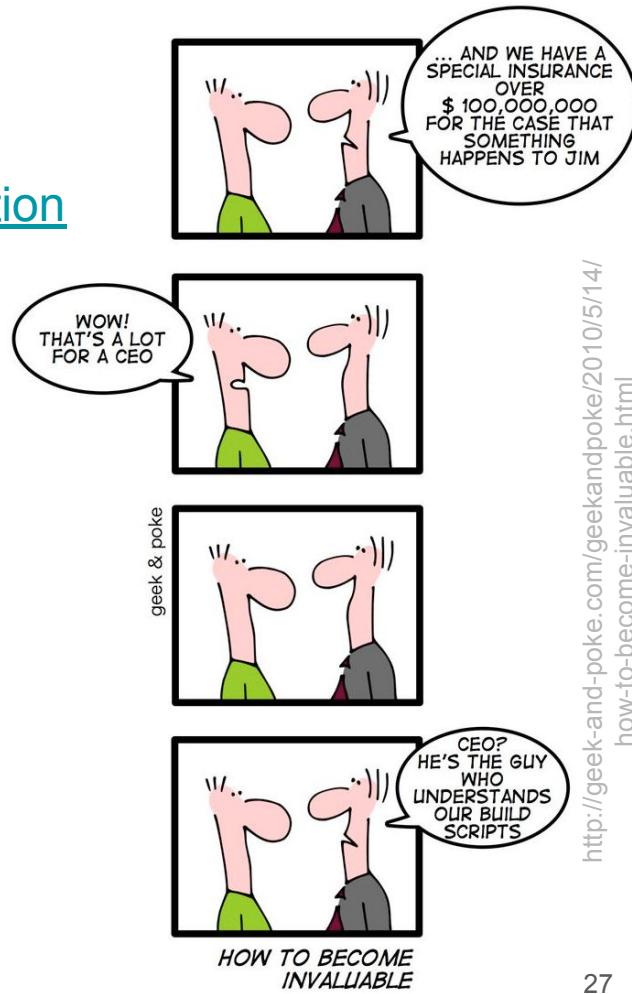
Mini hamburger button to
access tutorial section contents



General introduction to EasyBuild

<https://easybuilders.github.io/easybuild-tutorial/introduction>

- What is EasyBuild?
- Terminology
- Focus points



Installing EasyBuild



<https://easybuilders.github.io/easybuild-tutorial/installation>

Installing EasyBuild



<https://easybuilders.github.io/easybuild-tutorial/installation>

Recommended when using prepared container image:

```
export PATH=$HOME/.local/bin:$PATH  
export EB PYTHON=python3  
pip3 install --user easybuild
```

Configuring EasyBuild



<https://easybuilders.github.io/easybuild-tutorial/configuration>

Configuring EasyBuild



<https://easybuilders.github.io/easybuild-tutorial/configuration>

Recommended when using prepared container image:

```
export EASYBUILD_PREFIX=$HOME/easybuild  
export EASYBUILD_BUILDPATH=/tmp/$USER
```

Using pre-installed software stack



In prepared container image:

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

Basic usage



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

- Workflow
- Usage of **eb** command
- Installing software
- Exercises

```
$ eb SAMtools-1.10-GCC-9.3.0.eb
== temporary log file in case of crash /tmp/eb-zh7_fyre/easyb...
== found valid index for /home/example/.local/easybuild/easyb...
== processing EasyBuild easyconfig /home/example/.local/easyb...
== building and installing SAMtools/1.10-GCC-9.3.0...
== fetching files...
== creating build dir, resetting environment...
== unpacking...
== patching...
== preparing...
== configuring...
== building...
== testing...
== installing...
== taking care of extensions...
== restore after iterating...
== postprocessing...
== sanity checking...
== cleaning up...
== creating module...
== permissions...
== packaging...
== COMPLETED: Installation ended successfully (took 11 sec)
```

Short break



Next up:

[12:40 - 13:00] Troubleshooting (hands-on)



[13:00 - 13:20] Hierarchical module naming schemes

[13:20 - 14:00] Adding support for additional software (hands-on)

[14:00 - 14:10] (*short break*)

(times are in UTC)

Troubleshooting



<https://easybuilders.github.io/easybuild-tutorial/troubleshooting>

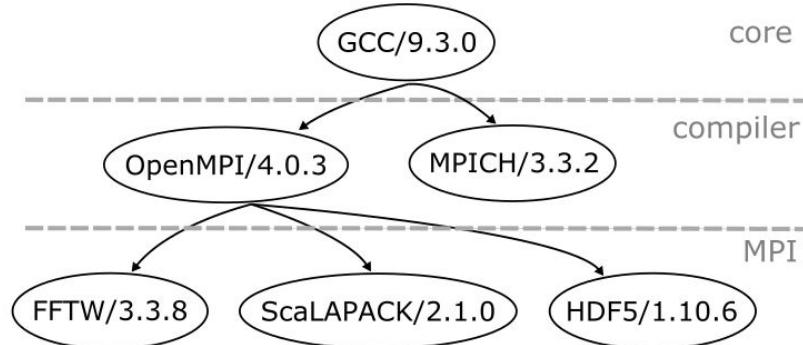
- EasyBuild error messages
- EasyBuild log files
- Build directory
- Exercises

Hierarchical module naming schemes



<https://easybuilders.github.io/easybuild-tutorial/hmns>

- Flat vs hierarchical module naming schemes
- Pros & cons
- Example (demo)
- Exercise



Note: you will run into problems if you are using Singularity because /easybuild is read-only!

Adding support for additional software



https://easybuilders.github.io/easybuild-tutorial/adding_support_software

- Easyconfigs vs easyblocks
- Writing easyconfigs
- Generating & copying easyconfigs
- Example (demo)
- Exercise

```
easyblock = 'CMakeMake'

name = 'eb-tutorial'
version = '1.0.0'

homepage = 'https://easybuilders.github.io/easybuild-tutorial'
description = "EasyBuild tutorial example"

source_urls = ['https://github.com/easybuilders/easybuild-tutorial']
sources = [SOURCE_TAR_GZ]
checksums = ['87643c9a950d02471fc283b31e8a088da7d5d49b']

toolchain = {'name': 'GCC', 'version': '9.3.0'}

builddependencies = [('CMake', '3.16.4')]

configopts = "-DEBTUTORIAL_MSG='Hello from the EasyBuild tutorial!'

sanity_check_paths = {
    'files': ['bin/eb-tutorial'],
    'dirs': [],
}

sanity_check_commands = ['eb-tutorial']
```

Short break



Next up:

[14:10 - 15:25] EasyBuild at the Jülich Supercomputing Centre

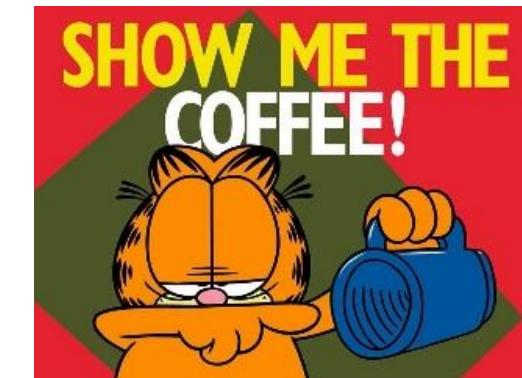
[14:25 - 15:40] EasyBuild at Compute Canada

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[15:15 - 16:00] Q&A



(times are in UTC)

EasyBuild at JSC



<https://easybuilders.github.io/easybuild-tutorial/jsc>

- by Alan O'Cais



Jülich Supercomputing Centre



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



Jülich Supercomputing Centre



- JSC is a German supercomputing centre since 1987
 - About 200 experts for all aspects of supercomputing and simulation sciences
- We have 3 primary systems at the moment
 - JUWELS - modular supercomputing, 70 petaflops in 2020
 - JURECA - CPU, GPU and KNL. To be replaced by in 2020
 - JUSUF - AMD, V100 GPU. Interactive workflows and community services





EasyBuild at JSC

- Geared towards *average* user experience
 - Hide lots of indirect software
 - Lots of toolchains => Module hierarchy
 - Renaming some modules, Lmod tweaks



EasyBuild at JSC

- Geared toward *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 remove this where possible



Upgrading and retiring software

- Provide latest software to new projects by default
 - **Stages** concept
 - Updates twice 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 twice 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)
- Enable user space installations
 - Can be leveraged to guide people on how to do this “properly”



EasyBuild at Compute Canada



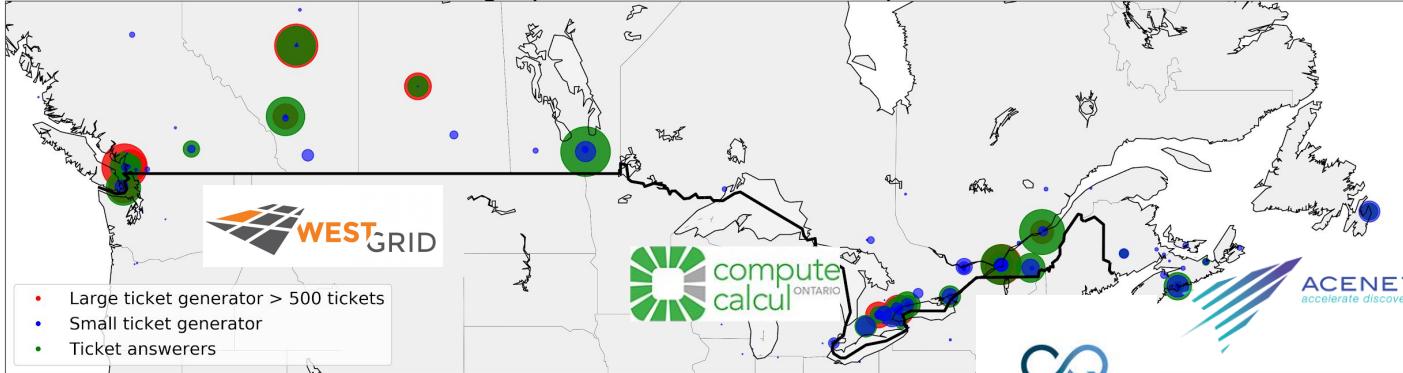
<https://easybuilders.github.io/easybuild-tutorial/computecanada>

- by Maxime Boissonneault



Compute Canada : the people

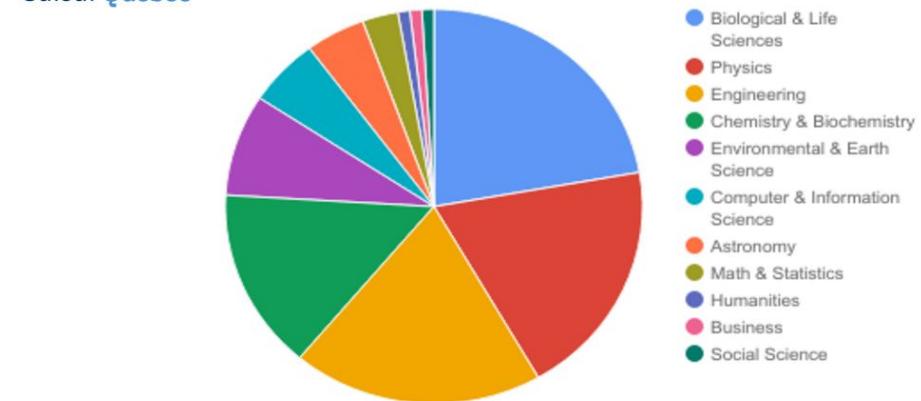
Network graph of ticket routes Compute Canada



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



Before 2015

- Around 30 Compute Canada sites hosting hardware
- Over 50 clusters or other hardware resources
- All configured differently

Compute Canada : the hardware



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

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

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**.

1. All software should be accessible on every site, reliably and performantly.
2. Software should be independent from the underlying OS stack.
3. Software installation should be tracked and reproducible via automation.
4. The user interface should make it easy to use a large and evolving
software stack.

What this means

All new Compute Canada sites

1. Need a distribution mechanism
 - a. CVMFS : CERN Virtual Machine File System

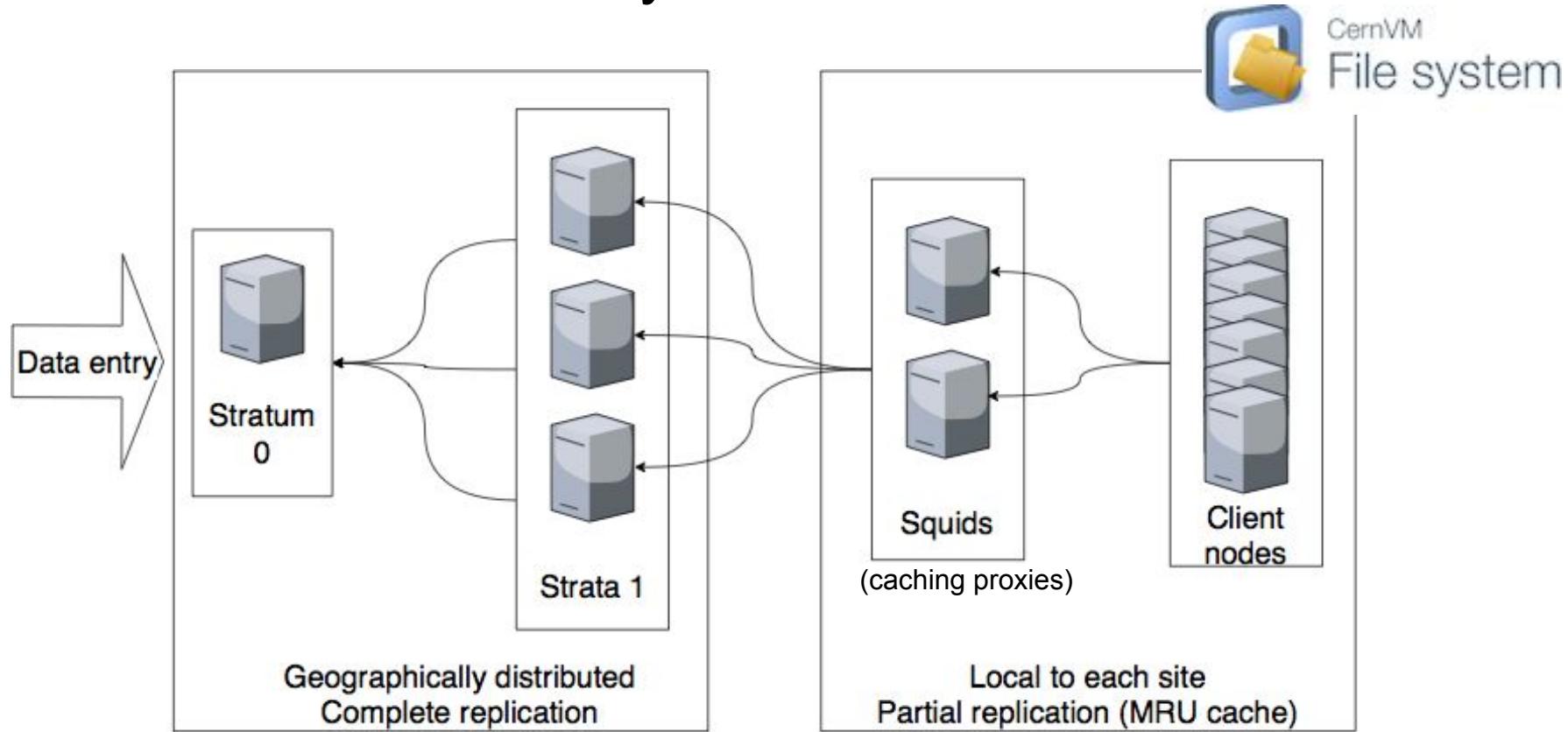
Consistency

2. Independent of the OS (Ubuntu, CentOS, Fedora, etc.)
 - a. Nix ==> Gentoo Prefix
3. Automated installation (humans are not so consistent)
 - a. EasyBuild

Easy to use

4. Needs a module interface that scale well
 - a. Lmod with a hierarchical structure

CVMFS content delivery



Software: design overview

Easybuild layer: modules for Intel, PGI, OpenMPI, CUDA, MKL, high-level applications.

Multiple architectures (sse3, avx, avx2, avx512)

`/cvmfs/soft.computecanada.ca/easybuild/{modules,software}/2017`

Easybuild-generated modules around Nix profiles (mostly deprecated):

GCC, Eclipse, Qt+Perl+Python no longer

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

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

`module nixpkgs/16.09 => $EBROOTNIXPKGS=`

`/cvmfs/soft.computecanada.ca/nix/var/nix/profiles/16.09`

Gray area: Slurm, Lustre client libraries, IB/OmniPath/InfiniPath client libraries (all dependencies of OpenMPI). In Nix 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

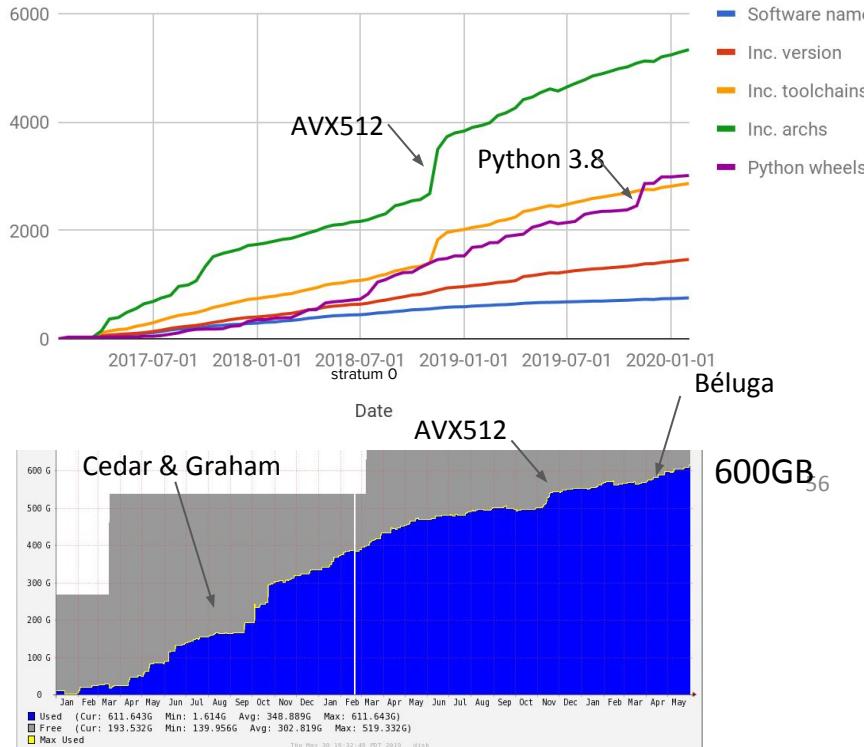
Available software

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](#)

Design choices / EB features



- Compatibility layer => filtering of a lot of dependencies (M4, cmake, etc.)
- Toolchains based combinations of
 - Intel/GCC, OpenMPI, MKL, Cuda
 - Not “foss” nor “intel”
 - => We are (ab)using the --try-toolchain, --try-software-version, --try-update-deps options
- Custom MNS :
 - Hierarchical, lower case
 - No version suffix at all
 - Toolchains are hidden
- No LD_LIBRARY_PATH

Hooks

- 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)

Handling Python



- 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 (see next slide)
- [Not supporting Anaconda](#)

Python wheels

What are wheels?

[Wheels](#) are [the new standard](#) of Python distribution and are intended to replace eggs. Support is offered in `pip >= 1.4` and `setuptools >= 0.8`.

Advantages of wheels

1. Faster installation for pure Python and native C extension packages.
2. Avoids arbitrary code execution for installation. (Avoids `setup.py`)
3. Installation of a C extension does not require a compiler on Linux, Windows or macOS.
4. Allows better caching for testing and continuous integration.
5. Creates `.pyc` files as part of installation to ensure they match the Python interpreter used.
6. More consistent installs across platforms and machines.
7. **You can compile your own wheels, linking against your compiled libraries**



You can use this too!

Mounting our software stack:

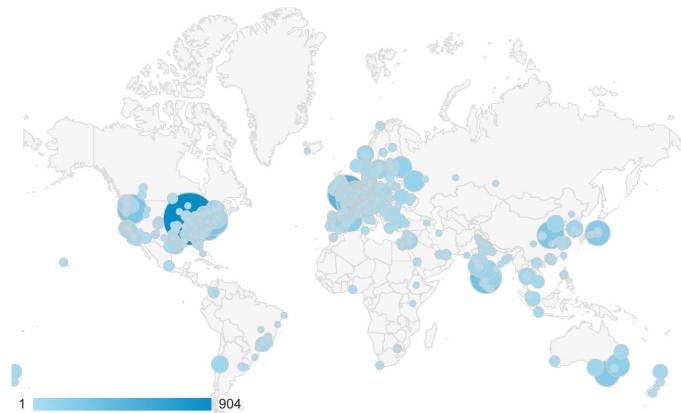
https://docs.computecanada.ca/wiki/Accessing_CVMFS

The EasyBuild community



<https://easybuilders.github.io/easybuild-tutorial/community>

- Brief history of the project
- Who is using EasyBuild?
- Who is maintaining EasyBuild?
- EasyBuild events



Contributing to EasyBuild



<https://easybuilders.github.io/easybuild-tutorial/contributing>

- Contribution workflow
- GitHub integration features in EasyBuild
- Contribution stats

GitHub

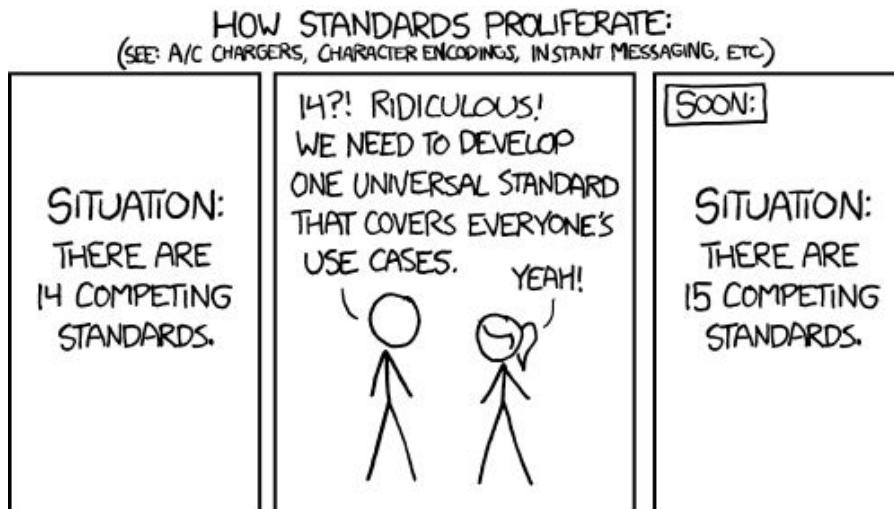


Comparison with other tools



https://easybuilders.github.io/easybuild-tutorial/comparison_other_tools

-  **Spack**
-  **Nix**
-  **Guix**
-  **CONDA**



<https://xkcd.com/927>

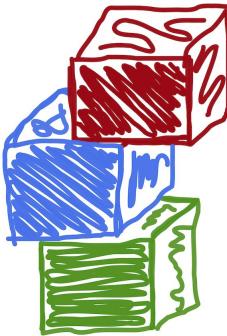
Getting help



https://easybuilders.github.io/easybuild-tutorial/getting_help

- Documentation
- GitHub
- Mailing list
- Slack
- Bi-weekly conf call





easybuild

Any more questions?

Please take a minute to fill out the evaluation survey !

<https://nl.surveymonkey.com/r/eb-tutorial>