



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...

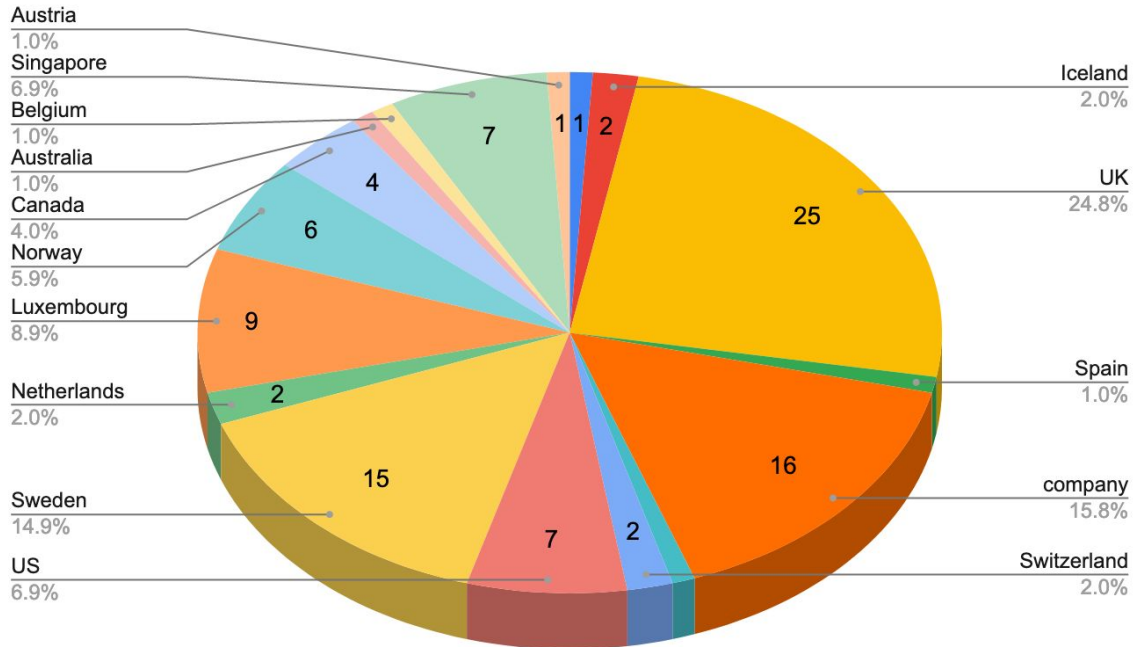


Attendance



- 101 registrations
- 7 companies
- 16 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: **FIXME FIXME FIXME**
- 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
- Questions or problems?

Speak up in #tutorial on EasyBuild Slack!

Prepared environment

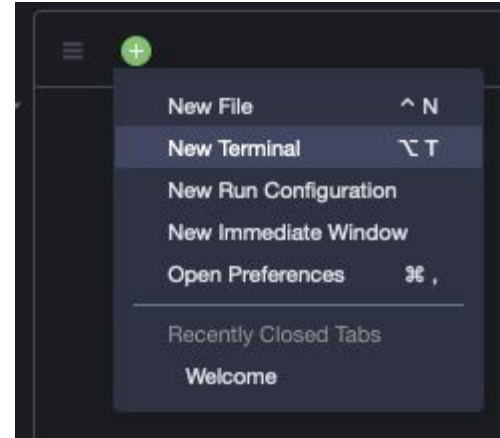
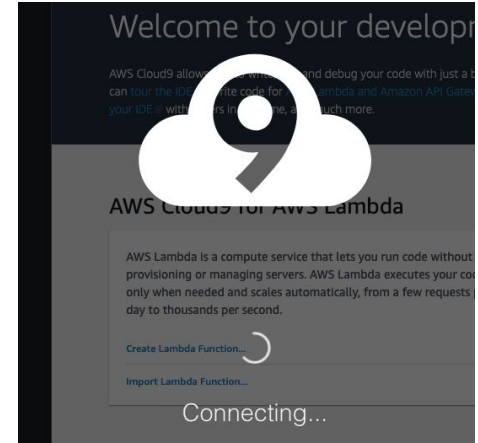


- Docker container image (also usable via Singularity)
 - also usable via Singularity
 - CentOS 7.8 + Lmod 8
 - Pre-installed software stack in `/easybuild`
 - Use `python3` to run EasyBuild
- Resources available in AWS Cloud9

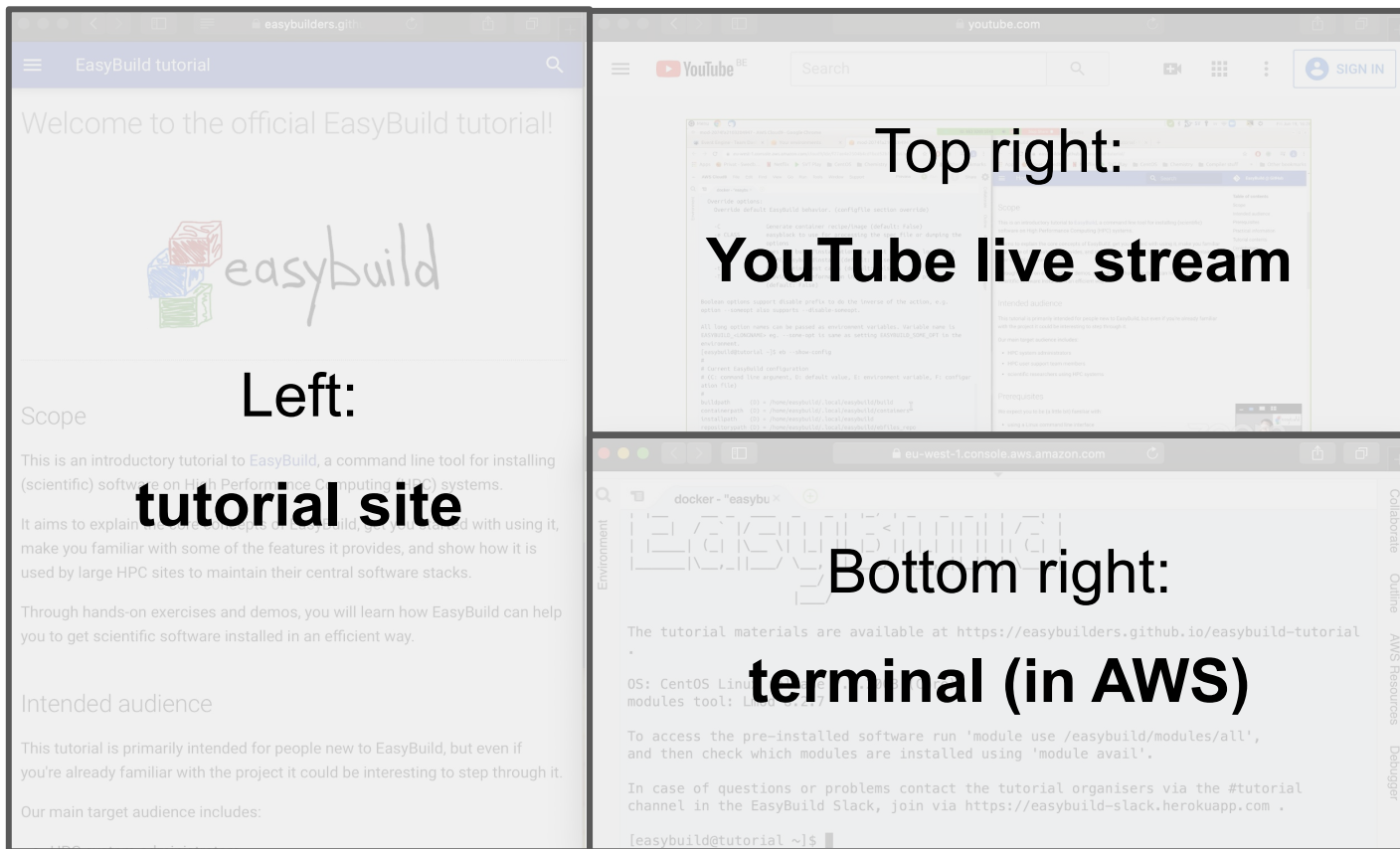


aws Cloud9 login procedure

- **Use login URL you received via email**
- Click “AWS console”
- Click “Open IDE”
- Search for Cloud 9
- Close welcome window
- Use “+” to start a Terminal session



Recommended screen setup

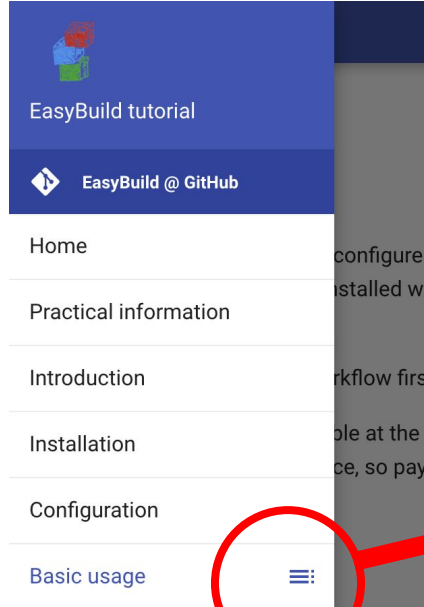


Tutorial site

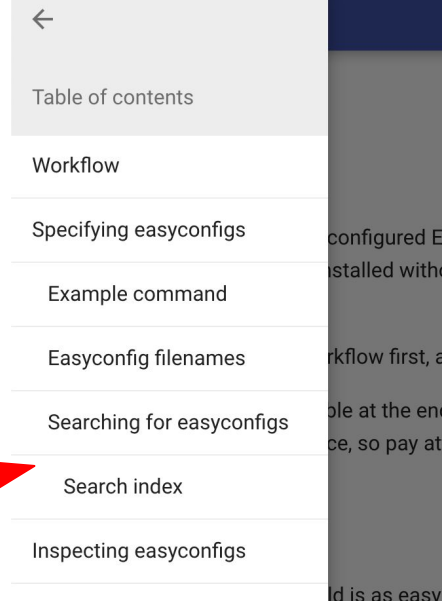
Hamburger button to
access tutorial overview



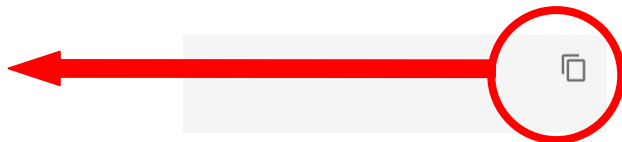
Welcome to the



Mini hamburger button to
access tutorial section contents



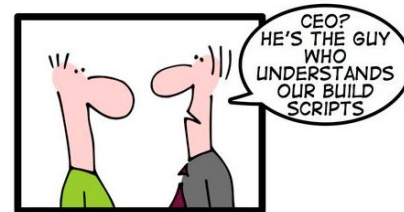
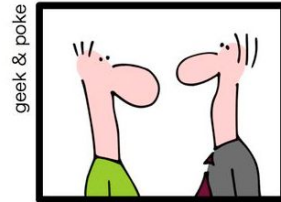
Copy button in
code snippets!



General introduction to EasyBuild

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

- What is EasyBuild?
- Terminology
- Focus points



HOW TO BECOME INVALUABLE

Installing EasyBuild



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

In 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>

In 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/easyco
== 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)

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Troubleshooting



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

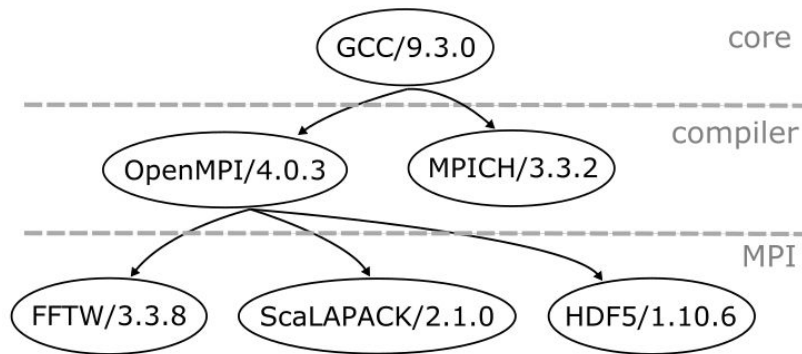
- EasyBuild error messages
- EasyBuild log files
- Build directory
- Exercises

Hierarchical module naming schemes



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

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



Adding support for additional software



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

- Easyconfigs vs easyblocks
- Writing easyconfigs
- Generating & copying easyconfigs
- Example
- 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']
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'"]

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

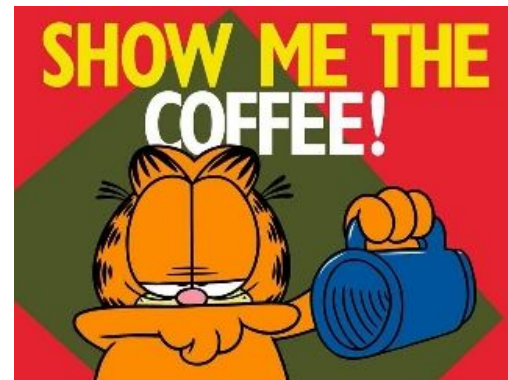
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EasyBuild at JSC



<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 toward *average* user experience
 - Hide lots of indirect software
 - Lots of toolchains => Module hierarchy
 - Renaming some modules, Imod 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
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 - 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 easybuild

- 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



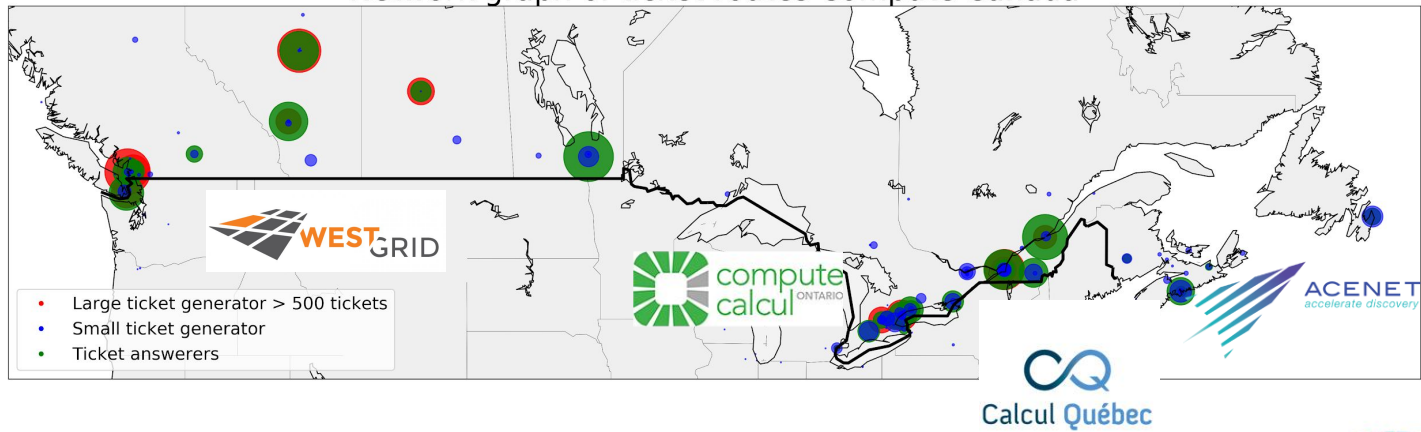
<https://easybuilders.github.io/easybuild-tutorial/computecanada>

- by Maxime Boissonneault



Compute Canada : the people

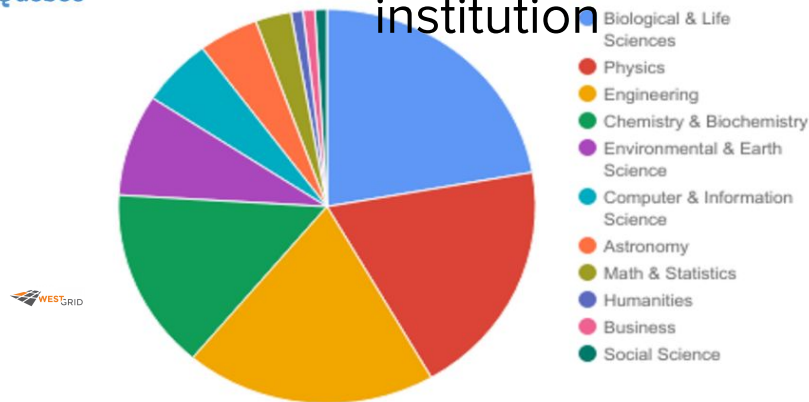
Network graph of ticket routes Compute Canada



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

All research disciplines supported

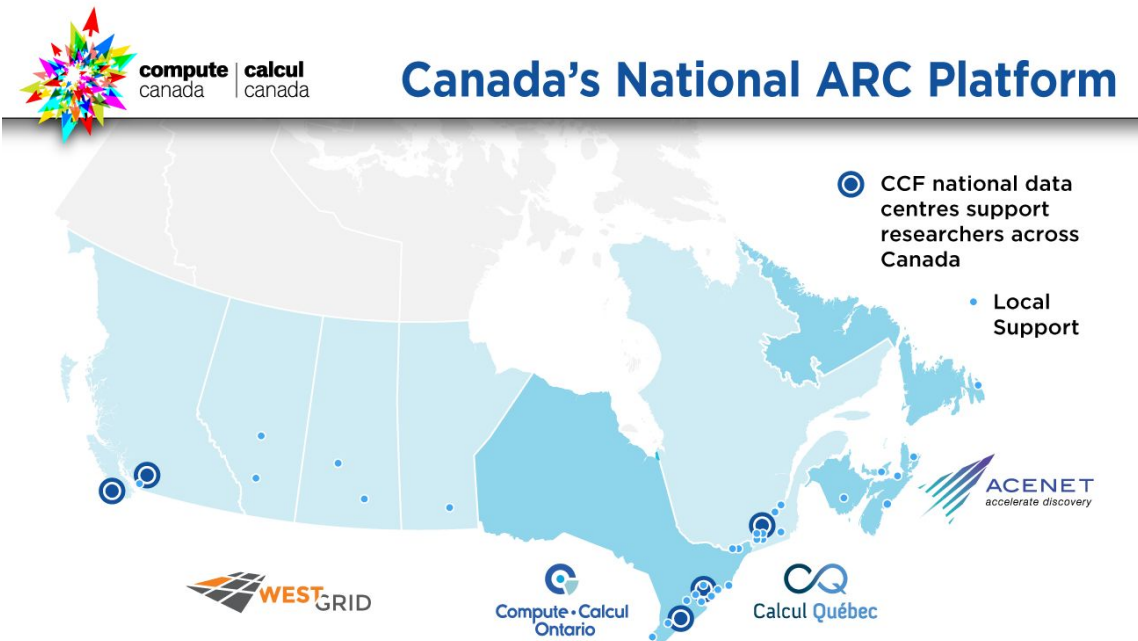
Free access for any researcher at a Canadian institution



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

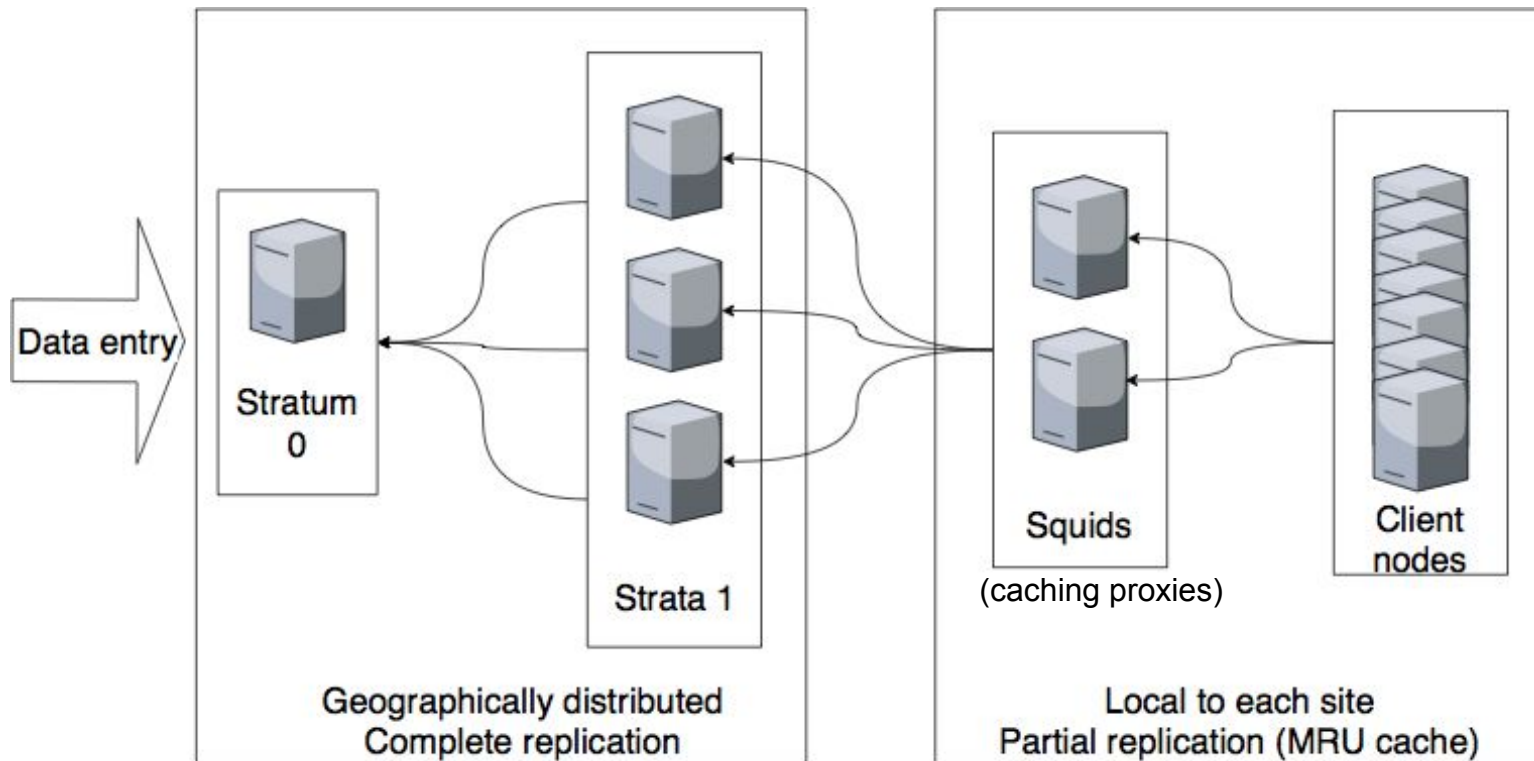
Consistency

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

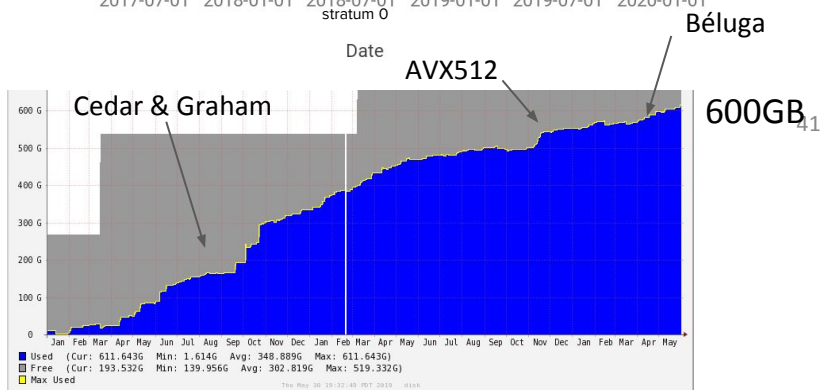
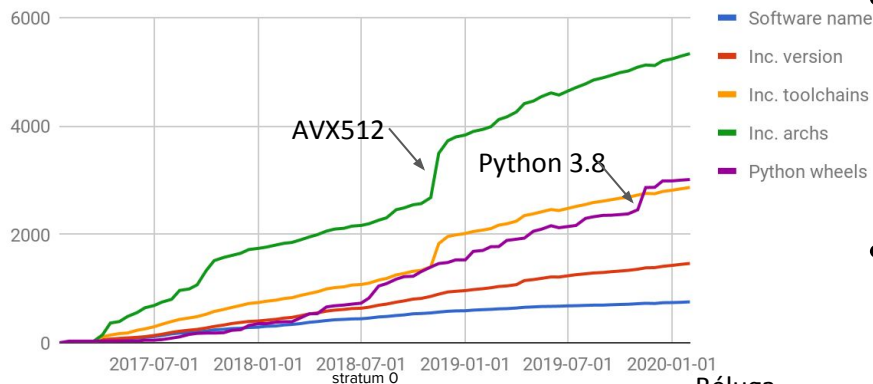
Available software

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

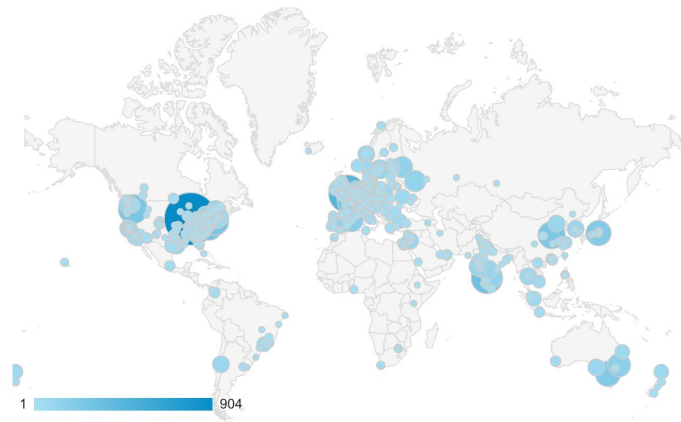
- Mounting our software stack
 - https://docs.computecanada.ca/wiki/Accessing_CVMFS

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

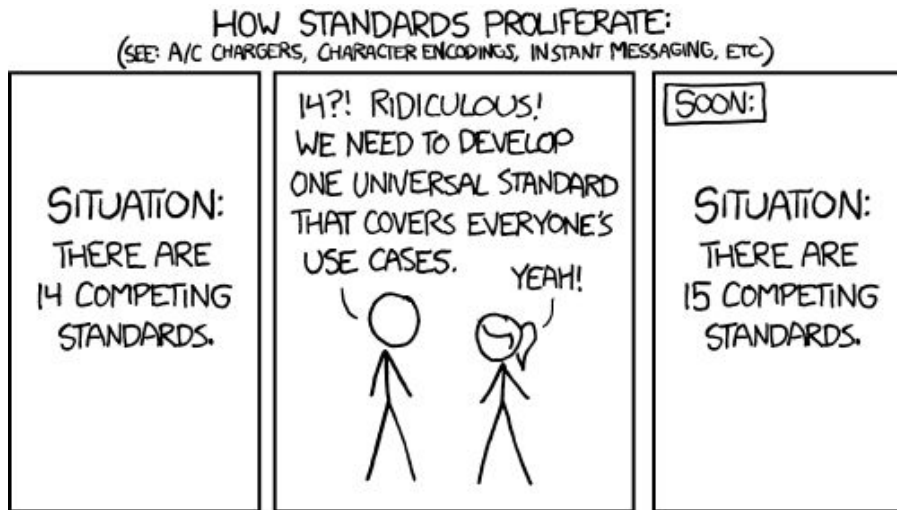


Comparison with other tools



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

- Spack
- Nix
- conda
- Gentoo



Getting help



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

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



Questions?

SURVEY LINK GOES HERE