Getting (your) scientific software installed using 

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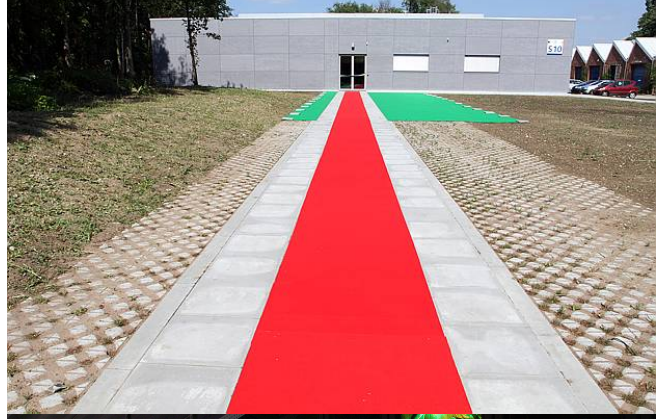
20190510 - CSCS Software Management Course

https://users.ugent.be/~kehoste/EasyBuild_20190510_CSCS_software_management.pdf

https://easybuilders.github.io/easybuild *https://easybuild.readthedocs.io*

HPC-UGent

GHENT UNIVERSITY



- part of central IT department of Ghent University (Belgium)
- centralised scientific computing services, training & support
- for researchers of UGent, industry & knowledge institutes
- 6 Tier-2 clusters (> 15k cores in total), ~2 PB shared storage
- 7+1 team members, > 3000 user accounts
- member of Flemish Supercomputer Centre (VSC)
  https://www.vscentrum.be

Vlaanderen
is computing

whoami

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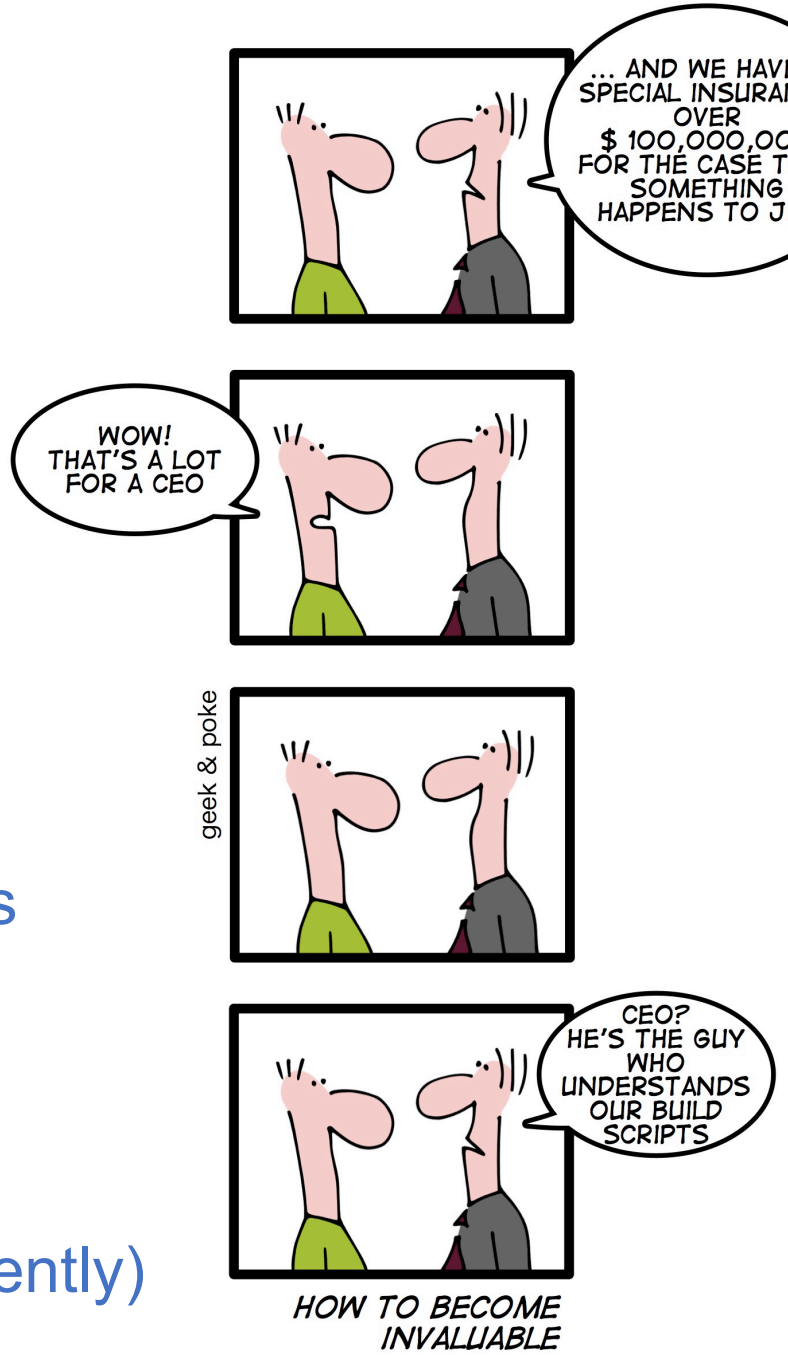
@boegel *(GitHub, IRC, Slack)*
@kehoste *(Twitter)*

- Masters & PhD in Computer Science from Ghent University
- PhD topic: machine learning applied to software performance, compilers, ...
- joined HPC-UGent team in October 2010
- main tasks: user support & training, *software installations*
- slowly also became  **lead developer & release manager**
- likes family, beer, loud music, FOSS, helping people, dad jokes, stickers, ...
- doesn't like CMake, SCons, Bazel, TensorFlow, OpenFOAM, ...

Getting scientific software installed

Installation of scientific software is a tremendous problem for HPC sites all around the world.

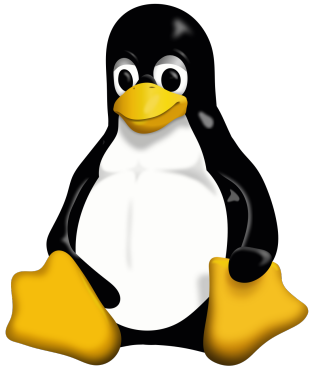
- ideally built from source (performance is key!)
- tedious, time-consuming, frustrating,
  sometimes simply not worth the (manual) effort...
- huge burden on researchers & HPC support teams
  - over 25% of support tickets at HPC-UGent,
    but consumes *way* more than 1/4th of support time...
- very little collaboration among HPC sites (until recently)



http://geekandpoke.typepad.com/geekandpoke/2010/05/how-to-become-invaluable.html

What about existing software installation tools? (1/2)

- **traditional package managers in Linux(-like) operating systems**
  - *yum* to install RPMs (Red Hat derivatives)
  - *apt* to install .deb files (Debian & derivatives)
  - *Homebrew* (macOS/Linux)
  - *Portage* (Linux), *pkgsrc* (*nix), ...



- **problems in context of scientific software & HPC:**
  - not well suited to idiosyncrasies of scientific software
  - not aware (enough) of MPI/BLAS/LAPACK/GPUs, other compilers (Intel, PGI, ...)
  - bad fit for multi-user HPC systems in general
  - little support for having multiple versions installed side-by-side
  - strong focus on generically optimised binaries (portability is important to limit effort)

What about existing software installation tools? (2/2)

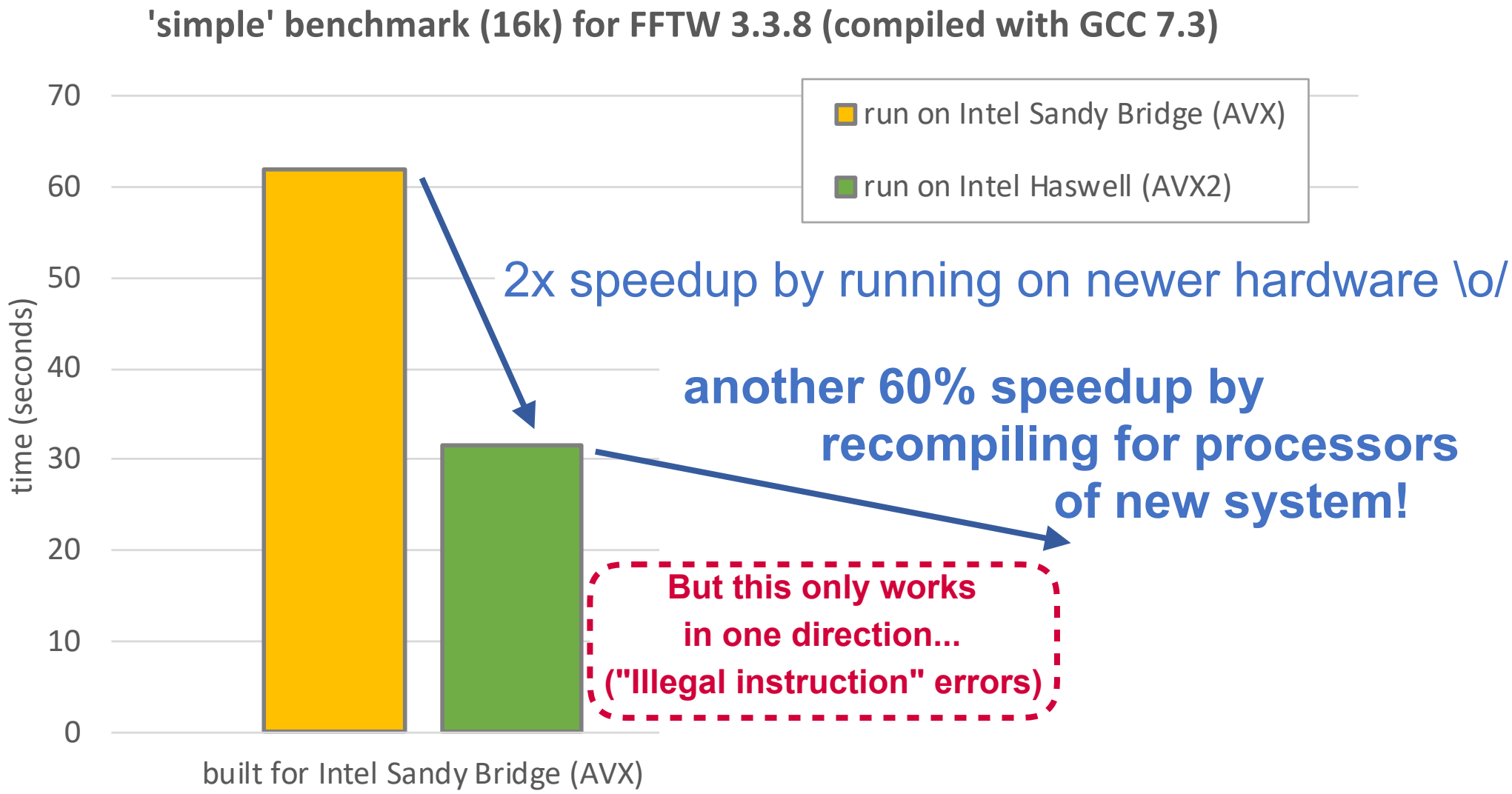
CONDA (installation tool for Anaconda distribution)

- very popular tool for installing scientific software, but mainly **targeted to individual users**
- **not well suited for centrally managing software** installations on multi-user HPC systems
- installing software with `conda` *usually* results in running **generically optimised binaries**
- hard to combine with software installed in other ways (e.g. centrally provided modules)

Containers (Docker/Singularity)  

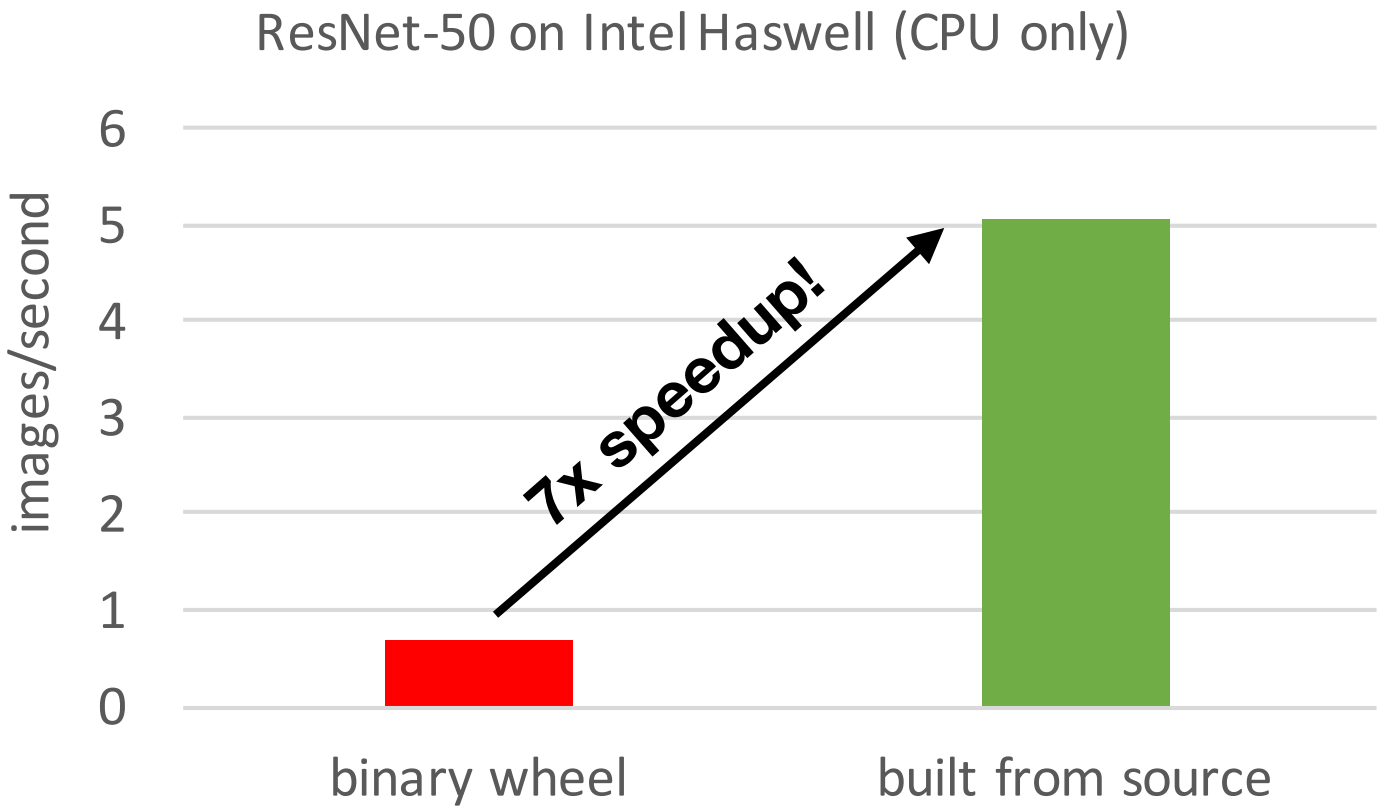
- **lack of attention to optimising for underlying hardware** ("mobility of compute")
- **integration with system resources** (MPI, CUDA, ...) is ***still a problem***
- **someone still needs to be build/maintain/update the container image you need/want !**
- in my opinion, containers are a *symptom*, not a cure...

Performance is key in HPC



(FFTW 3.3.8 installed in Singularity container, built from source)

"pip install tensorflow" works fine for me...



(disclaimer: old version of TensorFlow (1.4.x?), but point is still valid)

- installing pre-built generically optimised binaries is easy
- ... but **you may be paying a *significant* prize w.r.t. performance**

https://easybuilders.github.io/easybuild - https://easybuild.readthedocs.io

- **framework for installing scientific software** *(built from source when possible)*
- strong focus on Linux & HPC systems (and hence also performance)
- **by default builds/optimises specifically for host architecture**
- implemented in Python 2, lead development by HPC-UGent
- available under GPLv2 license via PyPI, GitHub
- supports different compilers & MPI libraries, x86_64/ARM/POWER, ...
- **good integration with Cray Programming Environment**
- active & helpful worldwide community

Almost 10 years of easybuild

- in-house development at HPC-UGent since summer 2009
- first public release in April 2012 (EasyBuild v0.5)
- **first stable release on November 13th 2012, during SC'12 (EasyBuild v1.0)**
- intention was to get feedback, but gradually a community emerged around it...
- **frequent stable releases** since then (latest: EasyBuild v3.9.0, Apr 12th 2019)
- community-driven development: bug reports, feature requests, contributions

Supported software

http://easybuild.readthedocs.io/en/latest/version-specific/Supported_software.html

- latest EasyBuild (v3.9.0) supports installing **over 1,700 different software packages**
  - including CP2K, NAMD, NWChem, OpenFOAM, TensorFlow, WRF, ...
  - a lot of bioinformatics software is also supported out of the box
  - + >1,000 extensions: Python packages, R libraries, Perl modules, X11 libraries, ...
  - built from source when possible, optimised by host architecture by default
- diverse toolchain support:
  - compilers: GCC, Intel, Clang, PGI, IBM XL, **Cray GNU/Intel/CCE**, CUDA
  - MPI libraries: OpenMPI, Intel MPI, MPICH, MPICH2, MVAPICH2, **Cray MPI**, ...
  - BLAS/LAPACK libraries: Intel MKL, OpenBLAS, ScaLAPACK, BLIS, **Cray LibSci**, ...

terminology

http://easybuild.readthedocs.io/en/latest/Concepts_and_Terminology.html

- **framework**
  - core of EasyBuild: Python modules & packages
  - provides supporting functionality for building/installing software, generating modules, ...
- **easyblock**
  - a Python module that serves as a build script, 'plugin' for the EasyBuild framework
  - implements a (generic or software-specific) build/install procedure
- **easyconfig file** (*.eb): build specification; software name/version, compiler toolchain, etc.
- **(compiler) toolchain***:* set of compilers + accompanying libraries (MPI, BLAS/LAPACK, ...)
- **extensions***:* additional packages for a particular applications (e.g., Python, R)

easybuild feature highlights (1)

- fully **autonomously** building and installing (scientific) software
  - automatic dependency resolution (via `--robot`)
  - automatic generation of environment module files (Tcl or Lua syntax)
- **no admin privileges required** (only write permission to installation target)
- thorough **logging** of executed build/install procedure
- **archiving** of easyconfigs, patches, easyblocks that were used
- highly **configurable**, via config files/environment/command line
- **dynamically extendable** with additional easyblocks, toolchains, etc.

feature highlights (2)

- support for **custom module naming schemes** (incl. hierarchical)
- **transparency** via support for 'dry run' installation & trace output
- **comprehensively tested**: lots of unit tests, frequent regression testing, ...
- actively developed, **frequent stable releases**
- **collaboration** between various HPC sites large & small
- integration with Torque/SLURM, FPM, Singularity, Docker, ...
- worldwide **community**

Integration with Cray Programming Environment

https://easybuild.readthedocs.io/en/latest/Cray-support.html

- initial (experimental) integration with Cray PE implemented April 2015
- declared stable in March 2016 (EasyBuild v2.7.0)
- custom `Cray*` toolchains leverage Cray-provided modules:

  `PrgEnv/*`, `cray-libsci`, `cray-mpich`, ...
- `--optarch` controls which `craype-*` module is used in build environment
- leveraging of Cray-provided "external" modules via provided metadata
- careful handling of Cray-provided modules in build environment & toolchains
- **used by CSCS since 2015 on Piz Daint & other Cray systems**

What  easybuild is *not*

- EasyBuild is ***not*** **YABT** (Yet Another Build Tool)

  it does *not* replace build tools like `cmake` or `make`; it wraps around them

- it is ***not*** **a replacement for package managers** (`yum`, `apt`, ...)

  it leverages some tools & libraries provided by the OS (glibc, OpenSSL, IB drivers, ...)

- it is ***not*** **a magic solution** to all your (software installation) problems...

  you will still run into compiler errors (unless somebody has already taken care of it)

What  easybuild is

- a **uniform interface** that wraps around software installation procedures
- a huge **time-saver**, by automating tedious/boring/repetitive tasks
- a way to provide a **consistent software stack** to your users
- an **expert system** for software installation on HPC systems
- a **platform for collaboration** with HPC sites worldwide
- a way to **empower *users* to self-manage their software stack** on HPC systems
- a tool that can be leveraged for **building *optimised* container images**

Installing easybuild

https://easybuild.readthedocs.io/en/latest/Installation.html

EasyBuild is already installed on Piz Daint!

```
$ module load daint-mc EasyBuild-custom
```

https://user.cscs.ch/computing/compilation/easybuild

- requirements:
  - GNU/Linux system + Python 2.6 or 2.7 (Python 3 will be supported soon)
  - environment modules tool (default configuration requires Lmod)
  - a system C/C++ compiler (only really needed to install toolchains)
- installation procedure (pick one):
  - `pip install easybuild` (or equivalent thereof using other Python installation tool)
  - bootstrap script (recommended)

```
$ python bootstrap_eb.py $EASYBUILD_PREFIX
$ module use $EASYBUILD_PREFIX/modules/all
$ module load EasyBuild
```

Updating easybuild

https://easybuild.readthedocs.io/en/latest/Installation.html#updating-an-existing-easybuild-installation

- new versions of EasyBuild 3.x are a drop-in replacement (for older EasyBuild 3.x)
  - upcoming EasyBuild 4.0 will have some minor backwards-incompatible changes
- recommend way to pick up new EasyBuild version & start using it:

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

```
kehoste@daint103:~> module load daint-gpu EasyBuild-custom
kehoste@daint103:~> eb --version
This is EasyBuild 3.8.1 (framework: 3.8.1, easyblocks: 3.8.1) on host daint103.

kehoste@daint103:~> eb --install-latest-eb-release
kehoste@daint103:~> module load EasyBuild/3.9.0
kehoste@daint103:~> eb --version
This is EasyBuild 3.9.0 (framework: 3.9.0, easyblocks: 3.9.0) on host daint103.
kehoste@daint103:~> which eb
/users/kehoste/easybuild/daint/haswell/software/EasyBuild/3.9.0/bin/eb
```

Configuring 

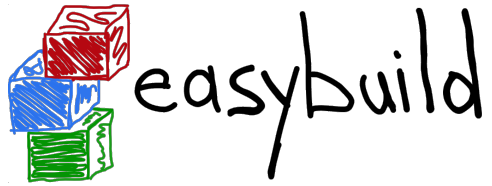
http://easybuild.readthedocs.io/en/latest/Configuration.html

EasyBuild is pre-configured on Piz Daint!

```
$ module load daint-mc EasyBuild-custom
```

https://user.cscs.ch/computing/compilation/easybuild

- default configuration (ab)uses `$HOME/.local/easybuild`
- configuring can be done via **config files**, **environment**, or **command line interface**
  - *all* configuration options are supported on all 3 levels
  - CLI overrides environment, which overrides configuration files
- easy to extend EasyBuild:
  - (also) use own easyconfigs repositories via `--robot-paths`
  - add additional easyblocks, toolchains, module naming schemes via --include-*
  - *http://easybuild.readthedocs.io/en/latest/Including_additional_Python_modules.html*

Inspecting the current configuration for 

http://easybuild.readthedocs.io/en/latest/Configuration.html

- use '`eb --show-config`' to get an overview of the current configuration
- only shows a couple of important settings + anything different from default
- output indicates via which configuration level each setting was specified
- full list of settings for current configuration via '`eb --show-full-config`'

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

Default  configuration on Piz Daint

(note: actual output has been trimmed for sake of clarity)

```
$ module load daint-mc EasyBuild-custom

$ eb --show-config
#
# Current EasyBuild configuration
# (C: command line argument, D: default value, E: environment variable, F: configuration file)
#
buildpath                 (E) = /run/user/23189/easybuild/build
external-modules-metadata (E) = /apps/common/UES/jenkins/production/easybuild/cray_external_...
hide-deps                 (F) = absl, ANTLR, APR, APR-util, Autoconf, Automake, Autotools, ...
hide-toolchains           (F) = CrayCCE, CrayGNU, CrayIntel, CrayPGI, GCCcore, ...
include-easyblocks        (E) = /apps/common/UES/jenkins/production/easybuild/easyblocks/*.py
installpath               (E) = /users/kehoste/easybuild/daint/broadwell
module-syntax             (F) = Tcl
modules-tool              (E) = EnvironmentModulesC
optarch                   (E) = broadwell
prefix                    (E) = /users/kehoste/easybuild/daint/broadwell
repositorypath            (E) = /users/kehoste/easybuild/daint/broadwell/ebfiles_repo
robot-paths               (E) = /apps/common/UES/jenkins/production/easybuild/easyconfigs/, ...
sourcepath                (E) = /users/kehoste/sources
tmpdir                    (E) = /run/user/23189/easybuild/tmp
```

Default  configuration on Piz Daint

(note: actual output has been trimmed for sake of clarity)

```
$ module load daint-mc EasyBuild-custom

$ eb --show-config
#
# Current EasyBuild configuration
# (C: command line argument, D: default value, E: environment variable, F: configuration file)
#
buildpath                  (E) = /run/user/23189/easybuild/build
external-modules-metadata  (E) = /apps/common/UES/jenkins/production/easybuild/cray_external_...
hide-deps                  (F) = absl, ANTLR, APR, APR-util, Autoconf, Automake, Autotools, ...
hide-toolchains            (F) = CrayCCE, CrayGNU, CrayIntel, CrayPGI, GCCcore, ...
include-easyblocks         (E) = /apps/common/UES/jenkins/production/easybuild/easyblocks/*.py
installpath                (E) = /users/kehoste/easybuild/daint/broadwell
module-syntax              (F) = Tcl
modules-tool               (E) = EnvironmentModulesC
optarch                    (E) = broadwell
prefix                     (E) = /users/kehoste/easybuild/daint/broadwell
repositorypath             (E) = /users/kehoste/easybuild/daint/broadwell/ebfiles_repo
robot-paths                (E) = /apps/common/UES/jenkins/production/easybuild/easyconfigs/, ...
sourcepath                 (E) = /users/kehoste/sources
tmpdir                     (E) = /run/user/23189/easybuild/tmp
```

User-specific '/run' directory is used for build and temporary directories.

Default  configuration on Piz Daint

(note: actual output has been trimmed for sake of clarity)

```
$ module load daint-mc EasyBuild-custom
$ eb --show-config
#
# Current EasyBuild configuration
# (C: command line argument, D: default value, E: environment variable, F: configuration file)
#
buildpath                (E) = /run/user/23189/easybuild/build
external-modules-metadata (E) = /apps/common/UES/jenkins/production/easybuild/cray_external_...
hide-deps                (F) = absl, ANTLR, APR, APR-util, Autoconf, Automake, Autotools, ...
hide-toolchains          (F) = CrayCCE, CrayGNU, CrayIntel, CrayPGI, GCCcore, ...
include-easyblocks       (E) = /apps/common/UES/jenkins/production/easybuild/easyblocks/*.py
installpath              (E) = /users/kehoste/easybuild/daint/broadwell
module-syntax            (F) = Tcl
modules-tool             (E) = EnvironmentModulesC
optarch                  (E) = broadwell
prefix                   (E) = /users/kehoste/easybuild/daint/broadwell
repositorypath           (E) = /users/kehoste/easybuild/daint/broadwell/ebfiles_repo
robot-paths              (E) = /apps/common/UES/jenkins/production/easybuild/easyconfigs/, ...
sourcepath               (E) = /users/kehoste/sources
tmpdir                   (E) = /run/user/23189/easybuild/tmp
```

Installation prefix for software & modules is set to $HOME/easybuild/daint/{broadwell,haswell} .

Sources are downloaded to $HOME/sources.

Default  configuration on Piz Daint

(note: actual output has been trimmed for sake of clarity)

Custom configuration for Piz Daint (1/2):

- **metadata for Cray-provided external modules**
- **Tcl-based environment modules tool** (Lmod is default)
- **target optimisation architecture** ('broadwell' or 'haswell')

```
$ module load daint-mc EasyBuild-custom
$ eb --show-config
#
# Current EasyBuild configuration
# (C: command line argument, D: default value, E: environment variable, F: configuration file)
#
buildpath                (E) = /run/user/23189/easybuild/build
external-modules-metadata (E) = /apps/common/UES/jenkins/production/easybuild/cray_external_...
hide-deps                (F) = absl, ANTLR, APR, APR-util, Autoconf, Automake, Autotools, ...
hide-toolchains          (F) = CrayCCE, CrayGNU, CrayIntel, CrayPGI, GCCcore, ...
include-easyblocks       (E) = /apps/common/UES/jenkins/production/easybuild/easyblocks/*.py
installpath              (E) = /users/kehoste/easybuild/daint/broadwell
module-syntax            (F) = Tcl
modules-tool             (E) = EnvironmentModulesC
optarch                  (E) = broadwell
prefix                   (E) = /users/kehoste/easybuild/daint/broadwell
repositorypath           (E) = /users/kehoste/easybuild/daint/broadwell/ebfiles_repo
robot-paths              (E) = /apps/common/UES/jenkins/production/easybuild/easyconfigs/, ...
sourcepath               (E) = /users/kehoste/sources
tmpdir                   (E) = /run/user/23189/easybuild/tmp
```

Default  easybuild configuration on Piz Daint

(note: actual output has been trimmed for sake of clarity)

Custom configuration for Piz Daint (2/2):
- **hiding dependencies & toolchain (in module avail)**
- **customised easyblocks maintained by CSCS**
- **additional easyconfig files (using Cray* toolchains)**

```
$ module load daint-mc EasyBuild-custom
$ eb --show-config
#
# Current EasyBuild configuration
# (C: command line argument, D: default value, E: environment variable, F: configuration file)
#
buildpath                (E) = /run/user/23189/easybuild/build
external-modules-metadata (E) = /apps/common/UES/jenkins/production/easybuild/cray_external_...
hide-deps                (F) = absl, ANTLR, APR, APR-util, Autoconf, Automake, Autotools, ...
hide-toolchains          (F) = CrayCCE, CrayGNU, CrayIntel, CrayPGI, GCCcore, ...
include-easyblocks       (E) = /apps/common/UES/jenkins/production/easybuild/easyblocks/*.py
installpath              (E) = /users/kehoste/easybuild/daint/broadwell
module-syntax            (F) = Tcl
modules-tool             (E) = EnvironmentModulesC
optarch                  (E) = broadwell
prefix                   (E) = /users/kehoste/easybuild/daint/broadwell
repositorypath           (E) = /users/kehoste/easybuild/daint/broadwell/ebfiles_repo
robot-paths              (E) = /apps/common/UES/jenkins/production/easybuild/easyconfigs/, ...
sourcepath               (E) = /users/kehoste/sources
tmpdir                   (E) = /run/user/23189/easybuild/tmp
```

Basic usage

http://easybuild.readthedocs.io/en/latest/Using_the_EasyBuild_command_line.html

http://easybuild.readthedocs.io/en/latest/Typical_workflow_example_with_WRF.html

- specify software name/version and toolchain to '`eb`' command
- usually done via easyconfig filename(s):

```
eb GCC-7.3.0-2.30.eb Clang-7.01-7.3.0-2.30.eb
```

- check whether required toolchain & dependencies are available using `--dry-run`/`-D`:

```
eb Python-3.7.0-foss-2018b.eb -D
```

- enable dependency resolution via `--robot`/`-r`:

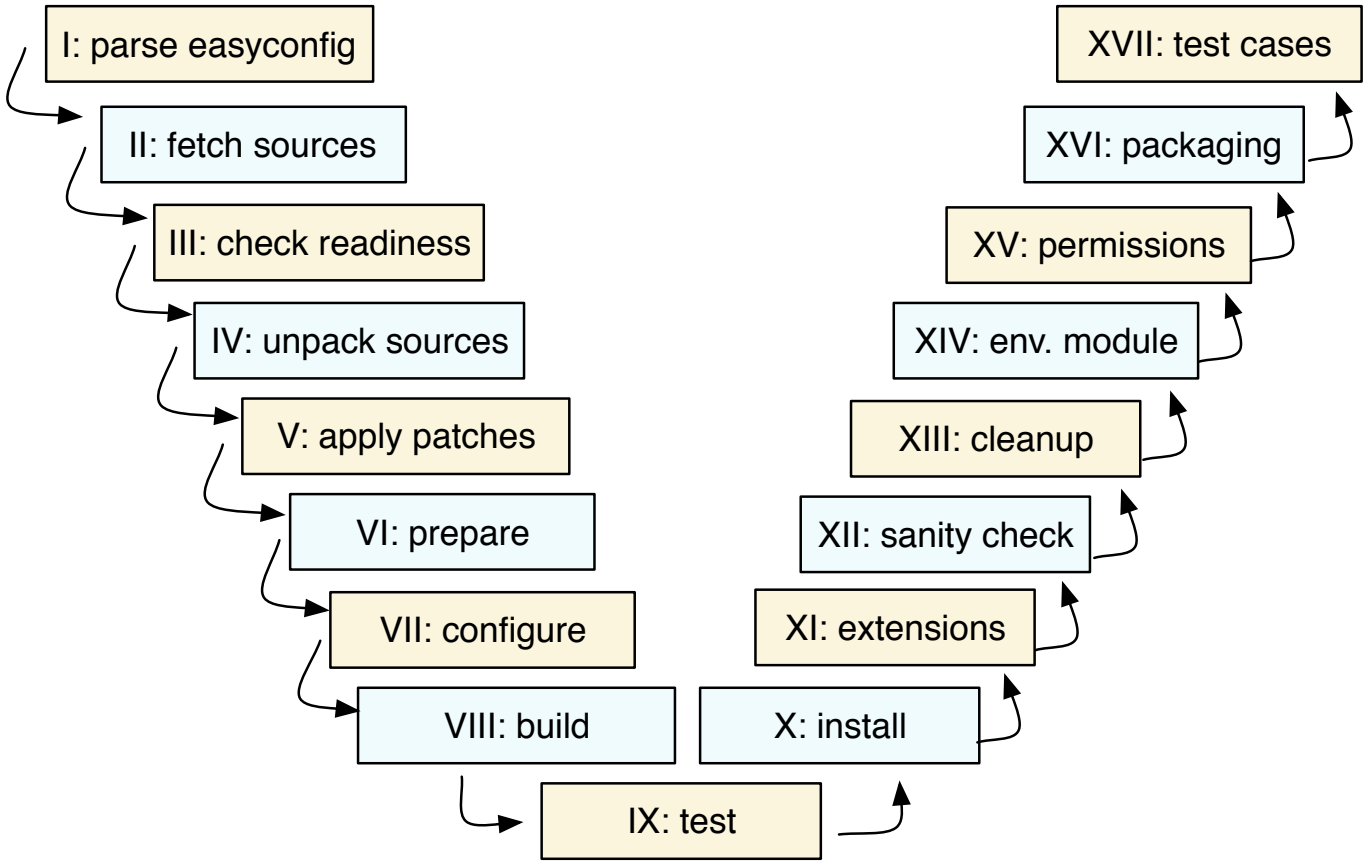
```
eb TensorFlow-1.13.1-foss-2018b-Python-3.6.6.eb -r
```

Installing TensorFlow from source with **one command**...


```
$ eb TensorFlow-1.13.1-foss-2018b-Python-3.6.6.eb
== temporary log file in case of crash /tmp/eb-GyvPHx/easybuild-U1TkEI.log
== processing EasyBuild easyconfig TensorFlow-1.13.1-foss-2018b-Python-3.6.6.eb
== building and installing TensorFlow/1.13.1-foss-2018b-Python-3.6.6...
== fetching files...
== creating build dir, resetting environment...
== unpacking...
== patching...
== preparing...
== configuring...
== building...
== testing...
== installing...
== taking care of extensions...
== postprocessing...
== sanity checking...
== cleaning up...
== creating module...
== permissions...
== packaging...
== COMPLETED: Installation ended successfully
== Results of the build can be found in the log file /opt/easybuild/software/Tensor...
== Build succeeded for 1 out of 1
== Temporary log file(s) /tmp/eb-GyvPHx/easybuild-U1TkEI.log* have been removed.
== Temporary directory /tmp/eb-GyvPHx has been removed.
```

Step-wise installation procedure

EasyBuild performs a step-wise installation procedure for each software:



- download sources (best effort)
- set up build directory & environment
  - unpack sources (& apply patches)
  - load modules for toolchain & deps
  - define toolchain-related env vars (`$CC`, `$CFLAGS`, ...)
- configure, build, (test), install, (extensions)
- perform simple sanity check on installation
- generate environment module file

each step can be customised via easyconfig parameters or an easyblock

Transparency of performed install procedure (1)

https://easybuild.readthedocs.io/en/latest/Tracing_progress.html

`eb --trace` shows more details while EasyBuild is performing installation(s)

- exact location of build and install directories
- list of source files & patches
- modules being loaded
- commands being executed
- pointer to temporary log file with output of commands
- timing information for each command (start time + how long it took)
- results of sanity check

Example output of `eb --trace`

```
$ eb TensorFlow-1.13.1-foss-2018b-Python-3.6.6.eb --trace
...
== preparing...
  >> loading toolchain module: foss/2018b
  >> loading modules for build dependencies:
  >>  * Bazel/0.20.0-GCCcore-7.3.0
  >>  * protobuf/3.6.1-GCCcore-7.3.0
  >> loading modules for (runtime) dependencies:
  >>  * Python/3.6.6-foss-2018b
  >>  * wheel/0.31.1-foss-2018b-Python-3.6.6
  >>  * h5py/2.8.0-foss-2018b-Python-3.6.6
  >> defining build environment for foss/2018b toolchain
...
== installing extension TensorFlow 1.13.1 (13/13)...
...
  >> running command:
        [started at: 2019-05-12 14:12:38]
        [output logged in /tmp/eb-pRHwkc/easybuild-run_cmd-SOINRV.log]
        bazel ... --jobs=6 --config=mkl //tensorflow/tools/pip_package:build_pip_package
  >> command completed: exit 0, ran in 00h41m22s
...
```

Transparency of performed install procedure (2)

https://easybuild.readthedocs.io/en/latest/Extended_dry_run.html

- **`eb --extended-dry-run`** (or '**`eb -x`**') reveals planned installation procedure
- runs in a matter of seconds
- shows commands that will be executed, build environment, generated module file, ...
- any errors that occur in used easyblock are ignored (but clearly reported)
- not 100% accurate since easyblock may require certain files to be present, etc.
- very useful when debugging easyblocks, instant feedback as a first pass
- implementation motivated by requests from the community
- helps to avoid impression that EasyBuild is a magic black box for installing software

Example output of --extended-dry-run (1/3)


```
$ eb WRF-3.8.0-intel-2016b-dmpar.eb -x

== temporary log file in case of crash /tmp/eb-Dh1wOp/easybuild-0bu9u9.log

== processing EasyBuild easyconfig /home/example/eb/easybuild-easyconfigs/easybuild/
easyconfigs/w/WRF/WRF-3.8.0-intel-2016b-dmpar.eb

...

*** DRY RUN using 'EB_WRF' easyblock (easybuild.easyblocks.wrf @ /home/example/eb/easybuild-
easyblocks/easybuild/easyblocks/w/wrf.py) ***

== building and installing WRF/3.8.0-intel-2016b-dmpar...
fetching files... [DRY RUN]

[fetch_step method]
Available download URLs for sources/patches:
  * http://www2.mmm.ucar.edu/wrf/src//$source
  * http://www.mmm.ucar.edu/wrf/src//$source

List of sources:
  * WRFV3.8.0.TAR.gz will be downloaded to /home/example/eb/sources/w/WRF/WRFV3.8.0.TAR.gz
```

Example output of `--extended-dry-run` (2/3)


```
$ eb WRF-3.8.0-intel-2016b-dmpar.eb -x
...

building... [DRY RUN]

[build_step method]
  running command "tcsh ./compile -j 4 wrf"
  (in /home/example/eb/software/WRF/3.8.0-intel-2016b-dmpar/WRF-3.8.0)
  running command "tcsh ./compile -j 4 em_real"
  (in /home/example/eb/software/WRF/3.8.0-intel-2016b-dmpar/WRF-3.8.0)
  running command "tcsh ./compile -j 4 em_b_wave"
  (in /home/example/eb/software/WRF/3.8.0-intel-2016b-dmpar/WRF-3.8.0)
...
[sanity_check_step method]
Sanity check paths - file ['files']
  * WRFV3/main/libwrflib.a
  * WRFV3/main/real.exe
  * WRFV3/main/wrf.exe
Sanity check paths - (non-empty) directory ['dirs']
  * WRFV3/main
  * WRFV3/run
Sanity check commands
  (none)
```

Example output of `--extended-dry-run` (3/3)


```
$ eb WRF-3.8.0-intel-2016b-dmpar.eb -x
...

[make_module_step method]
Generating module file /home/example/eb/modules/all/WRF/3.8.0-intel-2016b-dmpar,
with contents:

    #%Module
    proc ModulesHelp { } {
        puts stderr { The Weather Research and Forecasting (WRF) Model }
    }
    module-whatis {Description: WRF - Homepage: http://www.wrf-model.org}

    set root /home/example/eb/software/WRF/3.8.0-intel-2016b-dmpar

    conflict WRF

    if { ![ is-loaded intel/2016b ] } {
        module load intel/2016b
    }
    if { ![ is-loaded JasPer/1.900.1-intel-2016b ] } {
        module load JasPer/1.900.1-intel-2016b
    }
```

Log files

http://easybuild.readthedocs.io/en/latest/Logfiles.html

- **EasyBuild *thoroughly* logs the executed installation procedure**
  - active EasyBuild configuration
  - easyconfig file that was used
  - modules that were loaded + resulting changes to environment
  - defined environment variables
  - output + exit code of executed commands
  - informative log messages produced by easyblock
- log is file is copied to software installation directory for future reference
- can be used to debug build problems or see how installation was performed exactly

Log files: example


```
== 2019-05-13 13:34:31,906 main.EB_HPL INFO This is EasyBuild 3.9.0 (framework:
3.9.0, easyblocks: 3.9.0) on host example.
...
== 2019-05-13 13:34:35,503 main.EB_HPL INFO configuring...
== 2019-05-13 13:34:48,817 main.EB_HPL INFO Starting configure step
...
== 2019-05-13 13:34:48,823 main.EB_HPL INFO Running method configure_step part of
step configure
...
== 2019-05-13 13:34:48,823 main.run DEBUG run_cmd: running cmd /bin/bash
make_generic (in /tmp/easybuild_build/HPL/2.3/foss-2019a/hpl-2.3/setup)
== 2019-05-13 13:34:48,823 main.run DEBUG run_cmd: Command output will be logged
to /tmp/easybuild-W85p4r/easybuild-run_cmd-XoJwMY.log
== 2019-05-13 13:34:48,849 main.run INFO cmd "/bin/bash make_generic" exited with
exitcode 0 and output:
...
```

Easyconfig files as build specifications

http://easybuild.readthedocs.io/en/latest/Writing_easyconfig_files.html

- for each software installation, there is a corresponding easyconfig file
- **simple text files defining a set of easyconfig parameters** (in Python syntax)
- some are mandatory: software name/version, toolchain, metadata (homepage, descr.)
- other commonly used parameters:
  - easyblock to use
  - list of sources & patches
  - list of (build) dependencies
  - options for configure/build/install commands
  - files/directories that should be present, trivial commands that should work (sanity check)

Overview of supported easyconfig parameters:

```
$ eb -a
```

Include easyconfig parameters specific to a particular a particular easyblock:

```
$ eb -a -e PythonPackage
```

Example easyconfig file

no easyblock specified, which implies using a software-specific easyblock (`EB_WRF`)

software name and version

build variant (specific to WRF)
('dmpar': distributed, MPI)

software metadata

toolchain name & version

sources & patches

list of (build) dependencies
note: all versions are *fixed*!

```
name = 'WRF'
version = '3.8.0'

buildtype = 'dmpar'  # custom parameter for WRF
versionsuffix = '-' + buildtype  # part of module name

homepage = 'http://www.wrf-model.org'
description = "Weather Research and Forecasting (WRF) Model"

toolchain = {'name': 'intel', 'version': '2016b'}

source_urls = ['http://www.mmm.ucar.edu/wrf/src/']
sources = ['%(name)sV%(version_major_minor)s.TAR.gz']
patches = ['WRF-%(version)s_known_problems.patch']

builddependencies = [('tcsh', '6.20.00')]
dependencies = [
    ('JasPer', '2.0.10'),
    ('netCDF', '4.4.1'),
    ('netCDF-Fortran', '4.4.4'),
]
```

Adding support for additional software

- for each software installation, an **easyconfig file** is *required*
  - see ***https://easybuild.readthedocs.io/en/latest/Writing_easyconfig_files.html***
  - existing easyconfig files can serve as examples
  - tweaked easyconfig files can be *generated* via `eb --try-*`
- for 'standard' installation procedures, a **generic easyblock** can be used
  - installation can be controlled where needed via easyconfig parameters
- for custom installation procedures, a **software-specific easyblock** is required
  - see ***https://easybuild.readthedocs.io/en/latest/Implementing-easyblocks.html***

Tweaking existing easyconfigs via `--try-*`

- simple common use cases include:
  - updating to a more recent software version
  - installing with a different compiler toolchain
- dedicated CLI options: `--try-software-version`, `--try-toolchain`, ...
- success is not guaranteed... (hence the 'try')

```
kehoste@daint104:~> module load daint-mc EasyBuild-custom/cscs
kehoste@daint104:~> module avail CMake
----- /apps/daint/UES/jenkins/6.0.UP07/mc/easybuild/modules/all -----
CMake/3.12.0
kehoste@daint104:~> eb CMake-3.12.0.eb --try-software-version 3.14.3
...
kehoste@daint104:~> module avail CMake
----- /users/kehoste/easybuild/daint/broadwell/modules/all -----
CMake/3.14.3
----- /apps/daint/UES/jenkins/6.0.UP07/mc/easybuild/modules/all -----
CMake/3.12.0
```

Writing easyconfig files

https://easybuild.readthedocs.io/en/latest/Writing_easyconfig_files.html

- set of values for easyconfig parameters, written in Python syntax

  (strictly speaking order doesn't matter, but we maintain a preferred order & style)

- strictly required:

  `name`, `version`, `toolchain`, `homepage`, `description`

- commonly used:

  `easyblock`, `versionsuffix`, `source_urls`, `sources`,

  `(build)dependencies`, `(pre)configopts`, `(pre)buildopts`,

  `(pre)installopts`, `exts_list`, `sanity_check_paths`, `moduleclass`

Common generic easyblocks

http://easybuild.readthedocs.io/en/latest/version-specific/generic_easyblocks.html

- **`ConfigureMake`**
  standard '`./configure`' - '`make`' - '`make install`' installation procedure
- **`CMakeMake`**
  same as ConfigureMake, but using '`cmake`' for configuring
- **`PythonPackage`**
  installing an individual Python package ('`python setup.py install`', '`pip install`', ...)
- **`PythonBundle`**
  installing a bundle of Python packages
- **`MakeCp`**
  no (standard) configuration step, build with '`make`', install by copying binaries/libraries
- **`Tarball`**: just unpack sources and copy everything to installation directory
- **`Binary`**: run binary installer (specified via '`install_cmd`' easyconfig parameter)

Community (common) toolchains

http://easybuild.readthedocs.io/en/latest/Common-toolchains.html

- **`intel` and `foss`[1] toolchains** are most commonly used in EasyBuild community
- helps to focus efforts of HPC sites using one or both of these toolchains
- updated twice a year, clear versioning scheme: `<year>{a,b}` (`2017b`, `2018a`, ...)
- latest version:
  - `foss/2019a`

    binutils 2.31.1, GCC 8.2, OpenMPI 3.1.3,

    OpenBLAS 0.3.5, FFTW 3.3.8
  - `intel/2019a`

    binutils 2.31.1 + GCC 8.2 as base

    Intel compilers 2019.1.144, Intel MPI 2018.4.274, Intel MKL 2019.1.144

On Piz Daint, `Cray*` toolchains are typically used:

```
CrayCCE/18.08
CrayGNU/18.08
CrayIntel/18.08
CrayPGI/18.08
```

(1) FOSS: Free and Open Source Software

Easyconfig files vs easyblocks

http://easybuild.readthedocs.io/en/latest/Implementing-easyblocks.html

- thin line between using custom easyblock and 'fat' easyconfig with generic easyblock
- custom easyblocks are "do once and forget", **central solution to build peculiarities**
- reasons to consider implementing a software-specific easyblock include:
  - 'critical' values for easyconfig parameters required to make installation succeed
  - toolchain-specific aspects of the build and installation procedure (e.g., configure options)
  - interactive commands that need to be run
  - custom (configure) options for dependencies
  - having to create or adjust specific (configuration) files
  - 'hackish' usage of a generic easyblock

Demo: an easyconfig for Hello built with CMake


```
kehoste@daint104:~> module load daint-mc EasyBuild-custom
kehoste@daint104:~> ls
hello-cmake-1.0.tar.gz
kehoste@daint104:~> vim Hello.eb
kehoste@daint104:~> eb Hello.eb --trace
...
== configuring...
== building...
== testing...
== installing...
...
== sanity checking...
  >> file 'bin/hello' found: OK
  >> running command 'hello': OK
== cleaning up...
...
== COMPLETED: Installation ended successfully

kehoste@daint104:~> module load Hello/1.0-CrayGNU-18.08
kehoste@daint104:~> hello
Hello World!
```

Demo: an easyconfig for Hello built with CMake


```
kehoste@daint104:~> cat Hello.eb
easyblock = 'CMakeMake'

name = 'Hello'
version = '1.0'

homepage = 'https://example.com'
description = "Hello world!"

toolchain = {'name': 'CrayGNU', 'version': '18.08'}

sources = ['hello-cmake-%(version)s.tar.gz']

builddependencies = [('CMake', '3.14.3', '', True)]

sanity_check_paths = {
    'files': ['bin/hello'],
    'dirs': [],
}
sanity_check_commands = ["hello"]

moduleclass = 'tools'
```

Contributing to EasyBuild

http://easybuild.readthedocs.io/en/latest/Contributing.html

EasyBuild has improved significantly thanks to the community.

You too can contribute back, by:

- sending feedback
- reporting bugs
- joining the discussion (mailing lists, IRC/Slack, EasyBuild conf calls)
- sharing suggestions/ideas for enhancements & additional features
- contributing easyconfigs, enhancing easyblocks, adding support for new software...
- extending & enhancing documentation

How to contribute easyconfig files

https://easybuild.readthedocs.io/en/latest/Contributing.html

- open pull request (PR) to `develop` branch of `easybuild-easyconfigs` repository
- keep PRs limited in scope (rule of thumb: max. 10 easyconfigs touched per PR)
- if possible, submit test report to show the easyconfig(s) works for you
- take into account failing unit tests (if any) and comments by reviewer (if any)
- be patient...
- enjoy eternal glory once your pull request has been merged!

GitHub integration in easybuild

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

- goals:
  - **automate contribution workflow**
  - avoid direct interaction with git and

- initial implementation added support for:
  - opening new PRs & updating existing PRs `eb --new-pr` `eb --update-pr`
  - downloading & using easyconfigs from a PR `eb --from-pr`
  - uploading test reports to a PR `eb --upload-test-report`
- limited to easyconfig files, for now...
  - but implemented such that it is easy to extend to easyblocks, and even the EasyBuild framework itself

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
```

The easybuild community

group picture
4th EasyBuild User Meeting
@ UC Louvain (Feb 2019)

- EasyBuild community has been growing rapidly the last couple of years
- used by **hundreds of HPC sites and companies worldwide, incl. JSC, CSCS, SURFsara, Pfizer, ...**
- very welcoming & supportive to newcomers

mailing list: https://lists.ugent.be/wws/info/easybuild
Slack channel: easybuild.slack.com
IRC: #easybuild on FreeNode

easybuild maintainers

Damian Alvarez - `@damianam`
(Jülich Supercomputing Centre)

Miguel Dias Costa - `@migueldiascosta`
(National University of Singapore)

Pablo Escobar - `@pescobar`
(sciCORE, University of Basel)

Kenneth Hoste - `@boegel`
(HPC-UGent)

Adam Huffman - `@verdurin`
(Big Data Institute, University of Oxford)

Samuel Moors - `@smoors`
(Free University of Brussels)

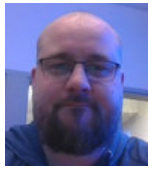
Alan O'Cais - `@ocaisa`
(Jülich Supercomputing Centre)

Bart Oldeman - `@bartoldeman`
(ComputeCanada)

Ward Poelmans - `@wpoely86`
(Free University of Brussels)

Åke Sandgren - `@akesandgren`
(Umeå University, Sweden)

Davide Vanzo - `@vanzod`
(Vanderbilt University)



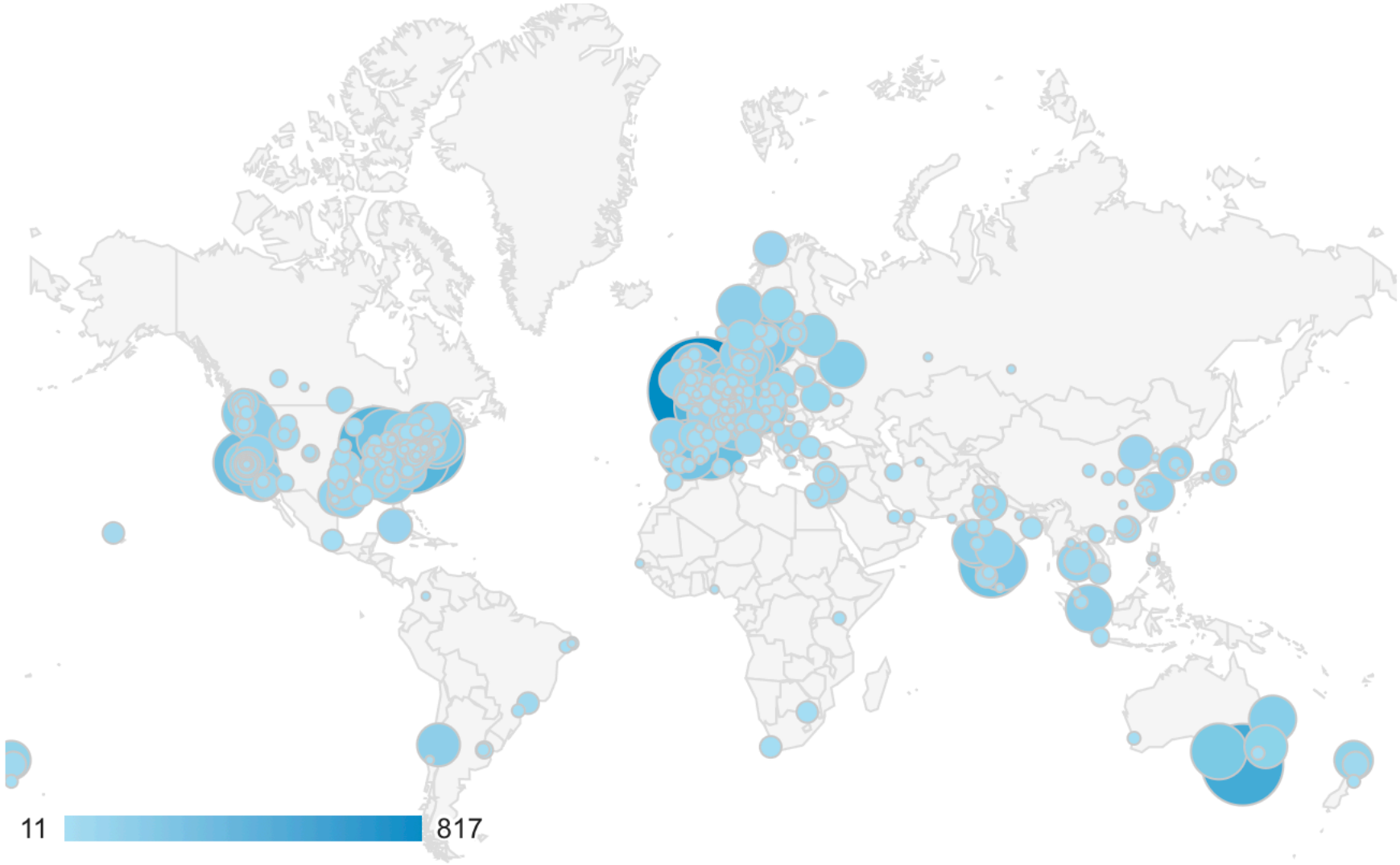
Mikael Öhman - `@micketeer`
(Chalmers University of Technology)

EasyBuild documentation visits

EasyBuild documentation at https://easybuild.readthedocs.io hitting **~500 weekly visitors**

(source: Google Analytics)

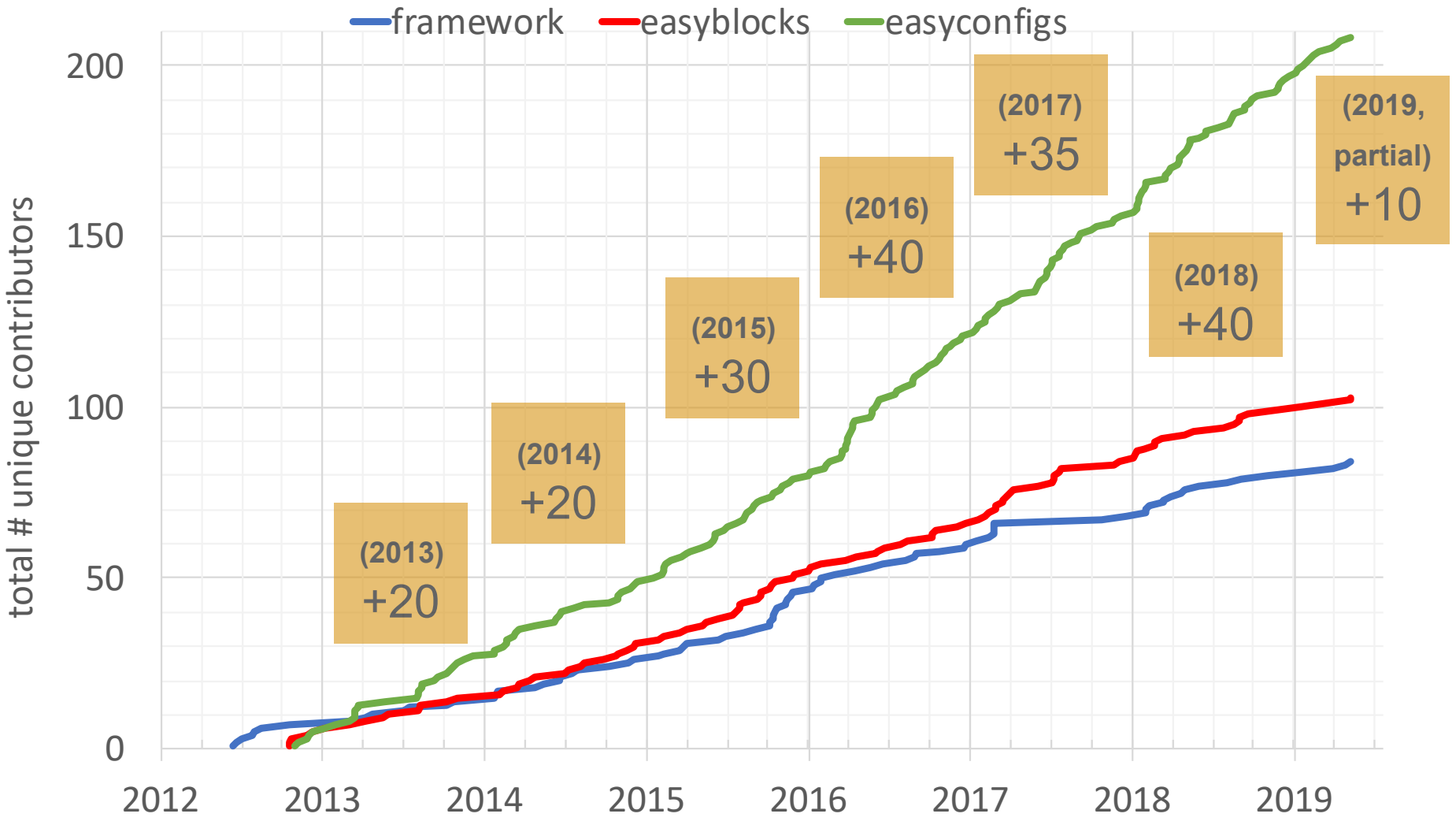
The sun never sets on EasyBuild...



cities from where https://easybuild.readthedocs.io was visited at least 10 times during the last year

(source: Google Analytics)

Unique contributors (total, per repository)

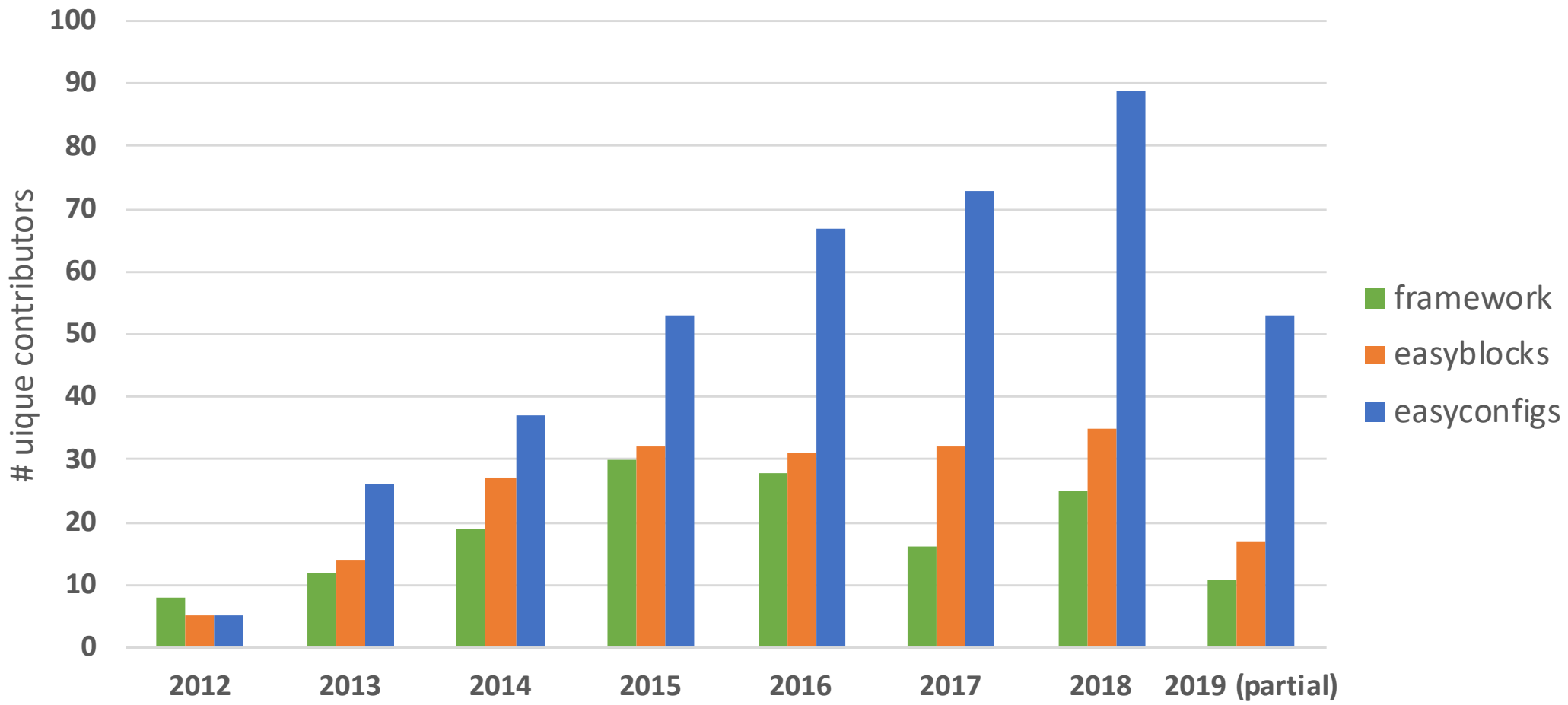


> 200 unique contributors for easyconfigs, > 100 for easyblocks, ~85 for framework

Unique contributors (per repository, per year)

Group of easyconfigs contributors is growing every year (reaching 100 in 2019?).

Stable group of easyblocks contributors, fluctuating a bit for framework.



Integration with Docker/Singularity

https://easybuild.readthedocs.io/en/latest/Containers.html

- (experimental) integration with Singularity since EasyBuild v3.6.0 (April 2018)
  - extended to also support Docker in EasyBuild v3.6.2 (July 2018)
- `eb --containerize` (or '`eb -C`') generates recipe to build container image
- generated recipe uses '`eb`' to build and install specified software in container image
- `--container-build-image` can be used to also build container image
  - makes `eb` call out to '`sudo singularity build`' (or '`sudo docker build`')
- **current implementation is experimental, has some rough edges...**

Integration with Docker/Singularity (demo)

https://easybuild.readthedocs.io/en/latest/Containers.html

```
$ export EASYBUILD_CONTAINER_BASE=shub:shahzebsiddiqui/eb-singularity:centos-7.4.1708
$ eb --experimental --containerize TensorFlow-1.13.1-foss-2018b-Python-3.6.6.eb
== temporary log file in case of crash /tmp/eb-sMtVBY/easybuild-1luKuM.log
== Singularity definition file created at /home/kehoste/containers/
Singularity.TensorFlow-1.13.1-foss-2018b-Python-3.6.6
== Temporary log file(s) /tmp/eb-sMtVBY/easybuild-1luKuM.log* have been removed.
== Temporary directory /tmp/eb-sMtVBY has been removed.
$ cat /home/kehoste/containers/Singularity.TensorFlow-1.13.1-foss-2018b-Python-3.6.6
Bootstrap: shub
From: shahzebsiddiqui/eb-singularity:centos-7.4.1708

%post
...
# change to 'easybuild' user
su - easybuild

eb TensorFlow-1.13.1-foss-2018b-Python-3.6.6.eb --robot --installpath=/app/ --prefix=/
scratch --tmpdir=/scratch/tmp

%environment
...
module load TensorFlow/1.13.1-foss-2018b-Python-3.6.6
```

Other features that were not covered in detail...

http://easybuild.readthedocs.io

- letting users manage their software stack on top of centrally provided modules
- installing hidden modules, hiding certain dependencies & toolchains
- support for using RPATH linking
- partial installations: only (re)generate module file, install additional extensions
- submitting installations as jobs to an HPC cluster via `--job` (distributed installation!)
- creating packages (RPMs, ...) for software installations done with EasyBuild
- installing (bundles of) Python packages for multiple Python versions in a single prefix

Outlook to  v4.0

https://github.com/easybuilders/easybuild/issues/447

Ongoing effort, see '4.x' branches in EasyBuild repositories on GitHub!

- ✓ support for running EasyBuild on top of Python 3.5 (or more recent Python 3)
- ✓ no more required dependencies (vsc-base has been ingested, setuptools no longer needed)
- WIP deprecated 'dummy' toolchain, replaced with 'system' toolchain (mostly about renaming)
  - custom easyblock for OpenMPI with more sensible default configuration
- WIP switch to using `pip` by default for installing Python packages (?)
  - (hopefully) stable integration with Singularity & Docker
  - **ETA: summer 2019**

vs

Spack

https://spack.rtfd.io

- EasyBuild: GPLv2 license; Spack: MIT/Apache 2.0 license
- **no stable releases yet for Spack (< 1.0), EasyBuild is stable since 2012**
- on par w.r.t. amount of supported software (but differences w.r.t. which software)
- (originally) targeted for different use cases: HPC support teams vs developers
- fixed dependency/toolchain versions in EasyBuild vs flexible CLI in Spack
- running EasyBuild on top of Python 3 is not supported yet (but coming really soon!)
- macOS support in EasyBuild is limited (no toolchains/testing for macOS)
- both projects are backed by an active & supportive community!

For a more detailed comparison,
see https://archive.fosdem.org/2018/schedule/event/installing_software_for_scientists

Papers on easybuild

Modern Scientific Software Management Using EasyBuild and Lmod

Markus Geimer (JSC), Kenneth Hoste (HPC-UGent), Robert McLay (TACC)

http://easybuilders.github.io/easybuild/files/hust14_paper.pdf

Making Scientific Software Installation Reproducible On Cray Systems Using EasyBuild

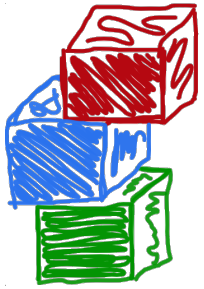
Petar Forai (IMP), Guilherme Peretti-Pezzi (CSCS), Kenneth Hoste (HPC-UGent)

https://cug.org/proceedings/cug2016_proceedings/includes/files/pap145.pdf

Scientific Software Management in Real Life:
Deployment of EasyBuild on a Large Scale System

Damian Alvarez, Alan O'Cais, Markus Geimer (JSC), Kenneth Hoste (HPC-UGent)

http://easybuilders.github.io/easybuild/files/eb-jsc-hust16.pdf



Questions?

Kenneth Hoste (HPC-UGent)

kenneth.hoste@ugent.be

20190510 - CSCS Software Management Course

https://users.ugent.be/~kehoste/EasyBuild_20190510_CSCS_software_management.pdf

https://easybuilders.github.io/easybuild

https://easybuild.readthedocs.io

Extra slides

(only used in case of time/interest)

Using a custom module naming scheme

- a couple of different module naming schemes are included in EasyBuild
  - see `--avail-module-naming-schemes`
  - specify active module naming scheme via `--module-naming-scheme`
  - default: `EasyBuildMNS` (`<name>/<version>-<toolchain>-<versionsuffix>`)
- **you can implement your own module naming scheme relatively easily**
  - specify how to compose module name using provided metadata
  - via Python module that defines custom derivative class of `ModuleNamingScheme`
  - make EasyBuild aware of it via `--include-module-naming-schemes`
- decouple naming of install dirs vs modules via `--fixed-installdir-naming-scheme`

Flat module naming scheme

- all modules are always available for loading
- long(er) module names
- '`module avail`' may be overwhelming for users
- too easy to load incompatible modules together

legend

(not available)

(available)

(loaded)

GCC/5.3.0

GCC/6.1.0

OpenMPI/1.10.2-GCC-5.3.0

OpenMPI/2.1.0-GCC-5.3.0

OpenMPI/1.10.3-GCC-6.1.0

OpenMPI/2.1.0-GCC-6.1.0

FFTW/3.3.4-gompi-2016.04

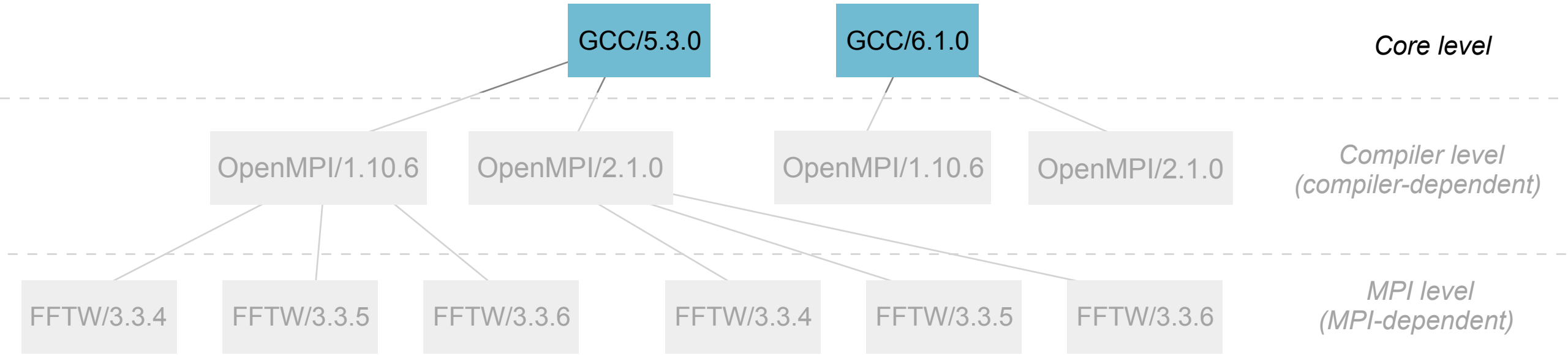
FFTW/3.3.6-gompi-2016.04

FFTW/3.3.4-gompi-2016.07

FFTW/3.3.6-gompi-2016.07

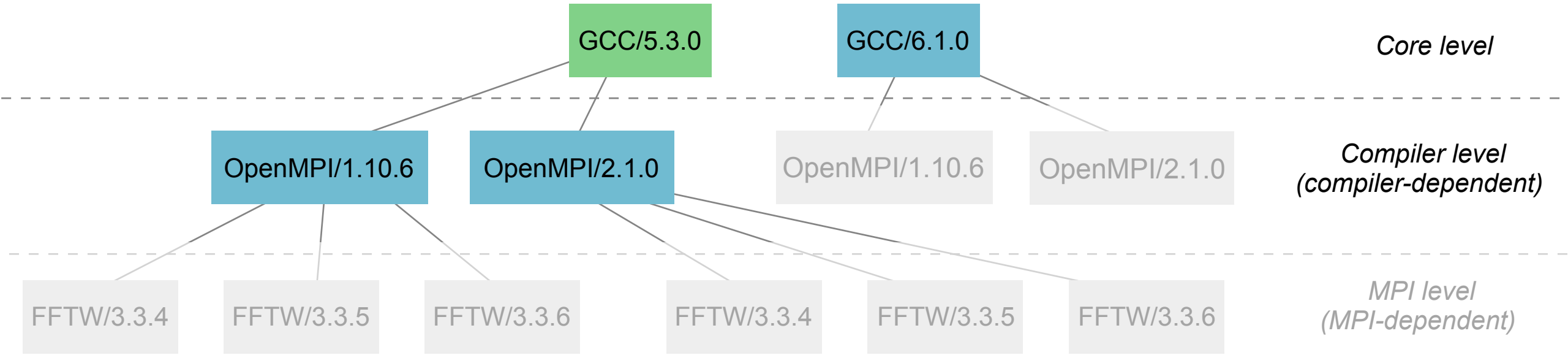
Hierarchical module naming scheme (1)

- modules are organised in a tree-like fashion
- initially, only 'core' modules are available for loading
- typically 3 hierarchy levels: core, compiler-dependent, MPI-dependent
- other modules are only visible via '`module spider`'



Hierarchical module naming scheme (2)

- Core modules may extend `$MODULEPATH` with an additional location
- loading a Core module may make more modules available
- in this example, loading a GCC module makes OpenMPI modules available



Hierarchical module naming scheme (3)

- even more modules may be made available by loading other modules
- for example, loading an OpenMPI modules reveals MPI-dependent modules
- EasyBuild can organise modules in hierarchy for you!