

EasyBuild 5.0

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EASYBUILD.io

building software with ease

Information

This talk will cover:

- what has been implemented
- what we aim to implement
- policy changes

It will also:

- provide background to decisions and changes
- tell you how you can contribute

information

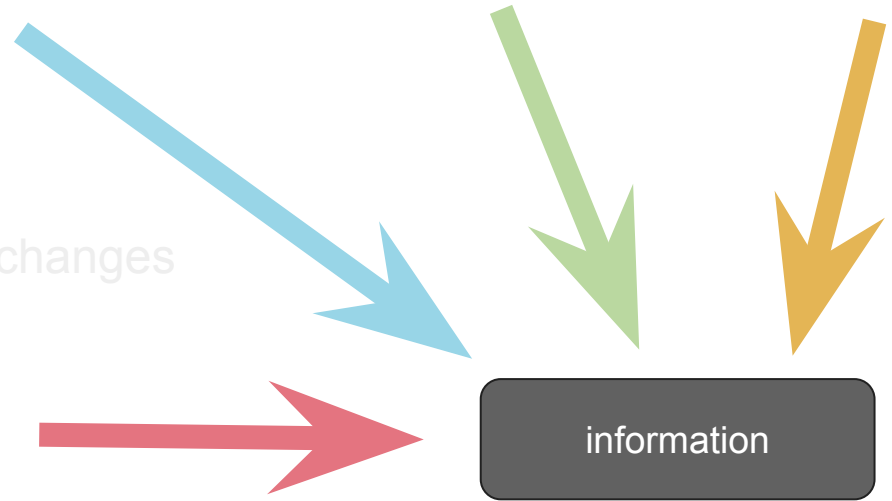
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Change Types

breaking change

A change in how EasyBuild works

- These may impact you / require changes

enhancement

A new feature

- To make using EasyBuild better or easier

code cleanup

Code enhanced or changes

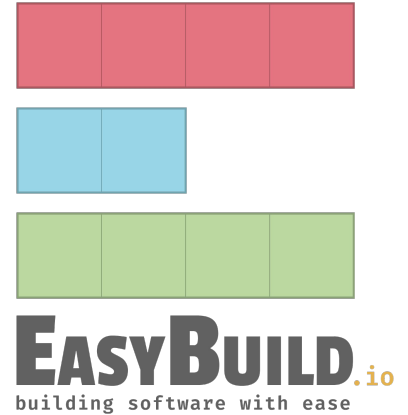
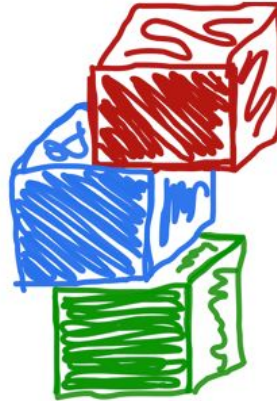
- No impact during use

information

EasyBuild

Major versions:

1. November 2012
2. March 2015
3. November 2016
4. September 2019
5. ? 2024



information

run_shell_cmd to replace run_cmd / run_cmd_qa

Improved interface

- Defaults for the standard use case
- Unified running of commands
- More modern Python
- Easier further enhancement
 - Save shell commands and environment
 - Improved logging
 - Error reporting

enhancement

run_shell_cmd to replace run_cmd / run_cmd_qa

Implemented in framework, with old functions deprecated

Use of run_cmd / run_cmd_qa

- Replaced in framework
- Replaced in CI / testsuite
- Nearly completed replacement in easyblocks
 - <https://github.com/easybuilders/easybuild-easyblocks/issues/3089>
- If you have custom easyblocks, hooks, etc., to convert
 - https://docs.easybuild.io/easybuild-v5/run_shell_cmd/
 - And the easyblock PRs

enhancement

Save shell commands and environment

Two additional files generated:

- env.sh - environment variables
- cmd.sh - script to enter environment

Then you can:

- rerun failing command(s)
- explore shell command history

To merge: <https://github.com/easybuilders/easybuild-framework/pull/4486>

enhancement

Standardise parameter and config names

Remove inconsistency

Standardise when to shorten a name and when not

Plan:

- Add new names as options
- Implement method for auto-renaming
- Switch to using new names in framework, easyblocks, easyconfigs
- Deprecate old names

enhancement

Enhance use of download_instructions

download_instructions enhanced

- Improved message when source(s) need manual download
- Information on where to place sources
- Provide a better user experience

Easyconfigs CI requires download_instructions to be specified where needed

enhancement

RPATH by default

Enabled RPATH linking

- <https://docs.easybuild.io/rpath-support>
- `$LD_LIBRARY_PATH` retained
 - `--filter-env-vars` available

Limited issue with mixed RPATH / non-RPATH stack

- e.g. seen in LAMMPS
- To fix: <https://github.com/easybuilders/easybuild-framework/pull/4475>

enhancement

--trace by default

Improved user experience

- Easier to see what command(s) are used
- Better understanding how EasyBuild operates

Most maintainers were using this as standard

enhancement

Python package installation

PythonPacakge defaults:

- `download_dep_fail`
- `use_pip`
- `sanity_pip_check`

Use `EBPYTHONPREFIXES`

- Instead of `PYTHONPATH`
- To merge: <https://github.com/easybuilders/easybuild-framework/pull/4496>

enhancement

Detect Fortran .mod files in GCCcore installations

GCCcore sub toolchain for Intel (and other) compilers

.mod files should not be mixed between compilers

- Warning if detected
- `--fail-on-mod-files-gcccore` to make this a failure
 - This will be enabled for PRs
- `ec` parameter: `skip_mod_files_sanity_check`
 - GeneMark-ET / CPLEX - .mod files are data files

enhancement

Python 3.12

Using EasyBuild on Python 3.12

- Working...
- Replaced distutils use

Building Python 3.12

- <https://github.com/easybuilders/easybuild-easyconfigs/pull/20407>
- Read the notes!

enhancement

Changed module options default

Lmod, with Lua syntax only

- --module-depends-on on by default
 - Improves module loading/unloading for dependencies
 - https://lmod.readthedocs.io/en/latest/098_dependent_modules.html
 - To merge: <https://github.com/easybuilders/easybuild-framework/pull/4500>
- --module-extensions on by default
 - “way to let users know that a package provides one or more extension”
 - https://lmod.readthedocs.io/en/latest/330_extensions.html
 - To merge: <https://github.com/easybuilders/easybuild-framework/pull/4501>

enhancement

Minimum versions

Python 3.6

- Python 2.7 usage <5%
- Python 3.5 usage ~1%

Lmod

- 8.0.0

Tmod

- (not yet merged) 4.3.0 if using ≥ 4

breaking change

Remove deprecated code

WARNING: Deprecated functionality, will no longer work in EasyBuild v5.0: `old_cmd` is deprecated, use `new_cmd` from `easybuild...` instead; see <https://docs.easybuild.io/deprecated-functionality/> for more information

In EB5 that code has been removed!

But you've been receiving warnings for this...

breaking change

New deprecations

Currently

- EnvironmentModulesC and EnvironmentModulesTcl
 - So Tmod < 4

Others will be added

- You'll receive warnings if used
- Removal in EB6
 - So you'll have some time!

information

Toolchain support policy

Central repository:

- References easyconfigs
- Generally one version of a software per toolchain generation
 - There are exceptions, but aim is to keep them limited

Site specific:

- Own repository
 - Add via robot paths
 - See https://docs.easybuild.io/using-easybuild/#robot_search_path

information

Toolchain support policy

<https://docs.easybuild.io/policies/toolchains/>

Example as of April 2024 when 2023b is the latest generation:

- Accept PRs only for the 6 most recent toolchain generations
 - Currently: 2023b, 2023a, 2022b, 2022a, 2021b, 2021a
- Deprecate toolchains generations 7 and 8
 - Closing PRs and issues for these toolchains.
 - Currently: 2020b, 2020a
- Archive easyconfigs for anything older
 - 2019b (and older)
 - Old SYSTEM toolchain easyconfigs

information

easyconfigs archive

Separate from the main easyconfigs repository

- Reduces size of the main easyconfigs repository
 - Faster git operations
 - Speeds up testsuite
- <https://github.com/easybuilders/easybuild-easyconfigs-archive>
- Will not be installed by default
- No support for these easyconfigs

code cleanup

Removing unused easyblocks

Removed: ACML, ALADIN, ARB, ATLAS, BiSearch, BLACS, CFDEMcoupling, CHARMM, cppcheck, DL_POLY_Classic, DOLFIN, Doris, ESPResSo, fastStructure, FreeFEM, HEALPix, IMOD, IronPython, libsmm, Modeller, Molpro, Mono, MSM, NEMO, PGI, pplacer, python_meep, samcef, SAS, SNPPhylo, TotalView, VSC-tools

- No easyconfigs in 5.0.x branch use these
- Mainly old, old software
- If you need support for these in the future, please contribute

breaking change

Remaining tasks

- Decide on remaining breaking changes for EB5
 - These items will need to be merged soon
- Decide on remaining non-breaking changes for EB5
 - More time to merge these
- Write documentation
 - <https://docs.easybuild.io/easybuild-v5/>
- Release candidate(s)
 - Test, test, test
- Release

information

Short term impact

Soon, we'll merge the 5.0.x branches into develop

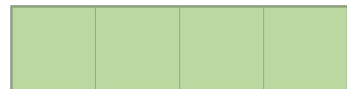
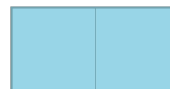
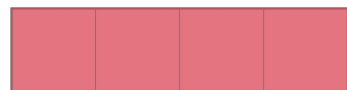
- Some easyconfigs will not build with EB 4.x
 - e.g. PythonPackage default changes
- Some easyblocks will fail with EB4.x
 - e.g. those using `run_shell_cmd`
- So when using
 - `--from-pr / --include-easyblocks-from-pr`
 - items merged in develop
- CI changes to reflect newly deprecated items

breaking change

So far...

PRs:

- 75 framework
 - New / changed functionality
- 170 easyblocks
 - Mainly related to `run_shell_cmd`
- 85 easyconfigs
 - Archiving old toolchains



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Observation

Survey is important

- Allows us a snapshot of usage
 - Architectures, Python, OS, etc.
 - Decisions are made from this information

information

Hands-on: Setting up environment

```
python3 -m venv eb5
```

```
source eb5/bin/activate
```

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

```
pip install https://github.com/easybuilders/easybuild-framework/archive/5.0.x.tar.gz
```

```
pip install https://github.com/easybuilders/easybuild-easyblocks/archive/5.0.x.tar.gz
```

```
pip install https://github.com/easybuilders/easybuild-easyconfigs/archive/5.0.x.tar.gz
```

```
eb --version
```

information

Hands-on: Testing

Test using EB

- If you run into something weird/broken, please report it

Don't hesitate to ask for help in the room

- Simon, Kenneth, Jasper, Adam, ...
- via EasyBuild Slack (#eum or #eb5 channel)

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