

Using Continuous Integration with EasyBuild in DEEP-SEA

Manoel Römmer, Jülich Supercomputing Centre

2023-12-01 - The DEEP-SEA Seminar Series

The Research leading to these results has received funding from the European Commission's FP7, H2020, and EuroHPC Programmes, under Grant Agreements nr 287530, 610476, 754304, and 955606



Continuous Integration in DEEP-SEA



Objective: Ensure a proper automated integration process by using software engineering techniques.



Continuous Integration in DEEP-SEA



Objective: Ensure a proper automated integration process by using software engineering techniques.

Currently done by employing general CI infrastructure by various Work Packages:

- Various automated checks and tests
- Automatically running benchmarks
- Automatically building and deploying software on DEEP



Continuous Integration in DEEP-SEA



Objective: Ensure a proper automated integration process by using software engineering techniques.

Currently done by employing general CI infrastructure by various Work Packages:

- Various automated checks and tests
- Automatically running benchmarks
- Automatically building and deploying software on DEEP

as part of an automated workflow, directly from GitLab.







Manoel Rommer – Using Continuous Integration with EasyBuild in DEEP-SEA, 2023-12-01







Build and deploy bleeding edge software stage from GitLab on the DEEP system







- Build and deploy bleeding edge software stage from GitLab on the DEEP system
- (Optionally) rebuild *reverse dependencies*, to keep every component in the Stage coherent







- Build and deploy bleeding edge software stage from GitLab on the DEEP system
- (Optionally) rebuild *reverse dependencies*, to keep every component in the Stage coherent

The software installations on DEEP are mostly handled by





The EasyBuild CI (cont'd)







The EasyBuild CI (cont'd)





This pipeline lives in the

deep-sea/wp3/software/easybuild-repository-deep-sea repository, and you can trigger it as a *downstream pipeline* from your own repository.



Prerequisites





EasyBuild Recipe



```
name = 'Scalasca'
version = '2.6.1'
toolchain = {'name': 'gpsmpi', 'version': '2022a'}
source_urls = [
    'https://apps.fz-juelich.de/scalasca/releases/scalasca/%(version_major_minor)s/dist'
sources = [SOURCELOWER_TAR_GZ]
checksums = ['a0dbc3de82a6c0fe598de9e340513cff2882c199410a632d3a7f073ba921c7e7']
dependencies = [
    ('CubeGUI', '4.8').
    ('CubeLib', '4.8').
    ('OTF2', '3.0.2').
    ('Score-P', '8.0').
```

Existing EasyBuild recipes used as a template to generate new recipes for CI run



6



The CI workflow lives in the JSC GitLab EasyBuild repository.





The CI workflow lives in the JSC GitLab EasyBuild repository.

• gitlab.jsc.fz-juelich.de/deep-sea/wp3/software/easybuild-repository-deep-sea





The CI workflow lives in the JSC GitLab EasyBuild repository.

- gitlab.jsc.fz-juelich.de/deep-sea/wp3/software/easybuild-repository-deep-sea
- Please have your EasyBuild recipes merged there in the 2023 branch





The CI workflow lives in the JSC GitLab EasyBuild repository.

- gitlab.jsc.fz-juelich.de/deep-sea/wp3/software/easybuild-repository-deep-sea
- Please have your EasyBuild recipes merged there in the 2023 branch

How use it then? You can *trigger* this pipeline from your own GitLab repository!





The CI workflow lives in the JSC GitLab EasyBuild repository.

- gitlab.jsc.fz-juelich.de/deep-sea/wp3/software/easybuild-repository-deep-sea
- Please have your EasyBuild recipes merged there in the 2023 branch

How use it then? You can *trigger* this pipeline from your own GitLab repository!

- Ideally: Your code repository in the JSC GitLab
- Alternatively: Create a repository just for your CI workflow



A Quick Word From Project Management



Public EasyBuild repository as Software Release: gitlab.jsc.fz-juelich.de/deep-sea/easybuild-repository-public-release

Internal EasyBuild repository:

gitlab.jsc.fz-juelich.de/deep-sea/wp3/software/easybuild-repository-deep-sea/

 \uparrow Please use this one to trigger Cl \uparrow



CI Configuration from YOUR y Repository



Manoel Römmer – Using Continuous Integration with EasyBuild in DEEP-SEA, 2023-12-01



÷.,

CI Configuration from YOUR y Repository



You need to configure a pipeline with the .gitlab-ci.yml

<pre>% main ∨ taz / + ∨</pre>	History Compare Find file Edit v	dia ≤ Cione ⇒
Name	Last commit	Last update
En vecode	Version 0.3	1 month ago
🗈 cmake	Enable support for use of system-wide SOCTCH and fla	3 weeks ago
En docs	Improve README	1 month ago
🗈 experiments	Improve failure color scheme	1 month ago
🗈 extern	Version 0.3	1 month ago
D generated_profile_headers_target	Version 0.3	1 month ago
🗈 scripts	Improvement of the Easyconfig	3 weeks ago
Es see	Add support for traffic-based mapping with reliability p	1 month ago
🗅 tests	Version 0.3	1 month ago
 .gitattributes 	Version 0.3	1 month ago
♦ .gitignore	Version 0.3	1 month ago
🤟 .gitlab-ci.yml	Try again	1 week ago
♦ .gitmodules	Version 0.3	1 month ago
CMakeLists.txt	Add install target	3 weeks ago
LICENSE-LGPL-2.1	Added license file (LGPL-2.1)	1 month ago
reaDME.md	Improve README	1 month ago
comperiment_multiple_mini128.sh	Version 0.3	1 month ago
c experiment_multiple_mini512.sh	Version 0.3	1 month ago



CI Configuration from YOUR y Repository

You need to configure a pipeline with the .gitlab-ci.yml

- If you already have a JSC GitLab repo with CI workflow, integrate it there
- If not, consider putting your code in JSC GitLab
- If not, create a repository with only your CI trigger

₽ main × taz / + ×		History Compare	Find file Edit v	do Y Cione Y
Name	Last commit			Last update
🗀 .vscode	Version 0.3			1 month ago
🖹 cmake	Enable support for use of system-wide SOCTCH a	nd fla		3 weeks ago
En doos	Improve README			1 month ago
🗈 experiments	Improve faiture color scheme			1 month ago
🗀 extern	Version 0.3			1 month ago
E: generated_profile_headers_target	Version 0.3			1 month ago
🗀 scripts	Improvement of the Easyconfig			3 weeks ago
🗁 sro	Add support for traffic-based mapping with reliab	lity p		1 month ago
🗈 tests	Version 0.3			1 month ago
♦ .gitattributes	Version 0.3			1 month ago
♦ .gitignore	Version 0.3			1 month ago
😝 .gitlab-ci.ymi	Try again			1 week ago
♦ .gitmodules	Version 0.3			1 month ago
CMakeLists.txt	Add install target			3 weeks ago
LICENSE-LGPL-2.1	Added license file (LGPL-2.1)			1 month ago
He README.md	Improve README			1 month ago
c experiment_multiple_mini128.sh	Version 0.3			1 month ago
C conscionant multiple minifile ab	Version 0.2			1 month and





How To Integrate





Upstream Workflow Summary



1. Have one EasyBuild recipe for your software merged in easybuild-repository-deep-sea Repository





Upstream Workflow Summary



- 1. Have one EasyBuild recipe for your software merged in easybuild-repository-deep-sea Repository
- 2. In your own pipeline:
 - Bundle your sources (e.g. .tar.gz) and move it somewhere well known /p/project/deepsea/ci-stage-sources





Upstream Workflow Summary



- 1. Have one EasyBuild recipe for your software merged in easybuild-repository-deep-sea Repository
- 2. In your own pipeline:
 - Bundle your sources (e.g. .tar.gz) and move it somewhere well known /p/project/deepsea/ci-stage-sources
- 3. Trigger the downstream CI pipeline:
 - For most, setting the \$SRC and \$SRC_URLS variable to your source file name should be enough
 - Some special care must be taken for Python EasyBuild recipes (and bundles in general). If you have one of these, talk to me!





```
stages: [prep, staging]
default:
   tags: [deep-sea, jacamar, shell]
```

create_tarball:

```
stage: prep
```

script:

- mkdir -p -m 777 /p/project/deepsea/ci-stage-sources/s/Score-P/
- tar -cvz --exclude=.git* -f /p/project/deepsea/ci-stage-sources/s/Score-P/\${CI_PIPELINE_ID}.tar.gz .
- chmod g+rw /p/project/deepsea/ci-stage-sources/s/Score-P/\${CI_PIPELINE_ID}.tar.gz

```
trigger-downstream:
```

```
stage: staging
variables:
EB_FILE_CURRENT: "Score-P-7.1-gpsmpi-2021b.eb"
SRC: "${CI_PFELINE_ID}.tar.gz"
SRC_URLS: "file:///p/project/deepsea/ci-stage-sources/s/Score-P/"
BUILD_INVERSE_DEPENDENCIES: "TRUE"
trigger:
project: deep-sea/wp3/software/easybuild-repository-deep-sea
strategry: depend
```

```
branch: ci-2023-dev
```





stages: [prep, staging]
default:
 tags: [deep-sea, jacamar, shell]





stages: [prep, staging]
default:
 tags: [deep-sea, jacamar, shell]

create_tarball:

stage: prep

script:

- mkdir -p -m 777 /p/project/deepsea/ci-stage-sources/s/Score-P/
- tar -cvz --exclude=.git* -f /p/project/deepsea/ci-stage-sources/s/Score-P/\${CI_PIPELINE_ID}.tar.gz .
- chmod g+rw /p/project/deepsea/ci-stage-sources/s/Score-P/\${CI_PIPELINE_ID}.tar.gz





stages: [prep, staging]
default:
 tags: [deep-sea, jacamar, shell]

create_tarball:

stage: prep

script:

- mkdir -p -m 777 /p/project/deepsea/ci-stage-sources/s/Score-P/
- tar -cvz --exclude=.git* -f /p/project/deepsea/ci-stage-sources/s/Score-P/\${CI_PIPELINE_ID}.tar.gz .
- chmod g+rw /p/project/deepsea/ci-stage-sources/s/Score-P/\${CI_PIPELINE_ID}.tar.gz

trigger-downstream:

```
stage: staging
variables:
EB_FILE_CURRENT: "Score-P-8.0-gpsmpi-2022a.eb"
SRC: "${CI_PIPELINE_ID}.tar.gz"
SRC_URLS: "file:///p/project/deepsea/ci-stage-sources/s/Score-P/"
BUILD_INVERSE_DEPENDENCIES: "TRUE"
```

trigger:

```
project: deep-sea/wp3/software/easybuild-repository-deep-sea
strategy: depend
branch: ci-2023-dev
```



Effect on EasyBuilds



Required:

• EB_FILE_CURRENT: A single EasyBuild recipe used as template



Effect on EasyBuilds



Required:

• EB_FILE_CURRENT: A single EasyBuild recipe used as template

Optional (kinda):

- SRC: Replaces the sources field in recipe
- SRC_URLS: Replaces the source_urls field in recipe
- BUILD_INVERSE_DEPENDENCIES: Enables reverse dependency rebuilt (value "TRUE" or "FALSE")



Effect on EasyBuilds



Required:

• EB_FILE_CURRENT: A single EasyBuild recipe used as template

Optional (kinda):

- SRC: Replaces the sources field in recipe
- SRC_URLS: Replaces the source_urls field in recipe
- BUILD_INVERSE_DEPENDENCIES: Enables reverse dependency rebuilt (value "TRUE" or "FALSE")

Also available:

• REBUILD_ONLY: Limits the reverse dependency rebuild by package names











\$ module use /p/project/deepsea/ci-stage-2023-dev/easybuild/modules/all
\$ module avail Score-P

------ /p/project/deepsea/ci-stage-2023-dev/easybuild/modules/all ------MPI/GCC/11.3.0/psmpi/5/Score-P/8.0.20231123.105500 (u) MPI/GCC/11.3.0/psmpi/5/Score-P/8.0.20231123.122040 (u, D)

Where:

```
g: built for GPU
```

u: Built by user

Use "module spider" to find all possible modules. Use "module keyword key1 key2 ..." to search for all possible modules matching any of the "keys".

\$ module load MPI/GCC/11.3.0/psmpi/5/Score-P/8.0.20231123.122040



Thank You For Your Attention



Manoel Rommer – Using Continuous Integration with EasyBuild in DEEP-SEA, 2023-12-01



÷.







Further Content





Continuous Integration Infrastructure







Reverse Dependency Rebuilding



- netCDF depends on HDF5
- When we push a new version of HDF5 we should also rebuild and test netCDF



Reverse Dependency Rebuilding

- netCDF depends on HDF5
- When we push a new version of HDF5 we should also rebuild and test netCDF

Reverse Dependency Rebuilding

EasyBuild CI needs to find reverse dependencies, update their dependency information and rebuild them







Reverse Dependency Resolution



- Not directly supported by EasyBuild
 - We dump EasyBuilds full dependency graph, use it to locate reverse dependencies
 - We actually need a present Easybuild (base-) recipe for that



Reverse Dependency Resolution



- Not directly supported by EasyBuild
 - We dump EasyBuilds full dependency graph, use it to locate reverse dependencies
 - We actually need a present Easybuild (base-) recipe for that
- Configurable by upstream user (that's You):
 - Do you need reverse dependency rebuild: Yes/No?
 - All your reverse dependencies or only a select few?
 - More flexible configuration options in the works!



Rewriting EasyBuild Recipes



```
name = 'Scalasca'
                                              name = 'Scalasca'
                                              version = 12.6.1.20230726.064424
version = 1261
toolchain = {
                                              toolchain = {
    'name': 'gpsmpi'.
                                                   'name': 'gpsmpi'.
    'version': '2022a'
                                                   'version': '2022a'
3
                                              3
dependencies = [
                                              dependencies = [
    ('CubeGUI', '4.8'),
                                                   ('CubeGUI', '4.8'),
    ('CubeLib', '4.8').
                                                   ('CubeLib', '4.8').
    ('OTF2', '3.0.2').
                                                   ('OTF2', '3.0.2'),
    ('Score-P', '8.0').
                                                   ('Score-P', '8.0.20230726.064424'),
```

We now have a robust and flexible solution to update EasyBuild Recipes!





In the previous design: Build job orchestration supposed to be done by JUBE







In the previous design: Build job orchestration supposed to be done by JUBE

Now: Moved to custom solution that generates downstream pipeline





In the previous design: Build job orchestration supposed to be done by JUBE

Now: Moved to custom solution that generates downstream pipeline

- Jacamar can directly submit (build) jobs to SLURM
- Jobs can be directly monitored from Gitlab CI/CD control panel
- Shell runners are available for other tasks





In the previous design: Build job orchestration supposed to be done by JUBE

Now: Moved to custom solution that generates downstream pipeline

- Jacamar can directly submit (build) jobs to SLURM
- Jobs can be directly monitored from Gitlab CI/CD control panel
- Shell runners are available for other tasks

Of course you can still, use JUBE to run your benchmarks on top of this stack!



How to Integrate?





Trigger?



workflow:

rules:

- if: \$CI_COMMIT_MESSAGE =~ /-draft\$/
 when: never
- if \$CI_PIPELIEN_SOURCE == "push"

When to trigger a rebuild?

- Depends on development workflow
- On push, merge request, release, manually,...

