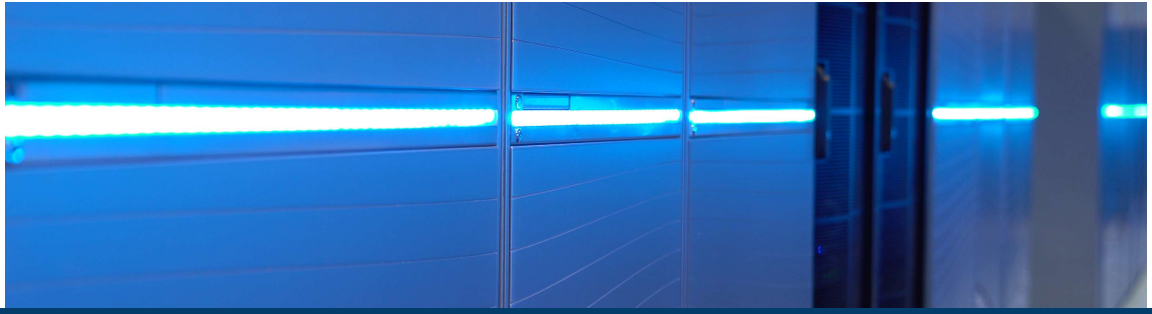


JSC site presentation
7th EasyBuild User Meeting

January 28, 2022 | Sebastian Achilles | Jülich Supercomputing Centre

easybuild

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

JUWELS Cluster + Booster

JUWELS Cluster

- 2271 standard, 240 large-mem and 56 GPU nodes
- 2× Intel Xeon Platinum 8168, 2× 24 cores, 2.7 GHz
- 96 GB (large mem and GPU 192 GB)
- InfiniBand EDR
- 56 nodes with 4× NVIDIA V100

JUWELS Booster

- 936 nodes
- 2× AMD EPYC Rome 7402, 2× 24 cores, 2.7 GHz
- 512 GB DDR4
- 4× NVIDIA A100
- 4× InfiniBand HDR200

JURECA-DC

JURECA-DC

- 768 nodes
- 2× AMD EPYC Rome 7742, 2× 64 cores, 2.25 GHz
- 512 GB DDR4 (large mem 1024 GB)
- 2× InfiniBand HDR200
- 96 large-memory nodes
- 192 GPU nodes with 4× NVIDIA A100

JURECA-Booster

- 1640 nodes
- 1× Intel Xeon Phi 7250-F, 1× 68 cores, 1.4 GHz
- 96 GiB + 16 GiB MCDRAM high-bandwidth memory
- Intel Omni-Path Architecture

JUSUF, HDFML

JUSUF

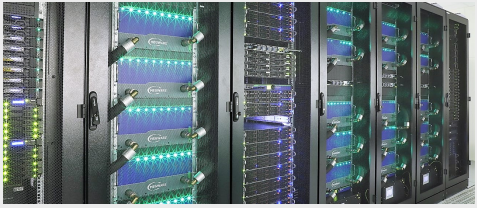
- 205 nodes
- 2× AMD EPYC Rome 7742, 2× 64 cores, 2.25 GHz
- 256 GB DDR4
- InfiniBand HDR100
- 61 nodes with 1× NVIDIA V100

HDFML

- 16 nodes
- 2× Intel Xeon Gold 6126, 2× 12 cores, 2.60 GHz
- 192 GB DDR4
- 4× NVIDIA V100
- InfiniBand HDR100

DEEP

DEEP-EST prototype



- 50 Cluster nodes: 2 x Intel Xeon Gold 6146, 192 GB
- 75 Extreme Scale Booster nodes: Intel Xeon Silver 4215, 48 GB, 1x NVIDIA V100
- 16 Data Analytics Module nodes: 2x Intel Xeon Platinum 8260M, 384 GB, 1x NVIDIA V100

Other systems

Other Prototypes

- ARM Cluster
- ...

JSC Clouds

- Jupyter-JSC
- virtual Test cluster(s)

JSC Software Team

- Software Core Team
  - 5 people
  - Responsible for core installation (GCCcore, compiler, MPI, Math)
  - Responsible for reviewing and merging PR into the JSC easybuild repository
- Software Group
  - Group of 36 people
  - Each module has has one responsible person which is applications/packages expert
  - Responsible for installation with EasyBuild (with ACLs), testing and validation as well as user questions

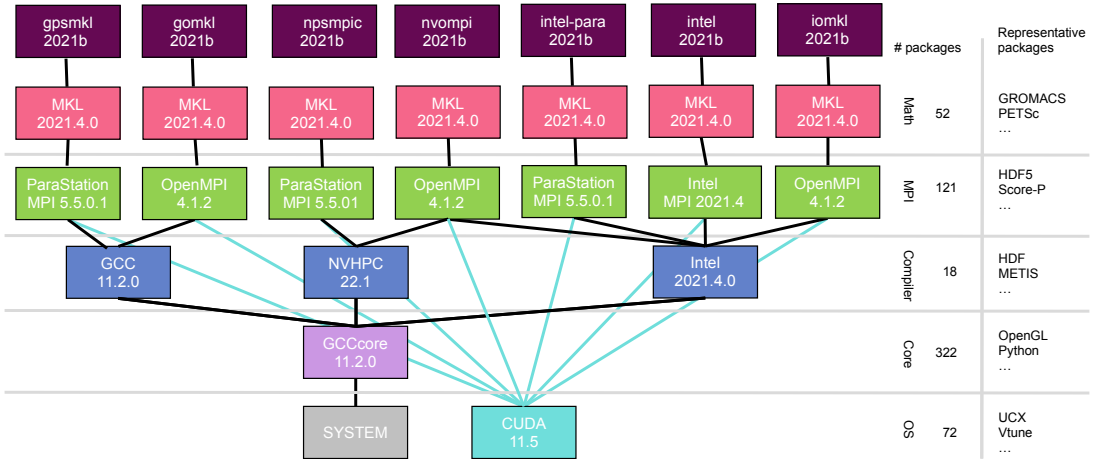
What is new at JSC?

- Beginning with `Stages/2022` increase overlap with upstream
- Allow users to install software with EasyBuild on-top of the available modules with `UserInstallations`

Stage 2022

- Based on `2021b` toolchain family
- Custom toolchains
- Reduced number of custom EasyBlocks (18 compared to 25 in 2021 stage)
- Extended hook

Stages 2022 toolchains



UserInstallations

Install packages in Production stage:

```
ml Stages/2022
ml Developers
eb packages-1.2.3.eb
```

Install packages in User space:

```
ml Stages/2022
ml UserInstallations
eb packages-1.2.3.eb
```

- currently used for testing and development
- Goal: Allow users to install easyconfigs from upstream (`--try-*`)

Usage of the hook in the JSC repo

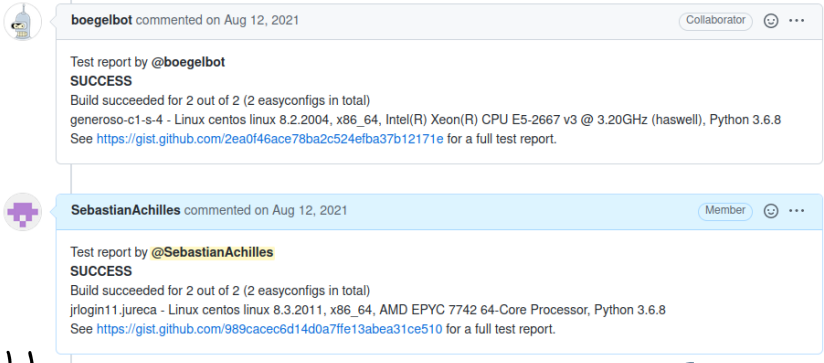
- Goal: increase overlap with upstream
- at the same time allow modification in JSC repo as well as allow to use easyconfigs from upstream (e.g. for users)
- Solution:
  - JSC hook can tweak dependencies, e.g. when you want to install an easyconfig from upstream
  - JSC CI is strict and only allows dependencies from JSC repo to maintain readability
- Some dependencies the hook currently tweaks:
  - `UCX` v1.12.0
  - `Mesa`, `glu`, `glew` → `OpenGL`
  - `CUDA` v11.5
  - `Boost` v1.78.0

Expanding the EB's shared test infrastructure

Virtual Cluster at JSC

Current situation

- One test cluster `generoso` based on Intel
- Other architectures or OS need to be manually tested by Maintainers



boegelbot commented on Aug 12, 2021 — Collaborator

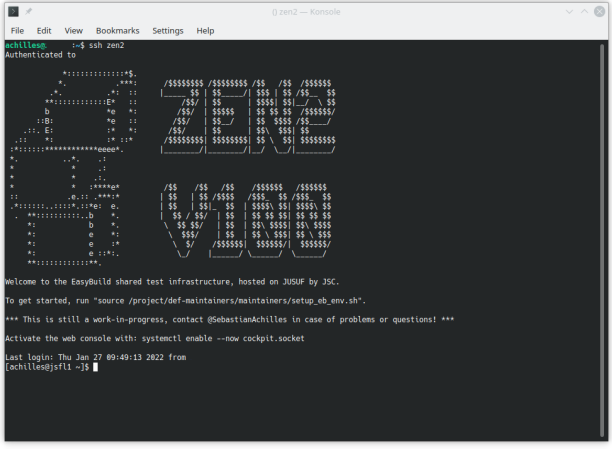
Test report by **@boegelbot**
SUCCESS
Build succeeded for 2 out of 2 (2 easyconfigs in total)
generoso-c1-s-4 - Linux centos linux 8.2.2004, x86_64, Intel(R) Xeon(R) CPU E5-2667 v3 @ 3.20GHz (haswell), Python 3.6.8
See https://gist.github.com/2ea0f46ace78ba2c524efba37b12171e for a full test report.

SebastianAchilles commented on Aug 12, 2021 — Member

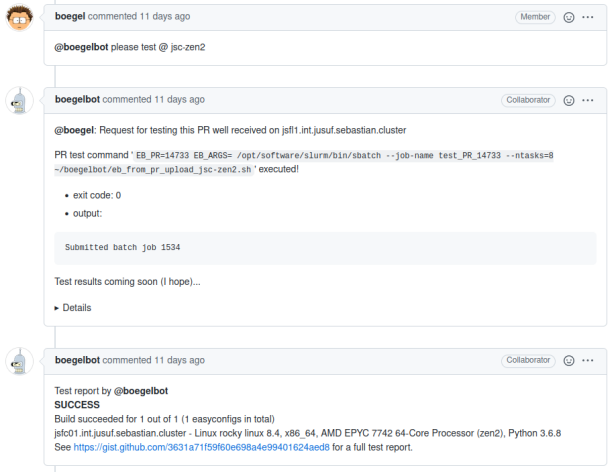
Test report by **@SebastianAchilles**
SUCCESS
Build succeeded for 2 out of 2 (2 easyconfigs in total)
jrlogin11.jureca - Linux centos linux 8.3.2011, x86_64, AMD EPYC 7742 64-Core Processor, Python 3.6.8
See https://gist.github.com/989cacec6d14d0a7ffe13abea31ce510 for a full test report.

Virtual Cluster with Magic Castle

- Virtual Cluster with Magic Castle: `https://github.com/ComputeCanada/magic_castle`
- JUSUF-Cloud: OpenStack, AMD EPYC 7742, NVIDIA V100
- boebelbot listening to submit test-reports



Now boegelbot can also run on AMD zen2



boegel commented 11 days ago — Member

@boegelbot please test @ jsc-zen2

boegelbot commented 11 days ago — Collaborator

@boegel: Request for testing this PR well received on jsfl1.int.jusuf.sebastian.cluster

PR test command '`EB_PR=14733 EB_ARGS= /opt/software/slurm/bin/sbatch --job-name test_PR_14733 --ntasks=8 ~/boegelbot/eb_from_pr_upload_jsc-zen2.sh`' executed!

- exit code: 0
- output:

```
Submitted batch job 1534
```

Test results coming soon (I hope)...

▸ Details

boegelbot commented 11 days ago — Collaborator

Test report by **@boegelbot**
SUCCESS
Build succeeded for 1 out of 1 (1 easyconfigs in total)
jsfc01.int.jusuf.sebastian.cluster - Linux rocky linux 8.4, x86_64, AMD EPYC 7742 64-Core Processor (zen2), Python 3.6.8
See https://gist.github.com/3631a71f59f60e698a4e99401624aed8 for a full test report.

Hardware for tests reports with boegelbot

CPU arch	system name	available
Intel Haswell	`generoso`	✓
AMD Zen2	`jsc-zen2`	✓

accelerators	system name	available
NVIDIA V100	`jsc-zen2`	(✓)

Hardware for tests reports with boegelbot

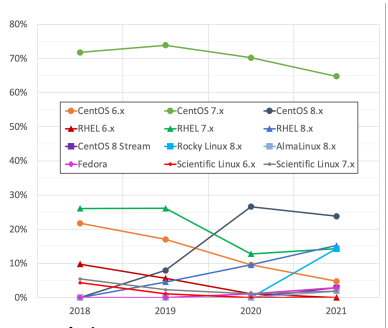
CPU arch	system name	available
Intel Haswell	`generoso`	✓
Intel Skylake		✗
AMD Zen2	`jsc-zen2`	✓
AMD Zen3		✗
ARM		✗
RISC-V		✗

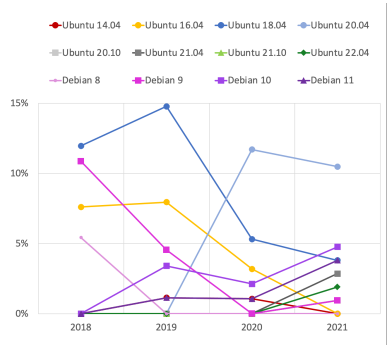
accelerators	system name	available
NVIDIA V100	`jsc-zen2`	(✓)
NVIDIA A100		✗
AMD MI100/MI200		✗
Intel Arc		✗

Testing different operating systems in container?

- Test reports by boegelbot currently done on RockyLinux
- However EasyBuild is used on many operating systems

⇒ Let boegelbot test different OS in containers





Thank you!

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