CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich

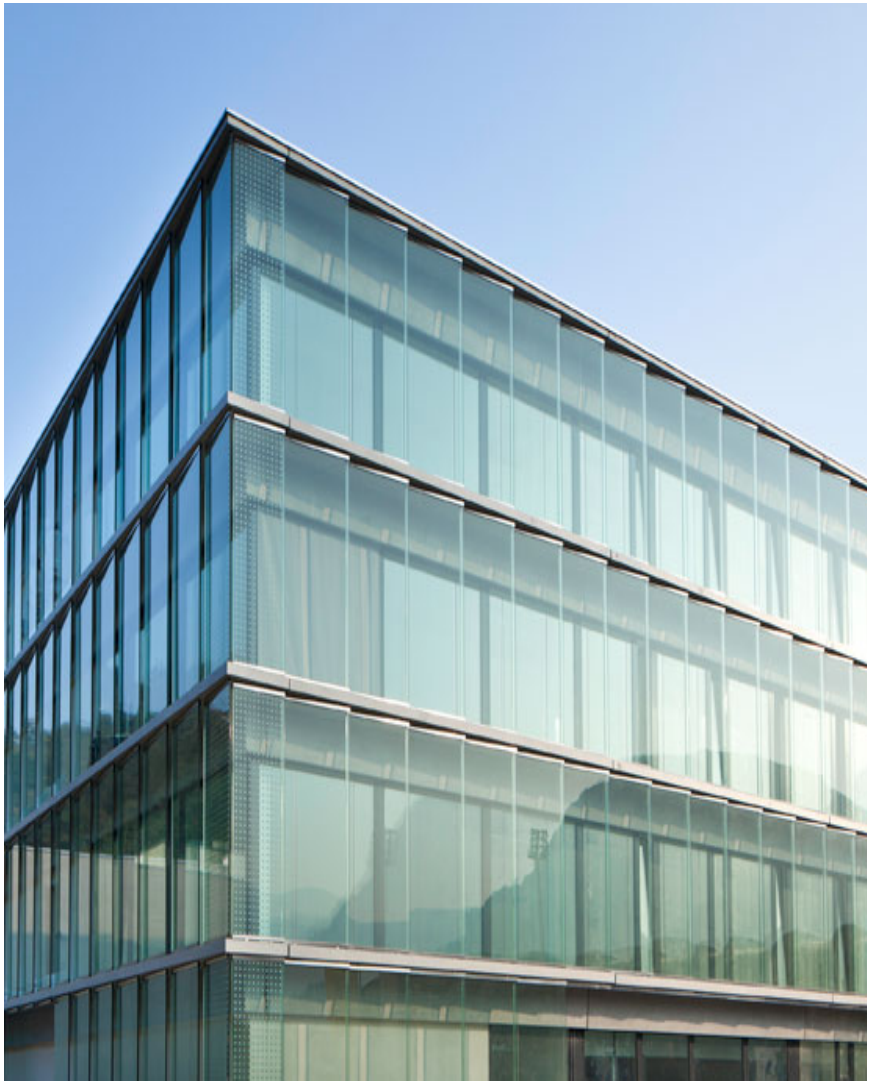
EasyBuild @ CSCS site update

3rd EasyBuild User Meeting
Jan 30th – Feb 1st 2018, Amsterdam

Guilherme Peretti-Pezzi
Theofilos Ioannis Manitaras

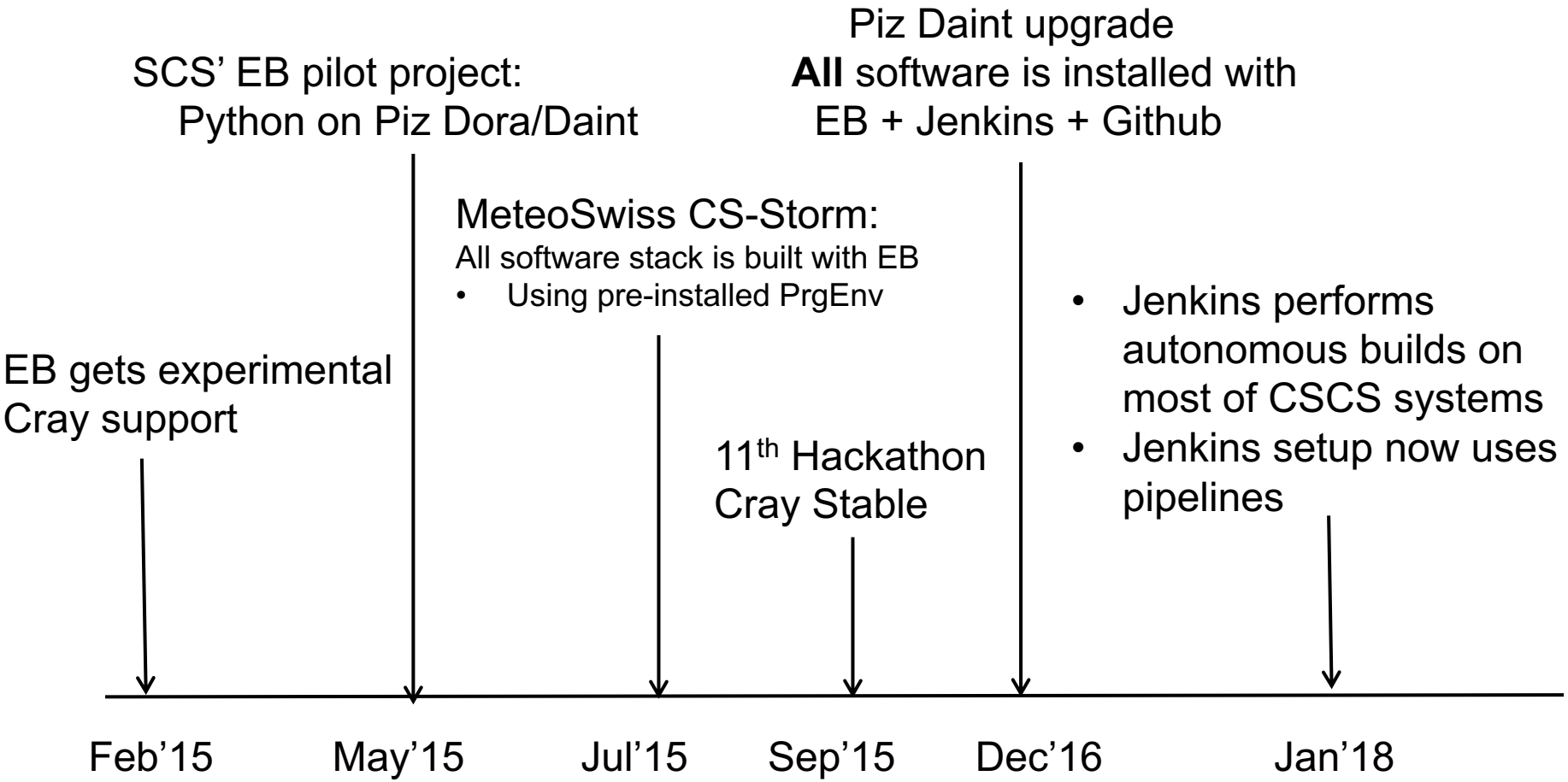
Scientific Computing Support (CSCS)

Outline



- **EB @ CSCS (Guilherme)**
  - **Timeline**
  - **Piz Kesch & Escha use case**
    - **Cray CS-Storm**
  - **Piz Daint**
    - **Cray XC**
- Using Jenkins with Easybuild at CSCS (Theo)
- Final remarks

EasyBuild timeline @ CSCS



EasyBuild Enhancements for Cray Systems

1. Support for external module files
2. Definition of Cray-specific toolchains
3. Custom easyblock for Cray toolchains

- Various smaller enhancements specific to the Cray environment

- **Thanks to Peter Forai & Kenneth Hoste**

Overview of CSCS HPC systems

System	Scope	Accelerators / node	Type
Piz Daint	User Lab	1 GPU	Cray XC50
Monch	PASC projects	0	NEC Intel IvyBridge
Escha	Meteo Swiss	16 GPU	Cray CS-Storm
Kesch	Meteo Swiss	16 GPU	Cray CS-Storm
Leone	Large Memory	1 GPU	HP DL 360 Gen 9

Piz Kesch & Escha use case (MeteoSwiss / Cray CS-Storm)

"Kesch" and "Es-cha" consist of identical systems (production and failover), each comprising:

Cray CS-Storm: 12 nodes

- 2 x Intel Haswell E5-2690v3 2.6 GHz 12-core CPUs per node
  - total of 24 E5-2690v3 processors
- 256 GB 2133 MHz DDR4 memory per node
  - total of 3 TB
- 8 NVIDIA® Tesla® K80 GPU devices per node
  - total of 192 GPUs

MeteoSwiss, the Swiss national weather forecasting service, hosts their dedicated production systems at Cray CS-Storm at CSCS, Lugano.

- EasyBuild software stack in production since September/2015
- (GCC initially provided by Cray was unable to assemble AVX2 instructions for haswell)

Piz Daint

Model	Cray XC50/XC40
XC50 Compute Nodes	Intel® Xeon® E5-2690 v3 (Haswell) @ 2.60GHz (12 cores, 64GB RAM) and NVIDIA® Tesla® P100 16GB
XC40 Compute Nodes	Intel® Xeon® E5-2695 v4 (Broadwell) @ 2.10GHz (18 cores, 64/128 GB RAM)
Login Nodes	Intel® Xeon® CPU E5-2650 v3 @ 2.30GHz (10 cores, 256 GB RAM)
Interconnect Configuration	Aries routing and communications ASIC, and Dragonfly network topology
Scratch capacity	6.2 PB (Lustre / Sonexion 3000)

Piz Daint

- #3 Top 500
  - #1 in Europe
  - 19.590 PFLOPS
- #10 Green 500
  - 10.398 MFLOPS/W

Available software on Cray using EasyBuild

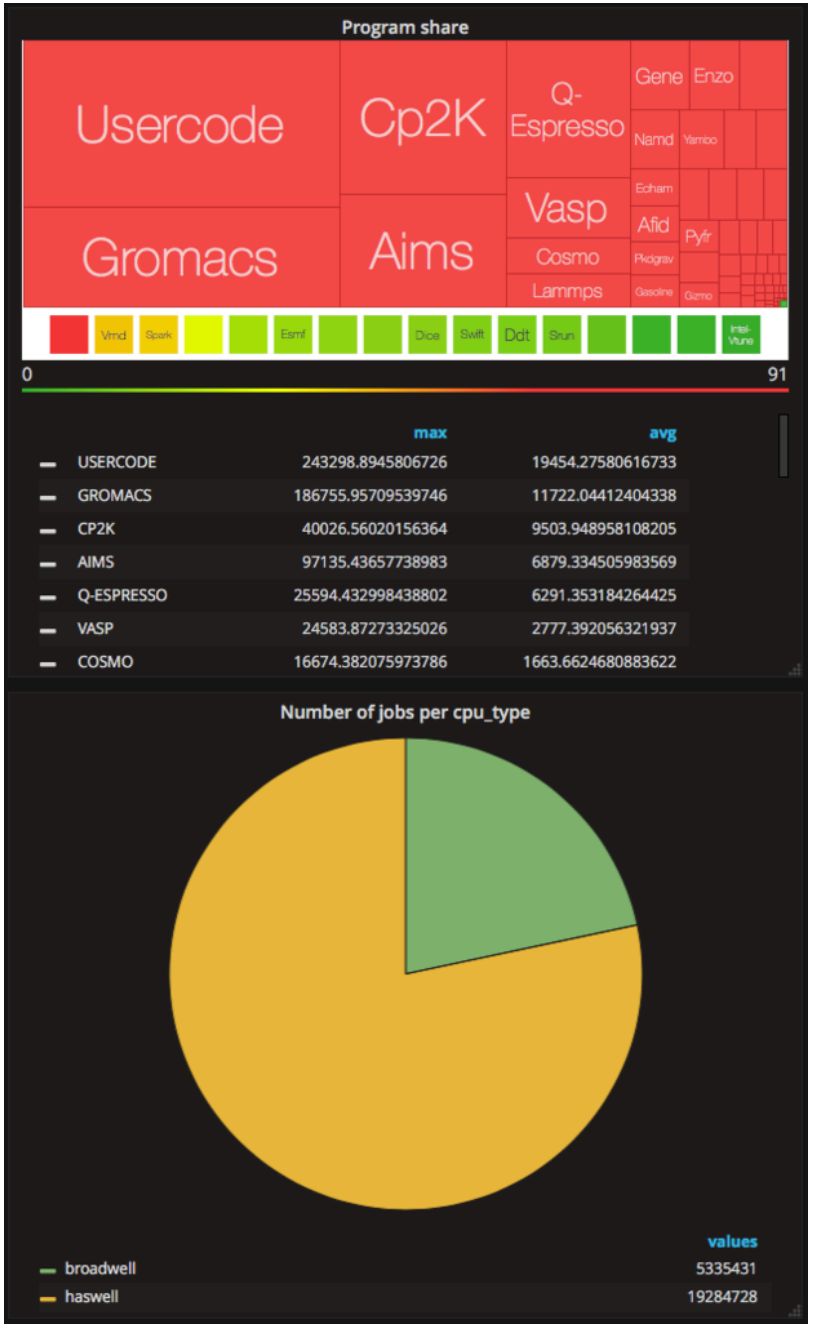
- Stock EasyBuild repository
  - Python, including
    - accelerated numpy + scipy, h5py, …
  - WRF
  - CP2K[*]
  - GROMACS[*]
  - Boost
  - GSL

[*] = GPU-enabled recipe available

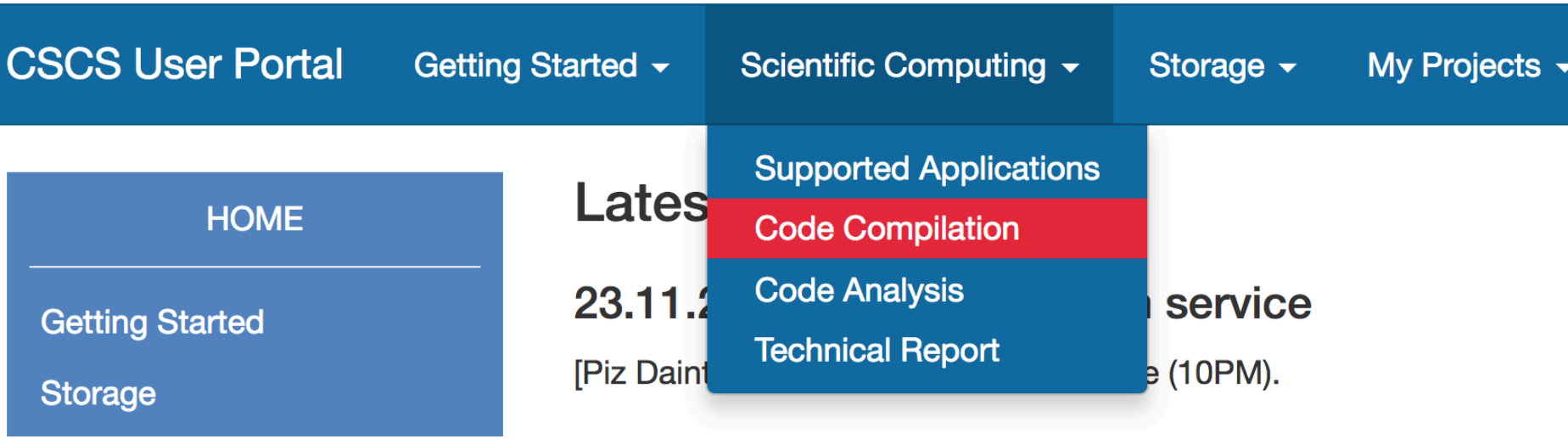
- CSCS Production Github repository
  - Amber[*]
  - CDO
  - CPMD
  - LAMMPS[*]
  - NCL
  - NCO
  - ParaView[*]
  - Octave
  - QuantumESPRESSO
  - R
  - Score-P/Scalasca/Extrae/Ipm
  - VASP[*]
  - Visit
  - VMD[*]
  - VTK[*]

  - TensorFlow[*], Theano[*]
  - CNTK[*], Caffe[*], Caffe2[*]

Apps and Users using xalt statistics



User instructions for EasyBuild (1)



User instructions for EasyBuild (2)

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CSCS User Portal | Getting Started | Scientific Computing | Storage | My Projects

SCIENTIFIC COMPUTING

Supported Applications

- ABCpy
- Amber
- CP2K
- CPMD

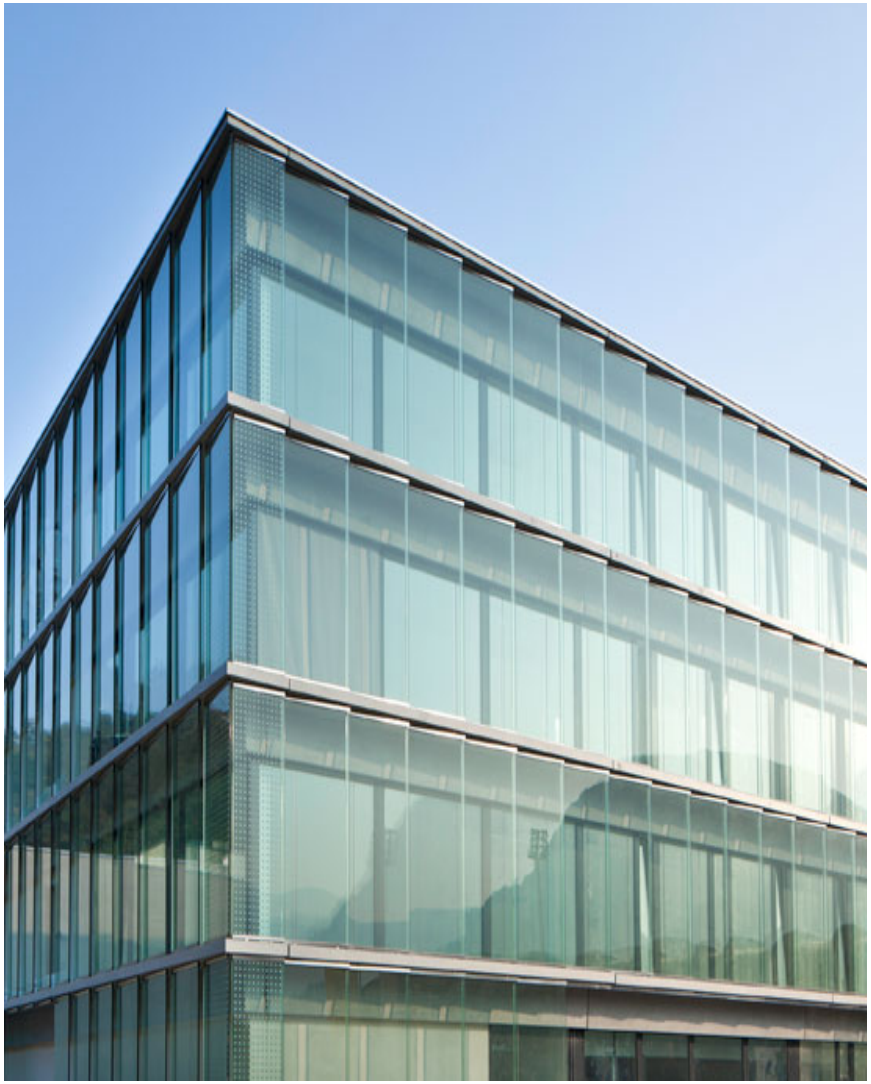
EasyBuild framework

Loading the environment

The EasyBuild framework is available at CSCS through the module `EasyBuild-custom`. This module defines the location of the EasyBuild configuration files, recipes and installation directories.

```
module load EasyBuild-custom
```

Outline



- EB @ CSCS (Guilherme)
  - Timeline
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    - Cray XC
- **Using Jenkins with Easybuild at CSCS (Theo)**
  - **Use of Jenkins with Easybuild at CSCS**
  - **Advantages of Jenkins pipelines**
  - **Demonstration of Testing pipeline**
  - **Demonstration of Regression pipeline**
- Final remarks

Jenkins at CSCS

- At CSCS Jenkins is the basic tool used for CI to test and deploy software packages which are defined as Easyconfigs and are built with Easybuild.

- Jenkins combined with Easybuild is used in three distinct projects:
  - Testing: tests a new Easyconfig submitted to Github.
  - Production: builds the software to be available as a module for users.
  - Regression: runs Easybuild for each installed Easyconfig.

- Recently we have migrated our Jenkins projects to `Pipelines` which offer:
  - Greater flexibility regarding the actions performed by Jenkins.
  - The `Jenkinsfile` of each project is version controlled.
  - Easily run the CI in parallel using all available resources.

Submitting a new PR

Contributing back

How to submit a pull request:

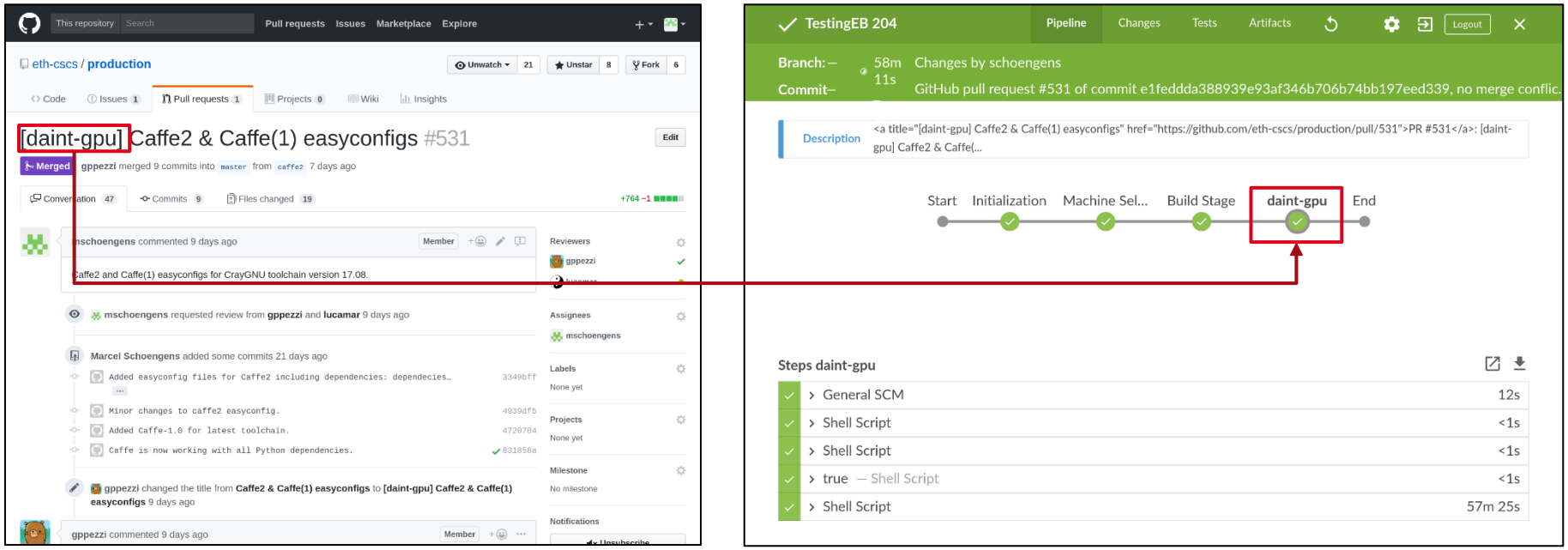
1. Add the EasyBuild configuration files to a **new branch**, including **all the required dependencies**
2. Create and **assign yourself a pull request** following this policy for the title:
   - the title **must match a supported system** in the list `daint dom kesch leone monch`, otherwise the build will fail immediately. The system names **have to be enclosed in square brackets** to be distinguished from the actual pull request title and be parsed by the corresponding Jenkins project.
   - if the title matches `WIP` ("Work In Progress"), then the test build will be aborted immediately, as work in progress is not supposed to be tested.
   - Dom and Piz Daint can test both software stacks `-gpu` and `-mc` at once:
     a. if the title matches only `${system}-gpu` or `${system}-mc`, only that software stack will be used:
        - `[dom-gpu] NAMD` will build using `-gpu`, `[dom-mc] NAMD` will use `-mc`.

     b. if the title matches both or none, then both will be used, one after another in a loop:
        - `[dom] NAMD` will build using both `-gpu` and `-mc` in a loop.
        - `[dom-gpu,dom-mc] NAMD` will do the same.
3. The CSCS Jenkins project `TestingEB` will test the build of new EasyBuild recipes with respect to the master. The corresponding pipeline of `TestingEB` is contained in the `jenkins/JenkinsfileTestingEB` script.
4. If the build is successful, you should **ask for a review**: the pull request will only be merged when approved.
5. In order to re-trigger the testing of the pull request without committing a change, add the comment `retest this please` which will notify the `TestingEB` Jenkins project.
6. (CSCS only) for production builds, please update the appropriate production build list here.

CI – Testing a new Easyconfig submitted to Github (1)

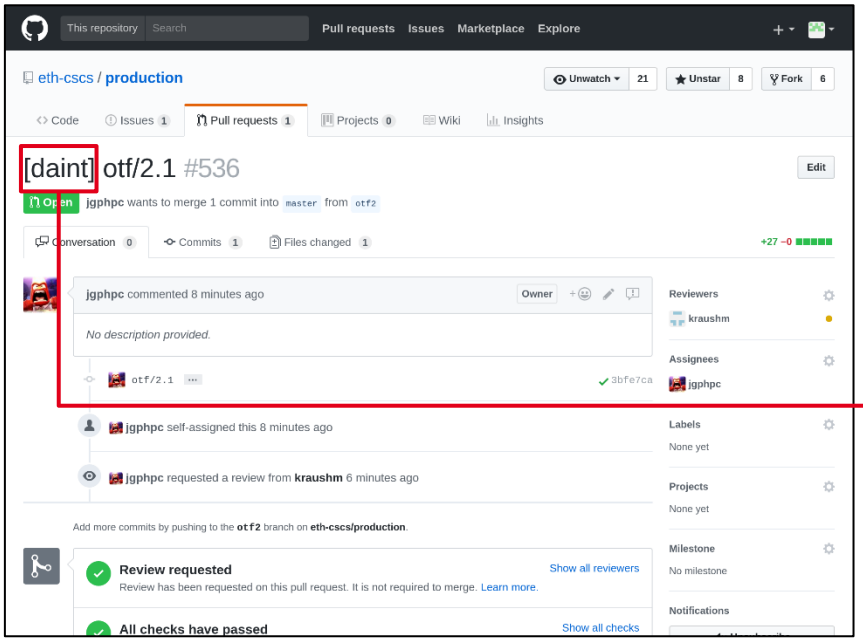
Github PR ([daint-gpu])

Triggered Pipeline

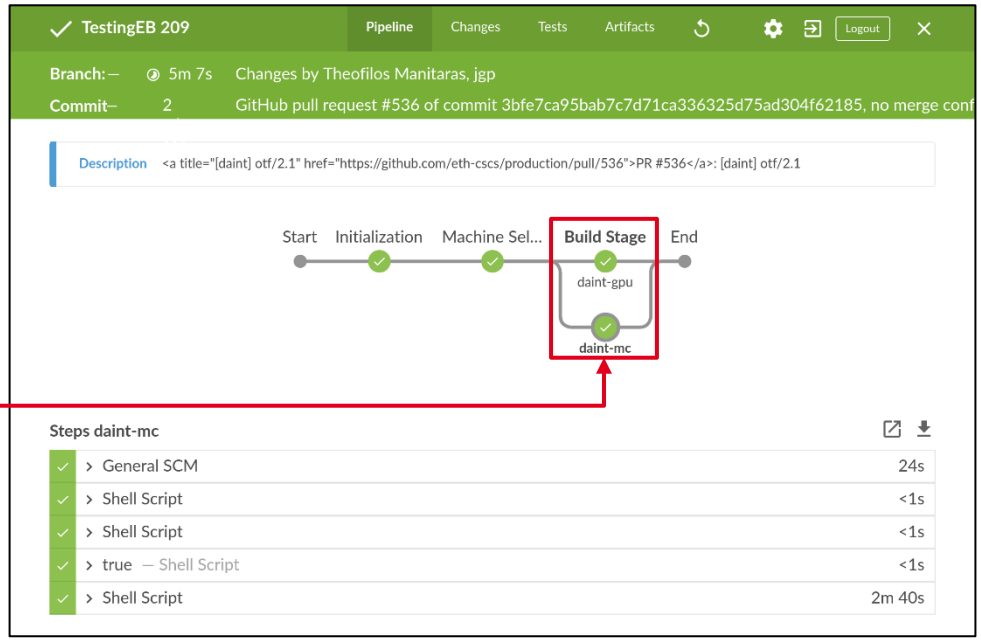


CI – Testing a new Easyconfig submitted to Github (2)

Github PR ([daint])

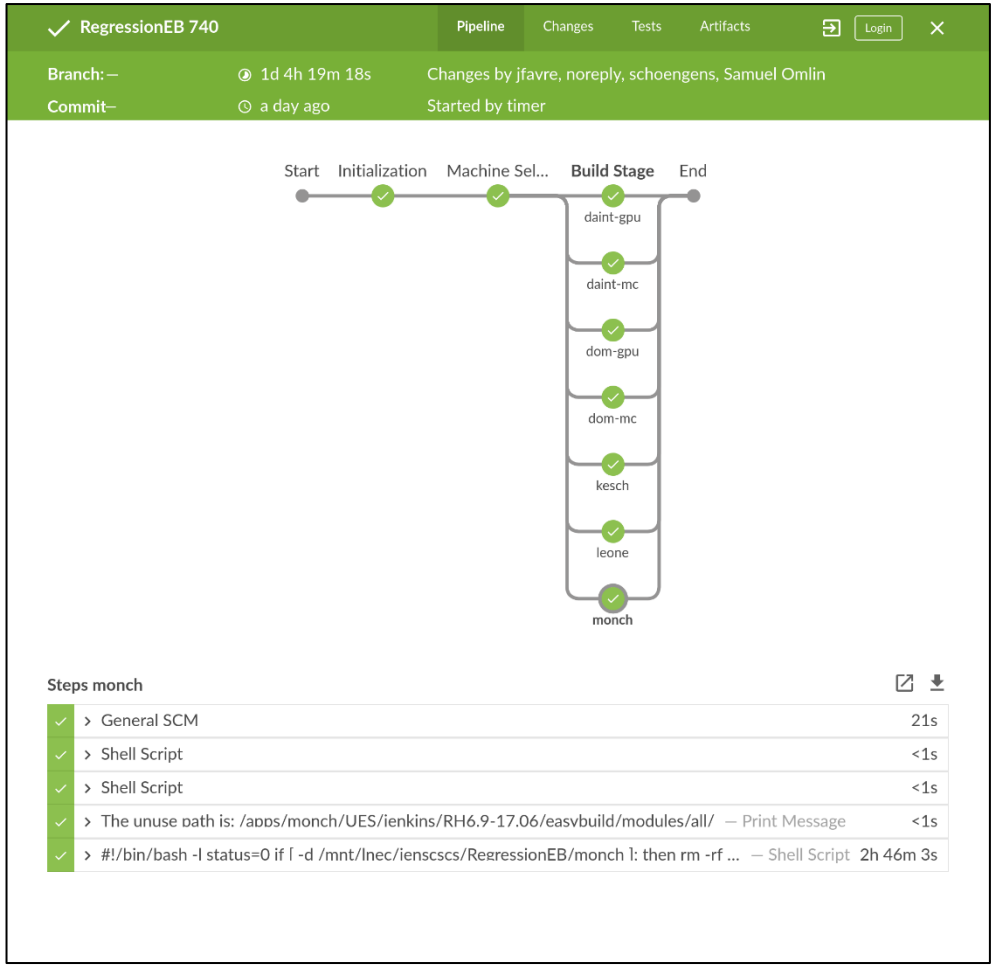


Triggered Pipeline

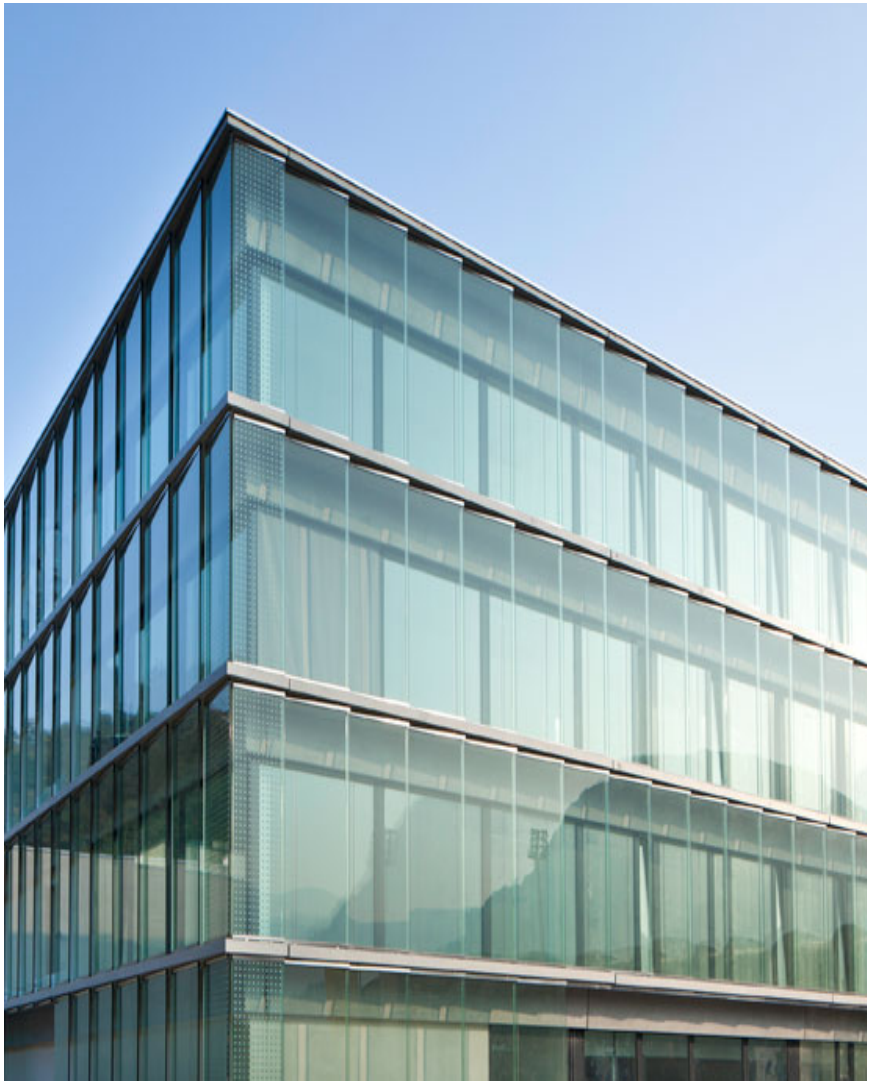


Regression Pipeline (All machines)

- Runs once a week and tests all Easyconfigs in production per machine in parallel.
- Ensure that each software package builds successfully.
- Through the Blue Ocean interface it is easy to inspect the console output of each machine.



Outline



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Final remarks

- Moving to EB at institution level takes time
  - Learning curve
  - Resistance to change
- EasyConfigs vs. EasyBlocks (my 5 cents)
  - EasyBlocks
    - (+) Reusable: Great for well packaged & stable software
    - (-) Too much overhead for bleeding edge software
    - (-) Reproducibility: how keep track of changes?
  - EasyConfigs
    - (-) Reuse by copy paste (=> duplication)
    - **(+++) Self contained recipes**

Final remarks (2)

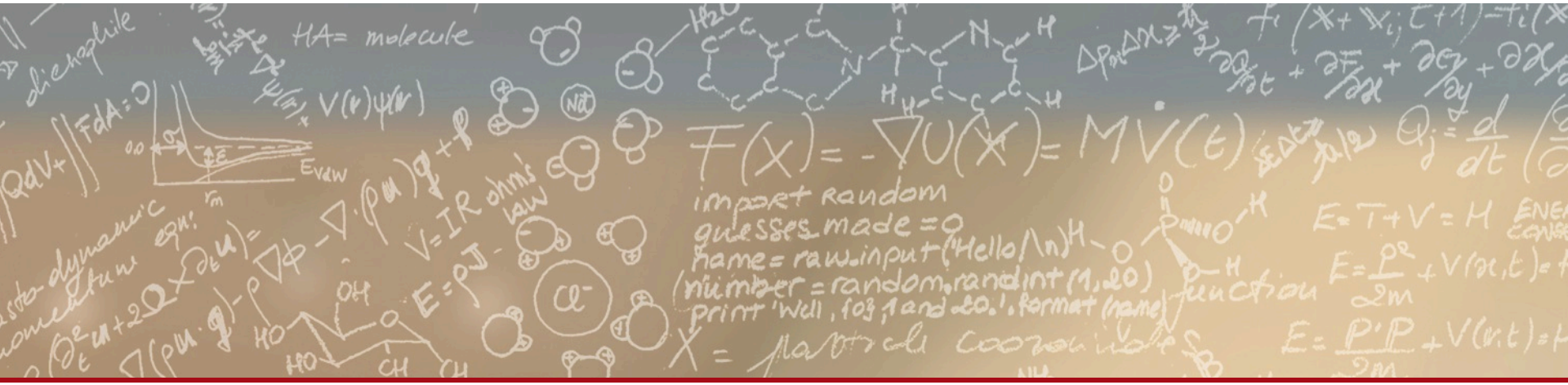
- Feature wish list
  - New command line options for dependencies
    - --try-dep-version ?
  - Have a separate log for command lines performed by EB
    - As complement to –extended-dry-run
  - Backup of custom easyblocks for reproducibility
  - External modules
    - Improve error reporting for missing modules
    - Generic/versionless entries on the metadata file

- Ongoing work
  - Deploying HPC OpenStack cluster with EB

Useful links for EasyBuild @ CSCS

- EasyBuild User Documentation at CSCS
  - https://user.cscs.ch/scientific_computing/code_compilation/easybuild_framework/

- Easyconfig files repositories
  - List of production builds performed by Jenkins
    - https://github.com/eth-cscs/production/tree/master/jenkins-builds
  - Custom easyconfigs:
    https://github.com/eth-cscs/production/tree/master/easybuild/easyconfigs
  - Custom easyblocks:
    - https://github.com/eth-cscs/production/tree/master/easybuild/easyblocks



Thank you for your kind attention