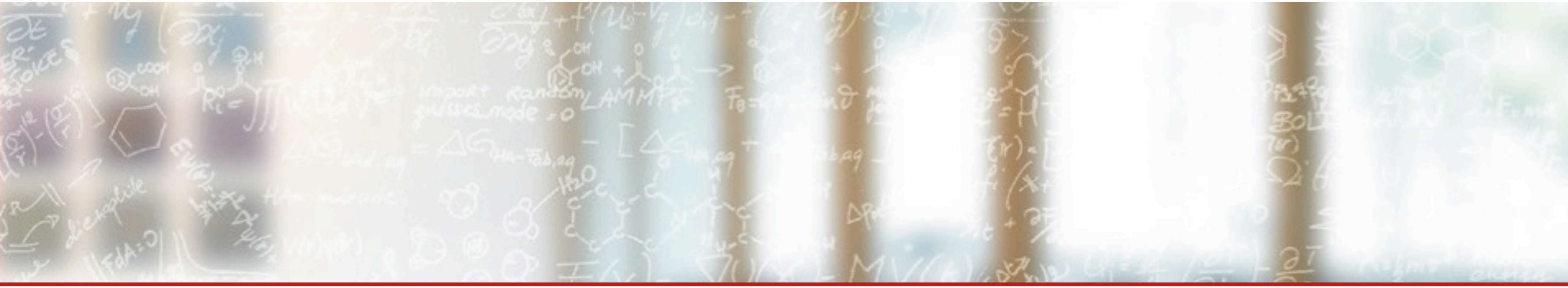
CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

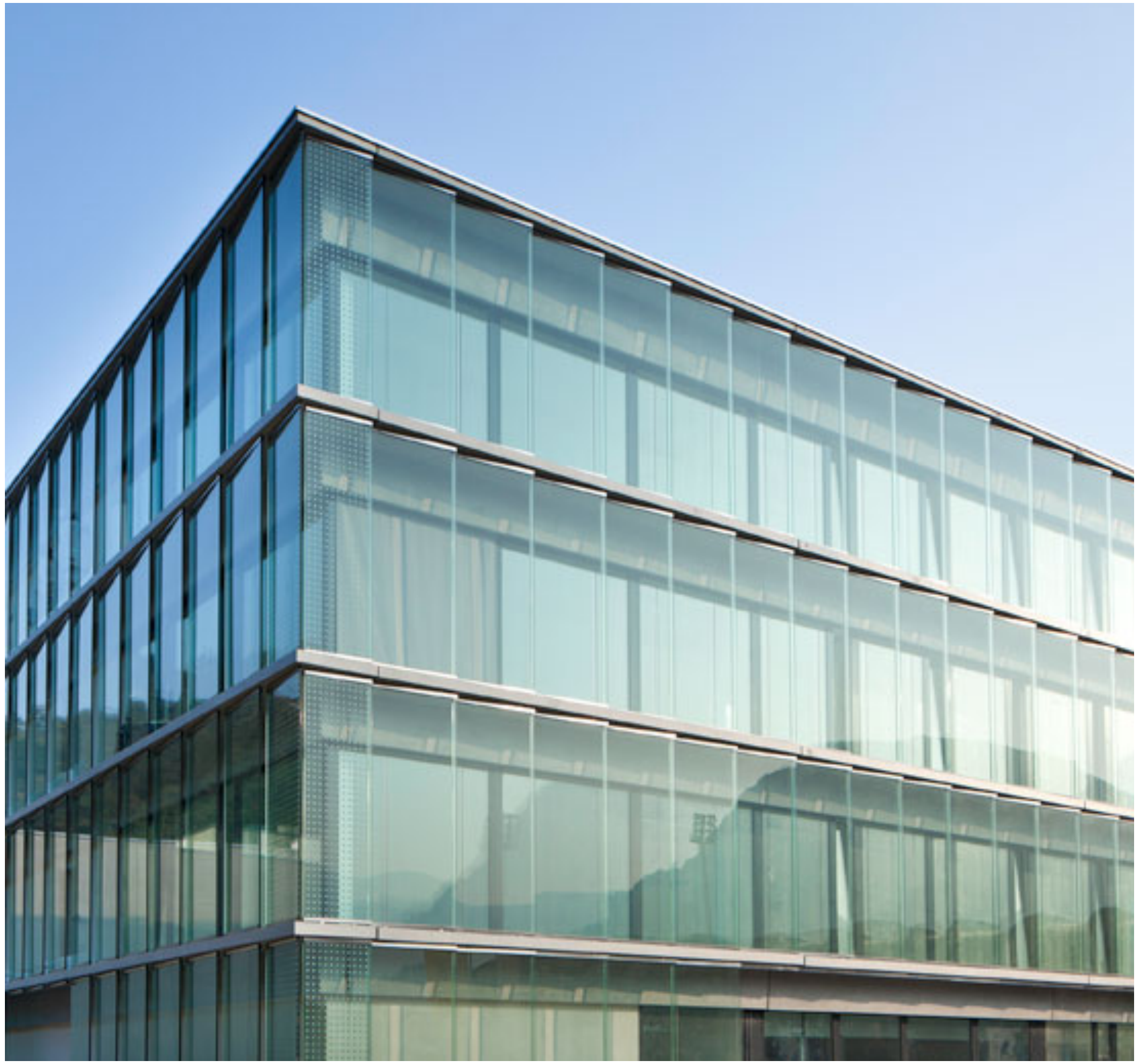
ETH zürich



EasyBuild @ CSCS: Current status and roadmap

EasyBuild Workshop
Guilherme Peretti-Pezzi, CSCS
September 8th, 2015

Outline



- Overview of EasyBuild setup @ CSCS
- Proposed workflow for using EB
- Python + MCH use cases
- Jenkins integration
- Final thoughts
- Intel use case ***new***
  - Luca Marsella

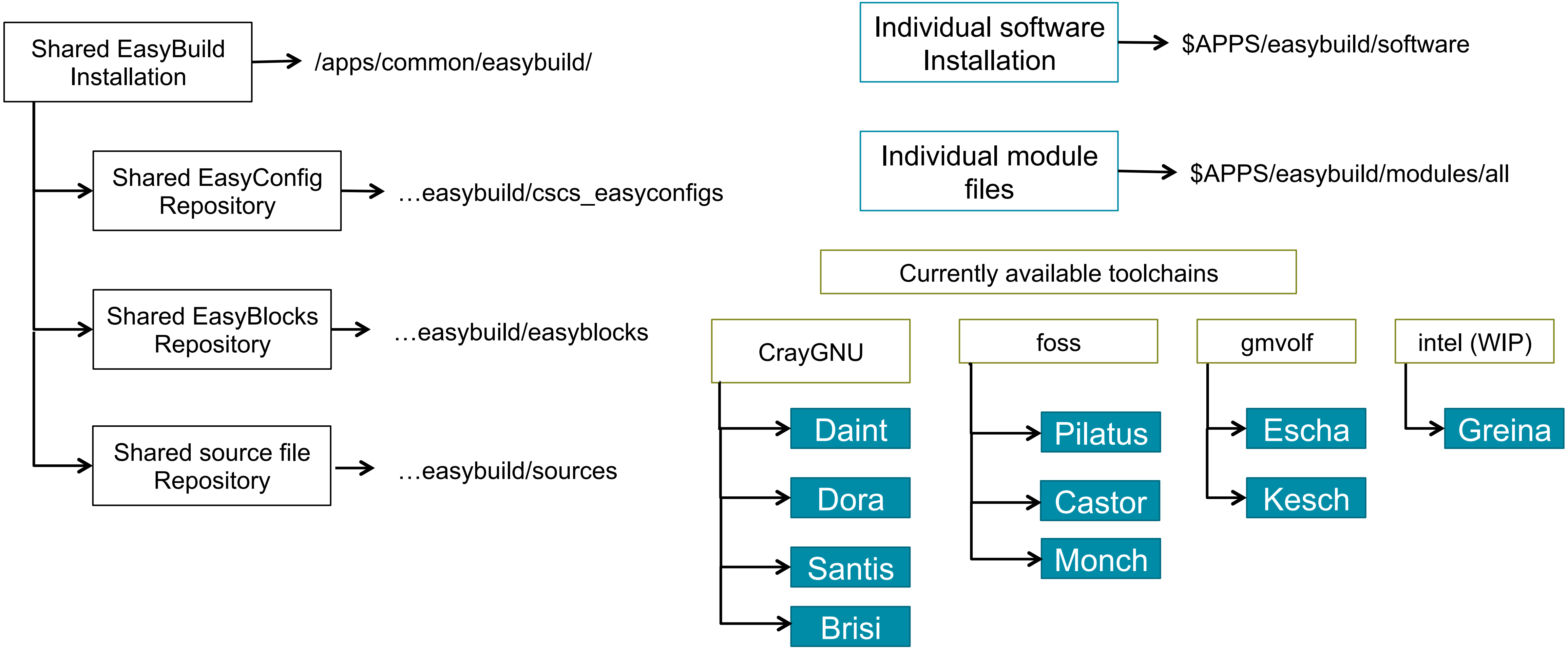
Some of the stock EasyBuild toolchains

- ClangGCC: Clang, GCC
- CrayCCE: PrgEnv-cray, fftw
- **CrayGNU: PrgEnv-gnu, fftw**
- CrayIntel: PrgEnv-intel, fftw
- GCC: GCC
- cgmpich: Clang, GCC, MPICH
- cgmvapich2: Clang, GCC, MVAPICH2
- cgompi: Clang, GCC, OpenMPI
- **dummy: (system libs and compilers)**
- **foss: BLACS, FFTW, GCC, OpenBLAS, OpenMPI, ScaLAPACK**
- gcccuda: CUDA, GCC
- **gmvapich2: GCC, MVAPICH2**
- gmvolf: BLACS, FFTW, GCC, MVAPICH2, OpenBLAS, ScaLAPACK
- gompic: CUDA, GCC, OpenMPI
- gpsolf: BLACS, FFTW, GCC, OpenBLAS, ScaLAPACK, psmpi
- iccifort: icc, ifort
- ictce: icc, ifort, imkl, impi
- **intel: icc, ifort, imkl, impi**
- iomkl: OpenMPI, icc, ifort, imkl
- iqacml: ACML, BLACS, FFTW, QLogicMPI, ScaLAPACK, icc, ifort

Remarks:

- Full list available with:
  - eb --list-toolchains
- GNU = GCC + binutils
- Since 2015b, foss and intel actually use GNU instead of GCC
  - so they secretly include binutils ;)
  - (not listed here but visible on the eb files)

EasyBuild setup @ CSCS



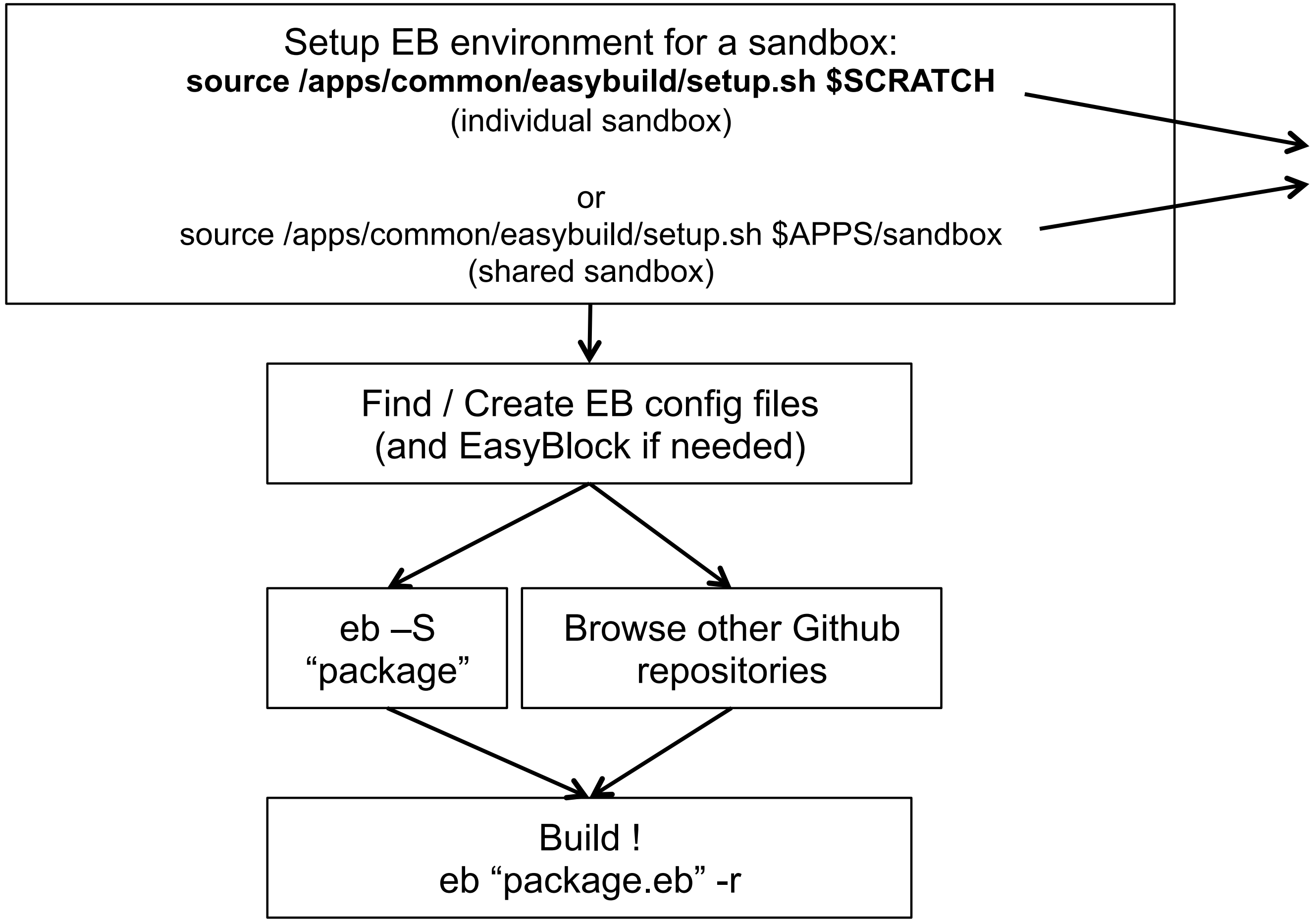
- Shared EasyBuild Installation → /apps/common/easybuild/
  - Shared EasyConfig Repository → …easybuild/cscs_easyconfigs
  - Shared EasyBlocks Repository → …easybuild/easyblocks
  - Shared source file Repository → …easybuild/sources

- Individual software Installation → $APPS/easybuild/software
- Individual module files → $APPS/easybuild/modules/all

Currently available toolchains

- CrayGNU → Daint, Dora, Santis, Brisi
- foss → Pilatus, Castor, Monch
- gmvolf → Escha, Kesch
- intel (WIP) → Greina

Proposed EasyBuild workflow for development (usable by all CSCS)



Setup EB environment for a sandbox:
source /apps/common/easybuild/setup.sh $SCRATCH
(individual sandbox)

or
source /apps/common/easybuild/setup.sh $APPS/sandbox
(shared sandbox)

Find / Create EB config files
(and EasyBlock if needed)

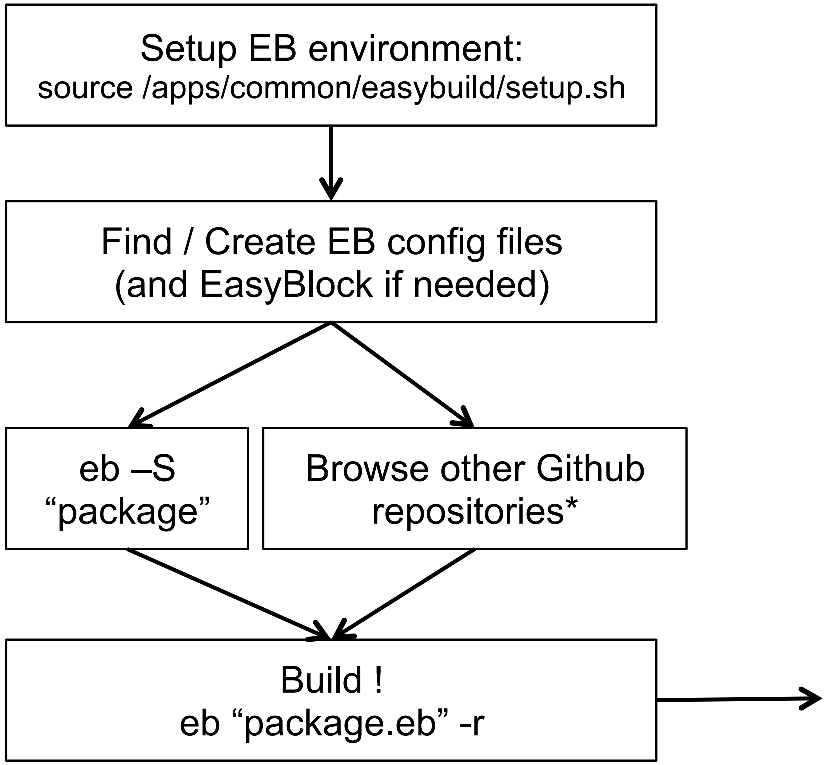
eb –S
“package”

Browse other Github
repositories

Build !
eb “package.eb” -r

Can be used for the hands on!

Proposed EasyBuild workflow for production builds (SCS):



Setup EB environment:
source /apps/common/easybuild/setup.sh

Find / Create EB config files
(and EasyBlock if needed)

eb –S
“package”

Browse other Github
repositories*

Build !
eb “package.eb” -r

What will happen:

- Build (+dependencies)
- Install
- Create module files
- If successful
  - Commit easyconfig file to CSCS Git repository!
    - Thanks to
      - Jens T. for Git support
      - Pablo E. for helping w/ setup

*Links on the last slide

Python use case

- Suported modules for Python 2 and 3
  - Setuptools 17.1.1, Pip 7.0.3, Nose 1.3.7, Numpy 1.9.2, Scipy 0.15.1, mpi4py 1.3.1, Cython 0.22, Six 1.9.0, Virtualenv 13.0.3, pandas 0.16.2, h5py 2.5.0 (serial/parallel), Matplotlib 1.4.3, pyCuda 2015.1, netcdf4 1.1.8

- Example Easyconfig files (for Python 2.7.10 on Cray)
  - Python-2.7.10-CrayGNU-5.2.40.eb
  - matplotlib-1.4.3-CrayGNU-5.2.40-Python-2.7.10.eb
  - netcdf4-python-1.1.8-CrayGNU-5.2.40-Python-2.7.10.eb
  - h5py-2.5.0-CrayGNU-5.2.40-Python-2.7.10-parallel.eb
  - h5py-2.5.0-CrayGNU-5.2.40-Python-2.7.10-serial.eb
  - pycuda-2015.1-CrayGNU-5.2.40-Python-2.7.10.eb
- Easyblocks
  - h5py.py, netcdf_python.py, pycuda.py

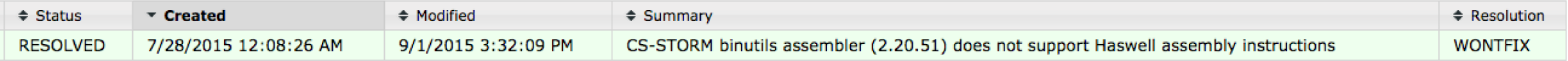
Now available on:
- Daint, Dora, Santis, Brisi (CrayGNU)
- Pilatus, Castor (foss)
- **Escha, Kesch (Python2/gmvolf) *new***

MCH CS-Storm use case (gmvolf/2015a)

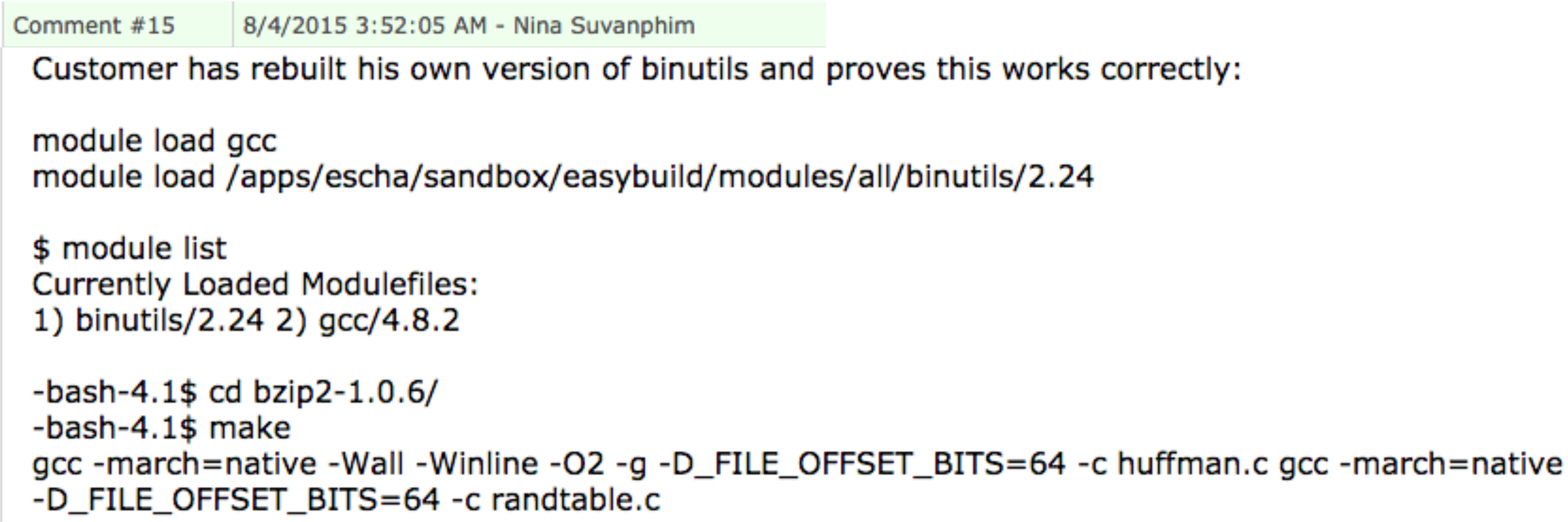
- **Autoconf/2.69**
- **Automake/1.15**
- **Autotools/20150215**
- binutils/2.25
- Bison/3.0.3
- Boost/1.49.0
- bzip2/1.0.6
- CDO/1.6.9
- CMake/3.2.2
- **Cube/4.3.2**
- cURL/7.40.0
- **ddt/5.0(default)**
- Doxygen/1.8.9.1
- FFTW/3.3.4
- flex/2.5.39
- freetype/2.5.5
- **GCC/4.8.2**
- gettext/0.18.2
- GLib/2.34.3
- gmvapich2/2015a
- gmvolf/2015a
- GSL/1.16
- HDF/4.2.8
- HDF5/1.8.15
- JasPer/1.900.1
- Java/1.7.0_80
- libffi/3.0.13
- libjpeg-turbo/1.4.0
- libpng/1.6.16
- libreadline/6.3
- libtool/2.4.6
- libxml2/2.9.1
- M4/1.4.17
- matplotlib/1.4.3
- **MVAPICH2/2.0.1_gnu48**
- NASM/2.11.06
- NCO/4.5.1
- ncurses/5.9
- ncview/2.1.5
- netCDF/4.3.3.1
- netCDF-Fortran/4.4.2
- netcdf-python/1.1.8
- OPARI2/1.1.4
- OpenBLAS/0.2.13
- OTF2/1.5.1
- Python/2.7.10
- R/3.1.3
- Ruby/2.2.2
- ScaLAPACK/2.0.2
- **Scalasca/2.2.2**
- **Score-P/1.4.2**
- SQLite/3.8.8.1
- Szip/2.1
- Tcl/8.6.3
- UDUNITS/2.1.24
- zlib/1.2.8

- **Blue**
  - **By JGP**
- **Green**
  - **By OPS/Cray**
- **Grey:**
  - **Grey zone**

MCH CS-Storm use case - fixing Cray's broken PrgEnv: gcc/4.8.2 lacks Haswell support (-march=native)



◆ Status	▾ Created	◆ Modified	◆ Summary	◆ Resolution
RESOLVED	7/28/2015 12:08:26 AM	9/1/2015 3:32:09 PM	CS-STORM binutils assembler (2.20.51) does not support Haswell assembly instructions	WONTFIX



Comment #15 8/4/2015 3:52:05 AM - Nina Suvanphim

Customer has rebuilt his own version of binutils and proves this works correctly:

```
module load gcc
module load /apps/escha/sandbox/easybuild/modules/all/binutils/2.24

$ module list
Currently Loaded Modulefiles:
1) binutils/2.24 2) gcc/4.8.2

-bash-4.1$ cd bzip2-1.0.6/
-bash-4.1$ make
gcc -march=native -Wall -Winline -O2 -g -D_FILE_OFFSET_BITS=64 -c huffman.c gcc -march=native
-D_FILE_OFFSET_BITS=64 -c randtable.c
```

Proposed "temporary" workaround: use assembler from cce!

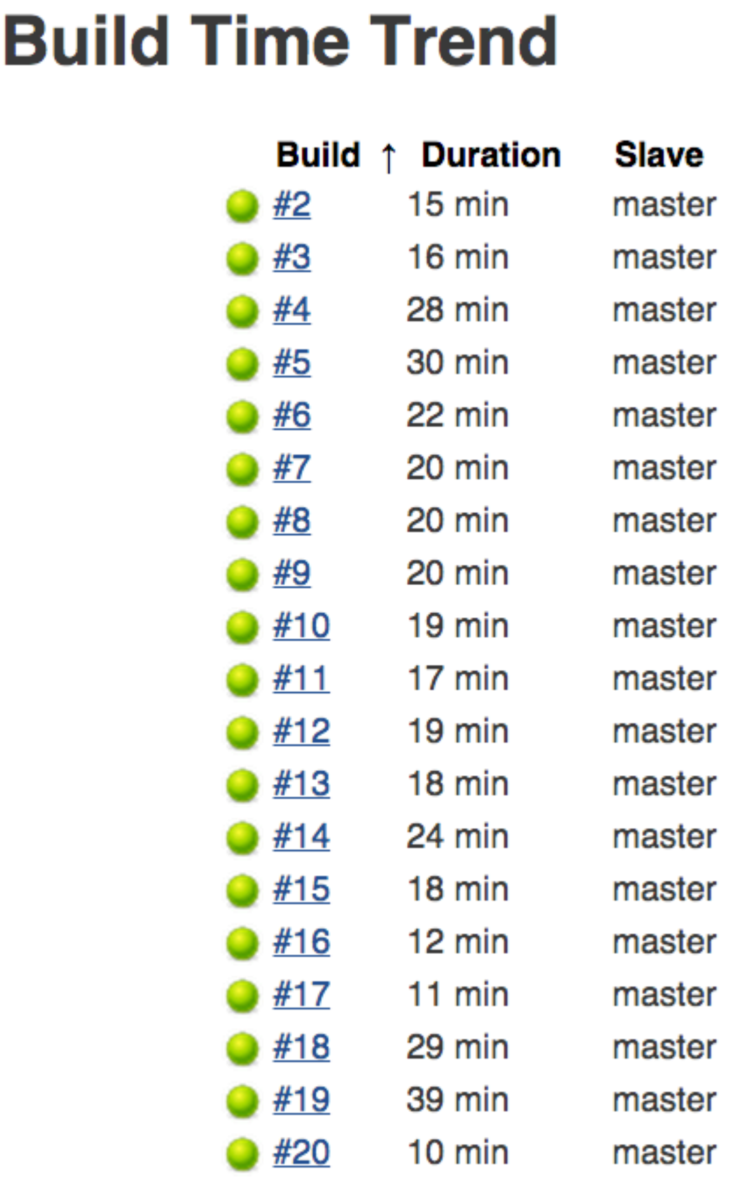
- export PATH=/opt/cray/cce/8.3.10/cray-binutils/x86_64-unknown-linux-gnu/bin:$PATH (before 'module load gcc')

Jenkins

- Jenkins is a tool designed for continuous integration/validation
- But it is much more powerful than that
  - Thousands of plugins are available
  - Can be easily configured to run tasks by ssh anywhere
  - You get logs for all of your executions for free
  - Info about running / past jobs and logs are always accessible through the web interface
- Some usage examples:
  - Development/Integration:
    - Checkout svn/git repositories to automatically build on different platforms
  - Validation
    - Periodically run unit tests
  - Monitoring
    - Periodically run sanity and performance tests (***regression***)
  - Run your favorite script or app
    - Use your creativity (example at CSCS: driving the acceptance of MCH machine)

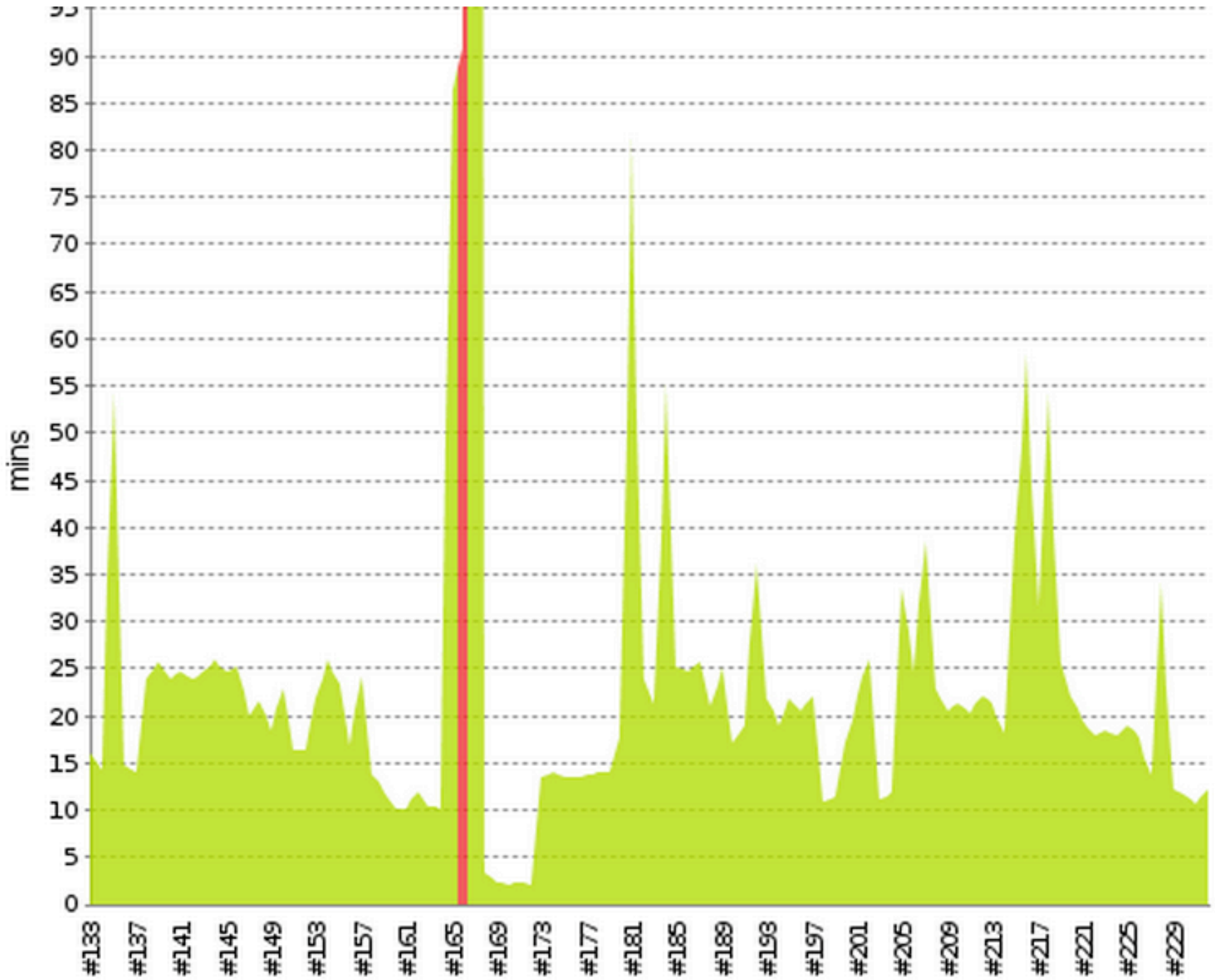
Jenkins example: Monitoring scratch performance for apps (netcdf5)

By lucamar™



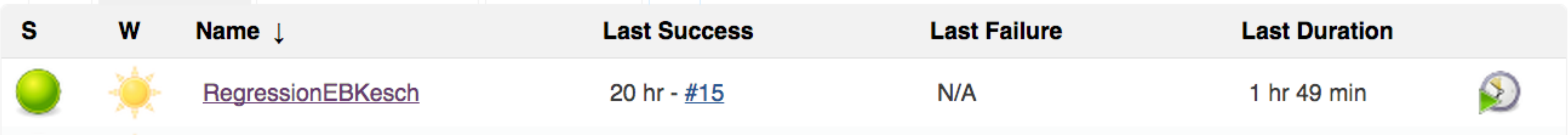
Build Time Trend

	Build ↑	Duration	Slave
●	#2	15 min	master
●	#3	16 min	master
●	#4	28 min	master
●	#5	30 min	master
●	#6	22 min	master
●	#7	20 min	master
●	#8	20 min	master
●	#9	20 min	master
●	#10	19 min	master
●	#11	17 min	master
●	#12	19 min	master
●	#13	18 min	master
●	#14	24 min	master
●	#15	18 min	master
●	#16	12 min	master
●	#17	11 min	master
●	#18	29 min	master
●	#19	39 min	master
●	#20	10 min	master

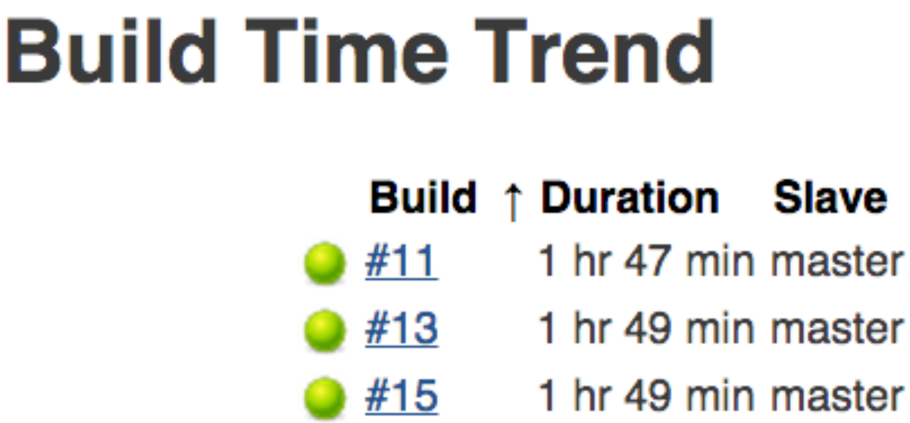


zürich

Jenkins example: Rebuilding all software stack for Escha/Kesch

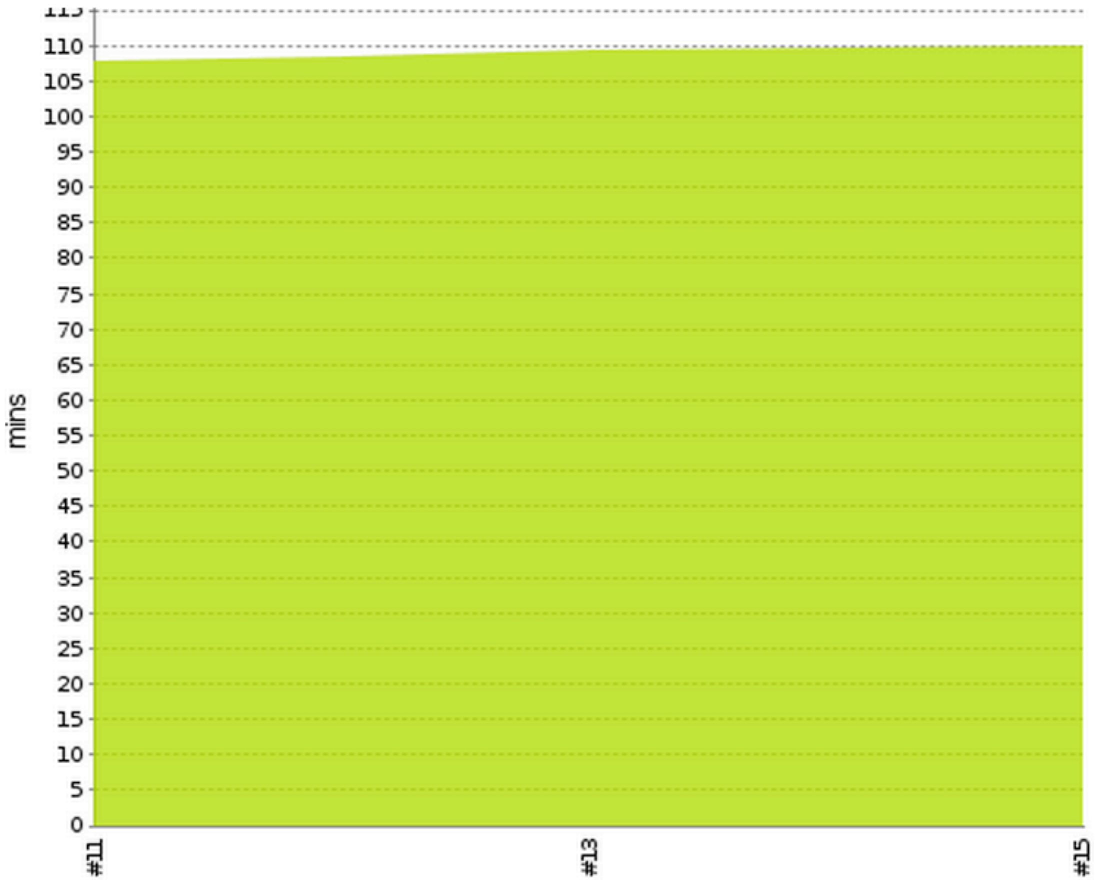


S	W	Name ↓	Last Success	Last Failure	Last Duration	
●	☀	RegressionEBKesch	20 hr - #15	N/A	1 hr 49 min	



Build Time Trend

	Build ↑	Duration	Slave
●	#11	1 hr 47 min	master
●	#13	1 hr 49 min	master
●	#15	1 hr 49 min	master

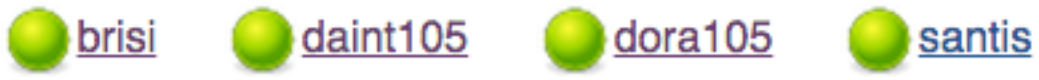


Jenkins + EB integration: workflow example for testing .eb files

- Testing new easyconfig files on all machines where the toolchain is available
- Workflow setup
  1. Create a folder accessible by jenscscs to store the .eb files
     - /path/to/eb-files/
  2. Create a jenkins project adding the target test systems
     - CrayGNU/5.2.40 = daint, dora, santis, brisi
     - foss/2015a = castor, pilatus
  3. Add the following commands to the “Execute shell”
     - source /apps/common/easybuild/setup.sh
     - find /path/to/eb-files/ -name '*CrayGNU-5.2.40*.eb' -exec eb {} "-r -f" \;
       - (foss/2015a: replace “*CrayGNU-5.2.40*” by “*foss-2015a*”)
- Usage
  1. Copy .eb files to /path/to/eb-files/
  2. Go to Jenkins and click on “Build now”

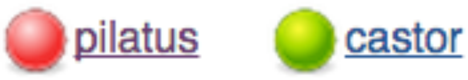
Jenkins: Example for testing .eb files

- /apps/common/tools/easybuild/jenkins/
- CrayGNU/5.2.40
  - CDO-1.6.9-CrayGNU-5.2.40.eb
  - NFFT-3.3.0-CrayGNU-5.2.40.eb



🟢 brisi 🟢 daint105 🟢 dora105 🟢 santis

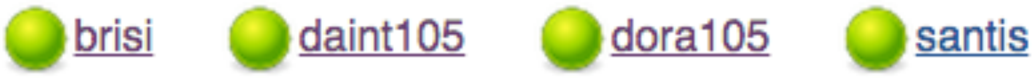
- foss/2015a
  - Ghostscript-9.10-foss-2015a.eb
  - HDF5-1.8.15-foss-2015a.eb



🔴 pilatus 🟢 castor

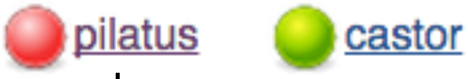
Jenkins: Example for testing .eb files

- /apps/common/tools/easybuild/jenkins/
- CrayGNU/5.2.40
  - CDO-1.6.9-CrayGNU-5.2.40.eb
  - NFFT-3.3.0-CrayGNU-5.2.40.eb



🟢 brisi 🟢 daint105 🟢 dora105 🟢 santis

- foss/2015a
  - Ghostscript-9.10-foss-2015a.eb
  - HDF5-1.8.15-foss-2015a.eb



🔴 pilatus 🟢 castor

↓

Red ball = ~~tomato~~ FAIL

Example projects available at https://jenkins.cscs.ch
- EasyBuildTest-foss
- EasyBuildTest-CrayGNU

Final thoughts

- Current EB installation is ready for application level
  - Validation with
    - Python use case: Daint, Dora, Santis, Brisi, Pilatus, Castor **and Escha/Kesch (new)**
    - **Escha/Kesch:** complete software stack built with gmvolf toolchain

- Continuous validation techniques can be easily applied
  - Testing builds across all systems with Jenkins
  - Changes/errors on the PrgEnv can be detected early

- In order to get the most out of EasyBuild
  - We need to have consistent PrgEnv on most systems
    - OK on Cray systems
    - Not currently true on non-Cray
      - Achievable with EasyBuild

Next steps (SCS)

- Try out EB for answering tickets requesting new software
  - Testing and feedback are very welcome
  - Can also be used to answer individual user requests
    - Builds that won’t be officially supported
    - Such as the famous RT ticket “#19610: nano editor for dora”

- Agree on toolchains for non-Cray systems
  - Stock toolchain (foss + intel for example)
    - Default “foss” toolchain works just fine for Python use case
    - Settings may be not optimal on all archs (for example concerning MPI, Slurm, …)
  - Tailored toolchain using existing PrgEnv (supported by HPC Operations team)
    - This approach was used on the new Storm MCH (gmvolf)
    - We might end up with a different toolchain on each system

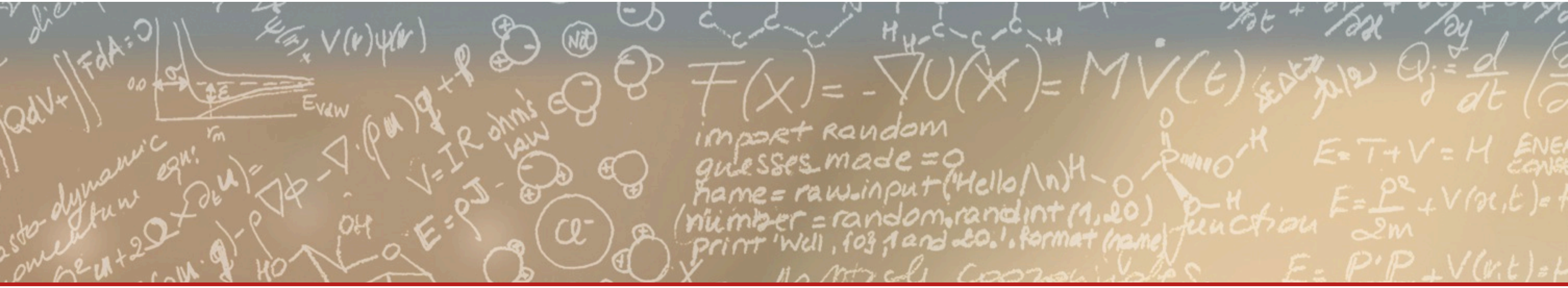
- Start contributing back
  - Open GitHub Pull Requests for new easyconfig files created by CSCS
  - Help to develop and test the stable Cray support

Links

- Easybuild Documentation
  - GitHub
    - https://github.com/hpcugent/easybuild
  - Workflow example (WRF)
    - http://easybuild.readthedocs.org/en/latest/Typical_workflow_example_with_WRF.html

- CSCS Internal doc
  - https://github.com/eth-cscs/tools/wiki/EasyBuild-at-CSCS

- Additional easyconfig files repositories
  - Development EasyBuild branch
    - https://github.com/hpcugent/easybuild-easyconfigs/tree/develop
  - Successful production builds at CSCS
    - https://github.com/eth-cscs/tools/tree/master/easybuild/ebfiles_repo



Thank you for your attention.