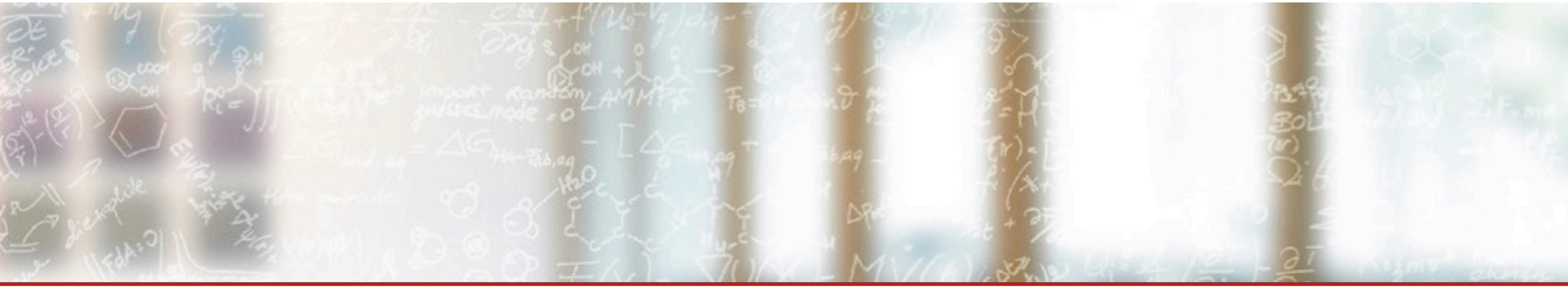
CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich



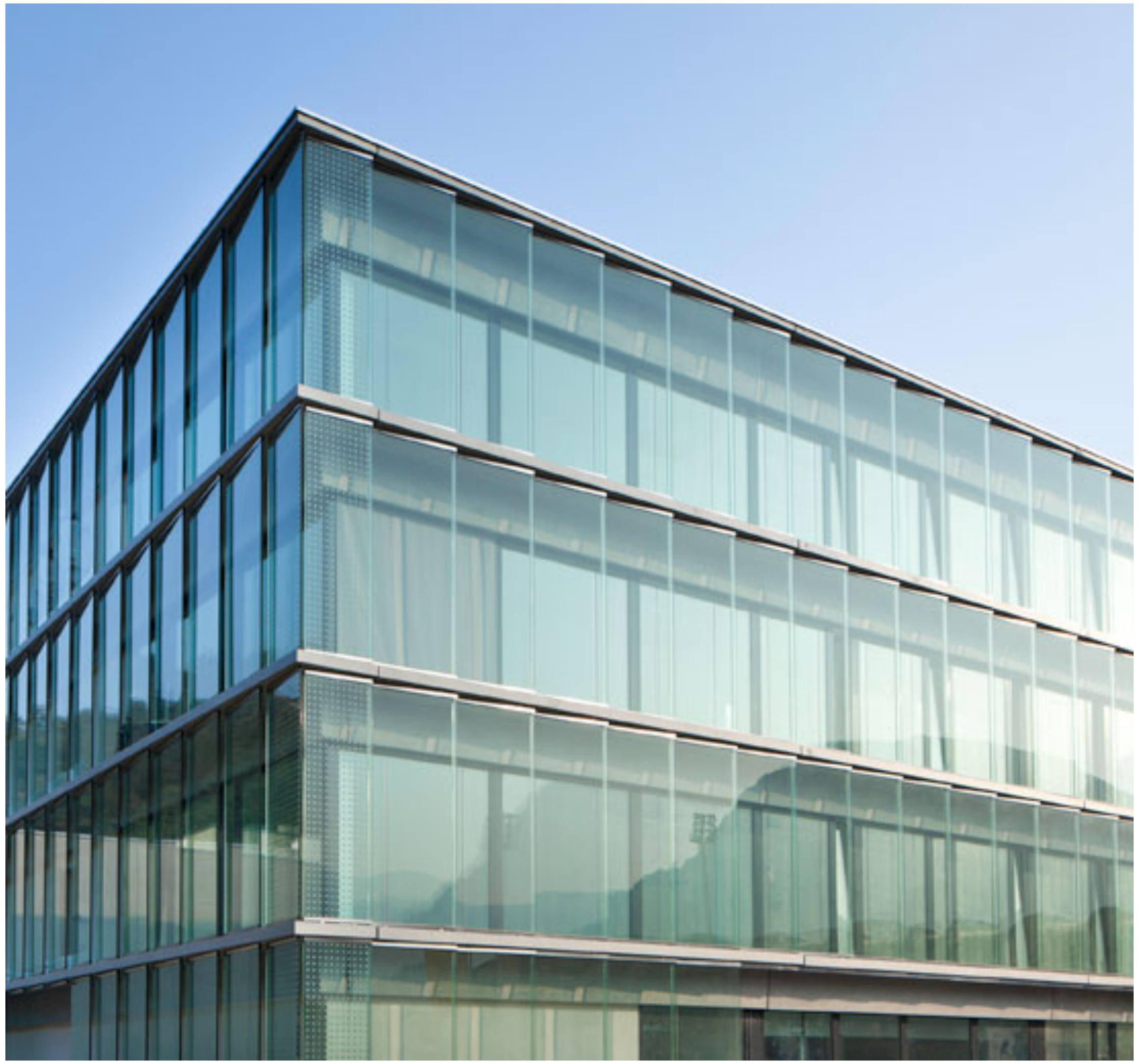
Site presentation: EasyBuild @ CSCS

1st EasyBuild User Meeting – Ghent, Belgium

Guilherme Peretti-Pezzi – Head of Scientific Computing Support (CSCS)

January 29th, 2016

Outline

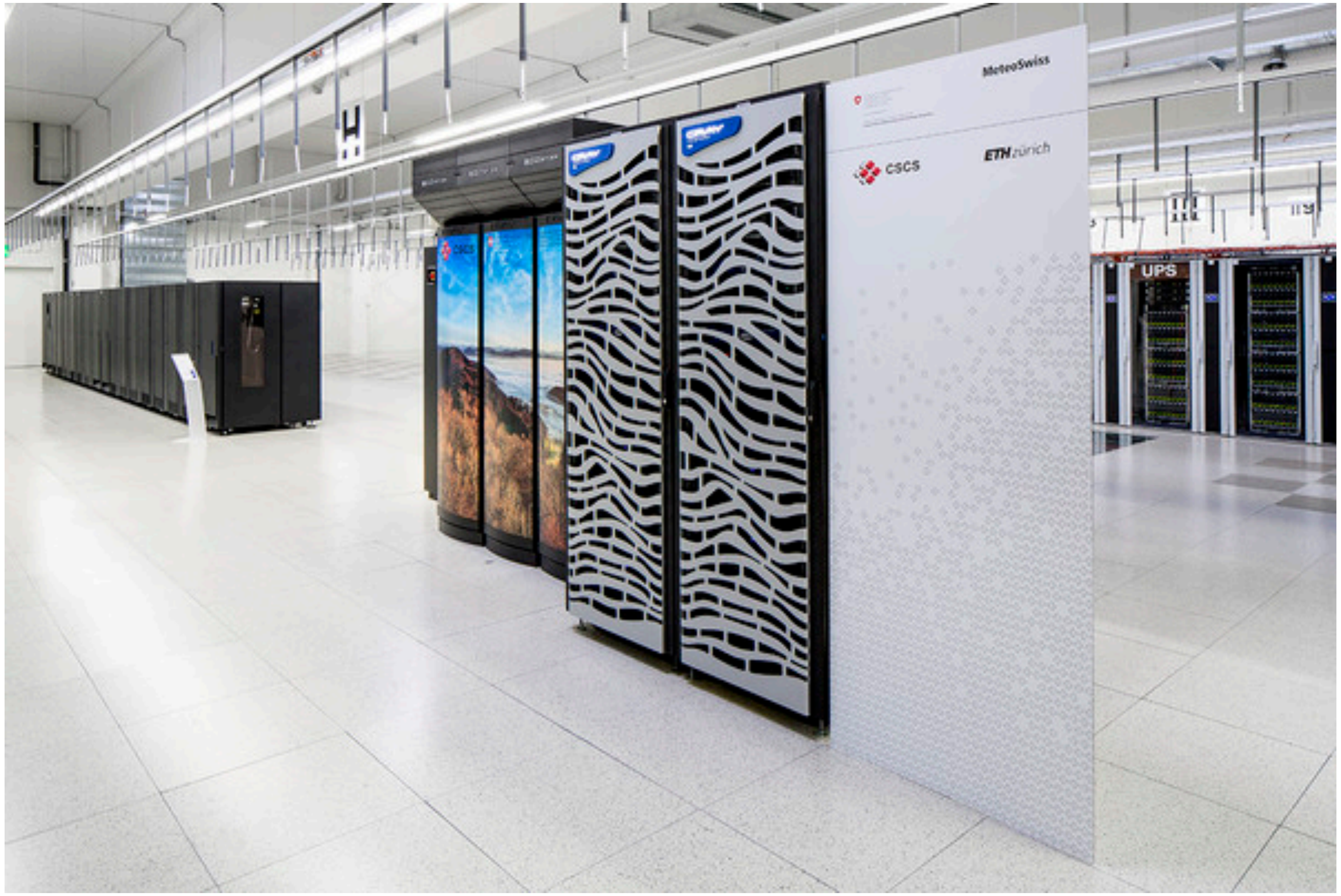


- Overview of systems @ CSCS
- Motivation to adopt EB
- EasyBuild setup / workflow @ CSCS
- Use cases
  - Python
  - Cray CS-Storm (MeteoSwiss)
- Uniform software stack at our systems
  - Using Jenkins to deploy and validate builds
- Final thoughts

Piz Daint (XC30) & Piz Dora (XC40)

#7 & #92 on Top500

Piz Escha & Piz Kesch (CS-Storm)



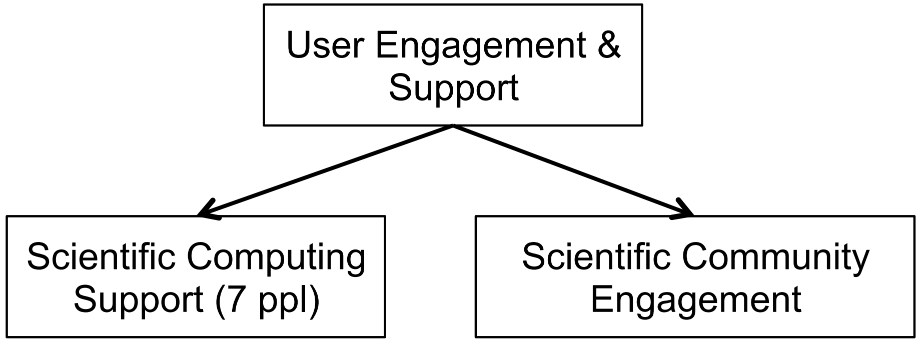
#353 on Top500

- 2 cabinets
  - 12 nodes
    - 8 x K80

Overview of systems (with EB) at CSCS

System	Type	# of nodes	# gpus/node	Cray?
Piz Daint	Production	5272	1	Y
Piz Dora	Production	1256	0	Y
Castor	Production	32	1	N
Pilatus	Production	38	0	N
Monch	Production	376	0	N
Escha	Production	12	16	Y (no PrgEnv)
Kesch	Production	12	16	Y (no PrgEnv)
Leone	Production	11	1 / 0	N
Santis	TDS	16	1	Y
Brisi	TDS	16	0	Y
Greina	R&D	---	---	N

Main groups doing HPC support @ CSCS


User Engagement & Support
Scientific Computing Support (7 ppl)
Scientific Community Engagement

Responsible for application support
- Now mostly using EB

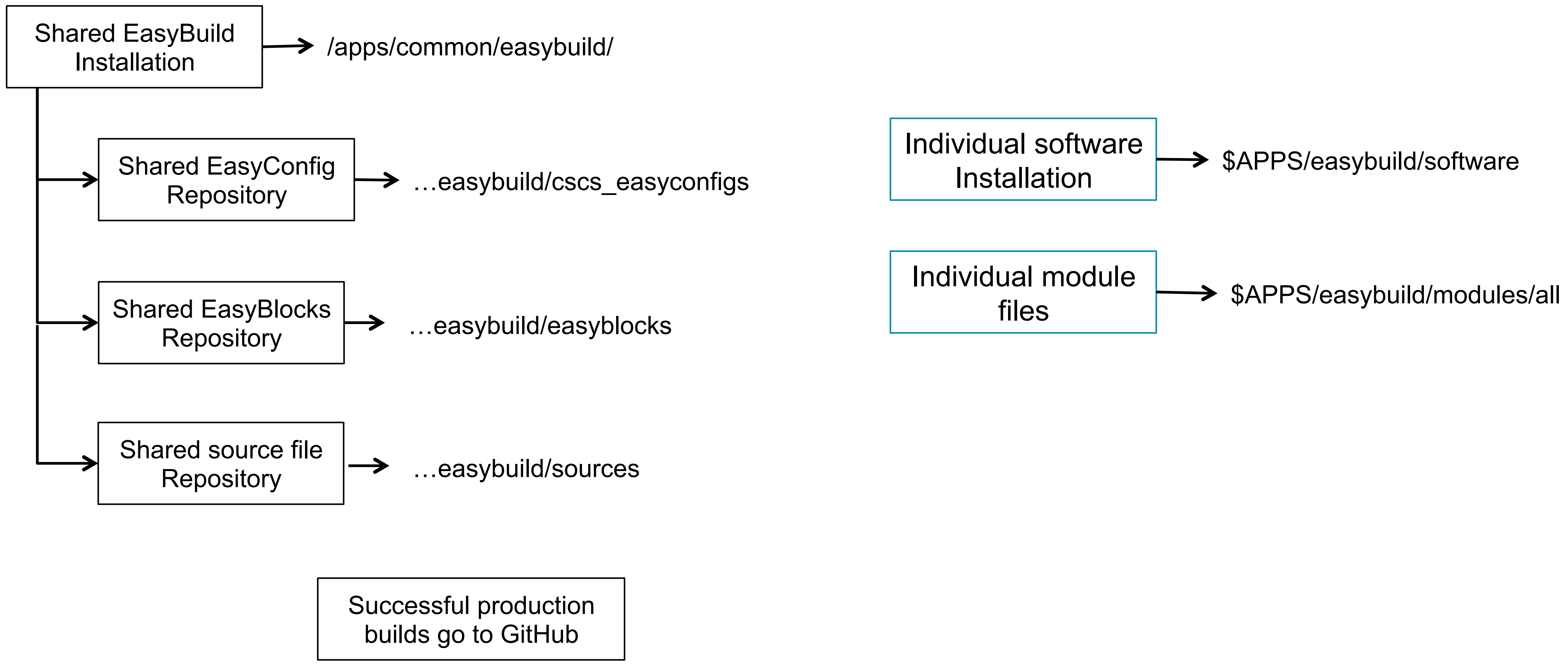
HPC Operations

Responsible for building Programming environment
- Gcc, intel, PGI, MPI
- Manual builds

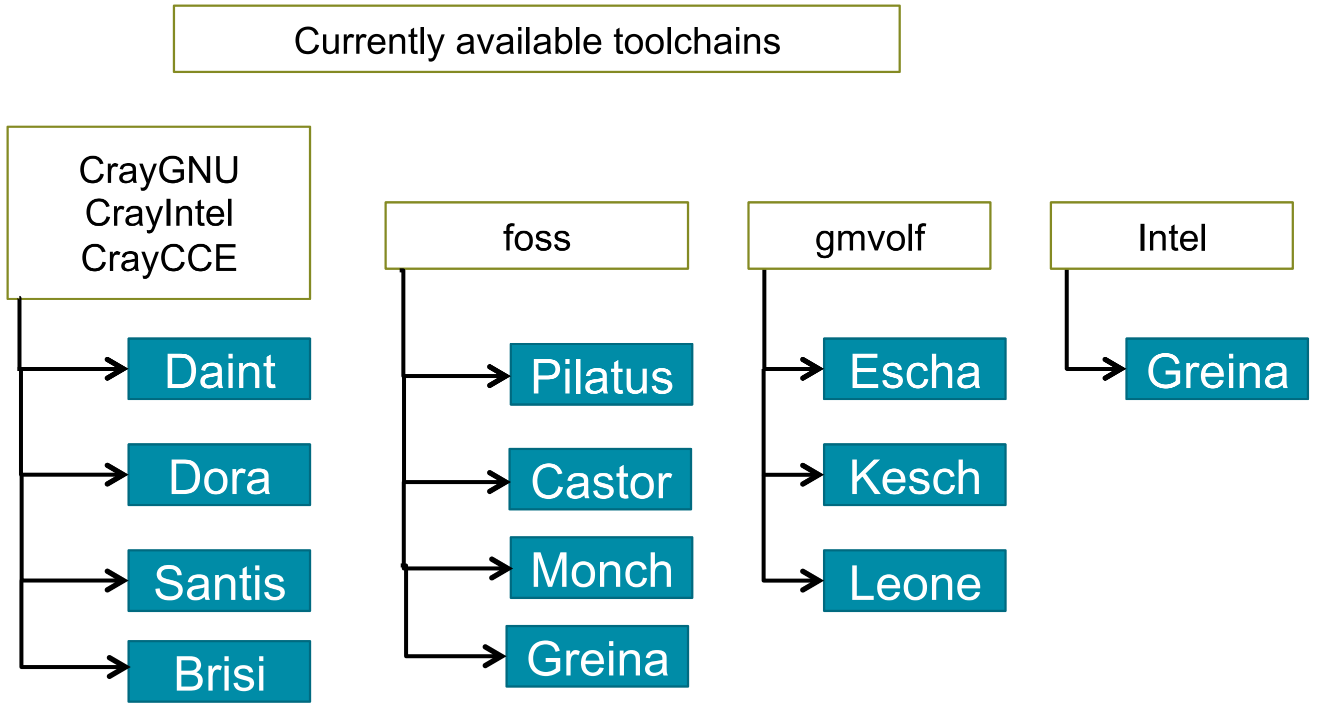
Motivation to adopt EasyBuild @ CSCS

- Lack of standard way to describe build recipes
  - Shell scripts, readme files, web/wiki pages, *invisible* docs
- Software available is very heterogeneous across systems
  - Moving users to a different machine requires a lot of work
- Systems upgrades are a huge overhead
  - Lots of manual work to re-deploy existing software
- Little collaboration with other sites doing the very same thing

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
Successful production builds go to GitHub
Individual software Installation
$APPS/easybuild/software
Individual module files
$APPS/easybuild/modules/all

EasyBuild setup @ CSCS



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

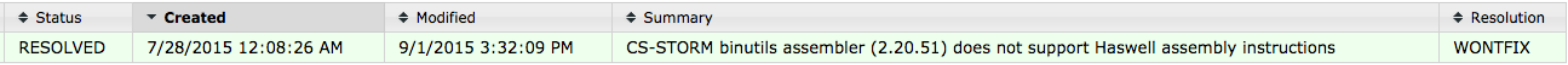
Now available on:
- Daint, Dora, Santis, Brisi (CrayGNU)
- Pilatus, Castor, Leone (foss)
- Escha, Kesch, Mönch (gmvolf)

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

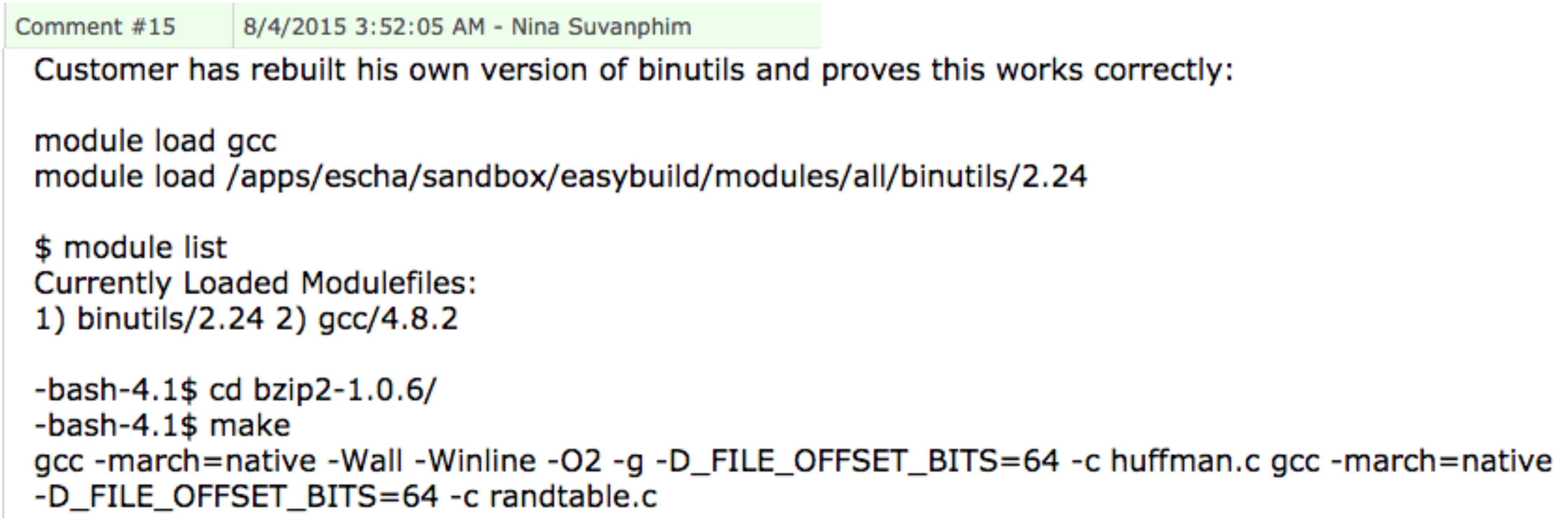
- Autoconf/2.69
- Automake/1.15
- Autotools/2015021**5**
- binutils/2.25
- Bison/3.0.3
- Boost/1.49.0
- bzip2/1.0.6
- CDO/1.6.9
- CMake/3.2.2
- Cube/4.3.2
- cURL/7.40.0
- ddt/5.0(default)
- Doxygen/1.8.9.1
- FFTW/3.3.4
- flex/2.5.39
- freetype/2.5.5
- **GCC/4.8.2**
- gettext/0.18.2
- GLib/2.34.3
- gmvapich2/2015a
- 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

- **Red**
  - **By OPS/Cray**

MCH CS-Storm use case - fixing Cray's unsupported 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!

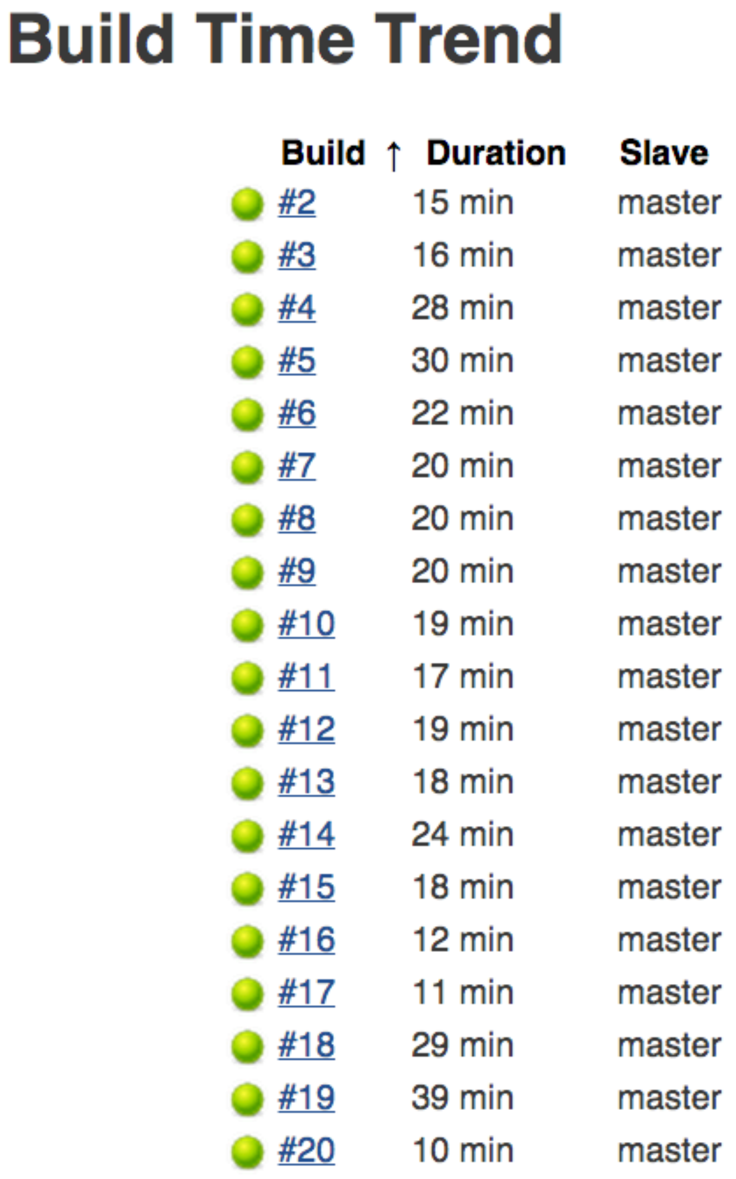
- export PATH=/opt/cray/cce/8.3.10/cray-binutils/x86_64-unknown-linux-gnu/bin:$PATH (before 'module load gcc')

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)

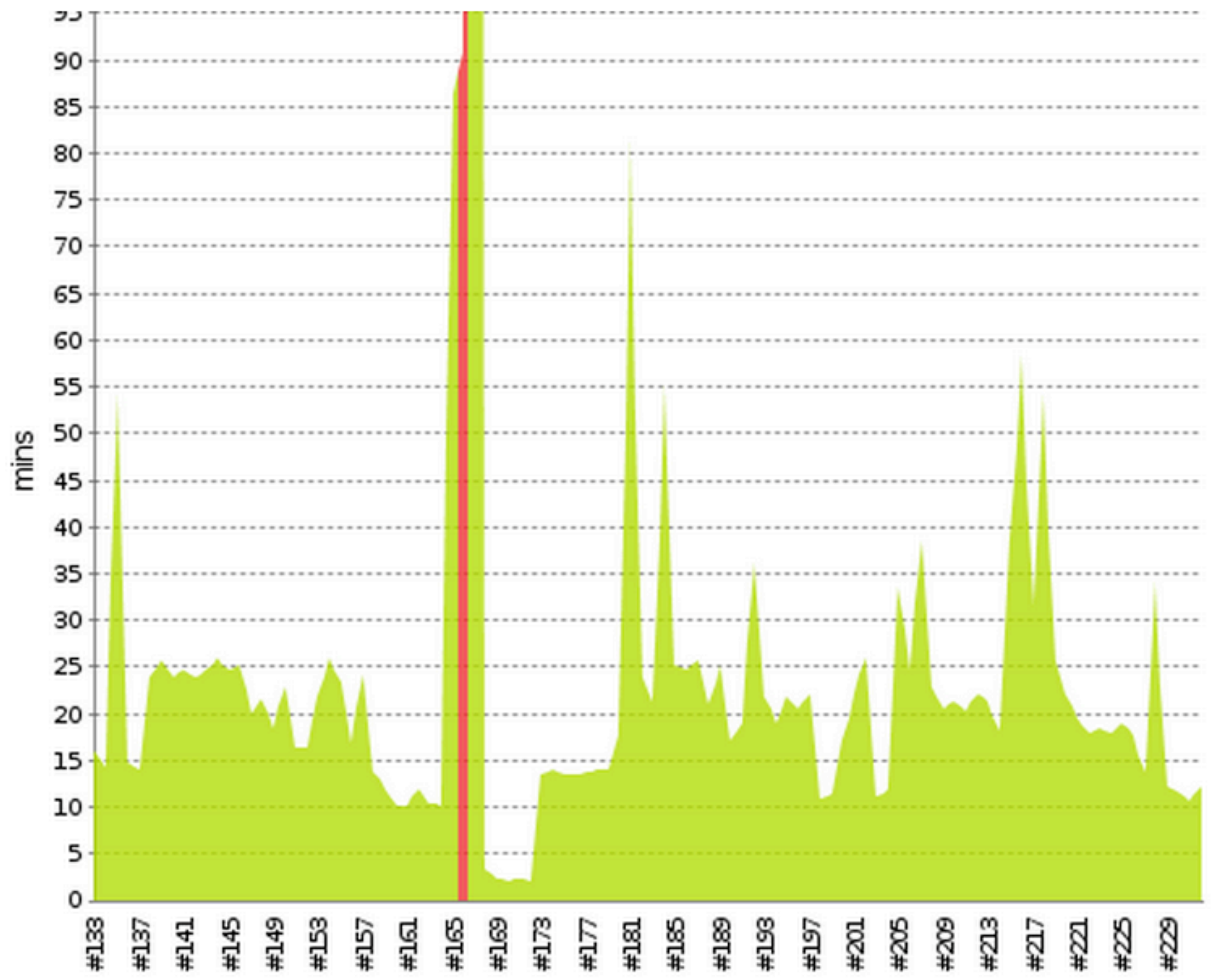
Jenkins example: Monitoring scratch performance for apps (netcdf5)

By lucamar™

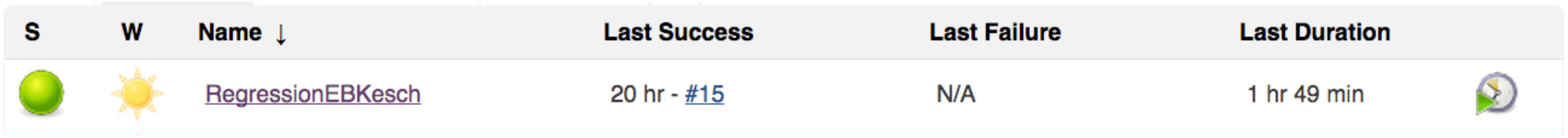


Build Time Trend

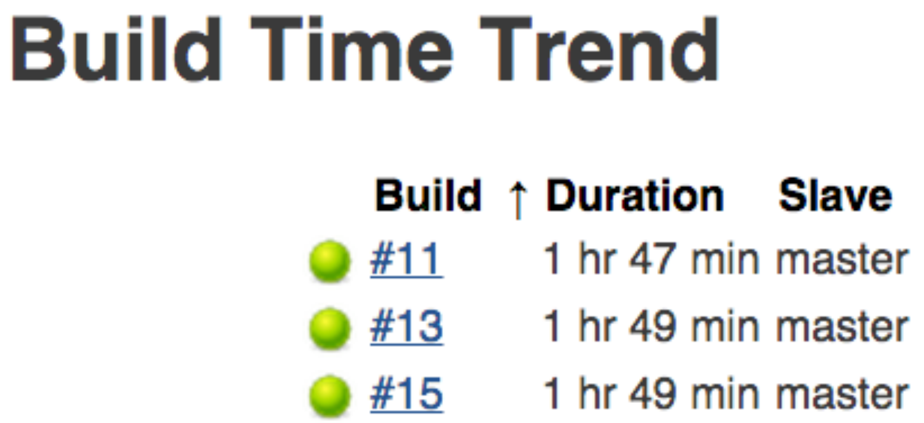
	Build ↑	Duration	Slave
●	#2	15 min	master
●	#3	16 min	master
●	#4	28 min	master
●	#5	30 min	master
●	#6	22 min	master
●	#7	20 min	master
●	#8	20 min	master
●	#9	20 min	master
●	#10	19 min	master
●	#11	17 min	master
●	#12	19 min	master
●	#13	18 min	master
●	#14	24 min	master
●	#15	18 min	master
●	#16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



Jenkins example: Rebuilding all software stack for Escha/Kesch

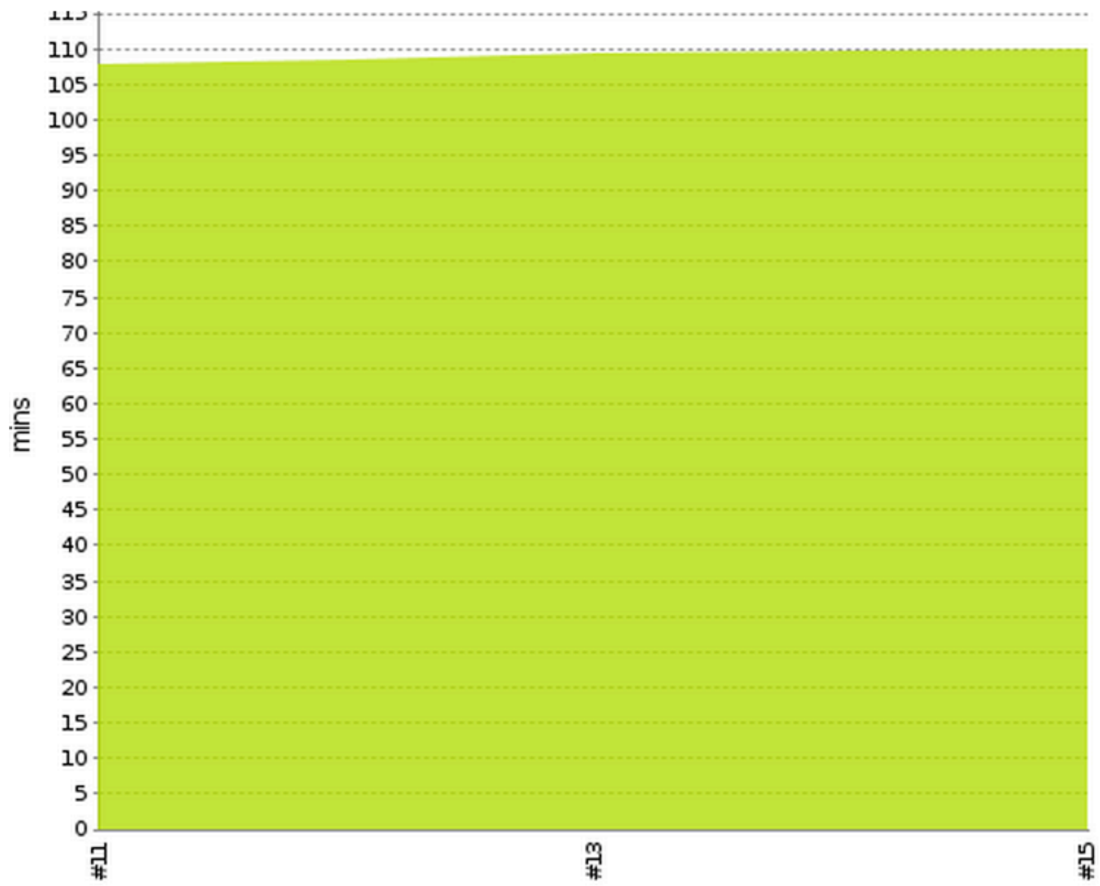


S	W	Name ↓	Last Success	Last Failure	Last Duration	
●	☀	RegressionEBKesch	20 hr - #15	N/A	1 hr 49 min	



Build Time Trend

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

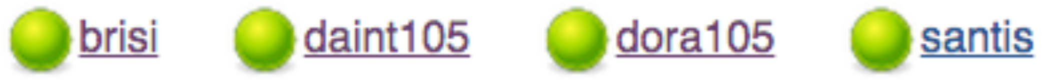


Jenkins + EB integration: workflow example for testing .eb files

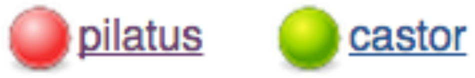
- Testing new easyconfig files on all machines where the toolchain is available
- Workflow setup
  1. Create a folder accessible by jenscscs to store the .eb files
     - /path/to/eb-files/
  2. Create a jenkins project adding the target test systems
     - CrayGNU = daint, dora, santis, brisi
     - foss/2015b = 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



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



Final thoughts

- Current EB installation is ready for application level
  - Validation with
    - Python use case: Daint, Dora, Santis, Brisi, Pilatus, Castor and Escha/Kesch
    - Escha/Kesch**:** complete software stack built with gmvolf toolchain
- Continuous validation techniques can be easily applied
  - Testing builds across all systems with Jenkins
    - weekly builds for every machine
  - Changes/errors on the PrgEnv can be detected early
- In order to get the most out of EasyBuild
  - We need to have consistent PrgEnv across
    - OK on Cray systems
    - Not currently true on non-Cray
      - Achievable with EasyBuild

Wish list

- Stable Cray support
  - Almost there: https://github.com/hpcugent/easybuild-framework/issues/1390
- +1 for Rpath support
- Backup of custom easyblocks for reproducibility
- Compatible build description with similar projects (Spack)
- Add more flexibility to toolchain definition
  - Possibility of creating custom (or modifying existing) without touching the framework
  - Possibility of (easily) using existing compilers
- Lower the bar for new users
  - To understand one build, user needs to look into easyconfig + easyblock + framework
  - Extended-dry-run is currently the best approach

Links

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

- Additional easyconfig files repositories
  - Successful production builds at CSCS
    - https://github.com/eth-cscs/tools/tree/master/easybuild/ebfiles_repo
  - Shared custom easyconfig files
    - https://github.com/eth-cscs/tools/tree/master/easybuild/easyconfigs
  - Shared custom easyblocks
    - https://github.com/eth-cscs/tools/tree/master/easybuild/easyblocks

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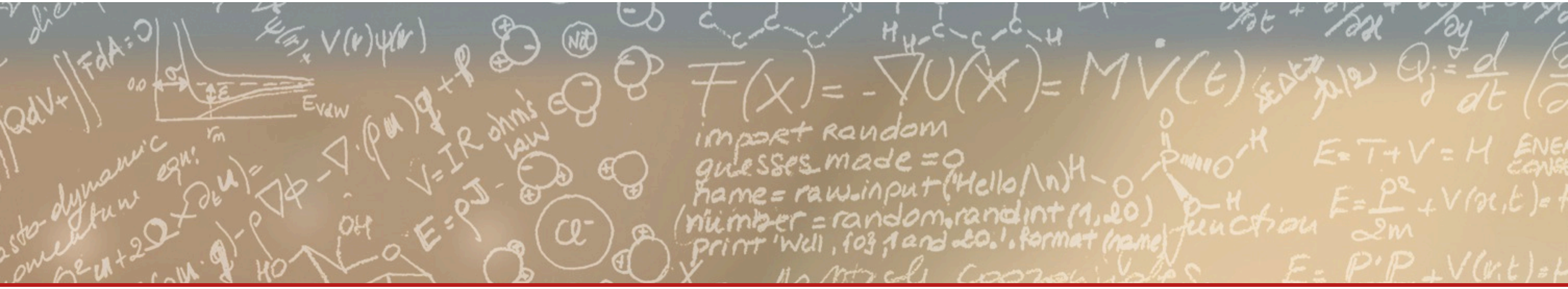

Thank you for your attention.