EasyBuild site presentations

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`http://users.ugent.be/~kehoste/EasyBuild-site-pres_20150209.pdf`

EasyBuild hackathon @ University of Basel
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HPC-UGent: general info

`http://ugent.be/hpc`

- HPC team at central IT dept. of Ghent University (Belgium)
- 9 team members: 1 manager, ∼3 user support, ∼5 sysadmin
- ∼1,500 user accounts, across all scientific domains
- tasks: hardware, system administration, user support/training, . . .

- member of Flemish Supercomputer Centre (VSC)
    - virtual centre, collaboration between Flemish university associations

HPC-UGent: systems

one Tier1 cluster ('muk')

- 528 nodes (8, 448 cores), Intel Sandybridge, FDR Infiniband, SL 6.6

6(+2) Tier2 clusters

- 3 batch clusters: Ethernet, SL 6.6
    - *gastly*: 42 nodes (336 cores), Intel Nehalem
    - *haunter*: 150 nodes (1, 200 cores), Intel Nehalem
    - *raichu*: 64 nodes (1, 024 cores), Intel SandyBridge

- 2 MPI clusters: Infiniband, SL 6.6
    - *gulpin*: 32 nodes (1, 024 cores), AMD Magny Cours, 2x QDR IB
    - *delcatty*: 160 nodes (2, 560 cores), Intel SandyBridge, FDR IB

- 1 ScaleMP vSMP system, (2x QDR Infiniband), SL 6.6
    - *dugtrio*: 16 nodes ($3 \times 48 + 2 \times 24$ cores), Intel Westmere

- 2 pre-production systems, Infiniband, *CentOS 7*
    - *golett*: 200 nodes (4, 800 cores), Intel Haswell, QDR IB
    - *phanpy*: 16 nodes, Intel Haswell, dual FDR IB, 512GB RAM + SSDs

HPC-UGent: EasyBuild configuration

- one dedicated install user, shared between multiple people :(
- flat module tree, default EasyBuild module naming scheme
- Tcl/C environment modules v3.2.10 as modules tool
  - pilot setup with Lmod v5.8.6 since last week
- Tier2: one shared filesystem for software + modules, NFS mounted
  - subdirectory per cluster, e.g., `/apps/gent/SL6/sandybridge`
  - software + modules for Tier1 system on 'local' GPFS filesystem
- installations are done by submitting jobs on the cluster
  - `module swap cluster/foo; eb ...  --job --robot`
- only install easyconfigs that have been merged into `develop` branch
- installed software is retained throughout lifetime of the system

'Common User Experience' VSC project

- collaboration between HPC sites @ Flemish universities
  - Ghent, Leuven, Antwerp, Brussels, Hasselt

- intention is to allow users to easily switch to a different VSC site

- important aspect: same module naming scheme
  - currently: default EasyBuild module naming scheme

- common toolchains: `intel/2015a`, `foss/2015a`
  - updated every 6 months (Dec/Jan, June/July)
  - different alternative compositions get evaluated/tested
  - other members of EasyBuild community also starting to pick these up

- minimal common divisor: toolchains, Python, Perl (bare), R (bare)

- sharing of easyconfig files, (enhancements to) easyblocks
  - via pull requests to main repository @ GitHub

- (my) intention is to also get Lmod included 'soon'

JSC: general info

- Jülich Supercomputer Centre (JSC) has $\sim$200 staff members
- hardware and system administration
  - division : High Performance Computing Systems with 16 staff
- user support and training
  - division : Application Support with 39 staff

- member of Gauss Centre for Supercomputing (GCS)
  virtual centre, combines the three national supercomputing centres
  in Germany

JSC: systems

Two Tier0 systems

- JUQUEEN - BG/Q
  - 28 racks (7 rows × 4 racks) - 28,672 nodes (458,752 cores)
  - main memory: 448 TB
  - overall peak performance: 5.9 PFLOPS (Linpack: 5.0 PFLOPS)
  - I/O Nodes: 248 (27x8 + 1x32) connected to 2 CISCO switches
- JURECA - cluster architecture (replaces JUROPA)
  - projected peak performance of about 1.8 PFLOPS
  - Intel Xeon E5-2680 v3 Haswell, 24 cores per node
  - latest InfiniBand with full fat tree

Number of additional research systems

- QPACE - hot cooling, Cell processors
- JUDGE - GPU cluster
- DEEP - cluster + booster

JSC: EasyBuild configuration

- shared installation group `software` with ~25 members
  - use GID permissions to control
- hierarchical module tree, default EasyBuild module naming scheme (currently)
- Lmod as modules tool
- one shared filesystem for software + modules
  - subdirectory per cluster
- installations are done by submitting jobs on the cluster
- software is provided in `stages`
  - new module hierarchy or features are built in new stage
  - dedicated user for rebuilds
  - deprecated toolchains and software versions are retired
  - soft links $\implies$ instant transition
  - previous stages can be loaded (installed software is retained)

Vienna Biocenter: general info

- Vienna Biocenter is a molecular biology cluster
- consists of 4 research institutes and $\sim$30 biotech companies
- research institutes: IMP, IMBA, MFPL, and GMI
- $\sim$450 scientists at IMP and IMBA, $\sim$100 at GMI, $\sim$700 at MFPL
- 1 person reponsible for HPC infrastructure at GMI
- 2 persons responsible for HPC infrastructure at IMP/IMBA
- no collaboration on HPC level

Vienna Biocenter: systems

Not realy high performance computing shops.

Almost all of workload is data analysis with R, Python, Perl, Java, etc.

GMI
- 1,600 cores Intel Sandy Bridge, IB FDR Torus, SLES11, Lustre
- 128 cores Intel Sandy Bridge, NUMALink6, SLES11, Lustre

IMP/IMBA
- 600 cores Intel SandyBridge, 1GbE and 10GbE, Debian7, 2PB Isilon

Vienna Biocenter: EasyBuild configuration

GMI

- set up the infrastructure there in 2011
- EasyBuild deployed since 1.0 in 2012
- default EasyBuild naming scheme, one install user
- Lmod in use sind 2012, flat module tree
- software and modules are on NetApp NFS cluster

IMP & IMBA

- inherited the setup in Dec 2014
- Tcl/C environment modules v3.2.10
- one install user, flat module tree
- no EasyBuild yet :(
- projects to deploy EasyBuild, Lmod, and XALT on the way
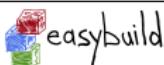
sciCORE: general info

- providing HPC facilities and support for the University of Basel

- 7 team members:
    - 1 manager
    - 3 user support/development
    - 3 sysadmin

- ∼350 user accounts

sciCORE: systems

- Maia cluster:
  - ~300 compute nodes
  - Intel Sandy Bridge & Ivy Bridge
  - ~4,000 cores
  - QDR infiniband
  - ~50TB BeeGFS (Fraunhofer)
  - CentOS 6.5
- BC2 cluster:
  - ~150 compute nodes
  - Intel Sandy Bridge, AMD Bulldozer
  - ~3,000 cores
  - Ethernet
  - ~2PB GPFS
  - CentOS 6.5

easybuild

sciCORE: EasyBuild configuration

- one dedicated install user, shared between multiple people
- flat module tree, EasyBuild default module naming scheme
- Lmod 5.7.4 (to be upgraded soon for performance improvements)
- default toolchains: `goolf-1.4.10` and `iomkl-2015.01`
- rely on system packages for common libraries like zlib, ncurses, libpng, bzip2, . . .
  - dependencies are filtered using "`eb --filter-deps`"
- BC2 cluster: one shared filesystem (GPFS) for software and modules
  - subdirectory per cpu type, e.g. `/import/bc2/apps/sandybridge`
  - every machine accesses the software in a common path (`/import/bc2/apps`) mapped with automounter
- Maia: software/modules is copied to local disk of each node
- compilation is done in login nodes (SGE support in EasyBuild?)