Alexander Grund
Center for Information Services and High Performance Computing (ZIH)

EasyBuild at ZIH - TU Dresden

5th EasyBuild User Meeting, Barcelona
31st January, 2020

TU (University of Technology) Dresden

— Since 1828/1961

— Ca. 32 000 students, 8 300 employees

— 18 faculties, 121 disciplines

— Focus on Biomedicine, Bioengineering, Materials sciences, Information technology, Microelectronics, Energy and Environment

— Since 2012 "University of Excellence" with Clusters

  – Center for Advancing Electronics Dresden (cfaed)

  – Physics of Life

  – Complexity and Topology in Quantum Materials

  – …

Center for Information Services and High Performance Computing (ZIH)

- Central scientific institution
- Member of the Gauß-Allianz
- Tasks:
  - Communication infrastructure
  - Operation of central IT infrastructure
  - Support for other departments
- Own Research and development work
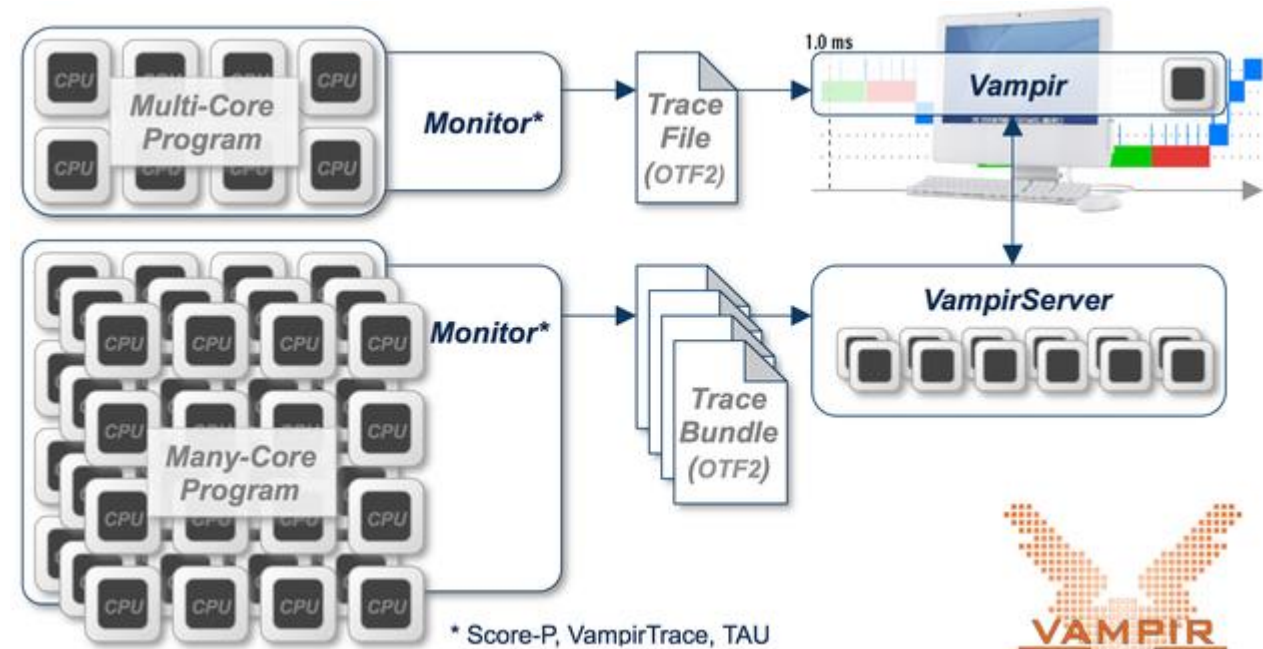
HPC Cluster

Main cluster: Taurus

— ~47 000 processors

— 270 Sandy Bridge nodes (gone)

— ~1600 Haswell nodes
  – 64 – 256 GB RAM
  – 128 GB local SSD

— 44 GPU nodes (2x K20), Sandy Bridge

— 64 GPU nodes (4x K80)

— 32 Power9 nodes (6x V100)

— Some consumer GPU nodes (GTX 1080Ti)

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ZIH – TU Dresden // Alexander Grund
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Folie 4

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HPC Cluster

Special Islands

— SMP nodes
  – 2 nodes @ 1 TB RAM
  – 4 nodes @ 2 TB RAM

— Intel Xeon Phi
  – 32 nodes w/ Knights Landing

— HPC Data Analytics
  – 90 nodes
  – 2 PB NVMe flash memory

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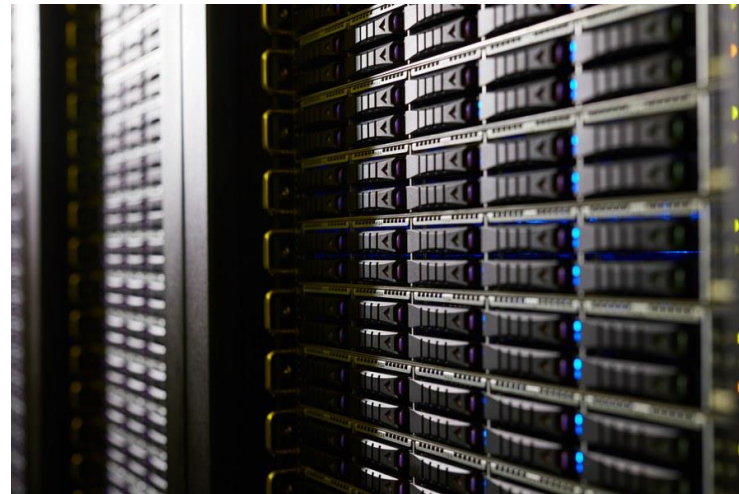
HPC Cluster

Upcoming:

— 192 nodes with AMD EPYC 7702 processors
  – 2 / node → 128 cores / node
— > 750 TFlops

"Superdome Flex"
— 32 Intel Cascade Lake 8276 → 896 cores
— 48 TB RAM in unified address space
— 400 TB NVMe memory

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Software environment

Previously:
— RHEL 6
— EnvironmentModules 3.2.1 (TCL/C Modules)
— Custom build software & modules

Since 10/2016:
— Lmod as alternative (opt-in)
— Separate EasyBuild environment: modenv/eb vs modenv/classic

Since 08/2017:
— Lmod as default
— New software build with EasyBuild (exceptions to modenv/classic)

Since 06/2018:
— Bull SCS5 w/ RHEL 7
— Clean new modenv/scs5 w/ EasyBuild modules (currently ~1300)
— Flat module structure due to user habits
— Some custom EasyConfigs, no custom EasyBlocks
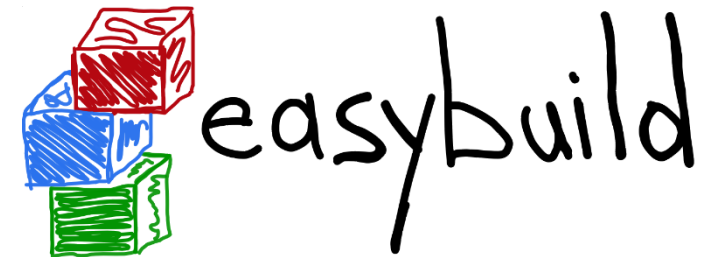
Module environment

Problem:
Heterogeneous cluster with multiple CPU architectures (westmere, sandy bridge, haswell, …)

Solution:
— Shared module folder
— Separate folders for software (binaries etc.)
— /sw/installed is symlinked to /sw/haswell or /sw/sandy on every node

➢ Most optimized builds w/ custom build settings possible
➢ Transparent for users
➢ Regression checks for "hardware dependent" bugs
o Symlinks may lead to trouble with build systems ➔ Better use bind mounts

Now mixture again:
— modenv/scs5 with Symlinks
— modenv/ml as separate module environment for Power9

User experience

— SLURM
 – 1 Architecture on every partition
— Lustre
 – Different storages (from SSD to tape)
 – Workspaces → Expire after given period
 – Some NFS
— Lmod

— Extensive wiki
 – Instructions for using SLURM
 – Examples for using certain software
 – List of installed modules

— Ticket system
 – Issues with system
 – Software requests
 – General help

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Software support

— For long time only 1 person allowed to install software
— Some exceptions for particular software, e.g. Vampir

— Now 2-3 people supporting the software stack

— Mostly official EasyConfigs used
— Some custom ones required (minor changes, different version)
— Some user-provided EasyConfigs
— No EasyBlocks written so far
— Some software still installed manually (LS-DYNA, STAR-CCM+)

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Software support – EasyBuild extensions

Helper script for installation: eb_zih
— Determine architecture and set up install targets (/sw/{haswell,sandy,ml})
— Load EasyBuild module and settings
— Set up group write permissions
— Add --group-writable-installdir to eb command

Separate script:
— Copies module files to user-visible location
— Check for module availability on all architectures

— EB Hooks for CMAKE_PREFIX_PATH in module files
— Shared folder for custom ECs, migration to git repo planned

Conclusion

— EasyBuild greatly simplifies software installation

— Community EasyConfigs save a lot of time

— Toolchain concept of EasyBuild makes cutting-edge software installation hard

    – Lot's of EasyConfigs to create on toolchain update

    – --try-* options nice but doesn't handle dependencies well

    – Trainee project for a webapp in work to help

— Mid term goal: Hierarchical module structure

    – Already in use in CLARA cluster from DLR

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