EasyBuild on IT4Innovations national supercomputing center
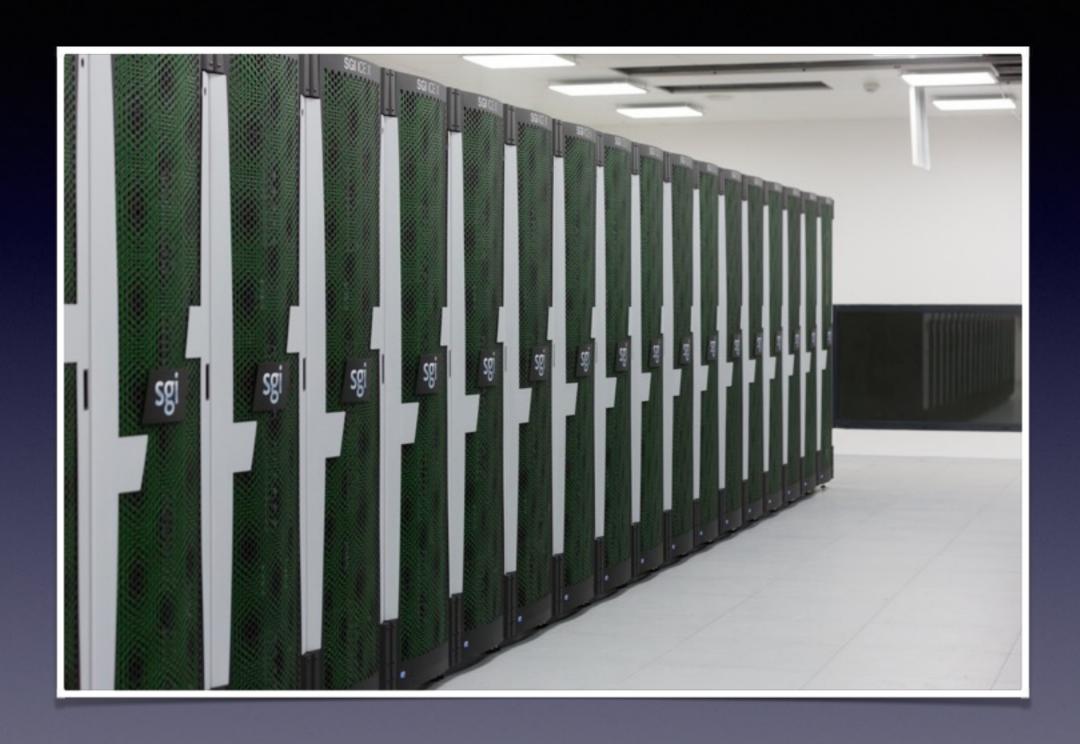
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About IT4Innovations

Salomon in Numbers

- Currently Nr. 48 in TOP500

- 1008 compute nodes

- 24 Haswell cores per node (24192 cores)

- 128 GB RAM per node

- 864 Intel Xeon Phi 7120P (52704 cores)

What did we use before EasyBuild

- Simple shell scripts called "p" scripts

- They contained all necessary information about software build

- Typically ./configure (options), make, make install

What was wrong with "p" scripts

- Manual module file creation was necessary

- OS dependencies were not captured

- Logging wasn't perfect

- Process wasn't always automatically repeatable

- A lot of manual work

Why do we use EasyBuild

- Repeatable installation process

- Automatic module creation

- Track (ideally) all dependencies

- Responsive community

- Actively developed

- And many other reasons

Our EasyBuild Environment

- We have our branch of easyconfigs, push to the branch triggers CI (GitLab CI)

- If build is successful, it goes to production

- Whole EasyBuild setup is managed by Ansible, same as OS on a cluster to be sure we have captured all changes to the cluster

- We are using currently TCL/C environmental modules (considering Lmod)

Problems with EasyBuild

- Users had problems with toolchains concept at first

- Complicated module naming (Lmod,HierarchicalMNS?)

- Rpath support missing (yet)

- We can't trust easyconfigs blindly, we have to check / modify it if necessary (EB is a layer)

- Lot of duplicated basic modules like Bash, zlib (minimal toolchains solve this?)

- intel/foss 2015b toolchains incompatibility

Our customisation

- Module naming scheme (IT4IModuleNamingScheme)

- Automatically append cluster modifications to the easyconfigs (modextravars for example)

Contribution back

- Some easyconfigs

- Intel 2016 easyblocks

- Bugfixes

- More to come…

Future

- Try Lmod

- Improve tests and build environment

- Prepare benchmarking tool for users to improve modules optimisation

Comments and Questions