



Software Environment on JURECA

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Why a hierarchy (using Lmod)?

- Compilers X MPI-Versions = module explosion
 - How to simplify naming and user view?
 - How to enforce consistency?
- Tcl/C modules not really developed any more and features very limited
 - Speed: Imod has a cache
 - Search: Imod has *spider*
 - Support for hidden modules
 - Additional features: Properties, Families,...



MPI Software

Compiler Software

User View





Why Stages?

- Newest hardware means compiler upgrades can have large impact
- New toolchains and versions means spider output gives too many choices
- Use Stages to retire outdated software and manage the user view
- Stages allow trivial transition to entirely new software stacks
 - Including changes to EasyBuild and naming scheme

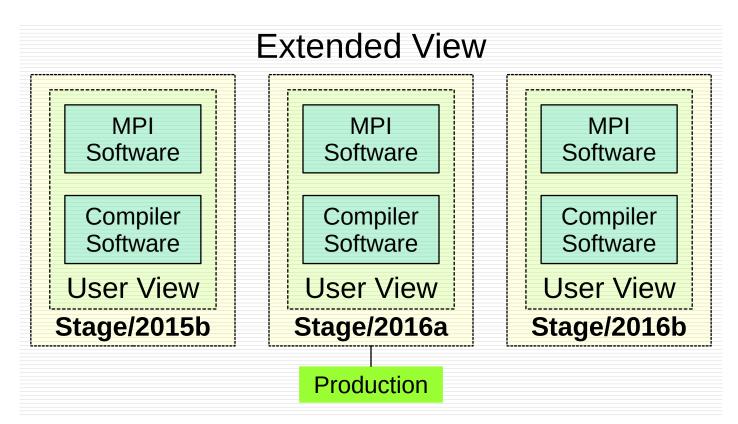


MPI Software

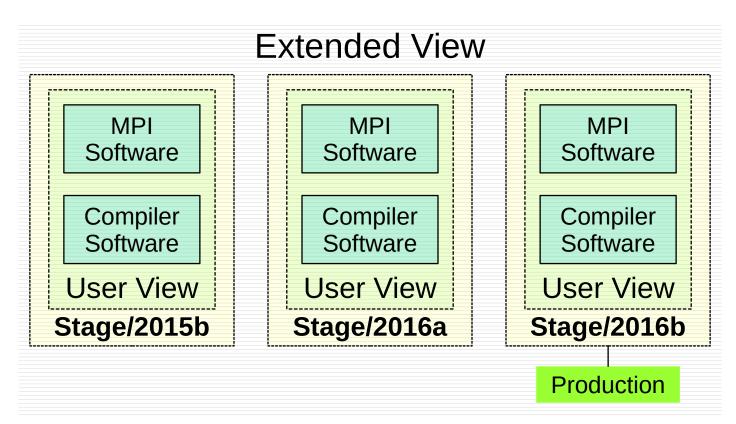
Compiler Software

User View

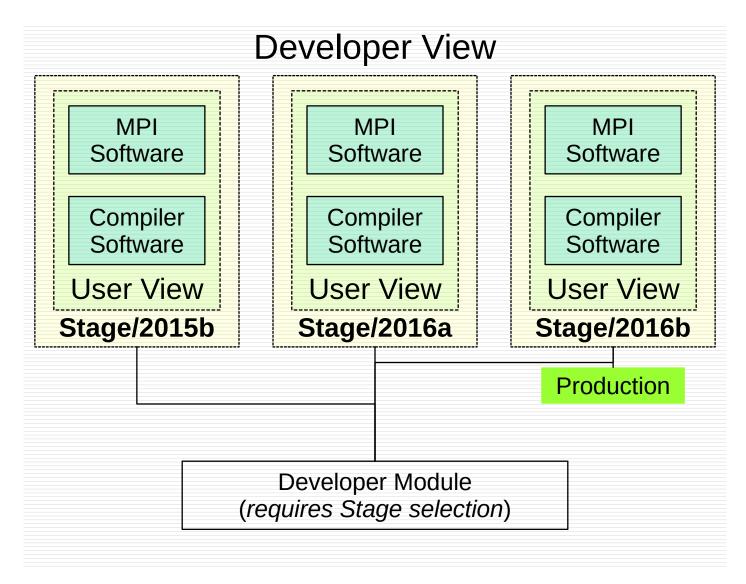
















Developer module

- Documentation and advice
- Permissions
 - EASYBUILD_SET_GID_BIT
 - EASYBUILD_STICKY_BIT
 - EASYBUILD_UMASK
 - EASYBUILD_GROUP_WRITABLE_INSTALLDIR
 - EASYBUILD **READ ONLY** INSTALLDIR
- Software is built in RAM
 - EASYBUILD BUILDPATH "/dev/shm/\$USER"





Developer Module (2)

- Where are things installed?
 - EASYBUILD_INSTALLPATH (Stage)
- Resolving dependencies
 - EASYBUILD_ROBOT controls where to look for dependencies
- Submitting builds as jobs (using –job)
- All things module related
- Licences, restrictions,...





Typical software issues:

- EasyBuild is not that easy
 - Learning curve
 - Failed builds have to be restarted from scratch
 - XYZ software doesn't fit the model
- No place for static installations within Stages
- What about long term software support?
- Software responsibility, testing and maintenance?





Moving Forward

- Maintain our own Golden EasyBuild repo
 - Easyconfigs in this branch have priority
 - Development in Stages/Devel only
 - Code review by swmanage
 - Only easyconfigs in golden repo installed to Production
 - Keep a legacy repository of all previously installed easyconfigs from Production
 - Distinguish between supported software and dependencies
 - Actively search for updates to supported software
 - Hide dependency modules by default?



Standards in module files

- Relevant to supported software
- Maintainer and email contact should be listed
- Configuration of installation (installed modules, compiler options used...)
- Should provide usage information
- What else?
- EasyBuild will soon (?) support templates to enforce this (restrict enforcing to supported?)



What has JSC contributed?

- GCCcore concept
- Minimal toolchains
- MNS independent installation directories
- Configurable default optimisation
- Hierarchical module naming scheme
- Bug fixes and support



What do we worry about?

- Environment explosion
- Dependencies creating clutter
- Version minimisation
- GPU-enabled software
- inodes!!





Comments and Questions



27/01/16