



EasyBuild @SURF

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SURF

- ✦ Supercomputing
- ✦ Clustercomputing
- ✦ Scientific visualisation
- ✦ Data services
- ✦ Research Cloud
- ✦ Grid/Spider
- ✦ HPML
- ✦ Digital platforms
- ✦ Security, trust & identity
- ✦ Network connectivity
- ✦ Training, consultancy
- ✦ ...

SURF

HPCV group

- ✦ **Supercomputing**
- ✦ **Clustercomputing**
- ✦ **Scientific visualisation**

- ✦ Data services
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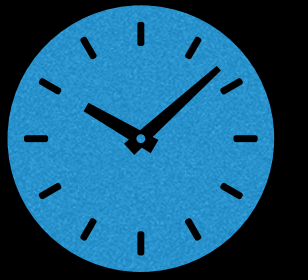
- ✦ HPML
- ✦ Digital platforms
- ✦ Security, trust & identity
- ✦ Network connectivity
- ✦ **Training, consultancy**
- ✦ ...

Systems

- **Cartesius** - former national supercomputer (Broadwell, Haswell, Ivy Bridge, Sandy Bridge, KNL)
- **Snellius** - new national supercomputer (Ice Lake, AMD ROME)
- **Lisa** - national cluster (Skylake, Cascade Lake)
- **ESC** - test system (Cascade Lake, AMD ROME)



Problems



- ✦ Large number of modules (we provide software stacks for our users)
- ✦ Some modules are “unique” for a particular users group or project (software may not comply with our software policy)
- ✦ Heterogeneous systems (different architectures, features)
- ✦ Multiple systems (need to install software on all of them)

A bit of history

- The old way of installing/maintaining the software



Create new
username for a
specific software

Download
sources/binaries

Write bash script
for the installation
process

Write modulefile

Repeat for every system

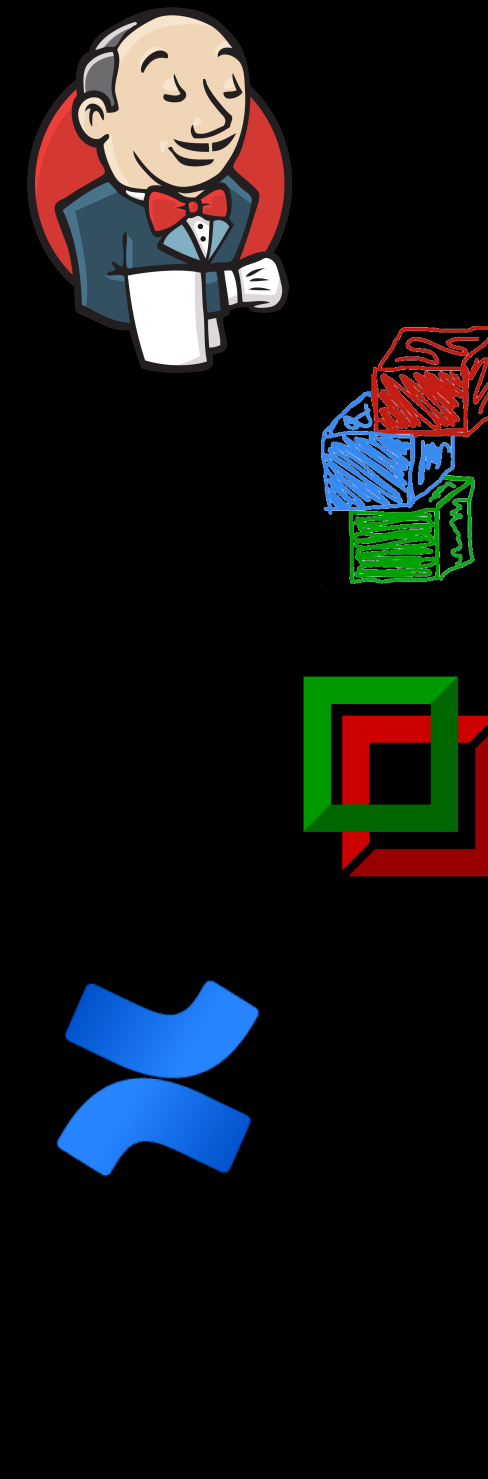
A bit of history

- ✦ Huge number of “software users”
- ✦ Manually written scripts
- ✦ Manually written modulefiles
- ✦ No tests or sanity checks
- ✦ Independent software environments on all systems
- ✦ Different module environments (Tmod, Lmod)
- ✦ ...

Current management

- ✦ **Lmod** - module environment
- ✦ **Jenkins** - automation
 - ✦ **EasyBuild** - software installation
 - ✦ **ReFrame** - software testing
 - ✦ **Confluence** - docs
- ✦ **Xalt** - usage monitoring

Lmod



Problem #1



- ✦ Large number of modules (we provide software stacks for our users)
- ✦ Some modules are “unique” for a particular users group or project (software may not comply with our software policy)
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Module environment



- ✦ Lmod - same module environment on all systems
 - ✦ Spider cache on (local and global)
 - ✦ **LMOD_EXACT_MATCH = yes**. Users have to specify full module names. Simplifies our helpdesk duties
 - ✦ **LMOD_EXTENDED_DEFAULT = no**. No partial match of a version
 - ✦ **LMOD_CASE_INDEPENDENT_SORTING = yes**. Simplifies module search for users

Module environment



- ✦ Global cache is updated at the end of Jenkins pipeline
- ✦ Local cache (in \$HOME) is updated after calling “eblocalinstall”
- ✦ “eblocalinstall” is a wrapper over the “eb” command. It re-defines EASYBUILD_INSTALLPATH_XXX envvars

```
$ cat /opt/lmod/lmod/init/lmodrc.lua | tail -n 10
scDescriptT = {
  {
    dir = "/sw/arch/lmod_cache/cacheDir",
    timestamp = "/sw/arch/lmod_cache/system.txt",
  },
  {
    dir = "~/.lmod.d/.cache",
    timestamp = "~/.lmod.d/users.txt",
  },
}
```

```
$ cat eblocalinstall | tail -n 8
# Update the local cache (Lmod only)
read module_system_version < <( _check_module_system ) || exit 1
if [ "$module_system_version" == "Lmod" ]
then
  $LMOD_PKG/libexec/update_lmod_system_cache_files \
  -d ~/.lmod.d/.cache -t ~/.lmod.d/users.txt \
  $EASYBUILD_INSTALLPATH_MODULES
fi

exit $exitcode
```


Software stacks

- ✦ One software stack release per year
- ✦ Release in August/September
- ✦ At most three software stacks on a system:
 - ✦ Production - full support, new software installation
 - ✦ PreviousProduction - limited support, patching
 - ✦ Deprecated - no support
- ✦ We use **Xalt** to track the software usage

```
$ module av
----- /sw/noarch/modulefiles/environment -----
2019      2020      2021      slurm-tools

$ module load 2020
$ module av
----- /sw/noarch/modulefiles/environment -----
2019      2020 (L)      2021      slurm-tools

---- /sw/arch/Debian10/EB_production/2020/modulefiles/phys ----
Elk/6.3.2-foss-2020a                      VASP5/5.4.4.pl2-intel-2020a
Elk/6.3.2-intel-2020a                     VASP5/5.4.4.pl2-intelcuda-2020a
UDUNITS/2.2.26-GCCcore-9.3.0             VASP6/6.1.1-intelcuda-2020a

---- /sw/arch/Debian10/EB_production/2020/modulefiles/perf ----
CubeGUI/4.4.4-GCCcore-9.3.0              OPARI2/2.0.5-GCCcore-9.3.0
CubeLib/4.4.4-GCCcore-9.3.0              OTF2/2.2-GCCcore-9.3.0
CubeWriter/4.4.3-GCCcore-9.3.0           PAPI/6.0.0-GCCcore-9.3.0
...
```

Software stacks

Year/Stack	2019	2020	2021	2022	2023	...
2019a	Production	Limited support	Deprecated	Deleted		
2020a		Production	Limited support	Deprecated	Deleted	
2021a			Production	Limited support	Deprecated	
2022a				Production	Limited support	
2023a					Production	
...						

Software stacks

- ✦ Prior to **2021a** we installed all software with both “foss” and “intel” toolchains
- ✦ Since **2021a** we install everything with “foss”. Only a few packages are still installed with “intel” (e.g. AMS, NWChem, OpenMolcas)
- ✦ We provide an additional set of compilers and development tools for experienced users: OneAPI, LLVM, NVHPC, AOCC
- ✦ We have relatively strict software policy

Software policy

- ✦ Requests for new software:
 - ✦ We **do not install** software that is older than 2 years unless the software is still maintained and relevant
 - ✦ We **don't install more than two different versions** of software per toolchain system-wide
 - ✦ We **don't install versions older than** the one already **available** system-wide (unless the software has no backward compatibility). These situations should be assessed on a case-by-case basis
 - ✦ Modules for **new versions** will **replace** the **existing** modules with older **versions** (unless the software has no backward compatibility)
 - ✦ The **default approach** is "users build software themselves in the local prefix". We may assist in installing software locally, but we avoid doing it ourselves (unless a user has consultancy hours added to the project)

Modules environment

- ✦ 2018 - approx. 700 modules
- ✦ 2019 - approx. 600 modules (introduced software policy)
- ✦ 2020 - approx. 470 modules (introduced Xalt)
- ✦ 2021 - approx. 380 modules (only foss toolchain)

Problem #2



- ✦ Large number of modules (we provide software stacks for our users)
- ✦ Some modules are “unique” for a particular users group or project (software installation may not comply with our software policy)
- ✦ Heterogeneous systems (different architectures, features)
- ✦ Multiple systems (need to install software on all of them)

Sub-stacks

- ✦ We are involved in multiple projects (Deltares, OSSC, CompBiomed, ReaxPro, etc.)
- ✦ Some projects require installation of additional software (e.g. proprietary software or software that depends on “intel” toolchain)
- ✦ We do not want to “spoil” our users by sharing additional software with them :)
- ✦ We want to avoid duplicates among the installed software

Sub-stacks

- ✦ We introduce **sub-stacks**
- ✦ The sub-stack depends on the basic software stack from the same year, but extends it
- ✦ Only some users can see/use a sub-stacks (ACLs)
- ✦ The MODULEPATH is populated in the sub-stack modulefile

```
$ module av
```

```
----- /sw/noarch/environment -----  
2020    2021    2021_Delft3D    2021_OSSC
```

Problem #3



- ✦ Large number of modules (we provide software stacks for our users)
- ✦ Some modules are “unique” for a particular users group or project (software may not comply with our software policy)
- ✦ Heterogeneous systems (different architectures, features)
- ✦ Multiple systems (need to install software on all of them)

Heterogeneity

- ✦ The “common” symlinks (Snellius):
 - ✦ AMD nodes:
 - ✦ `/sw/arch -> /gpfs/admin/hpc/sw/arch/AMD-ZEN2`
 - ✦ Intel nodes:
 - ✦ `/sw/arch -> /gpfs/admin/hpc/sw/arch/INTEL-AVX512`
 - ✦ All nodes (architecture agnostic modules/software):
 - ✦ `/sw/noarch -> /gpfs/admin/hpc/sw/arch/NOARCH`

```
/gpfs/admin/hpc/sw
├── arch
│   ├── AMD-ZEN2
│   ├── INTEL-AVX512
│   └── NOARCH
│       ├── Centos8.4
│       │   ├── 2021
│       │   │   ├── modulefiles
│       │   │   │   ├── all
│       │   │   │   │   ├── EasyBuild
│       │   │   │   │   └── eb
│       │   │   │   └── tools
│       │   │   │       └── EasyBuild
│       │   │   └── software
│       │   │       ├── EasyBuild
│       │   │       │   ├── 4.5.0
│       │   │       └── eb
│       │   │           └── 4.5.0
│       └── environment
├── easybuild
│   ├── easyblocks-surfsara
│   └── easyconfigs-surfsara
└── ...
```

Problem #4



- ✦ Large number of modules (we provide software stacks for our users)
- ✦ Some modules are “unique” for a particular users group or project (software may not comply with our software policy)
- ✦ Heterogeneous systems (different architectures, features)
- ✦ Multiple systems (need to install software on all of them)

Jenkins



- ✦ Automated software installation (Groovy, Bash + EasyBuild)
- ✦ Automated regression tests (Groovy, Bash + ReFrame)
- ✦ Automated documentation generation (Groovy, Bash, Python + REST API)
- ✦ Ideal workflow: install -> test -> document
- ✦ Currently, all three are decoupled (WIP)

Jenkins



- ✦ Multiple pipelines
- ✦ Some are executed automatically (regression tests)
- ✦ Some must be started manually (sw installation)

EasyConfigDelft3D		-	-	☆
EasyConfigNextProduction		-	-	☆
EasyConfigOSSC		-	-	☆
EasyConfigPreviousProduction		-	-	☆
EasyConfigProduction		-	-	☆
EasyConfigRegression		-	-	☆
EasyConfigTest		-	-	☆
ReFrameOSUpgradeMajor		-	-	☆
ReFrameOSUpgradeMinor		-	-	☆
ReFrameProductionMonthly		-	-	☆
ReFrameProductionWeekly		-	-	☆
ReFrameProductionYearly		-	-	☆
ReFrameSABS2020		-	-	☆
ReFrameSlurmUpgrade		-	-	☆
ReFrameTestingPipeline		-	-	☆

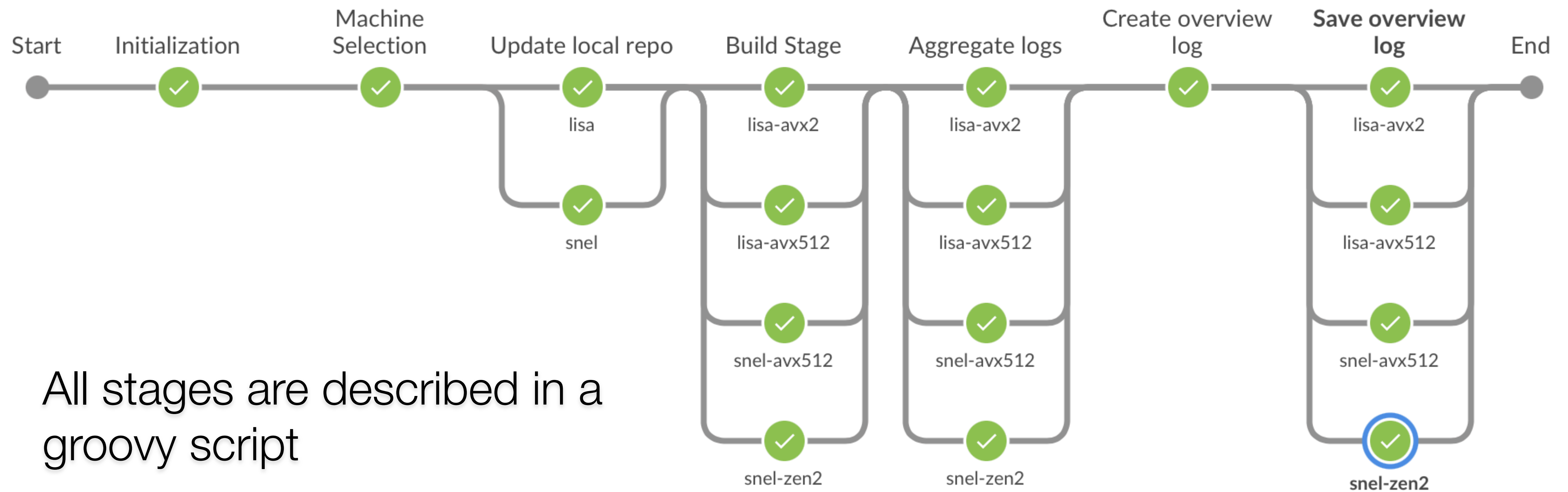
Jenkins

- ✦ Workflow (software installation):
 - ✦ parse a “buildlist” to check what should be installed
 - ✦ “buildlist” - plain text file with names of easyconfigs + some options (e.g. --from-pr)
 - ✦ allocate resources on a target machine and architecture
 - ✦ load modules (software stack + EasyBuild)
 - ✦ run installation
 - ✦ update global spider cache



```
#### Basic Compilers ####
GCCcore-10.3.0.eb
intel-compilers-2021.2.0.eb \
--accept-eula-for=Intel-oneAPI
#
#### Basic Components ####
binutils-2.36.1.eb
binutils-2.36.1-GCCcore-10.3.0.eb
pkg-config-0.29.2.eb
pkg-config-0.29.2-GCCcore-10.3.0.eb
Autotools-20210128-GCCcore-10.3.0.eb
ncurses-5.9.eb --from-pr 14144 \
# we need this specific version for Stata-17
ncurses-6.2-GCCcore-10.3.0.eb
git-2.32.0-GCCcore-10.3.0-nodocs.eb
Mercurial-5.8-GCCcore-10.3.0.eb
#### MPI Libraries ###
OpenMPI-4.1.1-GCC-10.3.0.eb \
--hooks=/sw/eb/easyconfigs-surf/hooks/\
mpi_hook.py --include-easyblocks=/sw/eb/\
easyblocks-surf/openmpi.py
OpenMPI-4.1.1-intel-compilers-2021.2.0.eb \
--hooks=/sw/eb/easyconfigs-surf/hooks/\
mpi_hook.py --include-easyblocks=/sw/eb/\
easyblocks-surf/openmpi.py
impi-2021.2.0-intel-compilers-2021.2.0.eb \
--accept-eula-for=Intel-oneAPI \
--hooks=/sw/\eb/ easyconfigs-surf/hooks/\
mpi_hook.py
MPICH-3.4.2-GCC-10.3.0.eb
#
...
```

Jenkins



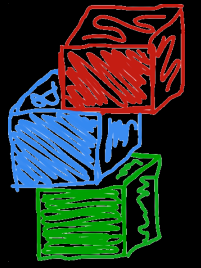
Jenkins



```
✓ Shell Script 1m 22s
3688 AMS-2021-101-intel-mpi1.eb ALREADY INSTALLED
3689 Gaussian-g16.c01-AVX2.eb ALREADY INSTALLED
3690 NAMD-2.14-foss-2021a-mpi.eb ALREADY INSTALLED
3691 NAMD-2.14-foss-2021a-mpi-memopt.eb ALREADY INSTALLED
3692 ORCA-5.0.1-gompi-2021a.eb ALREADY INSTALLED
3693 PLUMED-2.7.2-foss-2021a.eb ALREADY INSTALLED
3694 TURBOMOLE-7.5.1.eb ALREADY INSTALLED
3695 Libint-2.6.0-GCC-10.3.0-lmax-6-cp2k.eb ALREADY INSTALLED
3696 NWChem-7.0.2-intel-2021a.eb ALREADY INSTALLED
3697 CP2K-8.2-foss-2021a.eb ALREADY INSTALLED
3698 Lumerical-2021-R2.3-2834-e18f3c9-OpenMPI-4.1.1.eb ALREADY INSTALLED
3699 Lumerical-2021-R2.3-2834-e18f3c9-mpi-2021.2.0.eb ALREADY INSTALLED
3700 ANSYS-2021R2.eb ALREADY INSTALLED
3701 OpenFOAM-v2106-foss-2021a.eb ALREADY INSTALLED
3702 UDUNITS-2.2.28-GCCcore-10.3.0.eb ALREADY INSTALLED
3703 Elk-7.2.42-foss-2021a.eb ALREADY INSTALLED
3704 VASP5-5.4.4.pl2-foss-2021a-CUDA-11.3.1.eb ALREADY INSTALLED
3705 VASP5-5.4.4-intel-2021a-CUDA-11.3.1.eb ALREADY INSTALLED
3706 VASP6-6.2.1-foss-2021a-CUDA-11.3.1.eb ALREADY INSTALLED
3707 VASP6-6.2.1-intel-2021a-CUDA-11.3.1.eb ALREADY INSTALLED
3708 CubeWriter-4.6-GCCcore-10.3.0.eb ALREADY INSTALLED
3709 CubeLib-4.6-GCCcore-10.3.0.eb ALREADY INSTALLED
3710 CubeGUI-4.6-GCCcore-10.3.0.eb ALREADY INSTALLED
3711 gperftools-2.9.1-GCCcore-10.3.0.eb ALREADY INSTALLED
3712 HPL-2.3-foss-2021a.eb ALREADY INSTALLED
3713 OTF2-2.3-GCCcore-10.3.0.eb ALREADY INSTALLED
3714 PAPI-6.0.0.1-GCCcore-10.3.0.eb ALREADY INSTALLED
3715 Paraver-4.9.2-foss-2021a.eb ALREADY INSTALLED
3716 Score-P-7.0-gompi-2021a.eb ALREADY INSTALLED
3717 Scalasca-2.6-gompi-2021a.eb ALREADY INSTALLED
3718 HarfBuzz-2.8.1-GCCcore-10.3.0.eb ALREADY INSTALLED
3719 Pango-1.48.5-GCCcore-10.3.0.eb ALREADY INSTALLED
3720 ATK-2.36.0-GCCcore-10.3.0.eb ALREADY INSTALLED
3721 GTK+-2.24.33-GCCcore-10.3.0.eb ALREADY INSTALLED
3722 GdK-Pixbuf-2.42.6-GCCcore-10.3.0.eb ALREADY INSTALLED
3723 GTS-0.7.6-GCCcore-10.3.0.eb ALREADY INSTALLED
3724 Graphviz-2.47.2-GCCcore-10.3.0.eb ALREADY INSTALLED
3725 libgd-2.3.1-GCCcore-10.3.0.eb ALREADY INSTALLED
3726 SWIG-4.0.2-GCCcore-10.3.0.eb ALREADY INSTALLED
3727 Ffmpeg-4.3.2-GCCcore-10.3.0.eb ALREADY INSTALLED
3728 libGLU-9.0.1-GCCcore-10.3.0.eb ALREADY INSTALLED
3729 gnuplot-5.4.2-GCCcore-10.3.0.eb ALREADY INSTALLED
3730 matplotlib-3.4.2-foss-2021a.eb ALREADY INSTALLED
3731 VTK-9.0.1-foss-2021a.eb ALREADY INSTALLED
3732 wxWidgets-3.1.5-GCC-10.3.0.eb ALREADY INSTALLED
3733 Blender-2.93.7-lts.eb SUCCESS
3734 ParaView-5.9.1-foss-2021a-mpi.eb ALREADY INSTALLED
3735 TurboVNC-2.2.6-GCCcore-10.3.0.eb ALREADY INSTALLED
3736 VirtualGL-2.6.5-GCCcore-10.3.0.eb ALREADY INSTALLED
3737 OpenCV-4.5.3-foss-2021a-CUDA-11.3.1-contrib.eb ALREADY INSTALLED
3738 ASAP-2.0-foss-2021a-CUDA-11.3.1.eb ALREADY INSTALLED
3739 remotevis-git.eb ALREADY INSTALLED
3740 ncview-2.1.8-gompi-2021a.eb ALREADY INSTALLED
3741 WRF-4.3-foss-2021a-dmpar.eb ALREADY INSTALLED
3742 WPS-4.3.1-foss-2021a-dmpar.eb ALREADY INSTALLED
3743 ESMF-8.1.1-foss-2021a.eb ALREADY INSTALLED
3744 TensorFlow-2.6.0-foss-2021a-CUDA-11.3.1.eb ALREADY INSTALLED
3745 Horovod-0.22.1-foss-2021a-CUDA-11.3.1-TensorFlow-2.6.0.eb ALREADY INSTALLED
3746 PyTorch-1.10.0-foss-2021a-CUDA-11.3.1.eb ALREADY INSTALLED
3747 torchvision-0.11.1-foss-2021a-CUDA-11.3.1.eb ALREADY INSTALLED
3748 Horovod-0.23.0-foss-2021a-PyTorch-1.10.0.eb ALREADY INSTALLED
3749 IPython-7.25.0-GCCcore-10.3.0.eb ALREADY INSTALLED
3750 JupyterHub-1.4.1-GCCcore-10.3.0.eb ALREADY INSTALLED
3751 jupyter-server-proxy-3.1.0-GCCcore-10.3.0.eb ALREADY INSTALLED
3752 jupyterlmod-2.0.2-GCCcore-10.3.0.eb ALREADY INSTALLED
3753 IRkernel-1.2-foss-2021a.eb ALREADY INSTALLED
3754 supporting-utils.eb SUCCESS
3755 =====
3756 Built successfully: 2/215
3757 Already installed: 213/215
3758 Failed: 0/215
3759 Skipped: 0/215
3760 Missing easyconfigs: 0/215
3761 =====
3762 Return status: 0
```

```
✗ Shell Script 3m 15s
3379 OpenMolcas-21.06-intel-2021a.eb ALREADY INSTALLED
3380 Libint-2.6.0-GCC-10.3.0-lmax-6-cp2k.eb ALREADY INSTALLED
3381 libecpint-1.0.7-foss-2021a.eb FAILED
3382 Standard output: /gpfs/admin/_hpc/sw/arch/INTEL-AVX512/Centos8/EB_production/2021/logs/20220112_102349/libecpint-1.0.7-foss-2021a.stdout.log
3383 EasyBuild log: /gpfs/admin/_hpc/sw/arch/INTEL-AVX512/Centos8/EB_production/2021/logs/20220112_102349/libecpint-1.0.7-foss-2021a.ebout.log
3384 Last succesful build: Never build successfully
3385 =====
3386 CP2K-8.2-foss-2021a.eb ALREADY INSTALLED
3387 Lumerical-2021-R2.3-2834-e18f3c9-OpenMPI-4.1.1.eb ALREADY INSTALLED
3388 Lumerical-2021-R2.3-2834-e18f3c9-mpi-2021.2.0.eb ALREADY INSTALLED
3389 ANSYS-2021R2.eb ALREADY INSTALLED
3390 OpenFOAM-v2106-foss-2021a.eb ALREADY INSTALLED
3391 UDUNITS-2.2.28-GCCcore-10.3.0.eb ALREADY INSTALLED
3392 Elk-7.2.42-foss-2021a.eb ALREADY INSTALLED
3393 Crystal17-1.0.2-intel-2021a.eb ALREADY INSTALLED
3394 VASP5-5.4.4.pl2-foss-2021a-CUDA-11.3.1.eb ALREADY INSTALLED
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3400 CubeGUI-4.6-GCCcore-10.3.0.eb ALREADY INSTALLED
3401 gperftools-2.9.1-GCCcore-10.3.0.eb ALREADY INSTALLED
3402 HPL-2.3-foss-2021a.eb ALREADY INSTALLED
3403 HPL-2.3-intel-2021a.eb ALREADY INSTALLED
3404 OTF2-2.3-GCCcore-10.3.0.eb ALREADY INSTALLED
3405 Paraver-4.9.2-foss-2021a.eb ALREADY INSTALLED
3406 HarfBuzz-2.8.1-GCCcore-10.3.0.eb ALREADY INSTALLED
3407 Pango-1.48.5-GCCcore-10.3.0.eb ALREADY INSTALLED
3408 ATK-2.36.0-GCCcore-10.3.0.eb ALREADY INSTALLED
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3415 Ffmpeg-4.3.2-GCCcore-10.3.0.eb ALREADY INSTALLED
3416 libGLU-9.0.1-GCCcore-10.3.0.eb ALREADY INSTALLED
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3418 matplotlib-3.4.2-foss-2021a.eb ALREADY INSTALLED
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3425 OpenCV-4.5.3-foss-2021a-CUDA-11.3.1-contrib.eb ALREADY INSTALLED
3426 ASAP-2.0-foss-2021a-CUDA-11.3.1.eb ALREADY INSTALLED
3427 remotevis-git.eb ALREADY INSTALLED
3428 ncview-2.1.8-gompi-2021a.eb ALREADY INSTALLED
3429 WRF-4.3-foss-2021a-dmpar.eb ALREADY INSTALLED
3430 WPS-4.3.1-foss-2021a-dmpar.eb ALREADY INSTALLED
3431 ESMF-8.1.1-foss-2021a.eb ALREADY INSTALLED
3432 TensorFlow-2.6.0-foss-2021a-CUDA-11.3.1.eb ALREADY INSTALLED
3433 Horovod-0.22.1-foss-2021a-CUDA-11.3.1-TensorFlow-2.6.0.eb ALREADY INSTALLED
3434 PyTorch-1.10.0-foss-2021a-CUDA-11.3.1.eb ALREADY INSTALLED
3435 torchvision-0.11.1-foss-2021a-CUDA-11.3.1.eb ALREADY INSTALLED
3436 Horovod-0.23.0-foss-2021a-PyTorch-1.10.0.eb ALREADY INSTALLED
3437 IPython-7.25.0-GCCcore-10.3.0.eb ALREADY INSTALLED
3438 JupyterHub-1.4.1-GCCcore-10.3.0.eb ALREADY INSTALLED
3439 jupyter-server-proxy-3.1.0-GCCcore-10.3.0.eb ALREADY INSTALLED
3440 jupyterlmod-2.0.2-GCCcore-10.3.0.eb ALREADY INSTALLED
3441 IRkernel-1.2-foss-2021a.eb ALREADY INSTALLED
3442 supporting-utils.eb SUCCESS
3443 =====
3444 Built successfully: 1/215
3445 Already installed: 213/215
3446 Failed: 1/215
3447 Skipped: 0/215
3448 Missing easyconfigs: 0/215
3449 =====
3450 srun: error: gcn20: task 0: Exited with exit code 1
3451 srun: task 0: Terminating: Terminating stepid=304053.0
3452 Return status: 1
3453 script returned exit code 1
```

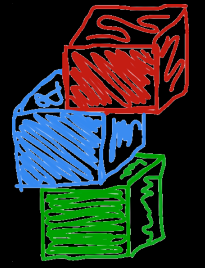
EasyBuild



✧ Old workflow:

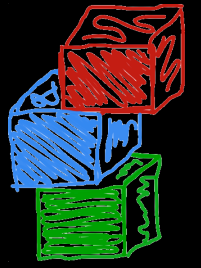
- ✧ download easyconfig from the public repo
- ✧ modify
- ✧ test installation locally
- ✧ push to the local repo
- ✧ execute a jenkins pipeline

EasyBuild



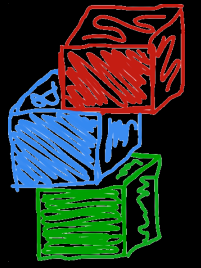
- ✦ A lot of site-specific easyconfigs and easyblocks in the local repo, almost no use of hooks
- ✦ Often only minor differences with the public repo (=> duplicated scripts)
- ✦ => easy to lost track of what version to use next time (public or local)
- ✦ Hardcoded “hot-fixes”
- ✦ Only local tests on locally available machine(s)

EasyBuild



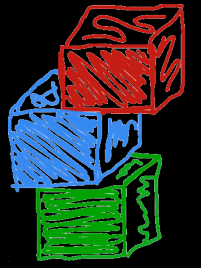
- ✧ **Current workflow:**
 - ✧ modify/write easyconfig or easyblock
 - ✧ test locally
 - ✧ create PR to the public repo
 - ✧ wait for acceptance / resolve reviews
 - ✧ use "--from-pr" in the build list

EasyBuild



- ✦ If site-specific modifications needed (e.g. “modextravars”) - write a hook
- ✦ Feedbacks and checks from the community
- ✦ Tests on different systems
- ✦ No duplicated scripts

EasyBuild



- ✧ Users can perform local installation using the wrapper-script (“eblocalinstall”)
 - ✧ `$HOME/.local/easybuild/...`
 - ✧ Generic installation (i.e. optimised for the least performant architecture)
 - ✧ The wrapper script supports all keys from the “eb” command (`--from-pr`, `--include-easyblock`, etc.)
- ✧ Users can also use site-specific easyconfigs and easyblocks and some hooks

Docs



- ✦ A simple Python script (~340 LoC)
- ✦ Atlassian python API (wrapper over REST API)
- ✦ The script parses modulefiles by category and generates/updates the wiki page
- ✦ Wiki lists description from the modulefile, all available versions of the software and all corresponding dependencies

LLVM

Description:

The LLVM Core libraries provide a modern source- and target-independent optimizer, along with code generation support for many popular CPUs (as well as some less common ones!) These libraries are built around a well specified code representation known as the LLVM intermediate representation ("LLVM IR"). The LLVM Core libraries are well documented, and it is particularly easy to invent your own language (or port an existing compiler) to use LLVM as an optimizer and code generator.

Homepage: <https://llvm.org/>

Version : 12.0.1

Dependencies :

- GCCcore/10.3.0
- ncurses/6.2-GCCcore-10.3.0
- zlib/1.2.11-GCCcore-10.3.0

Version : 12.0.0

Dependencies :

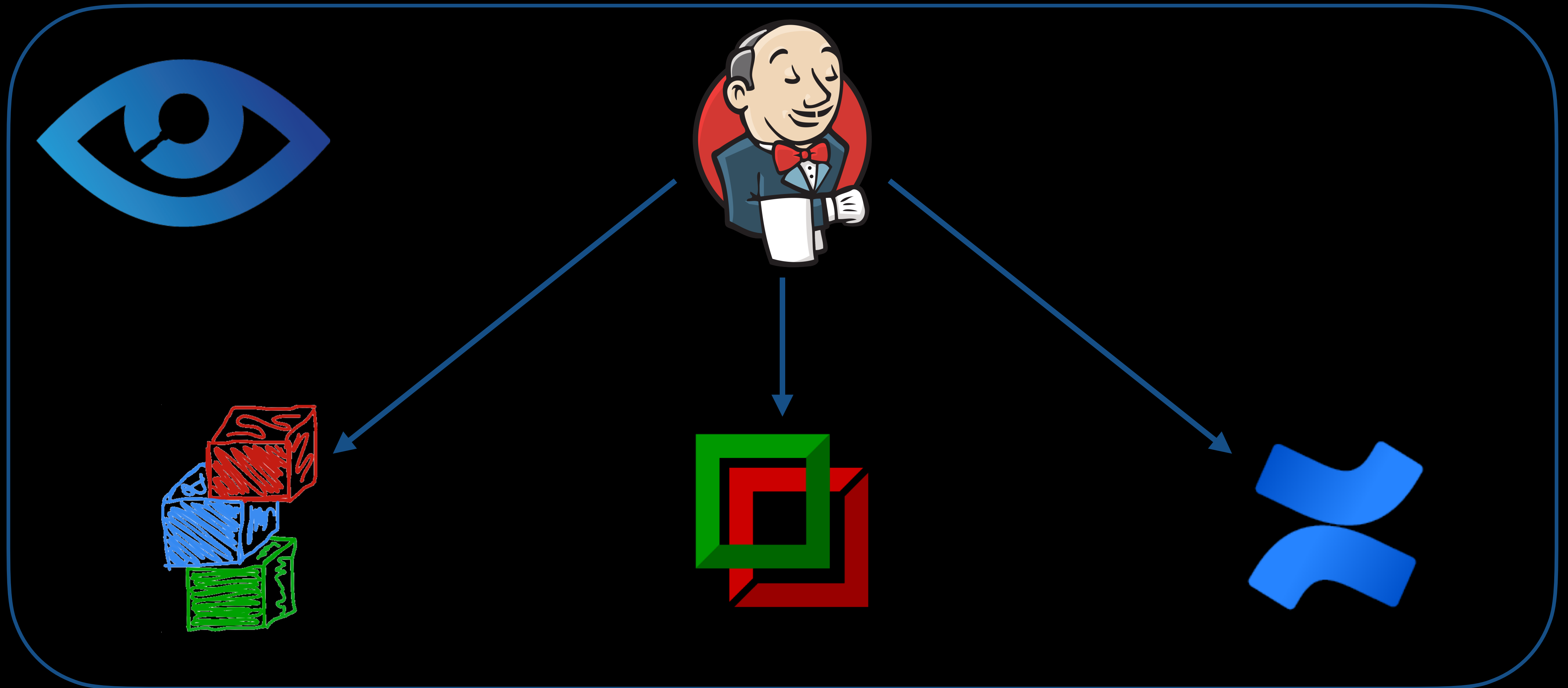
- GCCcore/10.3.0
- ncurses/6.2-GCCcore-10.3.0
- zlib/1.2.11-GCCcore-10.3.0

Version : 11.1.0

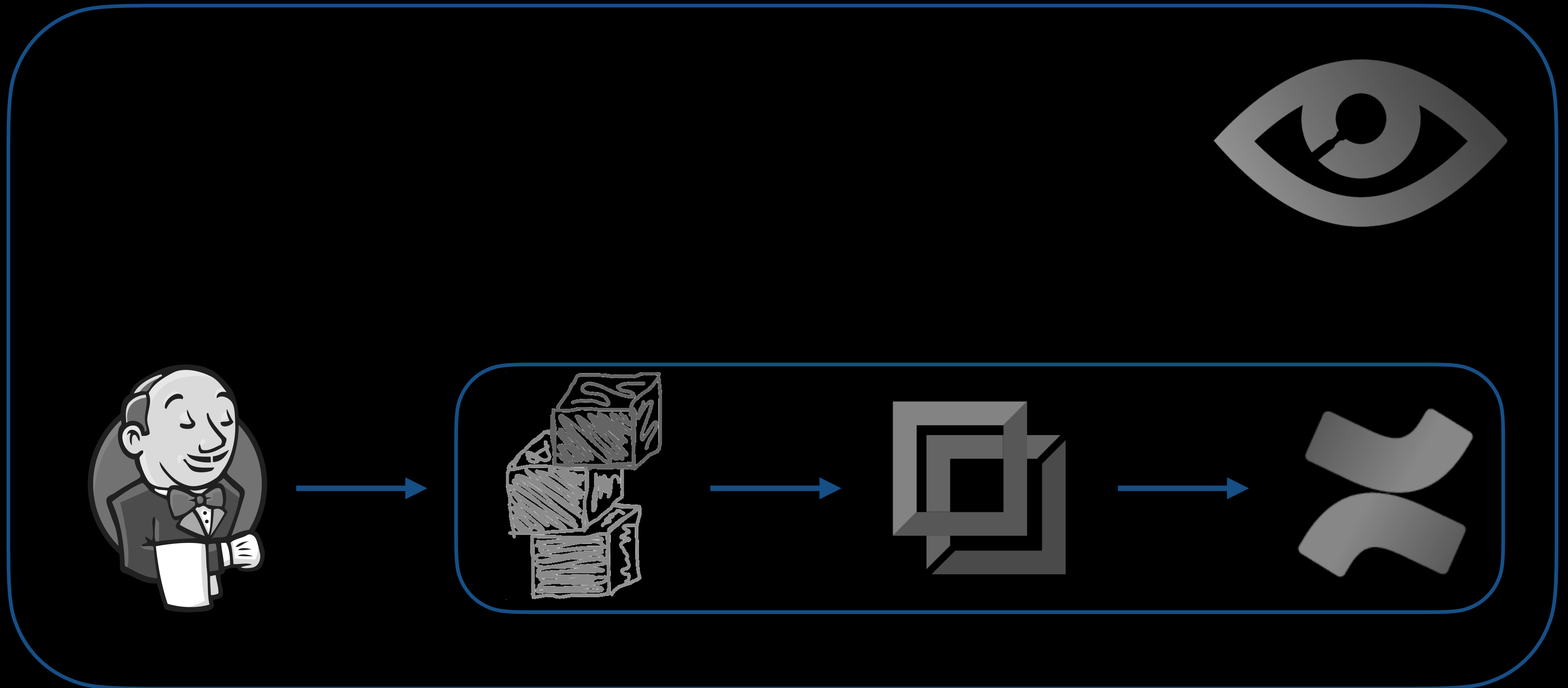
Dependencies :

- GCCcore/10.3.0
- ncurses/6.2-GCCcore-10.3.0
- zlib/1.2.11-GCCcore-10.3.0

Current workflow



Workflow we aim for



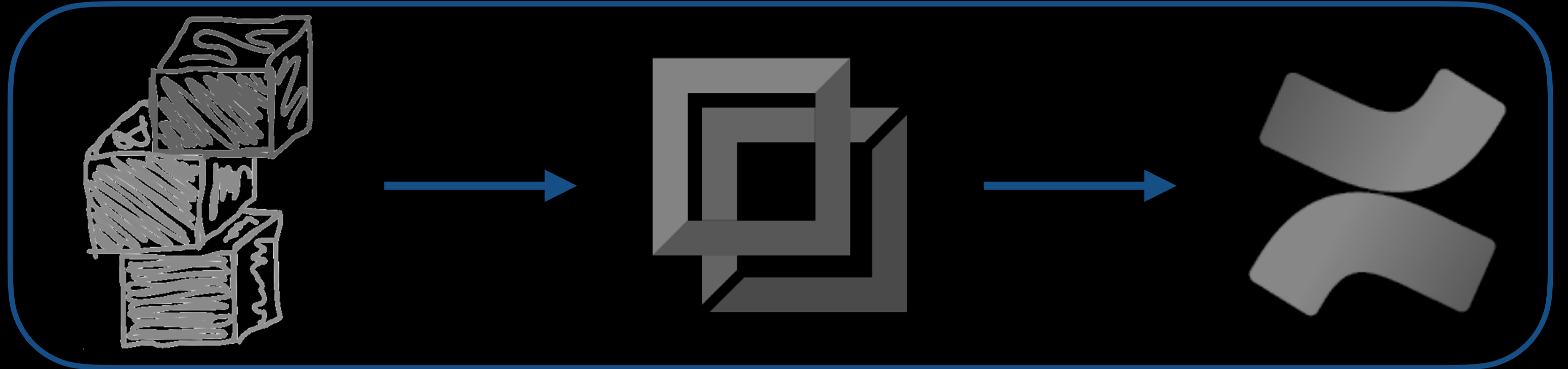
Workflow we aim for

- Analyse software usage with Xalt



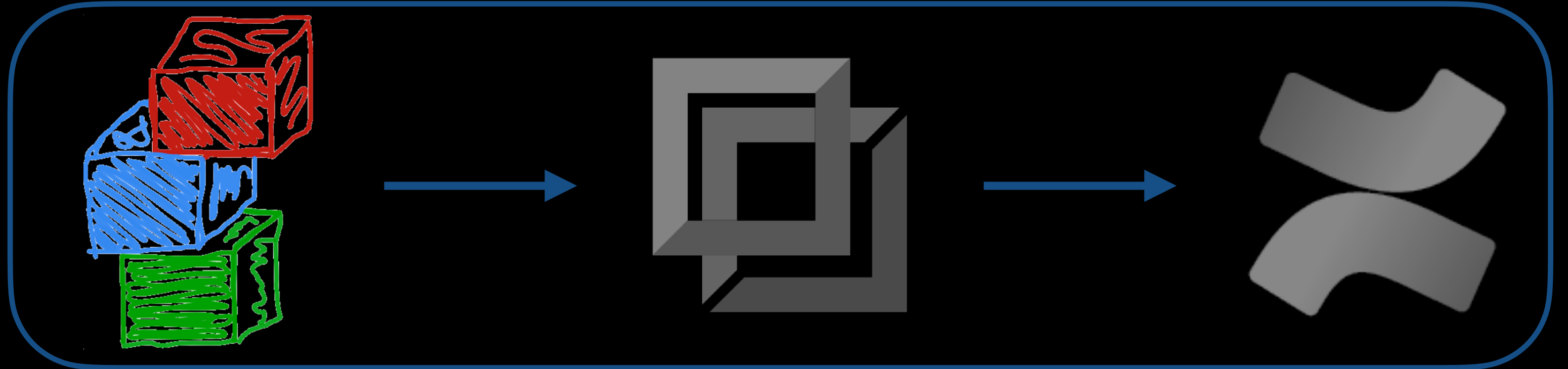
Workflow we aim for

- Analyse software usage with Xalt
- Automate all processes with Jenkins



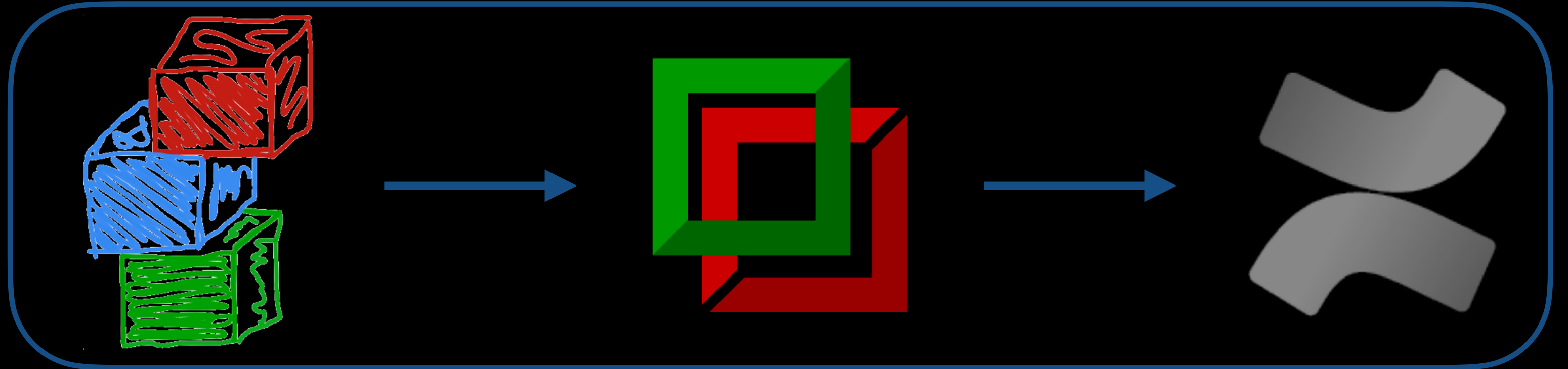
Workflow we aim for

- Analyse software usage with Xalt
- Automate all processes with Jenkins
- Modify/create easyconfigs/easyblocks, PR



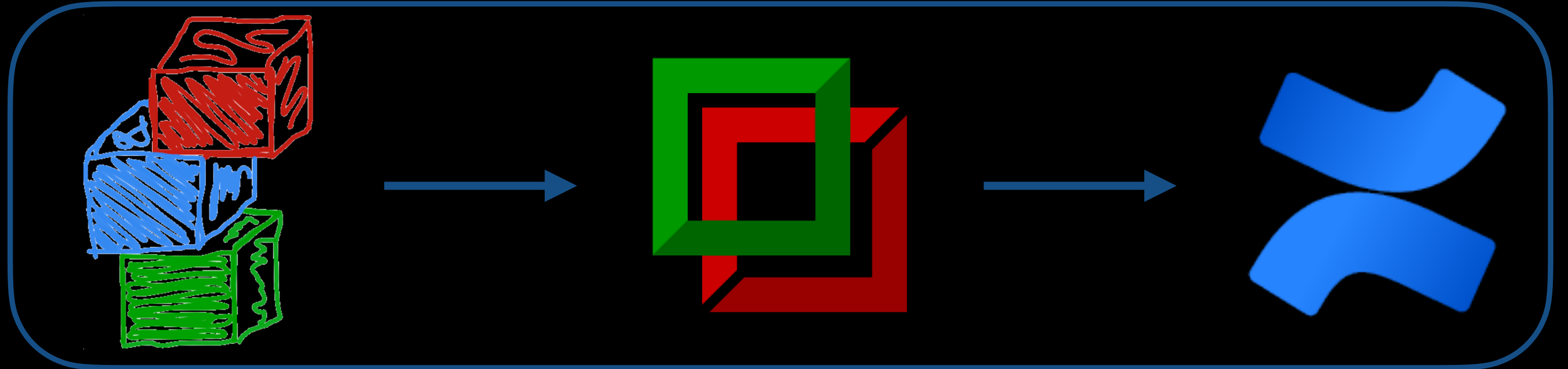
Workflow we aim for

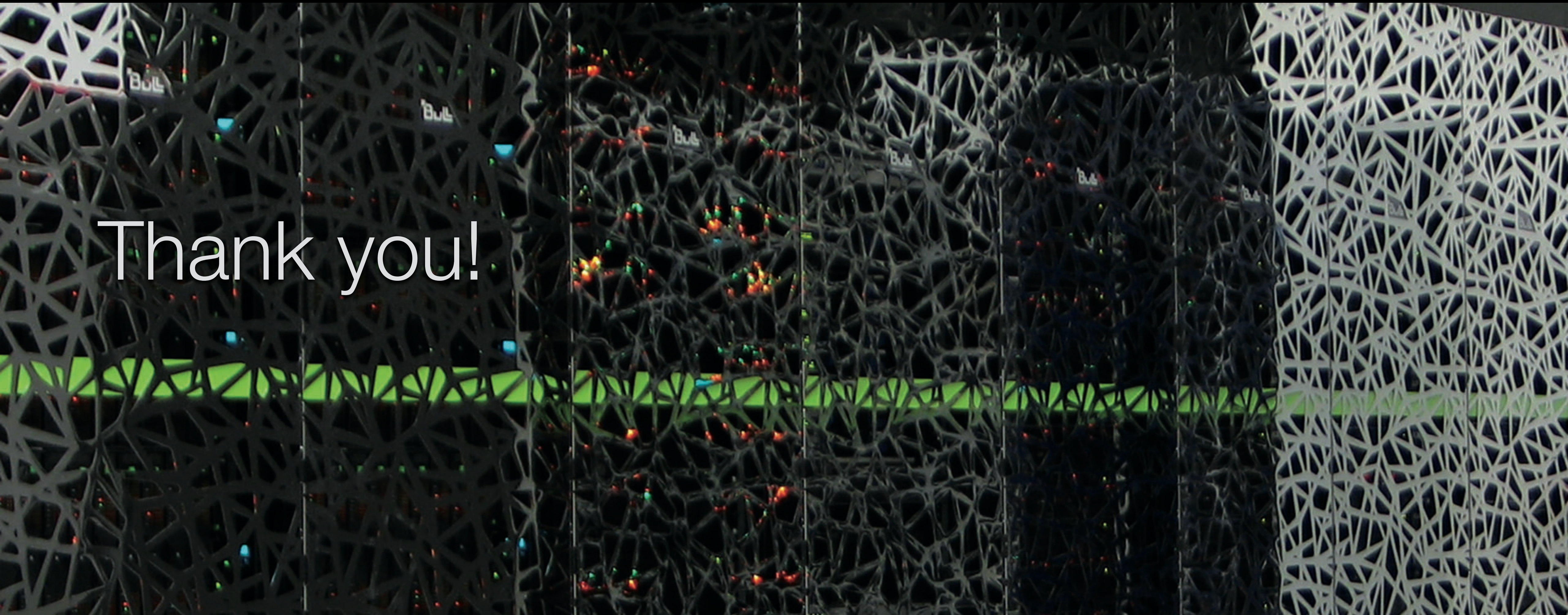
- Analyse software usage with Xalt
- Automate all processes with Jenkins
- Modify/create easyconfigs/easyblocks, PR
- Run regression tests



Workflow we aim for

- Analyse software usage with Xalt
- Automate all processes with Jenkins
- Modify/create easyconfigs/easyblocks, PR
- Run regression tests
- Create documentation





Thank you!