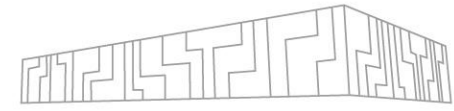




EASYBUILD MODULES

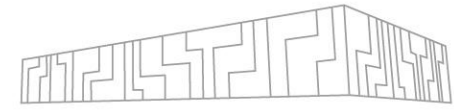
Milan Jaros, Ondrej Vysocky,
Lukas Krupcik

EASYBUILD & MODULES



Scientific Software Installation

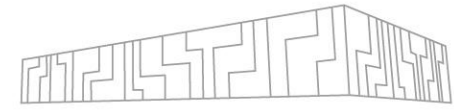
- | User request / critical updates / new software
- | All software on shared storage
- | Long-term support of installed software
- | Optimized for HPC cluster
 - | Built from source codes
 - | Linked with optimized libraries
 - | Build Optimization
 - | Host instruction set



Common Issues with Scientific Software

- | Incorrect use of build tools (make, cmake...)
- | Non-standard installation scripts
- | Incomplete build procedure (no configure)
- | Interactive installation scripts
- | Hardcoded paths and parameters
- | Dependent on specific version of library
- | ...

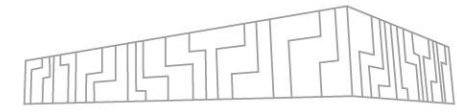
EASYBUILD & MODULES



Compilation Challenges

- | cmake, cmake --build
- | cmake, make, make install
- | make, make install
- | make
- | configure, make
- | configure, make, make install
- | autogen, configure, make, make install
- | install.sh
- | setup.py
- | and many other compilation procedures...

EASYBUILD & MODULES



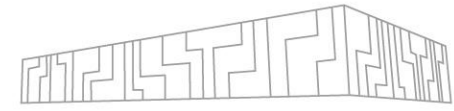
Environment Modules

- | Canonical way to access installed software
- | Module files specify user environment settings
- | LMOD 8.7.37 is installed on Karolina

/apps/modules/OS			
CentOS/6.9-GPU (s)	CentOS/7.4-GPU (s)	CentOS/7.5-VarROC (s,D)	Debian/8.0 Singularity-wrappers/master (s,D)
CentOS/6.9 (s)	CentOS/7.4 (s)	Debian/8.0-GPU (s)	Ubuntu/16.04-GPU (s)
Ubuntu/16.04 (s,D)			
/apps/modules/bio			
ABYSS/2.0.2-foss-2018a	GATK/4.0.2.1-Java-1.8.0_144	GROMACS/5.1.2-Intel-2016a-hybrid	RELION/2.1-foss-2017a-SP (G)
GROMACS/5.1.2-Intel-2015b-hybrid-single-cuda	GROMACS/2016.5-Intel-2017b	RELION/2.1-foss-2017a-SP (G,D)	
GROMACS/5.1.2-Intel-2015b-hybrid-single-cuda-7.5-PLUMED-2.2.1-test (G)	GROMACS/2018.1-Intel-2017c-hybrid-single-PLUMED (D)	alMost/2.1.0-foss-2015g	
GROMACS/5.1.2-Intel-2015b-hybrid-single-cuda-7.5-PLUMED-2.2.1 (G)	PLUMED/2.3b-foss-2016a	alMost/2.1.0-foss-2016a (D)	
		bowtie2/2.2.3	
/apps/modules/cae			
COMSOL/5.2-COM	COMSOL/5.2-EDU (D)	OpenFOAM/4.1-Intel-2017a	OpenFOAM/5.0-Intel-2017a (D)
		deMonNano/4.3.6	
/apps/modules/chem			
ABINIT/8.2.2-Intel-2017a	LAMMPS/22Jun2018-Intel-2017a	PLUMED/2.4.2-Intel-2017c (D)	nand/2.8 (D)
ASE/3.15.0-Python-2.7.13-base (D)	NMChem/6.6.revision27746-Intel-2017a-2015-10-20-Python-2.7.13 (D)	QuantumESPRESSO/5.4.0-Intel-2017.00	xdrfile/1.1.4-foss-2015g
Amber/18-Intel-2017b	NMChem/6.6.revision27746-Lonkl-2017a-2015-10-20-Python-2.7.13 (D)	QuantumESPRESSO/6.1-Intel-2017a	xdrfile/1.1.4-foss-2016a
Amber/18-HPICH-3.2-GCC-4.9.3-2.25 (D)	ORCA/4.0.1.2	cd2k-mpl/2.5.1-gcc (D)	xdrfile/1.1.4-Intel-2015b (D)
CP2K/5.1	OpenBabel/2.4.1-Python-2.7.13	Lammps/28Jun14	
LAMMPS/17Jan2018-foss-2017a-CUDA (G)	PLUMED/2.2.1-Intel-2015b	libxc/3.0.0	
LAMMPS/17Jan2018-Intel-2017a		molpro/2010.1-p45-Intel	
/apps/modules/compiler			
Clang/5.0.0-GCC-6.3.0-2.27	CCcore/4.9.3	LLVM/7.0.0-GCC-6.3.0-2.27	lfort/2017.1.132-GCC-5.4.0-2.26
GCC/4.4.7-system	CCcore/5.3.0	LLVM/7.0.0-Intel-2017c	lfort/2017.1.132-GCC-6.3.0-2.27
GCC/4.7.0	CCcore/5.4.0	OpenCoarrays/1.8.10-GCC-6.3.0-2.27 (D)	lfort/2017.4.196-GCC-6.4.0-2.28
GCC/4.8.3	CCcore/6.3.0	PGI/17.9-GCC-6.3.0-2.27	lfort/2017.5.239-GCC-6.3.0-2.27
GCC/4.9.3-binutils-2.25	CCcore/6.4.0	PGI/18.5-GCC-6.3.0-2.27 (D)	lfort/2017.7.259-GCC-6.3.0-2.27
GCC/4.9.3-1f	CCcore/7.1.0	bupe/2.16.2	lfort/2018.1.163-GCC-6.4.0-2.28
GCC/4.9.3	CCcore/8.1.0 (D)	chicken/4.8.0.6	lfort/2018.3.222-GCC-8.1.0-2.30 (D)
GCC/4.9.3-2.25	LLVM/3.8.1-Intel-2017a	gcc/4.8.1	tspec/1.9.1
GCC/5.1.0-binutils-2.25	LLVM/4.0.0-GCC-6.3.0-2.27	gpc/4.8.0.3	java/1.7
GCC/5.3.0-2.26	LLVM/5.0.0-GCC-6.3.0-2.27	lcc/2015.3.187-GNU-4.9.3-2.25	
GCC/6.3.0-2.27	LLVM/6.0.0-Py-2.7	lcc/2015.3.187-GNU-5.1.0-2.25	
GCC/7.1.0-2.28 (D)	LLVM/6.0.1-GCC-6.3.0-2.27	lcc/2016.1.150-GCC-4.9.3-2.25	
		lcc/2016.1.150-GCC-4.9.3-2.25	
		lcc/2017.0.098-GCC-5.4.0-2.26	
/apps/modules/data			
GDAL/1.9.2-foss-2015g	HDFS/1.0.16-foss-2016a-serial	HDFS/1.8.17-Intel-2017a	netCDF/4.4.1-Intel-2017a
GDAL/2.1.0-foss-2015g	HDFS/1.8.16-foss-2016a	HDFS/1.8.18-Intel-2017a-serial	netCDF/4.4.1.1-Intel-2017a (D)
GDAL/2.1.0-GCC-6.3.0-2.27	HDFS/1.8.16-Intel-2015b	HDFS/1.8.18-patch1-Intel-2017a	netCDF/4.4.1.1-Intel-2017a
GDAL/2.1.3-Python-2.7.13 (D)	HDFS/1.8.16-Intel-2016.01	HDFS/1.10.1-GCC-6.3.0-2.27-serial	netCDF-Fortran/4.4.4-Intel-2017a
			netCDF/4.4.1-Intel-2017a
/apps/modules/debugger			
Forge/5.1-43967 (D)	Forge/6.0.6 (D)	Forge/7.0.2 (D)	Forge/7.0.5-test
Forge/5.7	Forge/6.1.2	Forge/7.0.3	Forge/7.1
Forge/6.0.5 (D)	Forge/7.0.1 (D)	Forge/7.0.4	Forge/7.0.5
			PerformanceReports/7.0.6
			PerformanceReports/7.1 (D)
			TotalView/2018.2.6 (D)
			TotalView/2018.1.12

| <https://docs.it4i.cz/en/docs/software/modules/lmod>

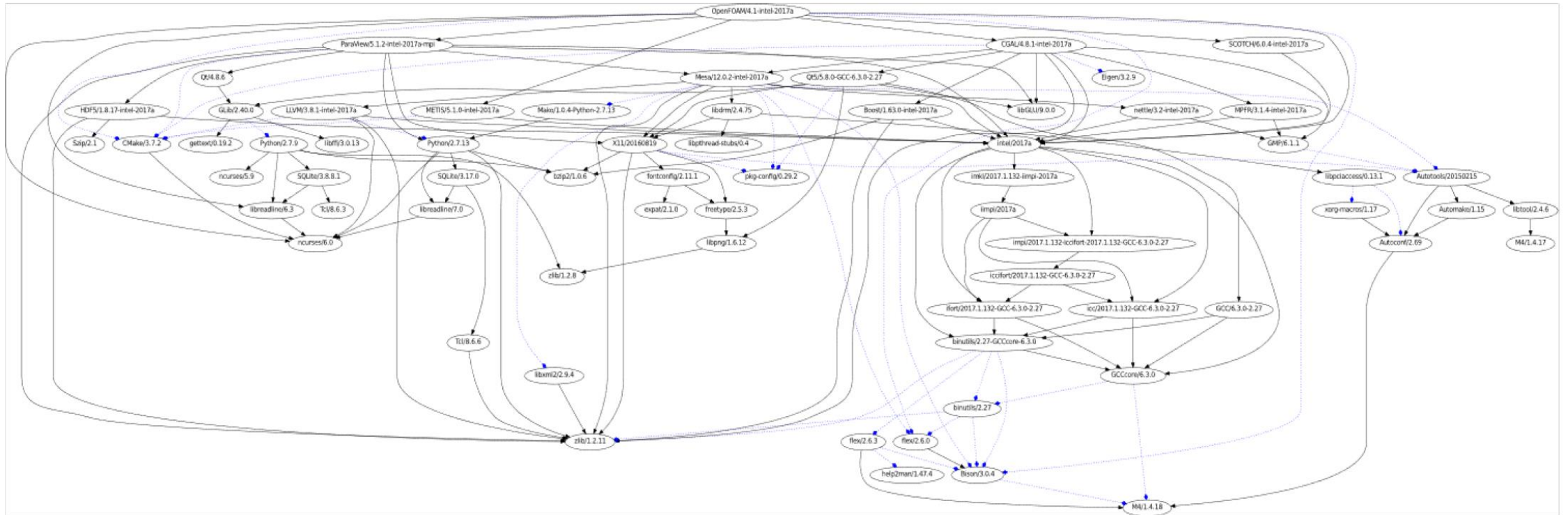
EASYBUILD & MODULES



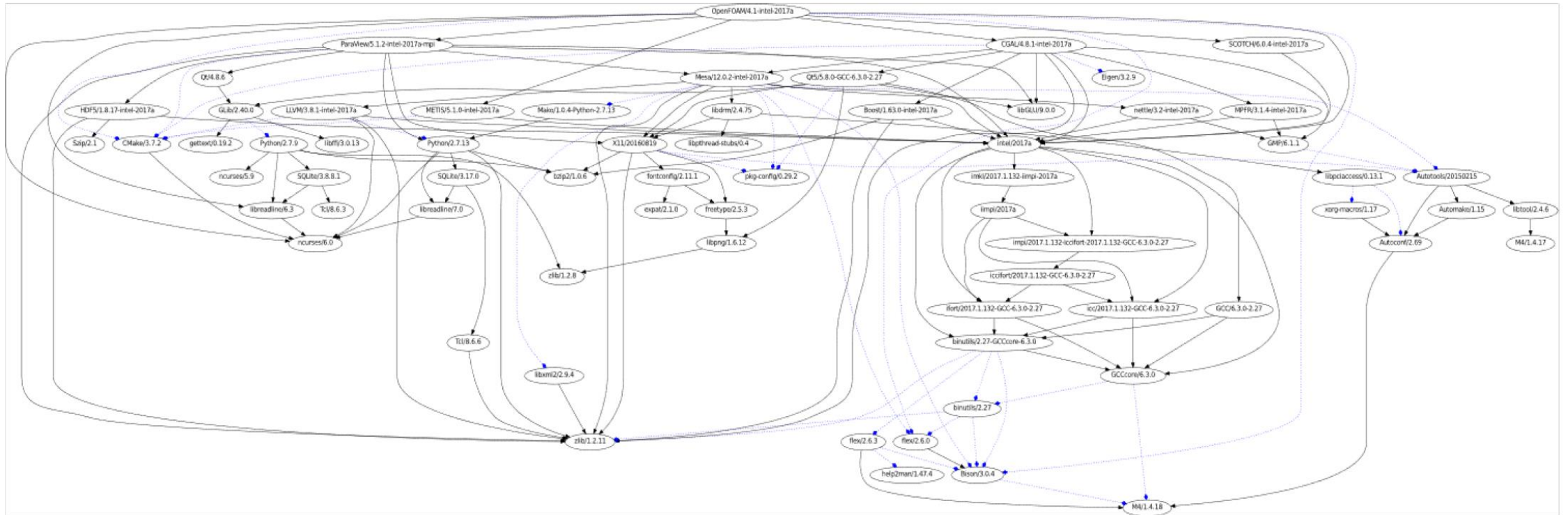
Challenges in Dependency Management

| OpenFOAM/4.1

OpenFOAM/4.1 - 67 dependencies

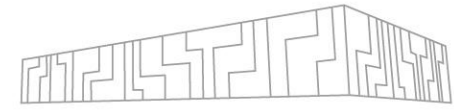


OpenFOAM/4.1 - 67 dependencies



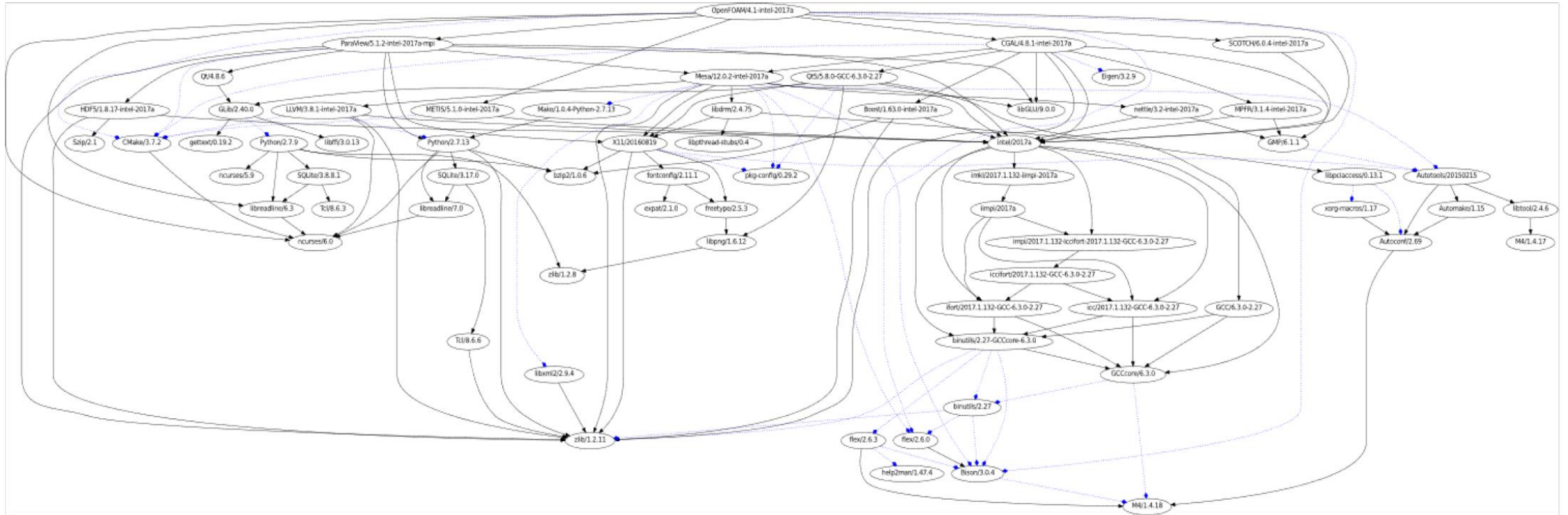
Manual installation?

EASYBUILD & MODULES



Challenges in Dependency Management

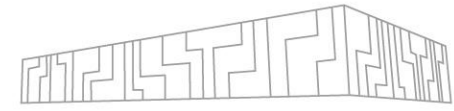
| OpenFOAM/4.1 - 67 dependencies



| Only one command...

| **eb OpenFOAM-4.1-intel-2017a.eb -r**

EASYBUILD & MODULES

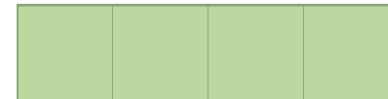
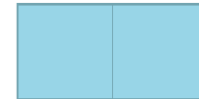
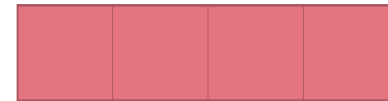


EasyBuild – Building Software With Ease

- | Framework for installing software
- | Collection of Python packages and modules
- | In development from 2009 at The Ghent University
- | Public from 2012

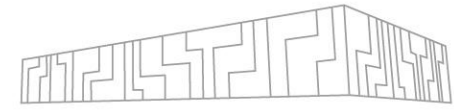
- | Massive community

| <https://docs.easybuild.io/>



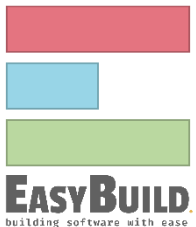
EASYBUILD.io
building software with ease

EASYBUILD & MODULES

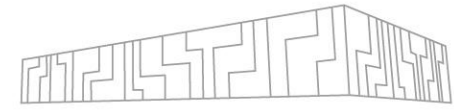


Features

- | Fully autonomous build and installation of SW
 - | Automatic dependency resolution
 - | Automatic module file generation
- | Logging of build/install procedure
- | Archiving of build specification
- | Extendable by user with additional easyblocks, toolchain, easyconfigs...
- | Actively developed
- | Each release comprehensively tested
- | Worldwide community



EASYBUILD & MODULES



Terminology

| EasyBuild framework

- | Core of EasyBuild, python modules and packages
- | Unpacking tarballs, applying patches...

| Easyblock

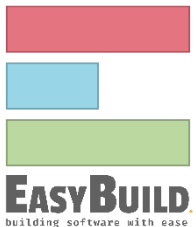
- | Implements build/install procedure
- | Python module, “plugin” for framework

| Easyconfig

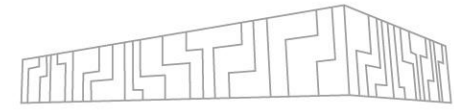
- | Build specification (software name, compiler...)

| Compiler toolchain

- | Compiler with accompanying libraries



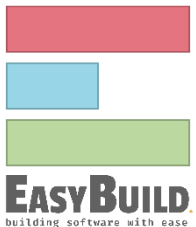
EASYBUILD & MODULES



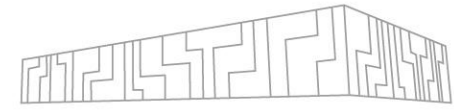
Installation Procedure

1. Parse easyconfig – process config, check dependencies
2. Fetch sources – download or search files
3. Check readiness – verify files, create build folder
4. Unpack sources – unpack tar/zip/rpm...
5. Apply patches – if any
6. Prepare – setup environment, dependencies
7. Configure – environment, libraries, optimization
8. Build – compile software
9. Test – check binaries/libraries
10. Install – to /apps/all/name/version...
11. Extensions – e.g. Python
12. Sanity checks – check folders/files/commands
13. Cleanup – remove temporary files
14. Environment module – create module file
15. Permissions – adjust access
16. Packaging – generate packages (FPM → RPM)
17. Test cases – run only for specific software

```
== processing EasyBuild easyconfig /apps/easybuild/easyconfigs-it4i/g/git/git-2.19.0.eb
== building and installing git/2.19.0...
== fetching files...
== creating build dir, resetting environment...
== unpacking...
== patching...
== preparing...
== configuring...
== building...
== testing...
== installing...
== taking care of extensions...
== postprocessing...
== sanity checking...
== cleaning up...
== creating module...
== permissions...
== packaging...
== COMPLETED: Installation ended successfully
```



EASYBUILD & MODULES

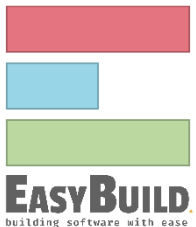


Commands:

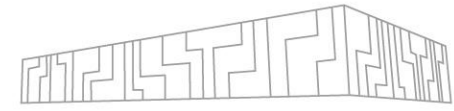
- | \$ eb git-2.19.0.eb
- | \$ eb ~/easyconfigs/git-2.19.0.eb
- | \$ eb --software=git,2.19.0 --toolchain=GCC,14.3.0

Options:

- | --robot/-r #dependency
- | --debug/-d #debug
- | --search/-S #search
- | --dry-run/-D #dry run
- | --extended-dry-run/-x #extended dry run



EASYBUILD & MODULES



Easyconfig Structure

```
easyblock = 'ConfigureMake'
```

```
name = 'git'
```

```
version = '2.19.0'
```

```
homepage = 'http://git-scm.com/'
```

```
description = """Git is a free and open source distributed version control system..."""
```

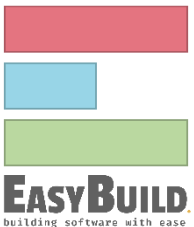
```
toolchain = {'name': 'dummy', 'version': ''}
```

```
sources = ['v%(version)s.tar.gz']
```

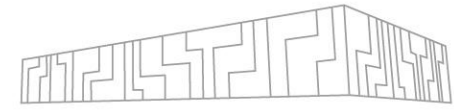
```
source_urls = ['https://github.com/git/git/archive']
```

| Other parameters: e.g. preconfigopts, sanity_check_paths, moduleclass

| Use: **ml git/2.19.0**



MODULES



"The Environment Modules package provides for the dynamic modification of a user's environment via module files."

- Preinstalled software ready to use for you
- **ml av module_name** – gives list of available modules
- **ml module_name** – loads the module
- **ml** – list of loaded modules
- **ml unload module_name** – remove of loaded module
- **ml purge** – removes all loaded modules



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