## Uni.lu HPC School 2018

PS3b: Software Build and Customization using Easybuild



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#### Latest versions available on Github:



UL HPC tutorials:

https://github.com/ULHPC/tutorials

**UL HPC School:** 

http://hpc.uni.lu/hpc-school/

PS3b tutorial sources:

ulhpc-tutorials.rtfd.io/en/latest/tools/easybuild/









2018













#### Introduction

# **Summary**

Introduction

2 Software/Modules Management





# Main Objectives of this Session

Discover Environment Modules and Lmod

•	Installation of EasyBuild	Part 2 (a)
•	Understanding local vs. global installation	Part 2 (b)
•	Build your own software on top of the provided	Part 2 (c)
	software set	
	→ local installation of HPL	
•	Write your own easyconfig file	Part 2 (d)

Part 1



## **Summary**

Introduction

2 Software/Modules Management



https://hpc.uni.lu/users/software/

- Based on Environment Modules / LMod
  - $\hookrightarrow$  convenient way to dynamically change the users environment \$PATH
  - → permits to easily load software through module command
- Currently on UL HPC:
  - $\rightarrow$  > 163 software packages, in *multiple* versions, within 18 categ.
  - → reworked software set for iris cluster and now deployed everywhere
     √ RESIF v2.0, allowing [real] semantic versioning of released builds

  - \$> module avail

- # List available modules
- \$> module load <category>/<software>[/<version>]





 $\bullet$  Key module variable: \$MODULEPATH / where to look for modules

 $\hookrightarrow$  altered with module use <path>. Ex:

export EASYBUILD\_PREFIX=\$HOME/.local/easybuild
export LOCAL\_MODULES=\$EASYBUILD\_PREFIX/modules/all
module use \$LOCAL\_MODULES





Key module variable: \$MODULEPATH / where to look for modules

→ altered with module use <path>. Ex:

```
export EASYBUILD_PREFIX=$HOME/.local/easybuild
export LOCAL_MODULES=$EASYBUILD_PREFIX/modules/all
module use $LOCAL MODULES
```

#### Main modules commands:

Command	Description
module avail	Lists all the modules which are available to be loaded
module spider <pattern></pattern>	Search for among available modules (Lmod only)
module load <mod1> [mod2]</mod1>	Load a module
module unload <module></module>	Unload a module
module list	List loaded modules
module purge	Unload all modules (purge)
module display <module></module>	Display what a module does
module use <path></path>	Prepend the directory to the MODULEPATH environment variable
module unuse <path></path>	Remove the directory from the MODULEPATH environment variable



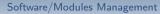




http://hpcugent.github.io/easybuild/

- Easybuild: open-source framework to (automatically) build scientific software
- Why?: "Could you please install this software on the cluster?"
  - → Scientific software is often difficult to build
    - √ non-standard build tools / incomplete build procedures
      - √ hardcoded parameters and/or poor/outdated documentation
  - $\hookrightarrow$  EasyBuild helps to facilitate this task
    - √ consistent software build and installation framework
    - √ includes testing step that helps validate builds
    - √ automatically generates LMod modulefiles
- \$> module use \$LOCAL MODULES
- \$> module load tools/EasyBuild
- \$> eb -S HPL # Search for recipes for HPL software
- \$> eb HPL-2.2-intel-2017a.eb # Install HPL 2.2 w. Intel toolchain







- RESIF: Revolutionary EasyBuild-based Software Installation Framework
  - → Automatic Management of software sets
  - → Fully automates software builds and supports all available toolchains
  - → Clean (hierarchical) modules layout to facilitate its usage

  - → Define options and software in easy to read yaml files
  - $\,\hookrightarrow\,$  Targeted at ULHPC sysadmins use case to build many softwares in one go





### Available software sets

- Gaia
  - → default: available by default
  - → bioinfo: load with

module use \$RESIF\_ROOTINSTALL/bioinfo/modules/all

- Iris
  - → default: available by default
  - → bioinfo: load with

module use /opt/apps/resif/data/stable/bioinfo/modules/all





### **Policies**

- We provide software that is used by many users on the cluster
- What the users should install themselves:
  - $\hookrightarrow$  Python packages
  - $\hookrightarrow \ \mathsf{R} \ \mathsf{packages}$
  - $\hookrightarrow$  Perl modules
  - $\hookrightarrow$  software only used by 1 or 2 persons



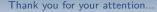


We provide several how-tos and tutorials for installing software as a user on the ULHPC website and in our HPC school tutorials:

- Installation with EasyBuild
- Installation from source with configure and make
- Installation of Python packages and usage of virtual environments
- Installation of Perl modules and how to set up a local library

Or just download precompiled binaries (see Bioinformatics tutorial) ;-)







### **Questions?**

http://hpc.uni.lu

#### High Performance Computing @ uni.lu

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