



UL HPC School 2017

PS3b: Software Build and Customization using Easybuild on the UL HPC Platform

UL High Performance Computing (HPC) Team

Sarah Peter

University of Luxembourg (UL), Luxembourg

<http://hpc.uni.lu>

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:

<https://github.com/ULHPC/tutorials/tree/devel/advanced/easybuild>





Summary

1 Introduction

2 Software/Modules Management



Main Objectives of this Session

- Understand LMod / Environment module
- Discover Easybuild
- Build you own software on top of the provided software set



Summary

1 Introduction

2 Software/Modules Management



Software/Modules Management

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

- Based on Environment Modules / **LMod**
 - ↪ convenient way to dynamically change the users' environment \$PATH
 - ↪ permits to easily load software through module command
- Currently on **UL HPC**:
 - ↪ **133 software packages**, in *multiple* versions, within **18 categories**
 - ↪ hierarchical organization **Ex:** toolchain/ictce

```
$> module avail
```

List available modules

```
$> module load <category>/<software>[/<version>]
```



Software/Modules Management

<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 are often **painful** to build
 - ✓ non-standard build tools / incomplete build procedure
 - ✓ hardcoded parameters and/or poor/outdated documentation
 - EasyBuild helps to facilitate this task
 - ✓ consistent software build and installation framework
 - ✓ automatically generates LMod modulefiles

```
$> module use /path/to/easybuild
$> module load tools/EasyBuild toolchain/intel
$> eb -S HPL      # Search for recipes for HPL software
$> eb HPL-2.2-intel-2017a.eb # Install HPC 2.2 w. Intel toolchain
```



Software/Modules Management

- **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
 - ↪ **Versioning** of software set builds
 - ↪ Easyconfig files from multiple sources
 - ↪ Define options and software in easy to read **yaml** files
 - ↪ Targeted at ULHPC sysadmins use case to build many softwares in one go



Available software sets

- Gaia

- ↪ **core**: available by default

- ↪ **lcsb**: load with

```
module use $RESIF_ROOTINSTALL/lcsb/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:
 - ↪ Python packages
 - ↪ R packages
 - ↪ Perl modules
 - ↪ software only used by 1 or 2 persons



DIY

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)
;-)



Thank you for your attention...

Questions?

<http://hpc.uni.lu>

The UL High Performance Computing (HPC) Team

University of Luxembourg, Belval Campus:

Maison du Nombre, 4th floor

2, avenue de l'Université

L-4365 Esch-sur-Alzette

mail: hpc@uni.lu



1 Introduction

2 Software/Modules Management