

UL HPC School 2017

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

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Latest versions available on Github:



UL HPC tutorials:

UL HPC School:

PS3b tutorial sources:

https://github.com/ULHPC/tutorials

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

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

















Summary

Introduction



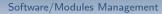




Main Objectives of this Session

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







Summary

Introduction







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

 - \$> module avail

List evailable modules

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





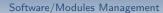
Software/Modules Management



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 - √ hardcoded parameters and/or poor/outdated documentation
 - $\hookrightarrow\,$ 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







- 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

 - → Easyconfig files from multiple sources
 - → 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

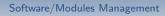
 - → Icsb: load with

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
 - \hookrightarrow R packages
 - → Perl modules
 - \hookrightarrow software only used by 1 or 2 persons



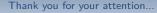


We provide several how-tos and tutorials for installing software as a user on the ULHPC website and in our HPC school tutorials:

- 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

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1 Introduction

