High Performance
Computing &
Big Data Services

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LET'S MAKE IT HAPPEN

Uni.lu HPC School 2020

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/

Summary

Main Objectives of this Session

- **Discover** Environment Modules and Lmod — Part 1
- **Installation** of EasyBuild — Part 2 (a)
- Understanding **local vs. global** installation — Part 2 (b)
- **Build your own software** on top of the provided software set — Part 2 (c)
  - ↪ local installation of a select software
  - ↪ using **existing** easyconfigs
- **Write your own easyconfig** file — Part 2 (d)
  - ↪ build the latest version of CMake
- Contribute back to Easybuild — Part 3

Summary

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: > **230 software packages**, in *multiple* versions, within **18 categ.**
  - ↪ reworked software set now deployed everywhere
    - ✓ RESIF v3.0, allowing [real] semantic versioning of released (arch-based) builds
  - ↪ hierarchical organization **Ex**: `toolchain/{foss,intel}`

```
$> module avail                                    # List available modules
```

```
$> module spider <pattern>          # Search for <pattern> within available modules
```

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

Software/Modules Management

- Key `module` variable: `$MODULEPATH` / where to look for modules.
  - ↪ **default** `iris`: `/opt/apps/resif/iris/<version>/{broadwell,skylake,gpu}/modules/all`
  - ↪ **default** `aion`: `/opt/apps/resif/aion/<version>/{epyc}/modules/all`
    - ✓ altered/prefix new path with `module use <path>`. **Ex** (to use **local** modules):

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

Software/Modules Management

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

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

ULHPC Toolchains and Software Set Versioning

- **Yearly** release based on Easybuid release of toolchains
  - ↪ see Component versions (**fixed per release**) in the foss and intel toolchains
    - ✓ count 6 months of validation/import *after* EB release before ULHPC release

Name	**Type**	2019[a] (prod/old)	**2019b** (devel)	**2020a** (next)
`GCCCore`	compiler	8.2.0	8.3.0	9.3.0
`foss`	toolchain	2019a	2019b	2020a
`intel`	toolchain	2019a	2019b	2020a
Python		3.7.2 (and 2.7.15)	3.7.4 (and 2.7.16)	3.8.2

```
# (new) 2019b software set - iris cluster
unset MODULEPATH
module use /opt/apps/resif/iris/2019b/broadwell/modules/all
# OR (when appropriate) skylake/GPU-specialized builds **ONLY** on skylake/GPU nodes
module use /opt/apps/resif/iris/2019b/skylake/modules/all
module use /opt/apps/resif/iris/2019b/gpu/modules/all
```

Practical Session Time

Your Turn!

Hands-on Easybuild

▶ url ◀ | github | src

- **Discover** Environment Modules and Lmod — Part 1
- Local Install/Update of EasyBuild in your `$HOME` — Part 2
- Search and build a missing/more recent software in your `$LOCAL_MODULES`
- Write your own easyconfig file
  ↪ build the latest version of a software you wish to test
- Contribute back to Easybuild — Part 3

Questions?

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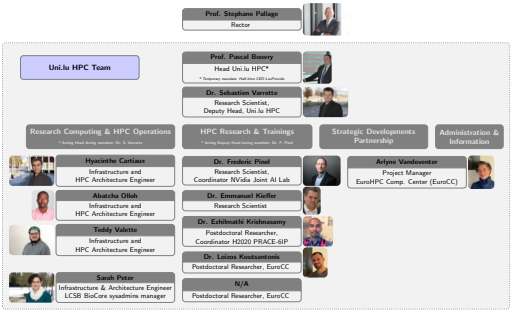

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