EasyBuild tutorial
Part 2: Using EasyBuild

For the LUMI User Support Team

Tue March 23rd 2021

EasyBuild tutorial for LUST

- Part I: **Introduction to EasyBuild** *(Tue March 9th 2021, 9am-12 CET)*
- Part II: **Using EasyBuild** *(Tue March 23rd 2021, 9am-12 CET)*

  today!
- Part III: **Advanced topics** *(Tue March 30th 2021, 9am-12 CET)*

  rescheduled!
- Part IV: **EasyBuild on Cray systems** *(to be planned)*

Practical information

- Tutorial website: **https://easybuilders.github.io/easybuild-tutorial**
  - Use LUMI version (see menu on the left)

- For hands-on demos and exercises, we will use **Puhti @ CSC**
  - `ssh username@puhti.csc.fi`
  - Small software stack installed with EasyBuild available in project space:

    ```
    module use /projappl/project_2003866/easybuild/modules/all
    ```
  - Load EasyBuild module: `module load EasyBuild/4.3.3`
  - Configure EasyBuild to use your home directory, except for build directories:

    ```
    export EASYBUILD_PREFIX=$HOME/easybuild
    export EASYBUILD_BUILDPATH=/tmp/$USER
    ```

Part II: Using EasyBuild

- [09:00-09:20 CET] Troubleshooting: errors, logs, build directories
- [09:20-09:40 CET] Hands-on exercise: fixing a broken easyconfig file
- [09:40-10:15 CET] Creating easyconfig files: what & how
- [10:15-10:30 CET] *(short break)*
- [10:30-11:00 CET] Creating easyconfig files: hands-on example + exercise
- [11:00-12:00 CET] Implementing easyblocks

Part II: Using EasyBuild - Troubleshooting

- Errors
- Log files
- Build directories
- Hands-on exercise: fix the easyconfig file for installing `Subread`!

Part II: Using EasyBuild - Troubleshooting

Hands-on exercise, part 1: **sources**

- `subread-2.0.1-source.tar.gz` is not available yet

Part II: Using EasyBuild - Troubleshooting

Hands-on exercise, part 1: **sources**

- `subread-2.0.1-source.tar.gz` is not available yet
- Two possible solutions:
  - Manual download + copy to EasyBuild `sourcepath`
  - Add source URL to let EasyBuild download the sources:

```
source_urls = ['https://download.sourceforge.net/subread/']
```

Part II: Using EasyBuild - Troubleshooting

Hands-on exercise, part 2: **toolchain**

- No module available for GCC version 8.5.0

Part II: Using EasyBuild - Troubleshooting

Hands-on exercise, part 2: **toolchain**

- No module available for GCC version 8.5.0

- Fix: change toolchain version to use existing GCC module:

```
toolchain = {'name': 'GCC', 'version': '10.2.0'}
```

Part II: Using EasyBuild - Troubleshooting

Hands-on exercise, part 3: **failing build**

- Compilation command fails, incorrect compiler flag `-fast`

Part II: Using EasyBuild - **Troubleshooting**

Hands-on exercise, part 3: **failing build**

- Compilation command fails, incorrect compiler flag `-fast`
- Easy solution: replace `-fast` with `-Ofast`
- Better solution: use `$CFLAGS` set by EasyBuild in build environment:

```
buildopts = '-f Makefile.Linux CFLAGS="$CFLAGS -fcommon"'
```

Part II: Using EasyBuild - Troubleshooting

Hands-on exercise, part 4: **sanity check**

- Sanity check command fails: `unrecognized option '--version'`

Part II: Using EasyBuild - Troubleshooting

Hands-on exercise, part 4: **sanity check**

- Sanity check command fails: `unrecognized option '--version'`
- Easily fixed by using correct option `-v` :

```
sanity_check_commands = ["featureCounts -v"]
```

Part II: Using EasyBuild - Easyconfig files

- Easyconfigs vs easyblocks
- Writing easyconfig files
- Generating tweaked easyconfigs
- Copying easyconfigs
- Hands-on example

Part II: Using EasyBuild - Easyconfig files

Hands-on exercise, part 1: **a personal message**

- Personalize the message that `eb-tutorial` prints using `$USER`

Part II: Using EasyBuild - Easyconfig files

Hands-on exercise, part 1: **a personal message**

- Personalize the message that `eb-tutorial` prints using `$USER`
- Requires tweaking configure option, careful with single vs double quotes!

```
configopts = '-DEBTUTORIAL_MSG="Hello $USER." '
```

Part II: Using EasyBuild - Easyconfig files

Hands-on exercise, part 2: **trivial version bump**

- Install eb-tutorial version 1.1.0 using existing easyconfig

Part II: Using EasyBuild - Easyconfig files

Hands-on exercise, part 2: **trivial version bump**

- Install eb-tutorial version 1.1.0 using existing easyconfig
- Manual: copy easyconfig file + edit, then install via `eb`
- Easy using `--try-software-version`:

```
eb example.eb --try-software-version 1.1.0
```

Part II: Using EasyBuild - Easyconfig files

Hands-on exercise, part 3: **py-eb-tutorial**

- Create an easyconfig file for py-eb-tutorial version 1.0.0

Part II: Using EasyBuild - Easyconfig files

Hands-on exercise, part 3: **py-eb-tutorial**

- Create an easyconfig file for py-eb-tutorial version 1.0.0
- Solution:
  - Use generic `PythonPackage` easyblock (and use “`use_pip = True`”)
  - Include required dependencies: `SciPy-bundle` + `eb-tutorial`
  - Customize sanity check

Part II: Using EasyBuild - Easyblocks

- Generic vs software-specific easyblocks
- Python class name, Python module filename
- Overall structure + derived easyblock
- Easyconfig parameters
- File operations, shell commands, environment variables
- Logging and errors, custom sanity check
- Version-specific parts
- Compatibility with `--extended-dry-run` and `--module-only`