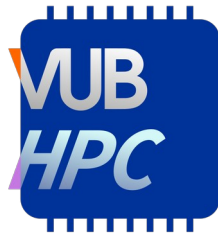


Controlling the shell environment in EasyBuild v5.0

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VLAAMS
SUPERCOMPUTER
CENTRUM



Vlaanderen
is supercomputing

WHO AM I?

Hi! I'm Alex (github: @lexming)

**Maintainer of EasyBuild
since 2020**

HPC sysadmin when not doing EB

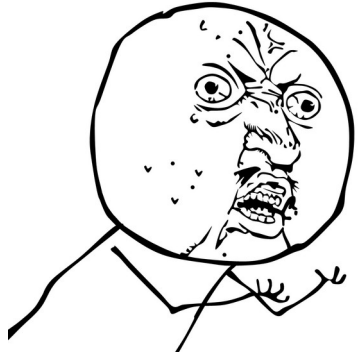
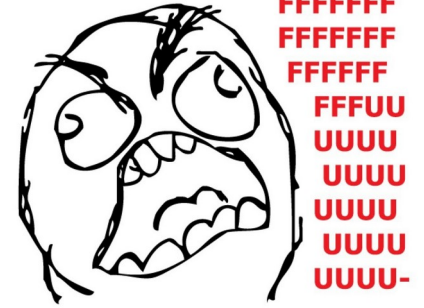
- ◆ HPC team of Vrije Universiteit Brussel (VUB) since 2019
- ◆ PhD in Computational Chemistry

This is me in Kraków using
EB 5.0, a world first!



WHAT IS THIS ABOUT?

```
$ ldd libawesome.so
libdl.so.2 => /lib/libdl.so.2 (0x00000000)
libz.so.1 => not found
```



```
/path/to/source.c:42: undefined reference to `GreatSymbol'
error: ld returned 1 exit status
```

```
error: colors.h: No such file or directory
```

```
$ python -c "import potato"
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ImportError: No module named potato
```

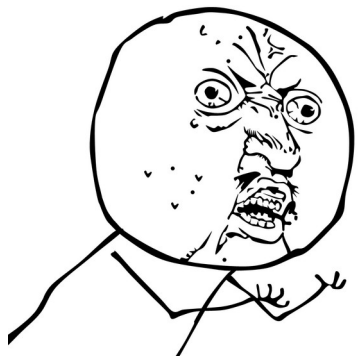
WHAT IS THIS ABOUT?

```
$ ldd libawesome.so  
    libdl.so.2 (0x00000000)  
    libz.so.1 (0x00000000)
```

\$LD_LIBRARY_PATH



FFFFFFF
FFFFFFF
FFFFFFF
FFFUU
UUUU
UUUU
UUUU
UUUU
UUUU



```
/path/to/source.c:42: undefined reference to `GreatSymbol'  
error: ld returned 1 exit status
```

\$LD_LIBRARY_PATH

```
error: colon is not a directory
```

\$CPATH

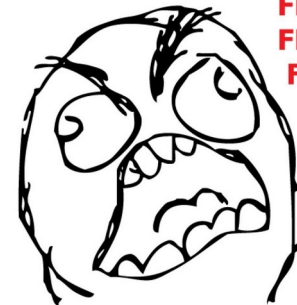
```
$ python -c "import potato"  
Traceback (most recent call last):  
  File "<stdin>", line 1, in <module>  
ImportError: No module named potato
```

\$PYTHONPATH

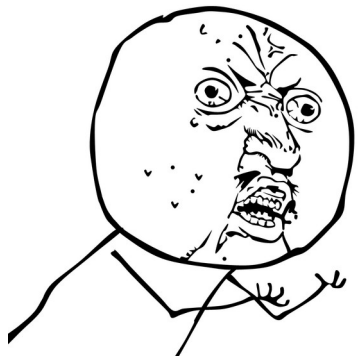
WHAT IS THIS ABOUT?

```
$ ldd libawesomeness.so  
lib...so.2 (0x00000000)  
li...
```

LIBRARY_PATH



FFFFFF
FFFFFF
FFFFFF
FFFUU
UUUU
UUUU
UUUU
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UUUU-



SEARCH PATHS

Environment variable that defines a list of paths that can potentially contain target files

PATH to 'GreatSymbol'

error: color... or directory

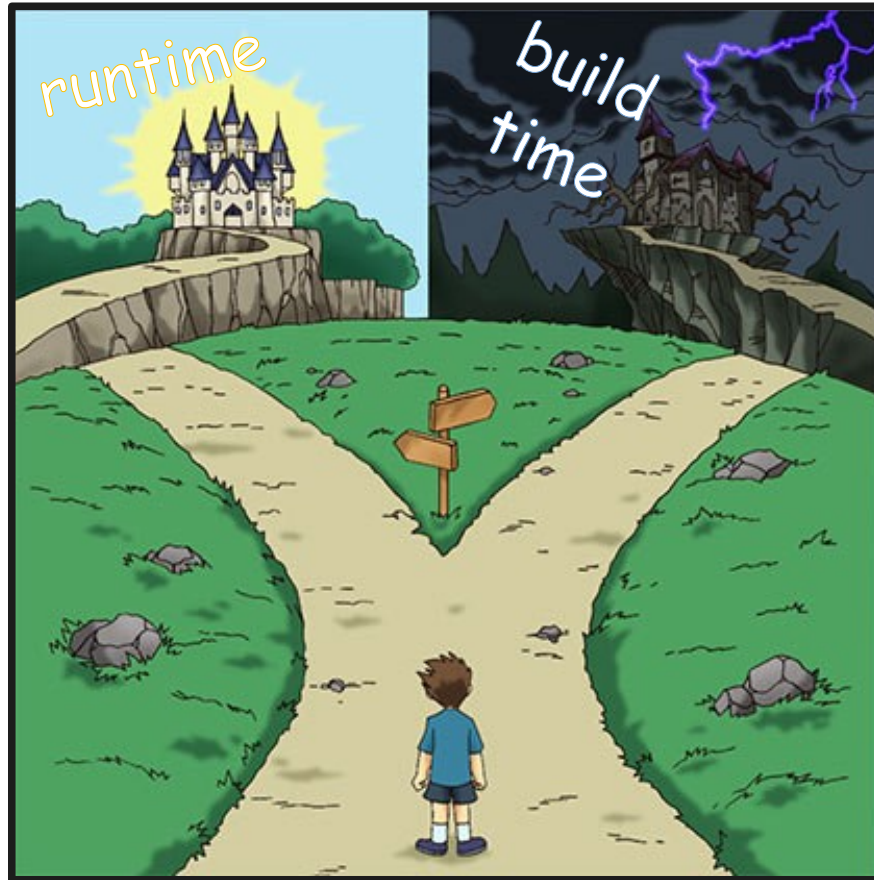
\$CPATH

Import... in <module>
module named potato

LD_LIBRARY_PATH

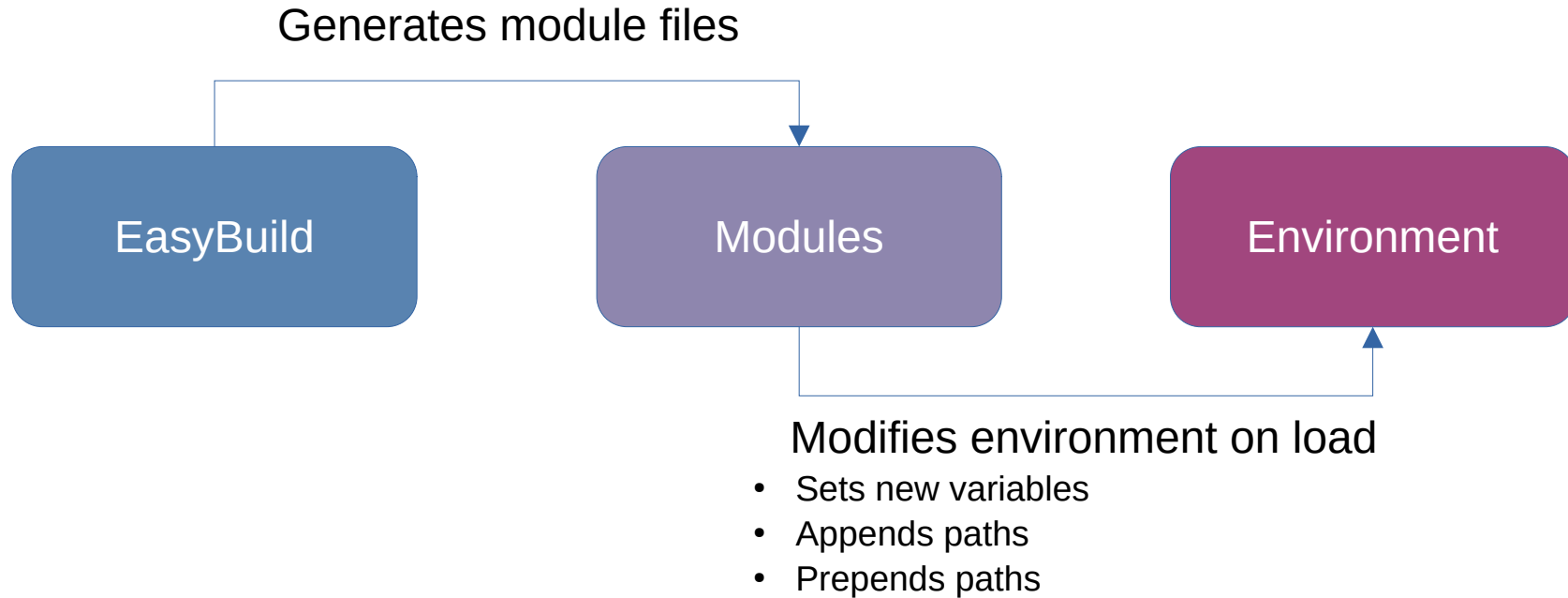
Runtime

- Modules are king
- EasyBuild is not even running
- Easy to check environment state



Build time

- Modules are still at play
- EasyBuild does its own tricks
- Tricky to check environment state



Framework

[easybuild.framework.easyblock]

EasyBlock.make_module_step()

- self.modules_header
- self.make_module_description()
- self.make_module_group_check()
- self.make_module_deppaths()
- self.make_module_dep()
- self.make_module_extend_modpath()
- **self.make_module_req()**
- self.make_module_extra()
- self.make_module_footer()

Framework

[easybuild.framework.easyblock]

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- self.make_module_footer()

EasyBuild v4.9

make_module_req()

- Parse dictionary from **make_module_req_guess()**
- Do many magic tricks about any possible content in the guess
- **!** No path expansion! **!**
- **!** Where is modextrapaths? **!**

make_module_req_guess()

- Populate dictionary with keys per environment variable
- Contains a default definition

Framework

[easybuild.framework.easyblock]

EasyBlock.make_module_step()

- self.modules_header
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- self.make_module_extend_modpath()
- **self.make_module_req()**
- self.make_module_extra()
- self.make_module_footer()

EasyBlock.module_load_environment

- Kind-of-dataclass that contains environment variable definitions
- Plus extra methods to easily manipulate environment variables

EasyBuild v5.0

make_module_req()

- Update environment with **modextrapaths**
- Read environment from **module_load_environment**
- Path expansion

Framework

[easybuild.tools.modules]

EasyBlock. module_load_environment

- Kind-of-dataclass that contains environment variable definitions
- Plus extra methods to easily manipulate environment variables

ModuleLoadEnvironment

- Contains collection of **ModuleEnvironmentVariable**
- Provides default environment definition
- Special getter, setter and other methods to manipulate the environment
- Capable of defining aliases of environment variables
- **No logic related to exporting environment variables into modules**

ModuleEnvironmentVariable

- Kind-of-dataclass for a single environment variable
- **Extra attributes:** type of variable, delimiter, placement
- Special getter, setter and other methods to manipulate the environment
- **No logic related to exporting environment variables into modules**

EasyBuild (framework)

- 1) EasyBlock gets from initialization
module_load_environment
- 2) Module step calls:
make_module_req()
- 3) Export module_load_environment
into module file
 - Inject modextrapaths
 - Expand paths
 - Generate module file code

Custom EasyBlocks

- Module load environment accessible at **all steps**:
self.module_load_environment
- If you need to check stuff in installation directory, use module step

```
self.module_load_environment.TBROOT = comp_libs_subdir_paths('tbb')
self.module_load_environment.LD_LIBRARY_PATH.append(os.path.join('lib', 'root'))
self.module_load_environment.remove('LIBRARY_PATH')
```

EasyBuild (framework)

- 1) EasyBlock gets from initialization `module_load_environment`
- 2) Module step calls: `make_module_req()`
- 3) Export `module_load_environment` into module file
 - Inject `modextrapaths`
 - Expand paths
 - Generate module file code

Custom EasyBlocks

- Module load environment accessible at **all steps**: `self.module_load_environment`
- If you need to check stuff in installation directory, use module step

Custom EasyConfigs

- Parameter `modextrapaths` is the **single interface** to manipulate `module_load_environment`

```
modextrapaths = {  
    'ENV_VAR_NAME': 'extra/subdir',  
    'WEIRD_ENV_VAR': {  
        'paths': ['another/subdir1', 'another/subdir2'],  
        'delimiter': '+',  
        'prepend': False,  
    },  
}
```

EVERYTHING SHOWED UP TO NOW DOES NOT MATTER!

Well, modules get loaded in the build environment. But then EasyBuild generates on its own the list of paths to passed to the compiler and linker.

- ◆ This is actually good, improves reliability of builds but not entirely relying on modules
- ◆ Modules still have a role, but (usually) with less precedence
- ◆ Where is that defined? In the **toolchain!**

Framework

[easybuild.tools.toolchain.toolchain]

Toolchains are not just a collection of dependencies. They have a lot of logic to run the build:

- ◆ Prepare step
 - Handle sysroot
 - Check dependencies
 - Load modules
 - **Add compiler/linker options for each dependency**
 - Prepare RPATH wrappers

--search-path-cpp-headers

- **flags**: CPPFLAGS environment variable, which translates into -I compiler options
- **cpath**: CPATH environment variable (less precedence)
- **include_paths**: C_INCLUDE_PATHS and co. environment variables (even less precedence)

--search-path-linker

- **flags**: LDFLAGS environment variable, which translates into -L compiler options
- **library_path**: LIBRARY_PATH environment variable (less precedence)

✨ **EasyBuild 5.0 is great!** ✨

- ◆ Clear and accessible definition of the environment that will be injected into module files
 - Use `self.module_load_environment` in easyblocks
 - Use `modextrapaths` in easyconfigs
- ◆ More control on how build environment is defined:
 - `--search-path-cpp-headers`
 - `--search-path-linker`

ACKNOWLEDGEMENTS



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Thank you for your attention!

