

# SITE PRESENTATION VUB

## 10th **EASYBUILD**. User Meeting

Vrije Universiteit Brussel (VUB)

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VRIJE  
UNIVERSITEIT  
BRUSSEL

VLAAMS  
SUPERCOMPUTER  
CENTRUM



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# THE VUB TIER-2



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- VUB is part of the VSC
- HPC team at the VUB Tier-2 cluster
  - Slurm scheduler
  - ~ 4,700 CPU cores (Intel + AMD)
  - ~ 30 NVIDIA GPUs
  - High-memory node with 1.5 TB of RAM
- We use EB4 and EB5 for our installations



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 **build\_tools** Public


 **vsc-software-stack** Public

 **easybuild-easyconfigs** Public

 site-vub  12 Branches  0 Tags

# WORKFLOW FOR INSTALL REQUESTS

- New easyconfig
- Add to VSC repository (site-vub)
- Create a PR in Easybuilders repo
- Install with a *submit script*
- Clean easyconfigs in site-vub

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 site-vub ▾  12 Branches  0 Tags

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easybuild-easyconfigs / contrib / easyconfig-templates / 2024a  
/ CMakeMake-minimalEb.tmpl

lexming remove checksums from templates 425610b · 2 weeks ago History

```

Code Blame 38 lines (27 loc) · 748 bytes
1 # Template for simple CMakeMake package in GCCcore 13.3.0
2 easyblock = 'CMakeMake'
3
4 name = 'softwareone'
5 version = '0.0.0'
6
7 homepage = 'https://www.domain.org'
8 description = ""
9 description in 80 chars long column
10 ""
11
12 toolchain = {'name': 'GCCcore', 'version': '13.3.0'}
13
14 source_urls = ['http://www.domain.org/download/']
15 sources = [SOURCELOWER_TAR_GZ]
16
17 builddependencies = [
18     ('binutils', '2.42'),
19     ('cmake', '3.29.3'),
20 ]
21
22 dependencies = [
23     ('dependencyname', '0.0.0'),
24 ]
25
26 sanity_check_paths = {
27     'files': ['bin/%(name)lower', 'lib/lib%(name)lower.s.(SHLIB_EXT)'],
28     'dirs': ['include'],
29 }
30
31 sanity_check_commands = [
32     "%(name)lower)s -v",
33     "%(name)lower)s -h 2>&1 | grep 'pattern.in.'output",
34 ]
35
36 moduleclass = 'module_class'
  
```

 build\_tools Public

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 site-vub ▾


 12 Branches

 0 Tags

# OUR SUBMIT SCRIPT

`submit_build.py`, submits jobs to install software with EasyBuild

- Determines which CPU architecture to use
- Creates Slurm job script dynamically
- If `--gpu` is specified, switches to a GPU partition
- Runs an Lmod cache update
- Some options:
  - Build location override (shared memory default)
  - `--bwrap` creates isolated namespace for software build
  - `--partition`, `--extra-flags`, `--rebuild`, etc.
- Keep it easy to use but flexible when needed

 `build_tools` Public `/bin/submit_build.py`

# DUMMY MODULES FOR GPU SOFTWARE

- ✗ Users get confused by GPU-only modules
- Generate dummy modules on CPU-only nodes
- Shows a clear message and points to documentation

???



```

506             #####
507             # ----- DUMMY MODULES ----- #
508             #####
509
510             is_cuda_software = 'CUDA' in self.name or 'CUDA' in self.cfg['versionsuffix']
511             if is_cuda_software and LOCAL_ARCH_FULL not in GPU_ARCHS:
512                 self.log.info("[pre-module hook] Creating dummy module for CUDA modules on non-GPU nodes")
513                 self.cfg['modluafooter'] = ""
514             if mode() == "load" and not os.getenv("BUILD_TOOLS_LOAD_DUMMY_MODULES") then
515                 LmodError([[
516                 This module is only available on nodes with a GPU.
517                 Jobs can request GPUs with the command 'srun --gpus-per-node=1' or 'sbatch --gpus-per-node=1'.
518
519                 More information in the VUB-HPC docs:
520                 https://hpc.vub.be/docs/job-submission/gpu-job-types/#gpu-jobs
521                 ]])
522             end""

```



build\_tools

Public

*/src/build\_tools/hooks\_hydra.py*



# ORGANIZING MODULES BY TOOLCHAIN GENERATION

- ✗ Users get confused by (sub)toolchain compatibility
- Set the `moduleclass` based on the toolchain generation
- Keep module tree clean and organized

???

```
129  def update_moduleclass(ec):
130      "update the moduleclass of an easyconfig to <tc_gen>/all"
131      tc_gen, log_msg = calc_tc_gen(
132          ec.name, ec.version, ec.toolchain.name, ec.toolchain.version, ec.easyblock)
133
134      if not tc_gen:
135          raise EasyBuildError("[parse hook] " + log_msg)
136
137      ec.log.info("[parse hook] " + log_msg)
138
139      ec['moduleclass'] = os.path.join(tc_gen, SUFFIX_MODULES_SYMLINK)
140
141      ec.log.info("[parse hook] updated moduleclass to %s", ec['moduleclass'])
```



build\_tools

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`/src/build_tools/hooks_hydra.py`

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```
✓ [15:50] vsc10800@login1 $VSC_SCRATCH $ ml av Python

----- /apps/brussel/RL8/skylake-ib/modules/2024a/all -----
Biopython/1.84-foss-2024a (D)
meson-python/0.16.0-GCCcore-13.3.0 (D)
netcdf4-python/1.7.1.post2-foss-2024a (D)
protobuf-python/5.28.0-GCCcore-13.3.0 (D)
Python-bundle-PyPI/2024.06-GCCcore-13.3.0 (D)
Python/3.12.3-GCCcore-13.3.0 (D)

----- /apps/brussel/RL8/skylake-ib/modules/2023a/all -----
Biopython/1.83-foss-2023a
Boost.Python/1.82.0-GCC-12.3.0
Brotli-python/1.0.9-GCCcore-12.3.0 (D)
bx-python/0.10.0-foss-2023a
CUDA-Python/12.1.0-gfbf-2023a-CUDA-12.1.1
flatbuffers-python/23.5.26-GCCcore-12.3.0 (D)
GitPython/3.1.40-GCCcore-12.3.0 (D)
graphviz-python/0.20.1-GCCcore-12.3.0
```

# FIX FOR INTEL COMPILERS ON AMD CPUs

## ✗ Intel compilers *get confused* by AMD CPUs

- Overrides with safe values:

Zen2 → `-march=core-avx2` ; Zen4 → `-march=rocketlake`

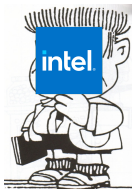
- Only applies for Intel-based toolchains

```

260     # set optarch for intel compilers on AMD nodes
261     optarchs_intel = {
262         'zen2': 'march=core-avx2',
263         # common-avx512 gives test failure for scipy
264         # see https://github.com/easybuilders/easybuild-easyconfigs/pull/18875
265         'zen4': 'march=rocketlake',
266     }
267     if LOCAL_ARCH in optarchs_intel and ec.toolchain.name in ['intel-compilers', 'iimpi', 'iimkl', 'intel']:
268         optarch = ec.toolchain.options.get('optarch')
269         # only set if not set in the easyconfig or if set to default value (i.e. True)
270         if not optarch or optarch is True:
271             ec.toolchain.options['optarch'] = optarchs_intel[LOCAL_ARCH]
272             ec.log.info(f"[parse hook] Set optarch in parameter toolchainopts: {ec.toolchain.options['optarch']}")

```

???



build\_tools

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# JAVA HEAP SIZING

- ✗ *Java gets confused* by Slurm memory limits
- Set max heap size to 80% of available memory
- No manual tuning needed for users

???

```
420         # set the maximum heap memory for Java applications to 80% of memory allocated to
421         # more info: https://projects.cc.vub.ac.be/issues/2940
422         if self.name == 'Java':
423             self.log.info("[pre-module hook] Set max heap memory in Java module")
424             self.cfg['modluafooter'] = ""
425         local mem = get_avail_memory()
426         if mem then
427             setenv("JAVA_TOOL_OPTIONS", "-Xmx" .. math.floor(mem*0.8))
428         end
429         ""
```



**build\_tools** Public

`/src/build_tools/hooks_hydra.py`

# Thank you!

Questions?