

- easybuilders/easybuild-easyconfigs {tools}[system/system] libtree v3.1.1 ✓ update  
#22193 by Thyre was merged on Jan 23 • Approved ↻ release after 4....
- easybuilders/easybuild-easyconfigs {perf}[impi/2024a] Add Score-P 8.4 (w/ CUDA 12.6.0) ✓ update  
#22143 by Thyre was merged on Jan 18 • Approved 1 task done ↻ 5.0.0
- easybuilders/easybuild-easyblocks Enhance Score-P EasyBlock for future releases and better oneAPI support. ✓ enhancement  
#3548 by Thyre was merged on Jan 18 • Approved ↻ 5.0
- easybuilders/easybuild-easyconfigs {devel}[GCCcore/14.2.0] CMake v3.31.3 × update  
#22107 by Thyre was closed on Jan 3 • Review required ↻ 1 task
- easybuilders/easybuild-easyconfigs {compiler}[system/system] NVHPC-24.11-CUDA-12.6.0 ✓ update  
#21877 by Thyre was merged on Nov 23, 2024 • Approved ↻ release after 4....
- easybuilders/easybuild-easyblocks enhance generic Bundle easyblock to transfer module requirements of components, but do not create logfile in components ✓ enhancement  
#3509 by Thyre was merged on Dec 26, 2024 • Approved 1 task done ↻ release after 4....

Annotations  
1 error and 2 warnings

```

System.IO.IOException: No space left on device : '/home/runner/runners/2.320.0/_diag/Worker_20241112-104429-utc.log'
at System.IO.RandomAccess.WriteAtOffset(SafeFileHandle handle, ReadOnlySpan`1 buffer, Int64 fileOffset)

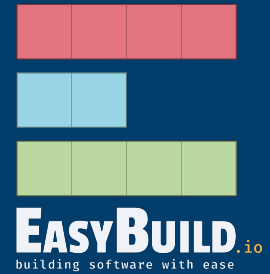
== building and installing GCCcore/13.3.0...
...
ERROR: Traceback (most recent call last):
  File "EasyBuild/4.9.3/[...]/easybuild/main.py", line 137, in build_and_install_software
    (ec_res['success'], app_log, err) = build_and_install_one(ec, init_env)
  File "EasyBuild/4.9.3/[...]/easybuild/framework/easyblock.py", line 4276, in build_and_install_one
    result = app.run_all_steps(run_test_cases=run_test_cases)
  File "EasyBuild/4.9.3/[...]/easybuild/easyblocks/g/gcc.py", line 1081, in run_all_steps
    return super(EB_GCC, self).run_all_steps(*args, **kwargs)
  File "EasyBuild/4.9.3/[...]/easybuild/framework/easyblock.py", line 4155, in run_all_steps
    self.run_step(step_name, step_methods)
  File "EasyBuild/4.9.3/[...]/easybuild/framework/easyblock.py", line 3990, in run_step
    step_method(self)()
  File "EasyBuild/4.9.3/[...]/easybuild/easyblocks/g/gcc.py", line 612, in configure_step
    cuda_cc = self.map_nvptx_capability()
  File "EasyBuild/4.9.3/[...]/easybuild/easyblocks/g/gcc.py", line 431, in map_nvptx_capability
    return sorted_gcc_cc[0]
IndexError: list index out of range

```

# 10th EasyBuild User Meeting

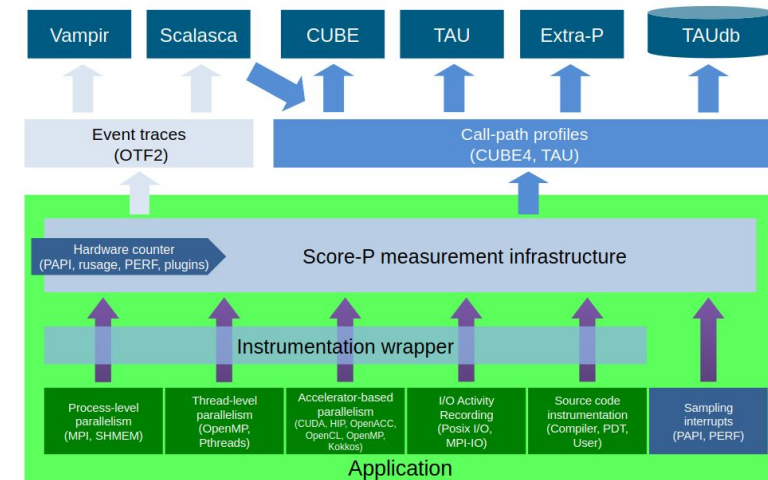
## Getting Started as EasyBuild Contributor

2025-03-25 | Jan André Reuter



# WHY DO I USE EASYBUILD?

- Software Developer for the performance measurement infrastructure **Score-P**
  - Main work focus: OpenMP, accelerators & compiler instrumentation
- Developing involves a lot of testing for different software versions, e.g.:
  - LLVM IR changes
  - New CUDA features
  - Changes in the OpenMP Tools Interface
  - ...



# WHY DO I USE EASYBUILD?

- Software Developer for the performance measurement infrastructure **Score-P**
  - Main work focus: OpenMP, accelerators & compiler instrumentation
- Developing involves a lot of testing for different software versions, e.g.:
  - LLVM IR changes
  - New CUDA features
  - Changes in the OpenMP Tools Interface
  - ...
- We have a CI for that, but...
  - HPC systems do have a limited amount of versions available
  - Doesn't really help for local development

test_tarball	
✓	docker_create_tarball_static
✓	docker_rocm
✓	eiger_PrgEnv-cray_shared
✓	eiger_PrgEnv-cray_static
🔄	eiger_PrgEnv-gnu_shared
🔄	eiger_PrgEnv-gnu_static
🔴	jureca_2024_aocc_parastation
🔄	jureca_2024_gcc_openmpi
🔄	jureca_2024_gcc_parastation
🔄	jureca_2024_intel_parastation
🔴	jureca_2024_nvhpc_openmpi
🔄	jureca_2024_nvhpc_parastation
🔄	jureca_2024_oneapi_parastation
🔄	jusuf_2024_gcc_openmpi
🔄	jusuf_2024_gcc_parastation
✓	jusuf_2024_gcc_static
🔄	jusuf_2024_intel_parastation
✓	jusuf_2024_intel_static
🔄	jusuf_2024_nvhpc_openmpi
🔄	jusuf_2024_nvhpc_parastation
🔄	juwels_2024_gcc_openmpi

# WHY DO I USE EASYBUILD?



- Software Developer for the performance measurement infrastructure **Score-P**
  - Main work focus: OpenMP, accelerators & compiler instrumentation
- **Solution: Have software locally available**
  - **EasyBuild:** Flexible, easily reproducible, and similar to software on HPC systems
  - In case where no EasyConfigs exist: Manual build...

-----  
CUDA :  
-----

Versions:  
CUDA/11.7.0  
CUDA/11.8.0  
CUDA/12.0.0  
CUDA/12.1.1  
CUDA/12.2.2  
CUDA/12.3.2  
CUDA/12.4.0  
CUDA/12.5.0  
CUDA/12.6.0  
CUDA/12.8.0

----- Core Compilers -----

AOCC/5.0	ROCm-LLVM/5.7.0
Clang/trunk	ROCm-LLVM/6.0.2
Clang/11.1.0	ROCm-LLVM/6.0.3
Clang/12.0.1	ROCm-LLVM/6.1.2
Clang/13.0.1	ROCm-LLVM/6.2.0
Clang/14.0.6	ROCm-LLVM/6.3.0
Clang/15.0.7	aomp/18.0-0
Clang/16.0.6	aomp/18.0-1
Clang/17.0.6	aomp/19.0-0
Clang/18.1.8	aomp/19.0-2
Clang/19.1.0	aomp/19.0-3
Clang/20.1.1	aomp/20.0-0

# NAIVE TRIES TO USE EASYBUILD...

- First tries to use EasyBuild on non-HPC system went... not well
- Unconventional OS (Arch Linux) not expected
- OS packages are picked up sometimes
  - Containers *can* help
- EasyBuild tutorial helped a lot for using it:
  - <https://tutorial.easybuild.io/>
- Started digging through EasyBuild & EasyConfigs to work around issues I ran into
- Lead to contributing fixes & local EasyConfigs

## Some GCCcore versions failing when building nvptx

```
make[1]: Entering directory '/data/EasyBuild-develop/build/GCCcore/12.3.0/system-system/gcc-12.3.0/build-nvptx-gcc'
mkdir -p -- ./fixincludes
mkdir -p -- ./libiberty
mkdir -p -- ./intl
mkdir -p -- ./gmp
mkdir -p -- ./zlib
Configuring in ./fixinc (took 28 mins 0 secs)
== Results of the build can be found in the log file(s) /tmp/eb-bbqft5x3/easybuild-GCCcore-12.3.0-20250227.184558.pg2BE.log
ERROR: Build of /data/EasyBuild/easybuild/easyconfigs/g/GCCcore/GCCcore-12.3.0.eb failed (err: 'build failed (first 300 chars): cmd " make
-j 8 " exited with exit code 2 and output:\nmake[1]: Entering directory \'/data/EasyBuild-develop/build/GCCcore/12.3.0/system-system/gcc
-12.3.0/build-nvptx-gcc'\nmkdir -p -- ./fixincludes\nmkdir -p -- ./libiberty\nmkdir -p -- ./intl\nmkdir -p -- ./gmp\nmkdir -p -- ./zlib\n
Configuring in ./fixinc')
```

## System dependencies not detected, as Arch Linux is not handled

```
jreuter@Linux ~$ eb --rebuild --installpath /tmp UCX-1.16.0-GCCcore-13.3.0.eb
== Temporary log file in case of crash /tmp/eb-zbyb8tif/easybuild-zyx96w6v.log
ERROR: Failed to process easyconfig /data/EasyBuild/easybuild/easyconfigs/u/UCX/UCX-1.16.0-GCCcore-13.3.0.eb: One or more OS dependencies
were not found: [['libibverbs-dev', 'libibverbs-devel', 'rdma-core-devel']]
x jreuter@Linux ~$ pacman -S libibverbs
cachyos-extra-znver4/rdma-core 56.0-1.1 [installed]
RDMA core userspace libraries and daemons
extra/rdma-core 56.0-1 [installed: 56.0-1.1]
RDMA core userspace libraries and daemons
jreuter@Linux ~$ find /usr -name "libibverbs.so"
/usr/lib/libibverbs.so
```



# Smaller contributions (Upstream & JSC)

- Main focus & interests:
  - Compilers (GCC, LLVM, AOCC, ...)
  - General accelerator support
  - Score-P, Scalasca and other performance tools
- For new software:
  - Used `eb --search` to find if ECs for dependencies exist (also checking PRs)
  - Create EasyConfig step by step
- For updating software:
  - Manual update, or
  - Use of `--try-toolchain --experimental --try-update-deps`

<a href="#">easybuilders/easybuild-easyconfigs {compiler}[system/system] NVHPC v25.1 w/ CUDA 12.6.0</a> ✓ <a href="#">update</a> #22207 by Thyre was merged last month • Approved <a href="#">👉</a> release after 4...
<a href="#">easybuilders/easybuild-easyconfigs {system}[system/system] CUDA v12.8.0</a> ✓ <a href="#">update</a> #22206 by Thyre was merged on Jan 26 • Approved <a href="#">👉</a> release after 4...
<a href="#">easybuilders/easybuild-easyconfigs {tools}[system/system] libtree v3.1.1</a> ✓ <a href="#">update</a> #22193 by Thyre was merged on Jan 23 • Approved <a href="#">👉</a> release after 4...
<a href="#">easybuilders/easybuild-easyconfigs {perf}[impi/2024a] Add Score-P 8.4 (w/ CUDA 12.6.0)</a> ✓ <a href="#">update</a> #22143 by Thyre was merged on Jan 18 • Approved <a href="#">🕒</a> 1 task done <a href="#">👉</a> 5.0.0
<a href="#">easybuilders/easybuild-easyblocks Enhance Score-P EasyBlock for future releases and better oneAPI support.</a> ✓ <a href="#">enhancement</a> #3548 by Thyre was merged on Jan 18 • Approved <a href="#">👉</a> 5.0
<a href="#">easybuilders/easybuild-easyconfigs {devel}[GCCcore/14.2.0] CMake v3.31.3</a> ✗ <a href="#">update</a> #22107 by Thyre was closed on Jan 3 • Review required <a href="#">📄</a> 1 task
<a href="#">easybuilders/easybuild-easyconfigs {compiler}[system/system] NVHPC-24.11-CUDA-12.6.0</a> ✓ <a href="#">update</a> #21877 by Thyre was merged on Nov 23, 2024 • Approved <a href="#">👉</a> release after 4...
<a href="#">easybuilders/easybuild-easyblocks enhance generic Bundle easyblock to transfer module requirements of components, but do not create logfile in components</a> ✓ <a href="#">enhancement</a> #3509 by Thyre was merged on Dec 26, 2024 • Approved <a href="#">🕒</a> 1 task done <a href="#">👉</a> release after 4...
<a href="#">easybuilders/easybuild-framework enhance EasyBlock class to allow passing in logfile</a> ✓ <a href="#">enhancement</a> #4707 by Thyre was merged on Dec 3, 2024 • Approved <a href="#">👉</a> release after 4...
<a href="#">easybuilders/easybuild-easyblocks let internal easyblock not create a log file in QuantumESPRESSO easyblock</a> ✓ <a href="#">bug fix</a> #3505 by Thyre was merged on Dec 18, 2024 • Approved <a href="#">🕒</a> 1 task done <a href="#">👉</a> release after 4...
<a href="#">easybuilders/easybuild-easyconfigs {tools}[system/system] VTune v2025.0.0</a> ✓ <a href="#">update</a> #21840 by Thyre was merged on Nov 13, 2024 • Approved <a href="#">👉</a> release after 4...
<a href="#">easybuilders/easybuild-easyblocks Fix oneAPI sanity check for ifort removal in 2025.0 and newer</a> ✓ <a href="#">update</a> #3495 by Thyre was merged on Nov 6, 2024 • Approved <a href="#">👉</a> release after 4...
<a href="#">easybuilders/easybuild-easyconfigs [system/system] Add Intel 2025.0.0 compilers</a> ✓ <a href="#">update</a> #21755 by Thyre was merged on Nov 6, 2024 • Approved <a href="#">👉</a> release after 4...
<a href="#">easybuilders/easybuild-easyblocks Enhance AOCC EasyBlock to correctly pass GCC toolchain and compiler driver</a> ✓ <a href="#">enhancement</a> #3480 by Thyre was merged on Oct 15, 2024 • Approved <a href="#">👉</a> release after 4...
<a href="#">easybuilders/easybuild-easyconfigs {devel,tools,lib,compiler}[system/system,GCCcore/14.2.0] Add pkgconf 2.3.0, XZ 5.6.3, ncurses 6.5, libxml 2.13.4, AOCC 5.0.0</a> ✓ <a href="#">2025a</a> <a href="#">update</a>

<a href="#">Fix HDF5 build on JEDI with NVHPC toolchain</a> 13061 • created 2 weeks ago by Jan André Reuter
<a href="#">Fix Autoconf for 'lic' flags by porting upstream patch</a> 12928 • created 1 month ago by Jan André Reuter
<a href="#">Fix Ascent-20250201-gpsmpi-2024a to use psmpi</a> 13042 • created 3 weeks ago by Jan André Reuter
<a href="#">Fix hashdeep-jsc configure patch checksum</a> 13043 • created 3 weeks ago by Jan André Reuter
<a href="#">2025: Update MNS for Intel with CUDA SYCL plugin</a> 12757 • created 3 months ago by Jan André Reuter
<a href="#">2025: Add VTune</a> 12762 • created 3 months ago by Jan André Reuter
<a href="#">2024: Replace VTune due to Rocky 9 incompatibility</a> 12763 • created 3 months ago by Jan André Reuter <a href="#">🔖</a> 2024
<a href="#">2025: Add Intel with CUDA SYCL plugin</a> 12755 • created 3 months ago by Jan André Reuter <a href="#">🕒</a> 2025 <a href="#">SYSTEM toolchain</a>
<a href="#">2025: Fix missing CUDA awareness for OpenMPI</a> 12716 • created 4 months ago by Jan André Reuter
<a href="#">2025: Fix AOCC EasyBlock with upstream changes</a> 12700 • created 4 months ago by Jan André Reuter <a href="#">🕒</a> 2025 <a href="#">easyblock bugfix</a>
<a href="#">2025: Generalize MNS hack for NVHPC versions</a> 12683 • created 4 months ago by Jan André Reuter
<a href="#">Fix OpenMPI/5.0.5 build for NVHPC/24.09 failure on JUWELS (Fixup to 12665)</a> 12678 • created 4 months ago by Jan André Reuter
<a href="#">2025: Add NVHPC 24.9 &amp; OpenMPI 5.0.5 for NVHPC</a> 12665 • created 5 months ago by Jan André Reuter <a href="#">🕒</a> 2025 <a href="#">Compiler toolchain</a> <a href="#">SYSTEM toolchain</a>
<a href="#">2025: Add AOCC 4.2.0 &amp; Custom EasyBlock</a> 12663 • created 5 months ago by Jan André Reuter <a href="#">🕒</a> 2025 <a href="#">GCCcore toolchain</a>
<a href="#">2024: Fix OTF2 Python bindings</a> 12602 • created 5 months ago by Jan André Reuter <a href="#">🔖</a> 2024
<a href="#">2025: Add NVPTX target to LLVM if cuda_compute_capabilities are set</a> 12593 • created 5 months ago by Jan André Reuter
<a href="#">2025: Add Intel compilers v2024.2.0</a> 12571 • created 6 months ago by Jan André Reuter
<a href="#">2025: CUDA 12.6.0, Z3 4.13.0, Clang 18.1.8</a> 12555 • created 6 months ago by Jan André Reuter <a href="#">🕒</a> 2025

# THE FIRST MAJOR CONTRIBUTION

easybuild-easyblocks#3396 : enhance custom easyblock for GCC to use **with-arch** option for nvptx with 13.1+

GCC 12.3.0 on JURECA-DC (AMD EPYC + NVIDIA A100):

```
[reuter1@jrlogin07 ~]$ gcc -fopenmp saxpy.c
ptxas fatal   : Value 'sm_35' is not defined for option 'gpu-name'
nvptx-as: ptxas returned 255 exit status
mkoffload: fatal error: x86_64-pc-linux-gnu-accel-nvptx-none-gcc returned 1 exit status
compilation terminated.
lto-wrapper: fatal error: /p/software/fs/jurecadc/stages/2024/software/GCCcore/12.3.0/bin/./libexec/gcc/x86_64-pc-linux-gnu/12.3.0//accel/nvptx-none/mkoffload returned 1 exit status
compilation terminated.
/p/software/jurecadc/stages/2024/software/binutils/2.40-GCCcore-12.3.0/bin/ld: error: lto-wrapper failed
collect2: error: ld returned 1 exit status
```

- Build issues when trying to use offloading in GCC
- Found release entry for GCC 13:

The default value for the `-march` option can be now changed when building GCC using the `--with-arch=` configure option. GCC's target libraries are then build both with `sm_30` and the specified target architecture. If not specified, GCC defaults to `sm_30`.

- Idea: Let's use it when building GCC 13.1+

GCC 13.3.0 on JEDI (NVIDIA GH200):

```
[reuter1@jpb1t-s01-01 jureca]$ gcc -fopenmp saxpy.c
lto1: internal compiler error: bytecode stream: string too long for the string table
0x6c35ff string_for_index
././././gcc/data-streamer-in.cc:53
0x6c35ff bp_unpack_indexed_string(data_in*, bitpack_d*, unsigned int*)
././././gcc/data-streamer-in.cc:97
0x935957 lto_input_mode_table(lto_file_decl_data*)
././././gcc/lto-streamer-in.cc:2061
0x6380db lto_file_finalize
././././gcc/lto/lto-common.cc:2275
0x6380db lto_create_files_from_ids
././././gcc/lto/lto-common.cc:2298
0x6380db lto_file_read
././././gcc/lto/lto-common.cc:2353
0x6380db read_cgraph_and_symbols(unsigned int, char const**)
././././gcc/lto/lto-common.cc:2801
0x625403 lto_main()
././././gcc/lto/lto.cc:654
Please submit a full bug report, with preprocessed source (by using -freport-bug).
Please include the complete backtrace with any bug report.
See <https://gcc.gnu.org/bugs/> for instructions.
nvptx mkoffload: fatal error: aarch64-unknown-linux-gnu-accel-nvptx-none-gcc returned 1 exit status
compilation terminated.
```



# THE FIRST MAJOR CONTRIBUTION

easybuild-easyblocks#3396 : enhance custom easyblock for GCC to use **with-arch** option for nvptx with 13.1+

```
def map_nvptx_capability(self):
    """
    Convert PTX ISA architecture passed via EasyBuild configs to a version which is understood by GCC.
    Valid architecture strings include 'sm_30', 'sm_35', 'sm_53', 'sm_70', 'sm_75', 'sm_80'.
    (as of GCC 14.1.0). Some additional architectures may be mapped.
    See: https://github.com/gcc-mirror/gcc/commit/de0ef04419e90eacf0d1ddb265552a1b08c18d4b

    As this list is updated regularly, try to parse the GCC source file (gcc/config/nvptx/nvptx.opt)
    and extract the supported architectures and their mapping. Based on the result, determine the lowest
    architecture required to support all 'cuda_compute_capabilities' and return this value.
    """
    cuda_cc_list = build_option('cuda_compute_capabilities') or self.cfg['cuda_compute_capabilities']
    architecture_mappings_file = os.path.join(self.cfg['start_dir'], 'gcc', 'config', 'nvptx', 'nvptx.opt')
    architecture_mappings_flag = "march-map="
    architecture_mappings_replacement = "misa="

    # Determine which compute capabilities are configured. If there are none, return immediately.
    if cuda_cc_list is None:
        return None
    cuda_sm_list = [f"sm_{cc.replace('.', '')}" for cc in cuda_cc_list]

    if not os.path.exists(architecture_mappings_file):
        warn_msg = f"Tried to parse nvptx.opt but file {architecture_mappings_file} was not found. " \
            "Please check the path and update the EasyBlock if necessary!"
        self.log.warning(warn_msg)
        return None

    # We want to read the mappings found in the GCC sources and create a map for this.
    # We're searching for the following pattern:
    # march-map=sm_32
    # Target RejectNegative Alias(misa=,sm_30)
    gcc_architecture_mappings = {}
    file_content = read_file(architecture_mappings_file).splitlines()
    for line_idx, line in enumerate(file_content):
        line = line.strip()
        if line.startswith(architecture_mappings_flag):
            key = line.split('=')[1]
            # Mapped architecture can be found in the following line
            line = file_content[line_idx + 1]
            if architecture_mappings_replacement not in line:
                warn_msg = "Tried to parse nvptx.opt but failed to extract mapped architectures! " \
                    f"Expected to find substring '{architecture_mappings_replacement}' in " \
                    f"line {line_idx + 1} but found '{line}'. Choosing default of GCC."
                self.log.warning(warn_msg)
                # Bail out, since results of mapping cannot be trusted
                return None
            value = line.split(architecture_mappings_replacement)[1].rstrip(')')
            gcc_architecture_mappings[key] = value
    self.log.info(f"Available architecture mappings in GCC {self.version}: \n {str(gcc_architecture_mappings)}")

    # Map compute capabilities to GCC ones
    # If no compute capability can be mapped, stick to default of GCC and return None
    gcc_cc = [gcc_architecture_mappings[cc] if cc in gcc_architecture_mappings else None for cc in cuda_sm_list]
    self.log.info(f"Mapped architectures: {str(cuda_sm_list)} -> {str(gcc_cc)}")
    if any(cc is None for cc in gcc_cc):
        self.log.info("At least one architecture could not be mapped. Choosing default of GCC.")
        return None

    # Get the lowest architecture mapping and return it
    sorted_gcc_cc = sorted(gcc_cc)
    self.log.info("Choosing first architecture in sorted list as default nvptx "
        f"architecture: {str(sorted_gcc_cc)}")
    return sorted_gcc_cc[0]
```

Thyre commented on Jul 26, 2024

### Motivation

GCC, like other compilers, allows users to use offloading via OpenMP & OpenACC for example to utilize accelerators in their written programs. While some compilers require the presence of CUDA for this e.g. Clang, GCC has no requirement for it to simply build and run an executable containing offloading code.

By default, GCC targets a very low architecture for NVIDIA GPUs though. In GCC 12.3.0, this was `sm_30`. In GCC 13.3.0, the default version is still the same, but [recent nvptx-tools](#) can bump this to `sm_50` when CUDA is detected. With this, GCC can work around the removal of `sm_3x` in more recent CUDA versions, avoiding the following error message:

#### GCC 12.3.0

```
$ gcc -fopenmp -foffload=nvptx-none test.c
ptxas fatal : Value 'sm_35' is not defined for option 'gpu-name'
nvptx-as: ptxas returned 255 exit status
mkoffload: fatal error: x86_64-pc-linux-gnu-accel-nvptx-none-gcc returned 1 exit status
compilation terminated.
lto-wrapper: fatal error: /p/software/fs/jurecad/stages/2024/software/GCCcore/12.3.0/bin/./libexec/gcc/x86_64-pc-linux-gnu/12.3.0/lto-wrapper: error: ld returned 1 exit status
collect2: error: ld returned 1 exit status
```

#### GCC 13.3.0

```
$ gcc --verbose -fopenmp -foffload=nvptx-none test.c
[...]
/p/software/fs/jurecad/stages/2025/software/GCCcore/13.3.0/bin/./libexec/gcc/x86_64-pc-linux-gnu/13.3.0/accel-nvptx-none-gcc: error: x86_64-pc-linux-gnu-accel-nvptx-none-gcc returned 1 exit status
Verifying sm_30 code with sm_50 code generation.
ptxas -c -o /dev/null /tmp/cc7PhNR.o --gpu-name sm_50 -00
[...]
```

However, this may break once again as soon as NVIDIA decides to remove the already deprecated support for `sm_50` (in CUDA 11.0). Fortunately, GCC has added a configure option to overwrite the default nvptx architecture. Beginning with GCC 13.1.0, one can pass `--with-arch=sm_[x]` to set the default option, as long as GCC can understand it.

In addition, choosing a newer architecture by default might bring performance improvements and access to additional features.

#### Scope of this PR

This pull request adds the new option `--with-arch=sm_[x]` to GCC builds starting with GCC 13.1.0 if offloading support via nvptx is enabled. To choose which architecture is being passed, a new function named `map_nvptx_capability` is implemented. This function retrieves `cuda_compute_capabilities` and matches them against the official GCC mappings (which can be found in [GCC\\_SRC/gcc/config/nvptx/nvptx.opt](#)) being used for the `-march-map=` argument.

Since GCC only allows to set a single default architecture, I decided to use the lowest one available. For example, JURECAD sets both 7.5 and 8.0 for EasyBuild. Therefore, 7.5 would be chosen.

If parsing the architecture mappings fails, for example because the file layout changed or the file was moved, a warning is returned. In this case, we stick to the default of GCC. This is also the case if the architectures in `cuda_compute_capabilities` cannot be mapped at all. This makes the additions more resilient to upstream changes.

Generally, this helps users as they are not required to pass architectures manually every single time as it is the case with CUDA 12 + GCC 12.3.0 right now. Here, one would need to pass `-foffload-options=-misa=sm_80`.

- 1.5 months in review
- Many additional safety nets added
- Tested on jsc-zen3, other JSC machines & by reviewers
- Merged before EB 4.9.3



# BREAKING AN EASYBUILD RELEASE

EasyBuild 4.9.3 came out on September 14th 2024.  
There was one small issue though...

```
== building and installing GCCcore/13.3.0...
...
ERROR: Traceback (most recent call last):
  File "EasyBuild/4.9.3/[...]/easybuild/main.py", line 137, in build_and_install_software
    (ec_res['success'], app_log, err) = build_and_install_one(ec, init_env)
  File "EasyBuild/4.9.3/[...]/easybuild/framework/easyblock.py", line 4276, in build_and_install_one
    result = app.run_all_steps(run_test_cases=run_test_cases)
  File "EasyBuild/4.9.3/[...]/easybuild/easyblocks/g/gcc.py", line 1081, in run_all_steps
    return super(EB_GCC, self).run_all_steps(*args, **kwargs)
  File "EasyBuild/4.9.3/[...]/easybuild/framework/easyblock.py", line 4155, in run_all_steps
    self.run_step(step_name, step_methods)
  File "EasyBuild/4.9.3/[...]/easybuild/framework/easyblock.py", line 3990, in run_step
    step_method(self)()
  File "EasyBuild/4.9.3/[...]/easybuild/easyblocks/g/gcc.py", line 612, in configure_step
    cuda_cc = self.map_nvptx_capability()
  File "EasyBuild/4.9.3/[...]/easybuild/easyblocks/g/gcc.py", line 431, in map_nvptx_capability
    return sorted_gcc_cc[0]
IndexError: list index out of range
```

Building GCC 13.1+ failed without a CUDA architecture.  
All tests were done with a CUDA architecture.

## Overview of tested easyconfigs (in order)

- SUCCESS GCCcore-10.2.0.eb
- SUCCESS GCCcore-12.3.0.eb
- SUCCESS GCCcore-14.2.0.eb

## EasyBuild info

- easybuild-framework version: 4.9.3.dev0-re0e04fb773a5cee26669211f563696da94455cfd
- easybuild-easyblocks version: 4.9.3.dev0-rc29c16dd9da0b9935a7fa4f041aacf0a76102453
- command line:

```
d-test-report --download-timeout=1000 GCCcore-10.2.0.eb GCCcore-12.3.0.eb GCCcore-14.2.0.eb --installpath /tmp.
```

- full configuration (includes defaults):

```
--accept-eula-for='*'
--accept-eula=''
--allow-loaded-modules='EasyBuild'
--buildpath='/tmp/boegelbot'
--check-ebroot-env-vars='warn'
--cleanup-builddir
--cleanup-easyconfigs
--cleanup-tmpdir
--color='auto'
--container-type='singularity'
--containerpath='/project/def-maintainers/boegelbot/rocky9/zen3/containers'
--cuda-compute-capabilities='8.0'
```

# BREAKING AN EASYBUILD RELEASE

```
easybuild/easyblocks/g/gcc.py
369 369     def map_nvptx_capability(self):
370 370         """
371 371         Convert PTX ISA architecture passed via EasyBuild configs to a version which is understood by GCC.
372 372         Valid architecture strings include 'sm_30', 'sm_35', 'sm_53', 'sm_70', 'sm_75', 'sm_80'.
373 373         (as of GCC 14.1.0). Some additional architectures may be mapped.
374 374         See: https://github.com/gcc-mirror/gcc/commit/de0ef04419e90eacfd0d1ddb265552a1b08c18d4b
375 375
376 376         As this list is updated regularly, try to parse the GCC source file (gcc/config/nvptx/nvptx.opt)
377 377         and extract the supported architectures and their mapping. Based on the result, determine the lowest
378 378         architecture required to support all 'cuda_compute_capabilities' and return this value.
379 379         """
380 380         cuda_cc_list = build_option('cuda_compute_capabilities') or self.cfg['cuda_compute_capabilities']
381 381         architecture_mappings_file = os.path.join(self.cfg['start_dir'], 'gcc', 'config', 'nvptx', 'nvptx.opt')
382 382         architecture_mappings_flag = "march-map="
383 383         architecture_replacement = "misa="
384 384
385 385         # Determine which compute capabilities are configured. If there are none, return immediately.
386 386         - if cuda_cc_list is None:
387 387         + if not cuda_cc_list:
388 388             return None
389 389         cuda_sm_list = [f"sm_{cc.replace('.', '')}" for cc in cuda_cc_list]
```

## Key takeaway:

Test EasyBlock changes with and without cuda-compute-capabilities



Thyre commented on Sep 16, 2024

Contributor

When no compute capability is set but NVPTX is enabled, trying to figure out the NVPTX architecture fails with the error:

```
File "easybuild/easyblocks/g/gcc.py", line 431, in map_nvptx_capability
    return sorted_gcc_cc[0]
IndexError: list index out of range
```

The error occurs because of an insufficient check for an unset CUDA compute capability. This commit changes the checked conditions, so that empty lists are also correctly handled.

# BREAKING THE EASYBUILD TEST SUITE

easybuild-easyblocks#3472 : Enhance generic Bundle easyblock to transfer module requirements of components

- **Idea:** Provide EasyConfig for Intel oneAPI with SYCL plug-in for NVIDIA GPUs (easybuild-easyconfigs#21582)
- Using Bundle EasyBlock failed: Additional module requirements not transferred...
- **Culprit:** `make_module_req_guess` was not implemented.
- **Solution:** Copy the requirements from all Bundle components.



Thyre commented on Oct 26, 2024 • edited ▾

Full (re-)installation

Test report by @Thyre

Overview of tested easyconfigs (in order)

- SUCCESS `builtdenv-default-foss-2023b.eb`
- SUCCESS `OpenSSL-3.eb`
- SUCCESS `Circuitscape-5.12.3-julia-1.9.2.eb`
- SUCCESS `Perl-bundle-CPAN-5.38.2-GCCcore-13.3.0.eb`
- SUCCESS `gfbf-2024a.eb`
- SUCCESS `crypt4gh-1.7-GCC-12.3.0.eb`
- SUCCESS `GCC-system.eb`
- SUCCESS `OpenMPI-system-GCC-system-2.29.eb`
- SUCCESS `X11-20240607-GCCcore-13.3.0.eb`

Build succeeded for 9 out of 9 (9 easyconfigs in total)  
datenlager - Linux Ubuntu 24.04, x86\_64, AMD Ryzen 7 37  
See <https://gist.github.com/Thyre/bbc3468bc740b0c511c>



boegelbot commented on Nov 8, 2024

Test report by @boegelbot

Overview of tested easyconfigs (in order)

- SUCCESS `X11-20240607-GCCcore-13.3.0.eb`
- SUCCESS `builtdenv-default-foss-2023b.eb`
- SUCCESS `OpenSSL-3.eb`
- SUCCESS `Circuitscape-5.12.3-julia-1.9.2.eb`
- SUCCESS `Perl-bundle-CPAN-5.38.2-GCCcore-13.3.0.eb`
- SUCCESS `crypt4gh-1.7-GCC-12.3.0.eb`
- SUCCESS `jiter-0.4.1-GCCcore-12.3.0.eb`
- SUCCESS `GCC-system.eb`
- SUCCESS `gfbf-2024a.eb`

Build succeeded for 9 out of 9 (9 easyconfigs in total)

jszen3c1.int.jsc-zen3.fz-juelich.de - Linux Rocky Linux 9.4, x86\_64, AMD EPYC-Milan Processor (zen3), Python 3.9.18  
See <https://gist.github.com/boegelbot/2df274b1d2731957ac6b0e5be8d36daf> for a full test report.

```
== Temporary log file in case of crash /tmp/eb-k6c_4924/easybuild-w2k6x1on.log
== processing EasyBuild easyconfig /tmp/eb-k6c_4924/files_pr21582/i/intel-compilers/intel-compilers-2024.2.0-CUDA-12.5.0.eb
== building and installing intel-compilers/2024.2.0-CUDA-12.5.0...
== fetching files...
== ... (took 2 secs)
== creating build dir, resetting environment...
== unpacking...
== ... (took 1 secs)
== patching...
== preparing...
== configuring...
== building...
== testing...
== installing...
== installing bundle component intel-compilers v2024.2.0 (1/2)...
== installing part 1/2 (l_dpccpp-cpp-compiler_p_2024.2.0.495_offline.sh)...
== installing part 2/2 (l_fortran-compiler_p_2024.2.0.426_offline.sh)...
== installing bundle component codeplay-oneapi-for-nvidia-gpus v2024.2.0 (2/2)...
== ... (took 55 secs)
== taking care of extensions...
== restore after iterating...
== postprocessing...
== sanity checking...
== FAILED: Installation ended unsuccessfully (build directory: /data/EasyBuild-develop/build/intelcompilers/2024.2.0/system-system-CUDA-12.5.0): build failed (first 300 chars): Sanity check failed: sanity check command icx --version exited with code 127 (output: /bin/bash: line 1: icx: command not found
)
sanity check command icpx --version exited with code 127 (output: /bin/bash: line 1: icpx: comm and not found
)
sanity check command ifx --version exited with code 127 (ou (took 59 secs)
== Results of the build can be found in the log file(s) /tmp/eb-k6c_4924/easybuild-intel-compilers-2024.2.0-20250310.094727.DcrBH.log
```

Custom module paths of oneAPI lost when using Bundle EasyBlock → Intel compilers not found



# BREAKING THE EASYBUILD TEST SUITE

easybuild-easyblocks#3472 : Enhance generic Bundle easyblock to transfer module requirements of components

## Annotations

1 error and 2 warnings

```
System.IO.IOException: No space left on device : '/home/runner/runners/2.320.0/_diag/Worker_20241112-104429-utc.log'
  at System.IO.RandomAccess.WriteAtOffset(SafeFileHandle handle, ReadOnlySpan`1 buffer, Int64 fileOffset)
  at System.IO.Strategies.BufferedFileStreamStrategy.FlushWrite()
  at System.IO.StreamWriter.Flush(Boolean flushStream, Boolean flushEncoder)
  at System.Diagnostics.TextWriterTraceListener.Flush()
  at GitHub.Runner.Common.HostTraceListener.WriteHeader(String source, TraceEventType eventType, Int32 id)
  at GitHub.Runner.Common.HostTraceListener.TraceEvent(TraceEventCache eventCache, String source, TraceEventType eventType, Int32 id, String message)
  at System.Diagnostics.TraceSource.TraceEvent(TraceEventType eventType, Int32 id, String message)
  at GitHub.Runner.Worker.Worker.RunAsync(String pipeIn, String pipeOut)
  at GitHub.Runner.Worker.Program.MainAsync(IHostContext context, String[] args)
System.IO.IOException: No space left on device : '/home/runner/runners/2.320.0/_diag/Worker_20241112-104429-utc.log'
  at System.IO.RandomAccess.WriteAtOffset(SafeFileHandle handle, ReadOnlySpan`1 buffer, Int64 fileOffset)
  at System.IO.Strategies.BufferedFileStreamStrategy.FlushWrite()
  at System.IO.StreamWriter.Flush(Boolean flushStream, Boolean flushEncoder)
  at System.Diagnostics.TextWriterTraceListener.Flush()
  at GitHub.Runner.Common.HostTraceListener.WriteHeader(String source, TraceEventType eventType, Int32 id)
  at GitHub.Runner.Common.HostTraceListener.TraceEvent(TraceEventCache eventCache, String source, TraceEventType eventType, Int32 id, String message)
  at System.Diagnostics.TraceSource.TraceEvent(TraceEventType eventType, Int32 id, String message)
  at GitHub.Runner.Common.Tracing.Error(Exception exception)
  at GitHub.Runner.Worker.Program.MainAsync(IHostContext context, String[] args)
Unhandled exception. System.IO.IOException: No space left on device : '/home/runner/runners/2.320.0/_diag/Worker_20241112-104429-utc.log'
  at System.IO.RandomAccess.WriteAtOffset(SafeFileHandle handle, ReadOnlySpan`1 buffer, Int64 fileOffset)
  at System.IO.Strategies.BufferedFileStreamStrategy.FlushWrite()
  at System.IO.StreamWriter.Flush(Boolean flushStream, Boolean flushEncoder)
  at System.Diagnostics.TextWriterTraceListener.Flush()
  at System.Diagnostics.TraceSource.Flush()
  at GitHub.Runner.Common.TraceManager.Dispose(Boolean disposing)
  at GitHub.Runner.Common.TraceManager.Dispose()
  at GitHub.Runner.Common.HostContext.Dispose(Boolean disposing)
  at GitHub.Runner.Common.HostContext.Dispose()
  at GitHub.Runner.Worker.Program.Main(String[] args)
```

Show less

- All CI jobs started failing due to disk space restriction on runners (14 GB)
- Affected develop, 5.x, and all pull requests
- Changes were reverted quickly

revert changes from PR #3472, seems to be leading to an infinite loop in easyconfigs test suite? #3504

Merged jfgrimm merged 1 commit into easybuilders:develop from boegel:20241112184552\_new\_pr\_bundle on Nov 12, 2024

- But what happened?

# WHAT HAPPENED?

## Late night analysis of what was going wrong

- Bundle EasyBlock was creating multiple log files, but closed only one of them.
- Same issue was visible with QuantumESPRESSO EasyBlock
  - Fortunate enough that this issue was not triggered earlier
- Several follow-up PRs:

[easybuilders/easybuild-easyblocks](#) enhance generic Bundle easyblock to transfer module requirements of components, but do not create logfile in components ✓  
enhancement  
#3509 by Thyre was merged on Dec 26, 2024 • Approved 1 task done ↻ release after 4...

[easybuilders/easybuild-framework](#) enhance EasyBlock class to allow passing in logfile ✓ enhancement  
#4707 by Thyre was merged on Dec 3, 2024 • Approved ↻ release after 4...

[easybuilders/easybuild-easyblocks](#) let internal easyblock not create a log file in QuantumESPRESSO easyblock ✓ bug fix  
#3505 by Thyre was merged on Dec 18, 2024 • Approved 1 task done ↻ release after 4...

### Annotations

1 error and 2 warnings

```
System.IO.IOException: No space left on device : '/home/runner/runners/2.320.0/_diag/Worker_20241112-104429-utc.log'
at System.IO.RandomAccess.WriteAtOffset(SafeFileHandle handle, ReadOnlySpan`1 buffer, Int64 fileOffset)
at System.IO.Strategies.BufferedFileStreamStrategy.FlushWrite()
at System.IO.StreamWriter.Flush(Boolean flushStream, Boolean flushEncoder)
at System.Diagnostics.TextWriterTraceListener.Flush()
at GitHub.Runner.Common.HostTraceListener.WriteHeader(String source, TraceEventType eventType, Int32 id)
at GitHub.Runner.Common.HostTraceListener.TraceEvent(TraceEventCache eventCache, String source, TraceEventType eventType, Int32 id, String message)
at System.Diagnostics.TraceSource.TraceEvent(TraceEventType eventType, Int32 id, String message)
at GitHub.Runner.Worker.Worker.RunAsync(String pipeIn, String pipeOut)
at GitHub.Runner.Worker.Program.MainAsync(IHostContext context, String[] args)
System.IO.IOException: No space left on device : '/home/runner/runners/2.320.0/_diag/Worker_20241112-104429-utc.log'
at System.IO.RandomAccess.WriteAtOffset(SafeFileHandle handle, ReadOnlySpan`1 buffer, Int64 fileOffset)
at System.IO.Strategies.BufferedFileStreamStrategy.FlushWrite()
at System.IO.StreamWriter.Flush(Boolean flushStream, Boolean flushEncoder)
at System.Diagnostics.TextWriterTraceListener.Flush()
at GitHub.Runner.Common.HostTraceListener.WriteHeader(String source, TraceEventType eventType, Int32 id)
at GitHub.Runner.Common.HostTraceListener.TraceEvent(TraceEventCache eventCache, String source, TraceEventType eventType, Int32 id, String message)
at System.Diagnostics.TraceSource.TraceEvent(TraceEventType eventType, Int32 id, String message)
at GitHub.Runner.Common.Tracing.Error(Exception exception)
at GitHub.Runner.Worker.Program.MainAsync(IHostContext context, String[] args)
Unhandled exception. System.IO.IOException: No space left on device : '/home/runner/runners/2.320.0/_diag/Worker_20241112-104429-utc.log'
at System.IO.RandomAccess.WriteAtOffset(SafeFileHandle handle, ReadOnlySpan`1 buffer, Int64 fileOffset)
at System.IO.Strategies.BufferedFileStreamStrategy.FlushWrite()
at System.IO.StreamWriter.Flush(Boolean flushStream, Boolean flushEncoder)
at System.Diagnostics.TextWriterTraceListener.Flush()
at System.Diagnostics.TraceSource.Flush()
at GitHub.Runner.Common.TraceManager.Dispose(Boolean disposing)
at GitHub.Runner.Common.TraceManager.Dispose()
at GitHub.Runner.Common.HostContext.Dispose(Boolean disposing)
at GitHub.Runner.Common.HostContext.Dispose()
at GitHub.Runner.Worker.Program.Main(String[] args)
```

Show less

```
Every 0,1s: ls -lah easyconfigs_test_*
total 106M
drwx----- 2 jreuter jreuter 820 27. Feb 16:48 .
drwxrwxrwt 17 root root 460 27. Feb 16:47 ..
-rw-r--r-- 1 jreuter jreuter 3,3M 27. Feb 16:48 easybuild-QuantumESPRESSO-5.3.0-20250227.164813.DMcBg.log
-rw-r--r-- 1 jreuter jreuter 3,3M 27. Feb 16:48 easybuild-QuantumESPRESSO-5.4.0-20250227.164813.WtkaM.log
-rw-r--r-- 1 jreuter jreuter 3,3M 27. Feb 16:48 easybuild-QuantumESPRESSO-5.4.0-20250227.164813.ZoarJ.log
-rw-r--r-- 1 jreuter jreuter 3,2M 27. Feb 16:48 easybuild-QuantumESPRESSO-6.0-20250227.164813.fTHHL.log
-rw-r--r-- 1 jreuter jreuter 3,2M 27. Feb 16:48 easybuild-QuantumESPRESSO-6.1-20250227.164813.bHwsA.log
```

# KEY TAKEAWAYS

The Good	The Bad
GitHub integration and testing <code>--new-pr</code> , <code>--upload-test-report</code>	Documentation, once working with EasyBlocks or Framework, e.g. how logging works
Creating / updating EasyConfigs is nicely documented, and often straight-forward.	Side-effects when changing EasyBlock / Framework. Additional tests necessary?
Great documentation to get started with using EasyBuild	(Long review times)
The large amount of software available!	

## Tips:

- Join EasyBuild conf. calls
- Don't hesitate to ask if you're running into issues!
- Look at logs to find out what failed



# PERSONAL WISH LIST

1. Also test aarch64:
  - a. Several build issues when setting up software stage on aarch64
2. Improved support for AMD GPUs / ROCm:
  - a. cuda-compute-capabilities only for NVIDIA
  - b. No (recent) ROCm packages
  - c. Many packages only built for NVIDIA
3. Additional toolchain support:
  - a. LLVM/Clang, AOCC, ROCm, ...

-  build\_software: [jedi]
-  build\_software: [jureca]
-  build\_software: [jusuf]
-  build\_software: [juwels]
-  build\_software: [juwels]
-  build\_software: [juwels\_boo...]
-  build\_software\_on\_compute...
-  build\_software\_on\_compute...



Thyre commented 2 hours ago

Contributor Author ...

Test report by [@Thyre](#)

Using easyblocks from PR(s) [easybuilders/easybuild-easyblocks#3657](#)

**SUCCESS**

Build succeeded for 3 out of 3 (2 easyconfigs in total)

Linux - Linux Arch Linux UNKNOWN, x86\_64, AMD Ryzen 7 7800X3D 8-Core Processor, 1 x AMD Navi 48 [RX 9070/9070 XT]

(model: 0x7550, driver: "6.13.5-arch1-1"), 1 x AMD Raphael (model: 0x164e, driver: "6.13.5-arch1-1"), Python 3.13.2

See <https://gist.github.com/Thyre/721906ee394b0dc5b9efa0a6b2991d9f> for a full test report.



```
class EB_Score_minus_P_minus_CPE(ConfigureMake):
    def configure_step(self, *args, **kwargs):

        comp_opts = {
            # assume that system toolchain uses a system-provided GCC
            toolchain.SYSTEM: 'gcc',
            toolchain.AMD: 'amdclang',
            toolchain.AOCC: 'aocc',
            toolchain.CCE: 'cray',
            toolchain.GCC: 'gcc',
            toolchain.IBMCOMP: 'ibm',
            toolchain.INTELCOMP: 'intel',
            toolchain.NVHPC: 'nvhpc',
            toolchain.PGI: 'pgi',
        }
```

**THANKS FOR  
YOUR TIME**