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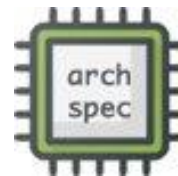
EESSI Happy Hour

Topic Series: EESSI Mix and Match

Mondays at 14:00 CEST



CernVM-FS



Current session: AMD ROCm support in EESSI

<https://www.eessi.io/docs/training/happy-hours-sessions>

Website: eessi.io

EESSI support portal:

gitlab.com/eessi/support



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Highlights:

- ISC'26 conference
22-26 June 2026 @ Hamburg
- EuroHPC User Days 2026
22-24 September 2026 in Dublin, Ireland.



Current Scenario:

- EESSI supports CUDA and ships the software stack that works with host_injections.
- CUDA is not redistributable as the site provides compiler/runtime.
- CUDA softwares are built as PTX fat binaries and codegen is deferred to the driver.

ROCm support is required as more HPC systems are being developed with AMD GPUs.
For eg. LUMI, JUPITER



Differences between ROCm and CUDA

- ROCm is Apache/MIT License -> completely redistributable. 🎉
- No PTX-equivalent mechanism -> one subtree per gfx target needed.
- Higher coupling between library and compiler/driver.
One year guaranteed support between ROCm and driver version.
-> Hard minimum version requirement for drivers on site.



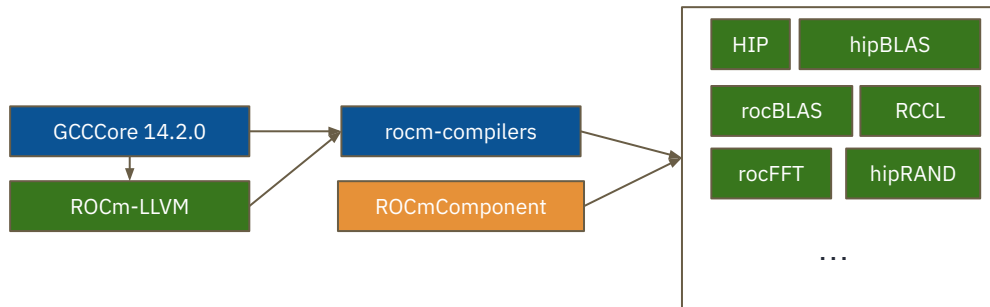
CernVM-FS



Lmod



ROCm 6.4.1 Stack



ROCm 6.4.1 stack will be available for all officially supported targets:

```

joglekar@nid007969 /c/s/v/2/s/L/x/a/z/a/amd $ pwd
/cvmfs/software.eessi.io/versions/2025.06/software/linux/x86_64/amd/zen3/accel/amd
joglekar@nid007969 /c/s/v/2/s/L/x/a/z/a/amd $ ls
gfx1030 gfx1100 gfx1101 gfx1200 gfx1201 gfx908 gfx90a gfx942
joglekar@nid007969 /c/s/v/2/s/L/x/a/z/a/amd $ █
  
```

AMD ROCm support in EESSI



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AMD's stock CMake assumes a monolithic /opt/rocm installation, EasyBuild prefers different dirs

Majority of the patches needed to build these libraries were to remove /opt/rocm hardcodings and point find_package commands to correct EasyBuild installations

Add ROCm-6.4.1 easyconfigs #25576

casparul merged 87 commits into easybuilders:develop from zerefwayne:and-working on Apr 22

Conversation 181 Commits 87 Checks 6 Files changed 52 +2,341 -1

Commits on Mar 22, 2026

Add CppHeaderParser-2.7.4-GCCcore-14.2.0	Verified	5b4894e	<>
zerefwayne committed on Mar 22			
Add rocm-compilers-19.0.0-ROCM-6.4.1.eb	Verified	b39f1e3	<>
zerefwayne committed on Mar 22			
Add rocm-cmake-0.14.0-rocm-compilers-19.0.0-ROCM-6.4.1.eb	Verified	6b6a77f	<>
zerefwayne committed on Mar 22			
Add HIP-6.4.1-rocm-compilers-19.0.0-ROCM-6.4.1.eb	Verified	6193daf	<>
zerefwayne committed on Mar 22			
Add hipBLAS-common-1.2.0-rocm-compilers-19.0.0-ROCM-6.4.1.eb	Verified	1cac1b2	<>
zerefwayne committed on Mar 22			
Add rocTracer-4.1.0-GCCcore-14.2.0-ROCM-6.4.1.eb	Verified	bdb4808	<>
zerefwayne committed on Mar 22			

<https://github.com/easybuilders/easybuild-easyconfigs/pull/25576/commits>

AMD ROCm support in EESSI

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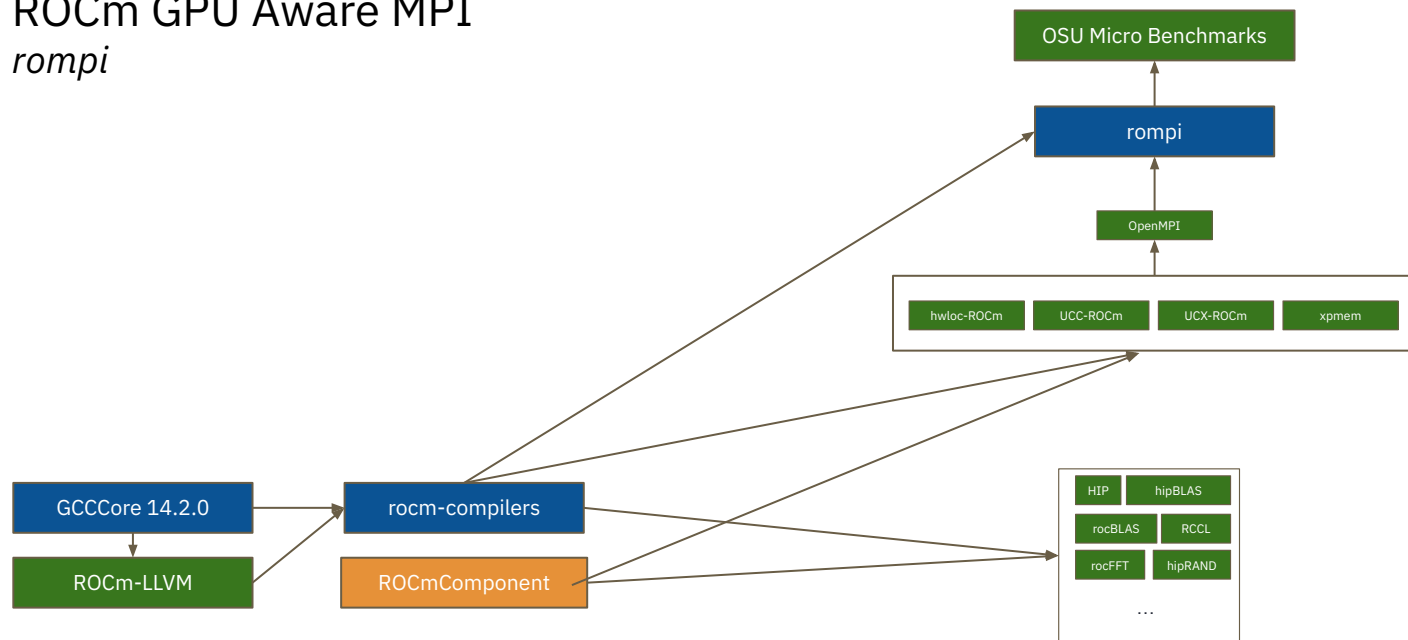


CernVM-FS



ROCm GPU Aware MPI

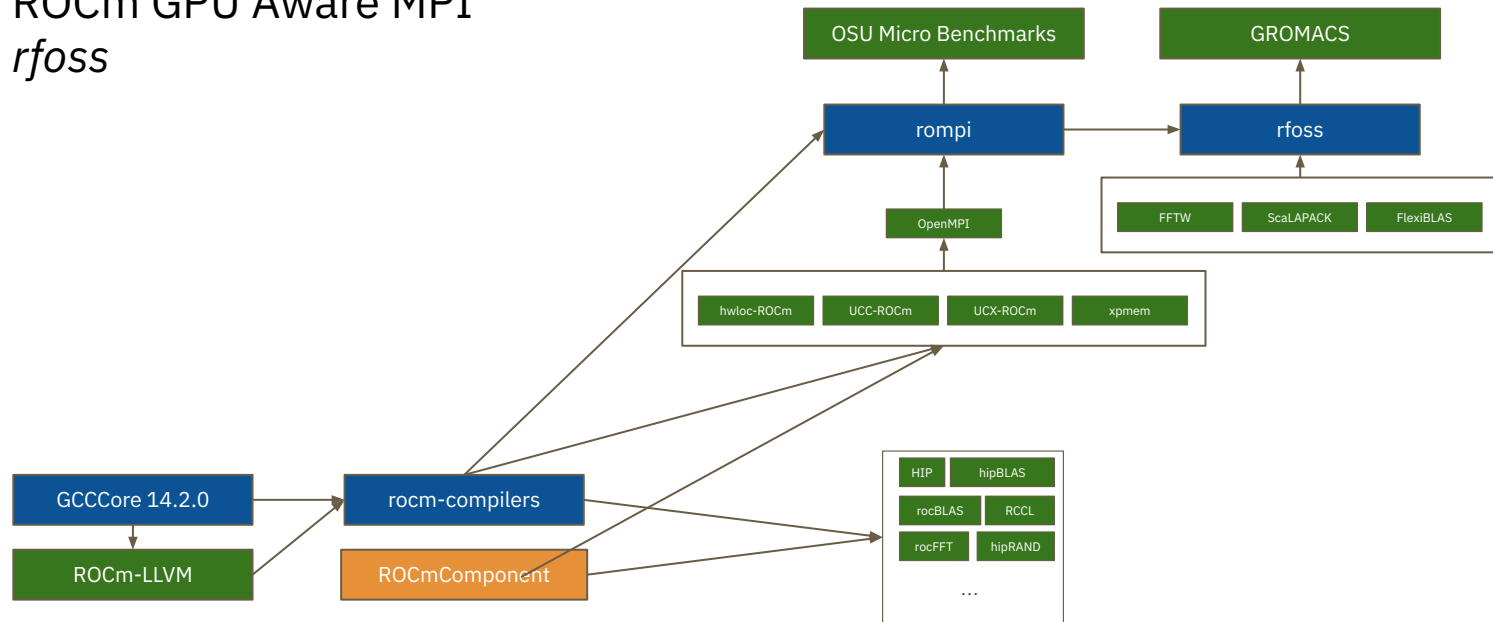
rompi



AMD ROCm support in EESSI



ROCm GPU Aware MPI rfoss

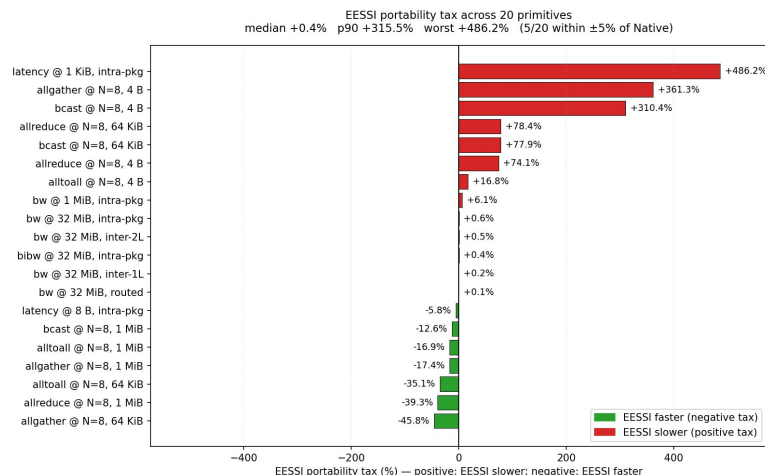




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These toolchains work as expected and provide an almost native performance on LUMI



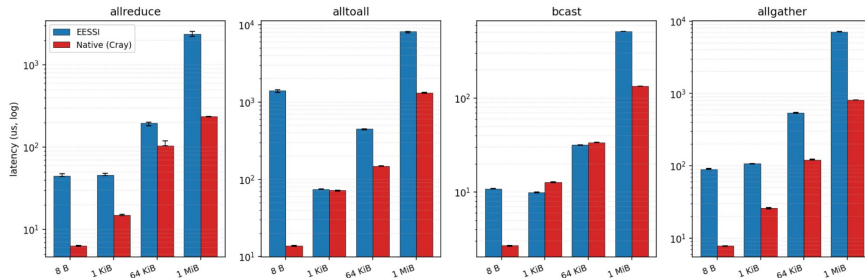
Except for small message sizes and inter-node communication on Slingshot-11 (LUMI)

AMD ROCm support in EESSI

Reason:

- OpenMPI + UCX cannot match the hardware optimisations done on LUMI for small message sizes
- Also, OpenMPI 5.0.7 exports libmpi.so.40 - not compatible with MPICH ABI Family which expects libmpi.so.12. We cannot do host injection as well since they aren't compatible.
- Hence, OpenMPI + UCX cannot utilise Slingshot-11 and fall back to primitive transfer mechanism

Inter-node collectives (2 nodes x 8 GCDs = 16 ranks) — EESSI vs Native at small/mid/large messages (error bars = min/max over runs)



Solution:

MPICH toolchain and LD_LIBRARY_PATH override to the rescue! 🚑

We build MPICH-4.3.2 with rocm-compilers toolchain.

rmphich toolchain (analogous to rompi) - includes rocm-compilers and MPICH-4.3.2 is built.

OSU and GROMACS are rebuilt against rmphich toolchain. Once the build succeeds we strip off the EasyBuild MPICH links from DT_RPATH, so override can work later.

We add /opt/cray MPI Libs to LD_LIBRARY_PATH before running and it access the vendor MPI installation



Before:

```
$ ldd $(which gmx_mpi) | grep -i mpi
libmpi.so.12      => /cvmfs/.../MPICH/4.3.2/lib/libmpi.so.12
libmpicxx.so.12  => /cvmfs/.../MPICH/4.3.2/lib/libmpicxx.so.12
```

After:

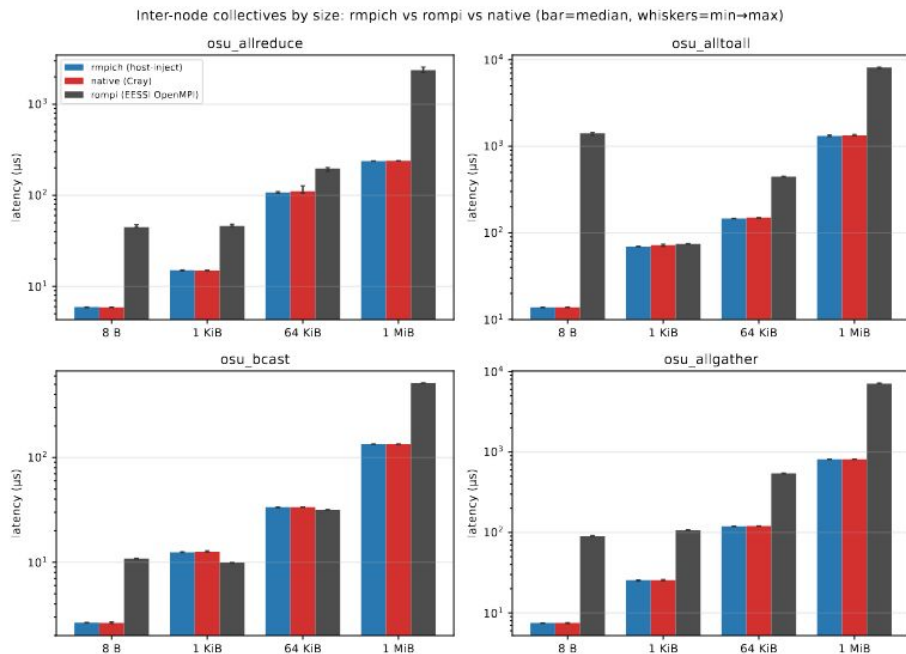
```
$ ldd $(which gmx_mpi) | grep -iE 'mpi|fabric|gtl'
/opt/cray/pe/mpich/9.0.1/gtl/lib/libmpi_gtl_hsa.so.0 (LD_PRELOAD'd)
libmpicxx.so.12 => /opt/cray/pe/mpich/9.0.1/.../lib-abi-mpich/libmpicxx.so.12
libfabric.so.1  => /opt/cray/libfabric/1.22.0/lib64/libfabric.so.1
```



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Results:



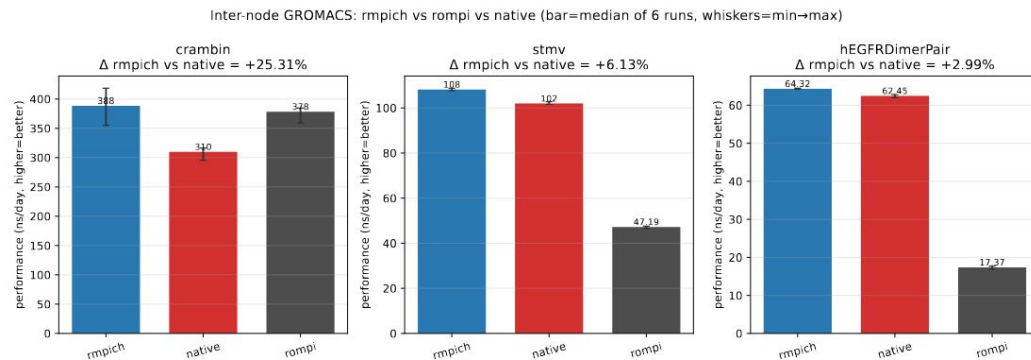
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Lmod



Results:



CernVM-FS



Lmod



For an actual host_injections solution:

We need to point OSU and GROMACS to placeholder paths in cvmfs repository

A script which would link those placeholder paths to /opt/cray MPI libs



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- NVIDIA and AMD GPU support in EasyBuild / EESSI have been a joint effort. Some notable contributions:
- LLVM toolchain in EasyBuild: Davide Grassano
- Exploratory ROCm work in EasyBuild & EESSI: Inuits (funded by Microsoft)
- ROCm-LLVM, ROCmComponent and rocm-compilers: Kenneth Hoste, Jan Andre Reuter, Bob Dröge, Caspar van Leeuwen, and others



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Lmod





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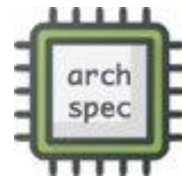
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Next session: Revisit the EESSI bot 

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