

NVIDIA HPC SDK RELEASE NOTES

RN-09976-001-V24.5 | May 2024



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Chapter 1. WHAT'S NEW

Welcome to the 24.5 version of the NVIDIA HPC SDK, a comprehensive suite of compilers and libraries enabling developers to program the entire HPC platform, from the GPU foundation to the CPU and out through the interconnect. The 24.5 release of the HPC SDK includes component updates as well as important functionality and performance improvements.

- Multiple features have been added to the 24.5 HPC Compilers to improve programming across various memory modes. See the documentation for further information.
 - The HPC Compilers' command line interface for controlling the memory modes during compilation and linking has been updated with new options that support separate, managed, and unified memory when using standard language parallelism, CUDA Fortran, OpenACC, and OpenMP.
 - The HPC Compilers have added diagnostics for mismatching GPU memory modes between compilation and linking, including use of the OpenMP requires directive with unified_shared_memory. The diagnostic is issued when programs are linked with different, incompatible memory mode options.
- When the compilation target is set to GPU, nvfortran now infers routines called from within DO CONCURRENT loops within a single compilation unit and compiles them for GPU without requiring explicit device routine annotations. Details can be found in the documentation.
- The HPC Compilers have implemented the -nvmalloc option. This option enables a general purpose memory allocation implementation that emphasizes fragmentation avoidance and scalable concurrency support. This work is based on the jemalloc memory allocator and is tuned for x86 CPUs and NVIDIA Grace Arm CPUs. When activated, it replaces malloc and the related memory allocating functions.
- NVPL has been updated to 24.03-beta in the HPC SDK 24.5. See NVIDIA Performance Libraries for more details.
 - With this update, the NVPL Tensor, ScaLAPACK, and BLACS libraries are now available.
 - The -Mnvpl flag has been improved for better integration with the HPC compilers:

- Without any sub-options, all NVPL libraries will be linked into the application on an as-needed basis as determined by the linker.
- Users may choose to override this behavior by specifying a list of NVPL libraries to link in, e.g. -Mnvpl=blas,lapack,fft,rand.
- -Mnvpl does not include NVPL ScaLAPACK unless -Mscalapack is also specified.
- The -Mscalapack flag has also been enhanced. When specified with -i8, it will now link in the ilp64 versions of the ScaLAPACK libraries now. When -Mscalapack is specified with -Mnvpl, the NVPL ScaLAPACK is used; Mscalapack without -Mnvpl will use Netlib ScaLAPACK, as before.
- The __int128 ABI has been updated for X86 to correctly pass i128 in either 2 registers or in a 16 byte stack slot if registers are not available. This matches the x86_64 SysV ABI specification. Object files that pass i128 will need to be recompiled.
- nvcpuid has been reworked to use the Linux kernel names and features as listed in / proc/cpuinfo.
- The HPC SDK version 24.5 is shipping with CUDA 12.4 and 11.8.

Chapter 2. RELEASE COMPONENT VERSIONS

The NVIDIA HPC SDK 24.5 release contains the following versions of each component:

	Linux_x86_64		Linux_aarch64		
	CUDA 11.8	CUDA 12.4	CUDA 11.8	CUDA 12.4	
nvc++	24.5		24.5		
nvc	24.5		24	24.5	
nvfortran	24	1.5	24.5		
nvcc	11.8.89	12.4.127	11.8.89	12.4.127	
NCCL	2.18.5	2.18.5	2.19.3	2.19.3	
NVSHMEM	2.11.0	2.11.0	N/A	2.11.0	
cuBLAS	11.11.4.17	12.4.2.65	11.11.3.6	12.4.2.65	
cuBLASMp	0.2.0	0.2.0	0.2.0	0.2.0	
cuFFT	10.9.0.58	11.2.1.3	10.9.0.58	11.2.1.3	
cuFFTMp	11.0.14	11.0.14	N/A	11.0.14	
cuRAND	10.3.0.86	10.3.5.147	10.3.0.86	10.3.5.147	
cuSOLVER	11.4.1.48	11.6.1.9	11.4.1.48	11.6.1.9	
cuSOLVERMp	0.5.0	0.5.0	0.5.0	0.5.0	
cuSPARSE	11.7.5.86	12.3.1.170	11.7.5.86	12.3.1.170	
cuTENSOR	2.0.1	2.0.1	2.0.1	2.0.1	
Nsight Compute	2024.1.1		2024.1.1		
Nsight Systems	2024.1.1		2024.1.1		
HPC-X	2.14	2.19	2.14	2.19	
OpenBLAS	0.3.23		0.3.23		
Scalapack		2.2.0 2.2.0		2.2.0	

Table 1 HPC SDK Release Components

	Linux_x86_64		Linux_aarch64	
	CUDA 11.8	CUDA 12.4	CUDA 11.8	CUDA 12.4
Thrust	1.15.1	2.3.2	1.15.1	2.3.2
CUB	1.15.1	2.3.2	1.15.1	2.3.2
libcu++	1.8.1	2.3.0	1.8.1	2.3.2

Chapter 3. SUPPORTED PLATFORMS

3.1. Platform Requirements for the HPC SDK

Architecture	Linux Distributions	Minimum gcc/ glibc Toolchain	Minimum CUDA Driver
x86_64	RHEL/CentOS 7.3 - 7.9 RHEL/CentOS/Rocky 8.0 - 8.7 RHEL 9.2 - 9.3 OpenSUSE Leap 15.2 - 15.4 SLES 15SP2, 15SP3, 15SP4 Ubuntu 18.04, 20.04, 22.04 Debian 10	C99: 4.8 C11: 4.9 C++03: 4.8 C++11: 4.9 C++14: 5.1 C++17: 7.1 C++20: 10.1	450.36.06
aarch64	RHEL/CentOS/Rocky 8.0 - 8.7 Rocky 9.2 - 9.3 Ubuntu 20.04, 22.04 SLES 15SP2, 15SP3, 15SP4 Amazon Linux 2 Amazon Linux 2023	C99: 4.8 C11: 4.9 C++03: 4.8 C++11: 4.9 C++14: 5.1 C++17: 7.1 C++20: 10.1	450.36.06

Table 2 HPC SDK Platform Requirements

Programs generated by the HPC Compilers for x86_64 processors require a minimum of AVX instructions, which includes Sandy Bridge and newer CPUs from Intel, as well as Bulldozer and newer CPUs from AMD. The HPC SDK includes support for v8.1+

Server Class Arm CPUs that meet the requirements appendix E specified in the SBSA 7.1 specification.

The HPC Compilers are compatible with gcc and g++ and use the GCC C and C++ libraries; the minimum compatible versions of GCC are listed in Table 2. The minimum system requirements for CUDA and NVIDIA Math Library requirements are available in the NVIDIA CUDA Toolkit documentation.

3.2. Supported CUDA Toolchain Versions

The NVIDIA HPC SDK uses elements of the CUDA toolchain when building programs for execution with NVIDIA GPUs. Every HPC SDK installation package puts the required CUDA components into an installation directory called [install-prefix]/ [arch]/[nvhpc-version]/cuda.

An NVIDIA CUDA GPU device driver must be installed on a system with a GPU before you can run a program compiled for the GPU on that system. The NVIDIA HPC SDK does not contain CUDA drivers. You must download and install the appropriate CUDA driver from NVIDIA, including the CUDA Compatibility Platform if that is required.

The nvaccelinfo tool prints the CUDA Driver version in its output. You can use it to find out which version of the CUDA Driver is installed on your system.

The NVIDIA HPC SDK 24.5 includes the following CUDA toolchain versions:

- ► CUDA 11.8
- CUDA 12.4

The minimum required CUDA driver versions are listed in the table in Section 3.1.

Chapter 4. KNOWN LIMITATIONS

- When a pointer is assigned to an array dummy argument with the target attribute, nvfortran may associate the pointer with a copy of the array argument instead of the actual argument.
- HPC-X users may notice longer startup overhead on MPI jobs that run for a very short period of time. The environment variable UCX_VFS_ENABLE=n can be set as a possible workaround.
- On some systems UCX can fail while parsing /proc/self/map information, resulting in the crash with the following trace: "sys.c:194 UCX FATAL failed to allocate maps buffer(size=32768)" To work around this issue, set UCX_MEM_EVENTS=n environment variable
- NVPL FFT respects the original OpenMP thread affinity mask. For applications built with OpenMP runtimes, controls of thread affinity (either via OMP_PROC_BIND or OMP_PLACES) could negatively impact the multi-threaded performance. Users are recommended to unset the two OpenMP environment variables or set OMP_PROC_BIND to false for better performance. Additional known issues related to NVPL are described in the NVPL documentation.
- The MPI wrappers in comm_libs/mpi/bin automatically detect the CUDA driver and select the matching MPI library from comm_libs/X.Y. Applications that require a full MPI directory hierarchy (e.g., bin, include, lib) or are launched via srun should bypass the MPI wrappers by loading the nvhpc-hpcx-cuda11 or the nvhpc-hpcxcuda12 environment module, depending on the installed CUDA driver version.
- Passing an internal procedure as an actual argument to a Fortran subprogram is supported by nvfortran provided that the dummy argument is declared as an interface block or as a procedure dummy argument. nvfortran does not support internal procedures as actual arguments to dummy arguments declared external.
- nvfortran only supports the Fortran 2003 standard maximum of 7 dimensions for arrays (Fortran 2008 raised the standard maximum dimensions to 15). This limit is defined in the standard CFI_MAX_RANK macro in the ISO_Fortran_binding.h C header file.
- Section "15.5.2.4 Ordinary dummy variables", constraint C1540 and Note 5 in the Fortran 2018 Standard allow Fortran compilers to avoid copy-in/copy-out argument passing provided that the actual and corresponding dummy arguments have the ASYNCHRONOUS/VOLATILE attribute, and the dummy arguments do not have

the VALUE attribute. This feature is fully supported in nvfortran with BIND(C) interfaces (i.e., Fortran calling C). Copy-in/copy-out avoidance with asynchronous/ volatile attributes may not be available in other cases with nvfortran.

- Some applications may see failures on Haswell and Broadwell with MKL version 2023.1.0 when running certain workloads with 4 or more OpenMP threads. The issue is resolved in MKL version 2023.2.0.
- cuSolverMp has two dependencies on UCC and UCX libraries in the HPC-X directory. To execute a program linked against cuSolverMP, please use the "nvhpc-hpcx-cuda11" environment module for the HPC-X library, or set the environment variable LD_LIBRARY_PATH as follows: LD_LIBRARY_PATH= \${NVHPCSDK_HOME}/comm_libs/11.8/hpcx/latest/ucc/lib:\${NVHPCSDK_HOME}/ comm_libs/11.8/hpcx/latest/ucx/lib:\$LD_LIBRARY_PATH
- To use HPC-X, please use the provided environment module files or take care to source the hpcx-init.sh script: \$. \${NVHPCSDK_HOME}/comm_libs/ X.Y/hpcx/latest/hpcx-init.sh Then, run the hpcx_load function defined by this script: hpcx_load. These actions will set important environment variables that are needed when running HPC-X. The following warning from HPC-X while running an MPI job – "WARNING: Open MPI tried to bind a process but failed. This is a warning only; your job will continue, though performance may be degraded" – is a known issue, and may be suppressed as follows: export OMPI_MCA_hwloc_base_binding_policy=""
- As of version 2.17.1, HPC-X does not have performance-optimal support for streamordered CUDA-allocated memory. In practical terms it means that IPC methods such as the MPI calls MPI_Send and MPI_Recv can have significantly degraded throughput when passed data allocated with the cudaMallocAsync function or its variants. This limitation will be removed in one of the future releases of HPC-X.
- Fortran derived type objects with zero-size derived type allocatable components that are used in sourced allocation or allocatable assignment may result in a runtime segmentation violation.
- When using -stdpar to accelerate C++ parallel algorithms, the algorithm calls cannot include virtual function calls or function calls through a function pointer, cannot use C++ exceptions, and must use random access iterators (raw pointers as iterators work best). When unified memory is not enabled, the algorithm calls can only dereference pointers that point to the heap. See the C++ parallel algorithms documentation for more details.

Chapter 5. DEPRECATIONS AND CHANGES

- Support for the Power CPU architecture in the HPC SDK has been discontinued.
- Support for the Amazon Linux 2 and RHEL 7-based operating systems will be removed in the HPC SDK version 24.9, corresponding with the upstream end-of-life (EOL).
- The -Mllvm command line option for nvc++, nvc, and nvfortran is no longer supported.
- The GNU extension macros linux and unix are no longer defined when in ANSI mode (e.g., -std=c++17 or -std=c99). If your code is compiled in ANSI mode and you rely on either of these macros, you will need to use one of the ANSI compliant macros __linux__ or __unix__.
- Arm (aarch64) only: The 23.9 version of nvfortran changes the calling/return sequence for Fortran complex functions to match GNU's gfortran convention. Prior to the 23.9 release, nvfortran functions returned complex values via the stack using a "hidden" pointer as the first parameter. Now, complex values are returned following the gfortan convention via the floating-point registers. All libraries released with NVIDIA HPC SDK for Arm have been updated to follow the "gfortran" method. Users linking against Arm's performance libraries will need to use the "gcc" version instead of the "arm" version. All Fortran code, including libraries, that uses complex numbers must be recompiled when using nvfortran on Arm systems.
- Support for CUDA Fortran textures is deprecated in CUDA 11.0 and 11.8, and has been removed from CUDA 12. The 23.9 release is the last version of the HPC Compilers to include support for CUDA Fortran texture.
- The OpenMPI 3 and 4 libraries will be removed from the HPC SDK in a future release.
- The -Minfo=intensity option is no longer supported.
- The CUDA_HOME environment variable is ignored by the HPC Compilers. It is replaced by NVHPC_CUDA_HOME.
- The -Mipa option has been disabled starting with the 23.3 version of the HPC Compilers.
- The -ta=tesla, -Mcuda, -Mcudalib options for the HPC Compilers have been deprecated.

- Starting with version 23.11, the HPC SDK bundles only CUDA 11.8 and the latest version of the CUDA 12.x series. Codepaths in the HPC Compilers that support CUDA versions older than 11.0 are no longer tested or maintained.
- cudaDeviceSynchronize() in CUDA Fortran has been deprecated, and support has been removed from device code. It is still supported in host code.
- Starting with the 21.5 version of the NVIDIA HPC SDK, the -cuda option for NVC+ + and NVFORTRAN no longer automatically links the NVIDIA GPU math libraries. Please refer to the -cudalib option.
- HPC Compiler support for the Kepler architecture of NVIDIA GPUs was deprecated starting with the 21.3 version of the NVIDIA HPC SDK.

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