

# **NVIDIA®** HPC Compilers

# OPENACC GETTING STARTED GUIDE

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# Chapter 1. OVERVIEW

The OpenACC Application Programming Interface (API) is a collection of compiler directives and runtime routines that allow software developers to specify loops and regions of code in standard Fortran, C++ and C programs that should be executed in parallel either by offloading to an accelerator such as a GPU or by executing on all the cores of a host CPU. The OpenACC API was designed and is maintained by an industry consortium. See the OpenACC website, http://www.openacc.org for more information about the OpenACC API.

This Getting Started guide provides examples of how to write, build and run programs using the OpenACC directives support in the NVIDIA HPC Compilers.

### 1.1. System Prerequisites

Using the OpenACC implementation in the NVIDIA HPC Compilers requires the following:

- An x86-64, OpenPOWER or Arm Server CPU-based system running Linux.
- For targeting GPUs, a CUDA-enabled NVIDIA GPU and an installed CUDA device driver, CUDA version 8.0 or later. See the NVIDIA CUDA webpage at http:// www.nvidia.com/cuda for more information on obtaining and installing a CUDA device driver.

### 1.2. Prepare Your System

To use the NVIDIA OpenACC compilers, follow these steps:

- **1.** Download the latest NVIDIA HPC SDK 23.9 packages from the NVIDIA download webpage at nvcompilers.com/downloads.
- **2.** Install the downloaded package in /opt/nvidia/hpc\_sdk or another directory of your choosing.
- **3.** Add the /opt/nvidia/hpc\_sdk/*target*/23.9/compilers/bin directory to your path, where *target* is one of Linux\_x86\_64, Linux\_ppcle64 or Linux\_aarch64.

**4.** Invoke the nvaccelinfo command to see that your GPU and drivers are properly installed and available. You should see output that looks something like the following:

0	
CUDA Driver Version:	10020
NVRM version:	NVIDIA UNIX x86_64 Kernel Module 440.33.01
Wed Nov 13 00:00:22 UTC 2019	
Device Number:	0
Device Name:	Tesla V100-PCIE-16GB
Device Revision Number:	7.0
Global Memory Size:	16945512448
Number of Multiprocessors:	80
Concurrent Copy and Execution:	
Total Constant Memory:	65536
Total Shared Memory per Block:	
Registers per Block:	65536
Warp Size:	32
Maximum Threads per Block:	1024
Maximum Block Dimensions:	1024, 1024, 64
Maximum Grid Dimensions:	2147483647 x 65535 x 65535
Maximum Memory Pitch:	2147483647B
Texture Alignment:	512B
Clock Rate:	1380 MHz
Execution Timeout:	No
Integrated Device:	No
Can Map Host Memory:	Yes
Compute Mode:	default
Concurrent Kernels:	Yes
ECC Enabled:	Yes
Memory Clock Rate:	877 MHz
Memory Bus Width:	4096 bits
L2 Cache Size:	6291456 bytes
Max Threads Per SMP:	2048
Async Engines:	7
Unified Addressing:	Yes
Managed Memory:	Yes
Concurrent Managed Memory:	Yes
Preemption Supported:	Yes
Cooperative Launch:	Yes
Multi-Device:	Yes cc70
NVIDIA Default Target:	

This tells you the driver version, the type of the GPU (or GPUs, if you have more than one), the available memory, the command-line flag you should use to target this GPU (in this case **-gpu=cc70**), and so on.

### 1.3. Supporting Documentation and Examples

You may want to consult the OpenACC 2.7 specification available at the OpenACC website, http://www.openacc.org. Simple examples appear in Using OpenACC with the HPC Compilers.

# Chapter 2. USING OPENACC WITH THE NVIDIA HPC COMPILERS

OpenACC directives are enabled by adding the -acc flag to the compiler command line. By default, the NVIDIA HPC compilers will parallelize and offload OpenACC regions to NVIDIA GPUs. You can specify -acc=multicore to parallelize for a multicore CPU, or -acc=host to generate an executable that will run serially on the host CPU.

Many aspects of GPU targeting and code generation can be controlled by adding the -gpu flag to the compiler command line. By default, the NVIDIA HPC compilers will target the NVIDIA GPU installed on the compilation host. You can specify -gpu=cc70 to exclusively target a Volta GPU, or specify multiple compute capabilities (ccXY) to generate GPU executables optimized for multiple generations of NVIDIA GPUs.

See the compiler man pages for a complete list of sub-options to -acc and -gpu compiler options. This release includes support for almost all of the OpenACC 2.7 specification. Refer to Implemented Features for details about which features are supported in this release.

### 2.1. CUDA Versions

The NVIDIA HPC compilers use components from NVIDIA's CUDA Toolkit to build programs for execution on an NVIDIA GPU. The NVIDIA HPC SDK puts the CUDA Toolkit components into an HPC SDK installation sub-directory; the HPC SDK typically bundles three versions of recently-released Toolkits.

You can compile a program for an NVIDIA GPU on any system supported by the HPC compilers. You will be able to run that program only on a system with an NVIDIA GPU and an installed NVIDIA CUDA driver. NVIDIA HPC SDK products do not contain CUDA device drivers. You must download and install the appropriate CUDA Driver from NVIDIA.

The NVIDIA HPC SDK utility **nvaccelinfo** prints the driver version as its first line of output. You can use it to find out which version of the CUDA Driver is installed on your system.

The NVIDIA HPC SDK 23.9 includes components from the following versions of the CUDA Toolkit:

- CUDA 11.0
- CUDA 11.8
- ► CUDA 12.2

If you are compiling a program for GPU execution on a system *without* an installed CUDA driver, the compiler selects the version of the CUDA Toolkit to use based on the value of the **DEFCUDAVERSION** variable contained in a file called **localrc** which is created during installation of the HPC SDK.

If you are compiling a program for GPU execution on a system *with* an installed CUDA driver, the compiler detects the version of the CUDA driver and selects the appropriate CUDA Toolkit version to use from those bundled with the HPC SDK.

The compilers look for a CUDA Toolkit version in the /opt/nvidia/hpc\_sdk/target/23.9/ cuda directory that matches the version of the CUDA Driver installed on the system. If an exact match is not found, the compiler searches for the closest match. For CUDA Driver versions up to and including 11.1, the compiler searches for the newest CUDA Toolkit version that is not newer than the CUDA Driver version. For CUDA Driver versions of 11.2 and later, the compiler searches for the closest version newer than the CUDA Driver version within the same major release sequence.

You can change the compiler's default selection of CUDA Toolkit version using a compiler option. Add the **cudaX**.**Y** sub-option to **-gpu** where **X**.**Y** denotes the CUDA version. Using a compiler option changes the CUDA Toolkit version for one invocation of the compiler. For example, to compile an OpenACC C file with the CUDA 11.0 Toolkit you would use:

nvc -acc -gpu=cuda11.0

# 2.2. Compute Capability

The compilers can generate code for NVIDIA GPU compute capabilities 3.5 through 8.6. The compilers construct a default list of compute capabilities that matches the compute capabilities supported by the GPUs found on the system used in compilation. If there are no GPUs detected, the compilers generate code for every supported compute capability.

You can override the default by specifying one or more compute capabilities using either command-line options or an rcfile.

To change the default with a command-line option, provide a comma-separated list of compute capabilities to the –gpu option.

To change the default with an rcfile, set the **DEFCOMPUTECAP** value to a blankseparated list of compute capabilities in the siterc file located in your installation's bin directory:

set DEFCOMPUTECAP=60 70;

Alternatively, if you don't have permissions to change the siterc file, you can add the **DEFCOMPUTECAP** definition to a separate .mynvrc file in your home directory.

The generation of device code can be time consuming, so you may notice an increase in compile time as the number of compute capabilities increases.

# 2.3. PTX JIT Compilation

As of HPC SDK 22.9, support for PTX JIT compilation is enabled in all compilers for relocatable device code mode. This means that applications built with -gpu=rdc (that is, with relocatable device code enabled, which is the default mode) are forward-compatible with newer GPUs thanks to the embedded PTX code. The embedded PTX code is dynamically compiled when the application runs on a GPU architecture newer than the architecture specified at compile time.

The support for PTX JIT compilation is enabled automatically, which means that you do not need to change the compiler invocation command lines for your existing projects.

Use scenarios

- As an example, you can compile your application targeting the Ampere GPU without having to worry about the Hopper GPU architecture. Once the application runs on a Hopper GPU, it will seamlessly use the embedded PTX code.
- In CUDA Fortran, or with the CUDA Interoperability mode enabled, you can mix in object files compiled with the CUDA NVCC compiler containing PTX code. This PTX code from NVCC will be handled by the JIT compiler alongside the PTX code contained in object files produced by the HPC SDK compilers. When using the CUDA NVCC compiler, the relocatable device code generation must be enabled explicitly using the NVCC --relocatable-device-code true switch, as explained in the CUDA Compiler Driver guide. For information about CUDA Interoperability, please refer to https://docs.nvidia.com/hpc-sdk/compilers/ hpc-compilers-user-guide/index.html#openmp-interop-cuda. The CUDA Fortran Programming Guide is available here: https://docs.nvidia.com/hpc-sdk/compilers/ cuda-fortran-prog-guide.

By default, the compiler will choose the compute capability that matches the GPU on the system where the code is being compiled. For code that is going to run on the system where it is compiled, we recommend letting the compiler set the compute capability.

When the default won't work, we recommend compiling applications for a range of compute capabilities that the application is expected to run against, for example, using the -gpu=ccall compiler option. When running the application on a system that supports one of those compute capabilities, the CUDA driver minor version is allowed to be less than the version of the CUDA toolkit used at compile time, as covered in section CUDA Versions.

#### Performance considerations

PTX JIT compilation, when it occurs, can have a start-up overhead for the application. The JIT compiler keeps a cached copy of the produced device code, which reduces the overhead on subsequent runs. Please refer to the CUDA Programming Guide for detailed information about how the JIT compiler works.

#### Known limitations

In general, in order for PTX JIT compilation to work, the CUDA driver installed on the deployment system must be at least of the version that matches the CUDA toolkit used to compile the application. This requirement is stricter than those explained in section CUDA Versions.

For example, as explained in that section, the compilers will use the CUDA 11.8 toolkit that is shipped as part of the HPC SDK toolkit when the CUDA driver installed in the system is at least 11.2. However, while the CUDA 11.2 driver is commonly sufficient to run the application, it will not be able to compile the PTX code produced by the CUDA 11.8 toolkit. This means that any deployment system where the PTX JIT compilation is expected to be used must have at least the CUDA 11.8 driver installed. Please refer to the CUDA Compatibility guide for further information about the CUDA Driver compatibility with CUDA Toolkits.

When the application is expected to run on a newer GPU architecture than specified at compile time, we recommend having a CUDA driver installed on the deployment system matching the CUDA toolkit used to build the application. One way to achieve that is to use the **NVHPC\_CUDA\_HOME** environment variable at compile time to provide a specific CUDA toolkit.

Below are a few examples of how the PTX version incompatibility can be diagnosed and fixed. As a general rule, if the CUDA driver is unable to run the application due to incompatible PTX, the application will terminate with an error message indicating the cause. OpenACC and OpenMP applications will in most cases suggest compiler flags to target the current CUDA installation.

#### OpenACC

Consider this program that we will compile for Volta GPU and attempt to run on an Ampere GPU, on a system that has CUDA 11.5 installed:

```
#include <stdio.h>
#define N 1000
int array[N];
int main() {
#pragma acc parallel loop copy(array[0:N])
   for(int i = 0; i < N; i++) {
      array[i] = 3.0;
   }
   printf("Success!\n");
}</pre>
```

When we build the program, HPC SDK will choose the CUDA 11.8 toolkit that is included as the default. When we attempt to run it, it fails because code generated with 11.8 does not work with the 11.5 driver:

```
$ nvc -acc -gpu=cc70 app.c
$ ./a.out
Accelerator Fatal Error: This file was compiled: -acc=gpu -gpu=cc70
Rebuild this file with -gpu=cc80 to use NVIDIA Tesla GPU 0
File: /tmp/app.c
Function: main:3
Line: 3
```

From the error message it follows that the system is unable to execute the Volta GPU instructions on the current system. The embedded Volta PTX could not be compiled, which implies a CUDA driver incompatibility. A way to fix this is to use the installed CUDA 11.5 toolkit at compile time:

```
$ export NVHPC_CUDA_HOME=/usr/local/cuda-11.5
$ nvc -acc -gpu=cc70 app.c
$ ./a.out
Success!
```

#### OpenMP

Likewise, an OpenMP program will compile but not run:

```
#include <stdio.h>
#define N 1000
int array[N];
int main() {
#pragma omp target loop
for(int i = 0; i < N; i++) {
    array[i] = 0;
    }
    printf("Success!\n");
}</pre>
```

```
$ nvc -mp=gpu -gpu=cc70 app.c
$ ./a.out
Accelerator Fatal Error: Failed to find device function 'nvkernel_main_F1L3_2'!
File was compiled with: -gpu=cc70
Rebuild this file with -gpu=cc80 to use NVIDIA Tesla GPU 0
File: /tmp/app.c
Function: main:3
Line: 3
```

We can also fix it by having **NVHPC\_CUDA\_HOME** point at the matching CUDA toolkit location:

```
$ export NVHPC_CUDA_HOME=/usr/local/cuda-11.5
$ nvc -acc -gpu=cc70 app.c
$ ./a.out
Success!
```

C++

In contrast to OpenACC and OpenMP applications that simply terminate when PTX JIT encounters an insufficient CUDA driver version, C++ applications throw a system exception when there is a PTX incompatibility:

```
#include <vector>
#include <algorithm>
#include <algorithm>
#include <iostream>
#include <assert.h>
int main() {
   std::vector<int> x(1000, 0);
   x[1] = -20;
   auto result = std::count(std::execution::par, x.begin(), x.end(), -20);
   assert(result == 1);
   std::cout << "Success!" << std::endl;
}
$ nvc++ -stdpar -gpu=cc70 app.cpp
</pre>
```

```
$ ./a.out
terminate called after throwing an instance of 'thrust::system::system_error'
what(): after reduction step 1: cudaErrorUnsupportedPtxVersion: the provided
PTX was compiled with an unsupported toolchain.
Aborted (core dumped)
```

The exception message contains a direct reference to an incompatible PTX, which in turn implies an mismatch between the CUDA toolkit and the CUDA driver version.

We can fix it similarly by setting **NVHPC CUDA HOME**:

```
$ export NVHPC_CUDA_HOME=/usr/local/cuda-11.5
$ nvc++ -stdpar -gpu=cc70 app.cpp
$ ./a.out
Success!
```

### 2.4. C Structs in OpenACC

Static arrays of struct and pointers to dynamic arrays of struct are supported in OpenACC regions by the NVIDIA C++ and C compilers.

```
typedef struct{
   float x, y, z;
}point;
extern point base[1000];
void vecaddgpu( point *restrict r, int n ){
   #pragma acc parallel loop present(base) copyout(r[0:n])
   for( int i = 0; i < n; ++i ){
        r[i].x = base[i].x;
        r[i].y = sqrtf( base[i].y*base[i].y + base[i].z*base[i].z );
        r[i].z = 0;
}</pre>
```

A pointer to a scalar struct is treated as a one-element array, and should be shaped as **r[0:1]**.

```
typedef struct{
    base[1000];
    int n;
    float *x, *y, *z;
}point;
extern point A;
void vecaddgpu(){
    #pragma acc parallel loop copyin(A) \
        copyout(A.x[0:A.n], A.y[0:A.n], A.z[0:A.n])
    for( int i = 0; i < A.n; ++i) {
        A.x[i] = A.base[i];
        A.y[i] = sqrtf( A.base[i] );
        A.z[i] = 0;
    }
}</pre>
```

In this example, the struct **A** is copied to the device, which copies the static array member **A**.**base** and the scalar **A**.**n**. The dynamic members **A**.**x**, **A**.**y** and **A**.**z** are then copied to the device. The struct **A** should be copied before its dynamic members, either by placing the struct in an earlier data clause, or by copying or creating it on the device in an enclosing data region or dynamic data lifetime. If the struct is not present on the device when the dynamic members are copied, the accesses to the dynamic members, such as **A**.**x**[**i**], on the device will be invalid, because the pointer **A**.**x** will not get updated.

A pointer to a struct is treated as a single element array. If the struct also contains pointer members, you should copy the struct to the device, then create or copy the pointer members:

```
typedef struct{
    int n;
    float *x, *y, *z;
}point;
void vecaddgpu( point *A, float* base ){
    #pragma acc parallel loop copyin(A[0:1]) \
        copyout(A->x[0:A->n], A->y[0:A->n], A->z[0:A->n]) \
        present(base[0:A->n])
    for( int i = 0; i < A->n; ++i ){
        A->x[i] = base[i];
        A->y[i] = sqrtf( base[i] );
        A->z[i] = 0;
}
```

Be careful when copying structs containing pointers back to the host. On the device, the pointer members will get updated with device pointers. If these pointers get copied back to the host struct, the pointers will be invalid on the host.

When creating or copying a struct on the device, the whole struct is allocated. There is no support for allocating a subset of a struct, or only allocating space for a single member.

Structs and pointer members can be managed using dynamic data directives as well:

```
typedef struct{
    int n;
    float *x, *y, *z;
```

```
}point;
void move to device ( point *A ) {
    #pragma acc enter data copyin(A[0:1])
    #pragma acc enter data create(A->x[0:A->n], A->y[0:A->n], A->z[0:A->n])
void move_from_device( point* A ) {
    #pragma acc enter data copyout(A->x[0:A->n], A->y[0:A->n], A->z[0:A->n])
    #pragma acc enter data delete(A[0:1])
void vecaddgpu( point *A, float* base ) {
    #pragma acc parallel loop present(A[0:1]) \
       present(A->x[0:A->n], A->y[0:A->n], A->z[0:A->n]) \
       present(base[0:A->n])
    for( int i = 0; i < A -> n; ++i ) {
       A \rightarrow x[i] = base[i];
       A->y[i] = sqrtf( base[i] );
       A - > z[i] = 0;
    }
```

### 2.5. C++ Classes in OpenACC

The NVIDIA C++ compiler supports use of C++ classes in OpenACC regions, including static array class members, member pointers to dynamic arrays, and member functions and operators. Usually, the class itself must be copied to device memory as well, by putting the class variable in a data clause outside the class, or the appropriately shaped **this**[0:1] reference in a data clause within the class. The entire class will be allocated in device memory.

```
// my managed vector datatype
template<typename elemtype> class myvector{
   elemtype* data;
    size_t size;
public:
   myvector( size t size ) { // constructor
       size = size ;
       data = new elemtype[size];
    }
    todev() { // move to device
        #pragma acc enter data copyin(this[0:1], data[0:size])
   fromdev() { // remove from device
        #pragma acc exit data delete( data[0:size], this[0:1])
    }
   void updatehost() { // update host copy of data
        #pragma acc update self( data[0:size] )
    }
   void updatedev() { // update device copy of data
        #pragma acc update device( data[0:size] )
    }
    ~myvector() { // destructor from host
       delete[] data;
   inline elemtype & operator[] (int i) const { return data[i]; }
    // other member functions
```

```
};
```

In the example below, the **this** pointer is copied to the device before **data**, so the pointer to **data** on the device will get updated. This is called an "attach" operation; the **class myvector** pointer **data** is attached to the device copy of the **data** vector.

Another class always creates device data along with host data:

```
// my managed host+device vector datatype
template<typename elemtype> class hdvector{
   elemtype* data;
    size t size;
public:
   hdvector( size t size ) { // constructor
       size = size_;
        data = new elemtype[size];
        #pragma acc enter data copyin(this[0:1]) create(data[0:size])
    }
   void updatehost() { // update host copy of data
        #pragma acc update self( data[0:size] )
    }
   void updatedev() { // update device copy of data
        #pragma acc update device( data[0:size] )
    }
    ~hdvector() { // destructor from host
        #pragma acc exit data delete( data[0:size], this[0:1] )
        delete[] data;
    inline elemtype & operator[] (int i) const { return data[i]; }
    // other member functions
};
```

The constructor copies the class in, so the **size** value will get copied, and creates (allocates) the **data** vector.

A slightly more complex class includes a copy constructor that makes a copy of the data pointer instead of a copy of the data:

```
#include <openacc.h>
// my managed vector datatype
template<typename elemtype> class dupvector{
   elemtype* data;
   size t size;
   bool iscopy;
public:
   dupvector( size_t size_ ) { // constructor
       size = size_;
       data = new elemtype[size];
       iscopy = false;
        #pragma acc enter data copyin(this[0:1]) create(data[0:size])
    }
   dupvector( const dupvector & copyof ) { // copy constructor
       size = copyof.size;
       data = copyof.data;
       iscopy = true;
        #pragma acc enter data copyin(this[0:1])
       acc attach( (void**)&data );
   }
   void updatehost() { // update host copy of data
        #pragma acc update self( data[0:size] )
    }
   void updatedev() { // update device copy of data
        #pragma acc update device( data[0:size] )
    ~dupvector() { // destructor from host
        if( !iscopy ) {
            #pragma acc exit data delete( data[0:size] )
            delete[] data;
```

```
}
#pragma acc exit data delete( this[0:1] )
}
inline elemtype & operator[] (int i) const { return data[i]; }
// other member functions
};
```

Note the call to the OpenACC runtime routine, acc\_attach, in the copy constructor. This routine takes the address of a pointer, translates the address of that pointer as well as the contents of the pointer, and stores the translated contents into the translated address on the device. In this case, it attaches the data pointer copied from the original class on the device to the copy of this class on the device.

In code outside the class, data can be referenced in compute clauses as expected:

```
dupvector<float> v = new dupvector<float>(n);
dupvector<float> x = new dupvector<float>(n);
...
#pragma acc parallel loop present(v,x)
for( int i = 0; i < n; ++i ) v[i] += x[i];</pre>
```

The example above shows references to the **v** and **x** classes in the parallel loop construct. The **operator[]** will normally be inlined. If it is not inlined or inlining is disabled, the compiler will note that the operator is invoked from within an OpenACC compute region and compile a device version of that operator. This is effectively the same as implying a **#pragma acc routine seq** above the operator. The same is true for any function in C++, be it a class member function or standalone function: if the function is called from within a compute region, or called from a function which is called within a compute region, and there is no **#pragma acc routine**, the compiler will treat it as if it was prefixed by **#pragma acc routine seq**. When you compile the file and enable – **Minfo=accel**, you will see this with the message:

In the above example the loop upper bound is the simple scalar variable **n**, not the more natural class member **v**.**size**. In the current implementation of the NVIDIA C+ + compiler the loop upper bound for a parallel loop or kernels loop must be a simple variable, not a class member.

The class variables appear in a **present** clause for the parallel construct. The normal default for a compute construct would be for the compiler to treat the reference to the class as **present\_or\_copy**. However, if the class instance were not present, copying just the class itself would not copy the dynamic data members, so would not provide the necessary behavior. Therefore, when referring to class objects in a compute construct, you should put the class in a **present** clause.

Class member functions may be explicitly invoked in a parallel loop:

```
template<typename elemtype> class dupvector{
    ...
    void incl( int i, elemtype y ){
        data[i] += y;
    }
}
...
#pragma acc parallel loop present(v,x)
    for( int i = 0; i < n; ++i ) v.incl( i, x[i] );</pre>
```

As discussed above, the compiler will normally inline **inc1**, when optimization is enabled, but will also compile a device version of the function since it is invoked from within a compute region.

A compute construct may contain compute constructs itself:

```
template<typename elemtype> class dupvector{
    ...
    void inc2( dupvector<elemtype> &y ){
        int n = size;
        #pragma acc parallel loop gang vector present(this,y)
        for( int i = 0; i < n; ++i ) data[i] += y[i];
    }
}
...
v.inc2( x );</pre>
```

Note again the loop upper bound of **n**, and the **this** and **y** classes in the **present** clause. A third example puts the parallel construct around the routine, but the loop itself within the routine. Doing this properly requires you to put an appropriate **acc routine** before the routine definition to call the routine at the right level of parallelism.

```
template<typename elemtype> class dupvector{
    ...
    #pragma acc routine gang
    void inc3( dupvector<elemtype> &y ){
        int n = size;
        #pragma acc loop gang vector
        for( int i = 0; i < n; ++i ) data[i] += y[i];
    }
}...
#pragma acc parallel
    v.inc3( x );</pre>
```

When the **inc3** is invoked from host code, it will run on the host incrementing host values. When invoked from within an OpenACC parallel construct, it will increment device values.

### 2.6. Fortran Derived Types in OpenACC

The NVIDIA Fortran compiler supports use of static and allocatable arrays of derived type in OpenACC regions.

```
module mpoint
type point
   real :: x, y, z
end type
type(point) :: base(1000)
end module
subroutine vecaddgpu( r, n )
use mpoint
 type(point) :: r(:)
 integer :: n
 !$acc parallel loop present(base) copyout(r(:))
 do i = 1, n
 r(i) %x = base(i) %x
 r(i)%y = sqrt( base(i)%y*base(i)%y + base(i)%z*base(i)%z )
 r(i)%z = 0
 enddo
```

end subroutine

You can explicitly reference array members of derived types, including static arrays and allocatable arrays within a derived type. In either case, the entire derived type must be placed in device memory, by putting the derived type itself in an appropriate data clause. In the current implementation, the derived type variable itself must appear in a data clause, at least a **present** clause, for any compute construct that directly uses the derived type variable.

```
module mpoint
type point
    real :: base(1000)
   integer :: n
   real, allocatable, dimension(:) :: x, y, z
end type
type(point) :: A
end module
subroutine vecaddqpu()
integer :: i
 !$acc parallel loop copyin(A) copyout(A%x,A%y,A%z)
do i = 1, n
 A\%x(i) = A\%base(i)
 A%y(i) = sqrt( A%base(i) )
 A\%z(i) = 0
enddo
end subroutine
```

In this example, the derived type **A** is copied to the device, which copies the static array member **A%base** and the scalar **A%n**. The allocatable array members **A%x**, **A%y** and **A%z** are then copied to the device. The derived type variable **A** should be copied before its allocatable array members, either by placing the derived type in an earlier data clause, or by copying or creating it on the device in an enclosing data region or dynamic data lifetime. If the derived type is not present on the device when the allocatable array members are copied, the accesses to the allocatable members, such as **A%x (i)**, on the device will be invalid, because the hidden pointer and descriptor values in the derived type variable will not get updated.

Be careful when copying derived types containing allocatable members back to the host. On the device, the allocatable members will get updated to point to device memory. If the whole derived type gets copied back to the host, the allocatable members will be invalid on the host.

When creating or copying a derived type on the device, the whole derived type is allocated. There is no support for allocating a subset of a derived type, or only allocating space for a single member.

Derived types and allocatable members can be managed using dynamic data directives as well:

```
module mpoint
type point
integer :: n
real, dimension(:), allocatable :: x, y, z
end type
contains
subroutine move_to_device( A )
type(point) :: A
!$acc enter data copyin(A)
!$acc enter data create(A%x, A%y, A%z)
```

```
end subroutine
subroutine move off device( A )
 type(point) :: A
 !$acc exit data copyout(A%x, A%y, A%z)
 !$acc exit data delete(A)
end subroutine
end module
subroutine vecaddgpu( A, base )
use mpoint
type(point) :: A
real :: base(:)
integer :: i
!$acc parallel loop present(A,base)
do i = 1, n
 A%x(i) = base(i)
 A%y(i) = sqrt( base(i) )
 A%z(i) = 0
enddo
end subroutine
```

### 2.7. Fortran I/O

The NVIDIA Fortran compiler includes limited support for **PRINT** statements in GPU device code. The Fortran GPU runtime library, which is shared between CUDA Fortran and OpenACC for NVIDIA GPU targets, buffers up the output and prints an entire line in one operation. Integer, character, logical, real and complex data types are supported.

The underlying CUDA **printf** implementation limits the number of print statements in a kernel launch to 4096. Users should take this limit into account when making use of this feature.

### 2.7.1. OpenACC PRINT Example

Here is a short example of printing character strings, integer, logical and real data within an OpenACC compute region:

```
program t
integer(4) a(10000)
a = [ (1+i,i=1,10000) ]
!$acc kernels
do i = 1, 10000
    if (a(i)/3000*3000.eq.a(i)) print *," located ",i,a(i),i.gt.5000,a(i)/5.0
end do
!$acc end kernels
end
```

# 2.8. OpenACC Atomic Support

The NVIDIA OpenACC compilers implement full support for atomics in accordance with the OpenACC specification. For example:

```
double *a, *b, *c;
. . .
#pragma acc loop vector
    for (int k = 0; k < n; ++k)</pre>
```

```
{
    #pragma acc atomic
    c[i*n+j] += a[i*n+k]*b[k*n+j];
}
```

The NVIDIA compilers also include support for CUDA-style atomic operations. The CUDA atomic names can be used in accelerator regions from Fortran, C, and C++. For example:

```
#pragma acc loop gang
for (j = 0; j < n1 * n2; j += n2) {
    k = 0;
    #pragma acc loop vector reduction(+:k)
    for (i = 0; i < n2; i++)
        k = k + a[j + i];
        atomicAdd(x, k);
}</pre>
```

# 2.9. OpenACC Declare Data Directive for Global and Fortran Module Variables

The compilers support the OpenACC declare directive with the copyin, create and device\_resident clauses for C global variables and Fortran module variables. This is primarily for use with the OpenACC routine directive and separate compilation. The data in the declare clauses are statically allocated on the device when the program attaches to the device. Data in a copyin clause will be initialized from the host data at that time. A program attaches to the device when it reaches its first data or compute construct, or when it calls the OpenACC acc\_init routine.

In C, the example below uses a global struct and a global array pointer:

```
struct{
  float a, b;
}coef;
float* x;
#pragma acc declare create(coef,x)
#pragma acc routine seq
void modxi( int i ) {
   x[i] *= coef.a;
void initcoef( float a, float b ) {
   coef.a = a;
   coef.b = b;
   #pragma acc update device(coef)
void allocx( int n ) {
   x = (float*)malloc( sizeof(float)*n );
   #pragma acc enter data create(x[0:n])
void modx( int s, int e ) {
   #pragma acc parallel loop
   for( int i = s; i < e; ++i ) modxi(i);</pre>
}
```

The declare create (coef, x) will statically allocate a copy of the struct coef and the pointer x on the device. In initcoef routine, the coefficients are assigned on the host, and the update directive copies those values to the device. The allocx routine allocates space for the x vector on the host, then uses an unstructured data directive to allocate that space on the device as well; because the x pointer is already statically present on the device, the device copy of x will be updated with the pointer to the device data as well. Finally, the parallel loop calls the routine modxi, which refers to the global x pointer and coef on the host, and when called on the device, such as in this parallel loop, this routine will access the global x pointer and coef struct on the device.

If the **modxi** routine were in a separate file, the declarations of **coef** and **x** would have the **extern** attribute, but otherwise the code would be the same, as shown below. Note that the **acc declare create** directive is still required in this file even though the variables are declared **extern**, to tell the compiler that these variables are available as externals on the device.

```
extern struct{
    float a, b;
}coef;
extern float* x;
#pragma acc declare create(coef,x)
. . .
#pragma acc routine seq
void modxi( int i ){
    x[i] *= coef.a;
}
```

Because the global variable is present in device memory, it is also in the OpenACC runtime *present* table, which keeps track of the correspondence between host and device objects. This means that a pointer to the global variable can be passed as an argument to a routine in another file, which uses that pointer in a **present** clause. In the following example, the calling routine uses a small, statically-sized global coefficient array:

```
float xcoef[11] = { 1.0, 2.0, 1.5, 3.5, ... 9.0 };
#pragma acc declare copyin(xcoef)
...
extern void test( float*, float*, float*, n );
...
void caller( float* x, float* y, int n ){
    #pragma acc data copy( x[0:n], y[0:n] )
    {
        ...
        test( x, y, xcoef, n );
        ...
    }
```

The **declare copyin** directive tells the compiler to generate code to initialize the device array from the host array when the program attaches to the device. In another file, the procedure **test** is defined, and all of its array arguments will be already present on the device; **x** and **y** because of the data construct, and **xcoef** because it is statically present on the device.

```
void test( float* xx, float* yy, float* cc, int n ){
    #pragma acc data present( xx[0:n], y[00:n], cc[0:11] )
    {
```

```
#pragma acc parallel loop
for( int i = 5; i < n-5; ++i ){
    float t = 0.0;
    for( int j = -5; j <= 5; ++j ){
        t += cc[j+5]*yy[i+j];
    }
    xx[i] /= t;
}
...
</pre>
```

In Fortran, module fixed-size variables and arrays, and module allocatable arrays which appear in declare directives at module scope will be available globally on the CPU as well as in device code. Module allocatable arrays that appear in a declare create, declare copyin or declare device\_resident will be allocated in host memory as well as in device memory when they appear in an allocate statement. The compiler manages the actual pointer to the data and a descriptor that contains array lower and upper bounds for each dimension, and the device copy of the pointer will be set to point to the array in device memory.

The following example module contains one fixed size array and an allocatable array, both appearing in a **declare create** clause. The static array **xstat** will be available at any time inside accelerator compute regions or routines.

```
module staticmod
integer, parameter :: maxl = 100000
real, dimension(maxl) :: xstat
real, dimension(:), allocatable :: yalloc
!$acc declare create(xstat,yalloc)
end module
```

This module may be used in another file that allocates the **yalloc** array. When the allocatable array **yalloc** is allocated, it will be allocated both in host and device memory, and will then be available at any time in accelerator compute regions or routines.

```
subroutine allocit(n)
use staticmod
integer :: n
allocate( yalloc(n) )
end subroutine
```

In another module, these arrays may be used in a compute region or in an accelerator routine:

```
module useit
use staticmod
contains
subroutine computer( n )
integer :: n
integer :: i
!$acc parallel loop
do i = 1, n
yalloc(i) = iprocess( i )
enddo
end subroutine
real function iprocess( i )
!$acc routine seq
integer :: i
iprocess = yalloc(i) + 2*xstat(i)
```

```
end function
end module
```

### 2.10. OpenACC Error Handling

The OpenACC specification provides a mechanism to allow you to intercept errors triggered during execution on a GPU and execute a specific routine in response before the program exits. For example, if an MPI process fails while allocating memory on the GPU, the application may want to call **MPI\_Abort** to shut down all the other processes before the program exits. This section explains how to take advantage of this feature.

To intercept errors the application must give a callback routine to the OpenACC runtime. To provide the callback, the application calls **acc\_set\_error\_routine** with a pointer to the callback routine.

The interface is the following, where **err msg** contains a description of the error:

```
typedef void (*exitroutinetype)(char *err_msg);
extern void acc set error routine(exitroutinetype callback routine);
```

When the OpenACC runtime detects a runtime error, it will invoke the callback\_routine.

This feature is not the same as error recovery. If the callback routine returns to the application, the behavior is decidedly undefined.

Let's look at this feature in more depth using an example.

Take the MPI program below and run it with two processes. Process 0 tries to allocate a large array on the GPU, then sends a message to the second process to acknowledge the success of the operation. Process 1 waits for the acknowledgment and terminates upon receiving it.

```
#include <stdio.h>
#include <stdlib.h>
#include "mpi.h"
#define N 2147483648
int main(int argc, char **argv)
 int rank, size;
 MPI Init(&argc, &argv);
 MPI Comm rank(MPI COMM WORLD, &rank);
 MPI Comm size (MPI COMM WORLD, & size);
  int ack;
  if(rank == 0) {
   float *a = (float*) malloc(sizeof(float) * N);
#pragma acc enter data create(a[0:N])
#pragma acc parallel loop independent
   for(int i = 0; i < N; i++) {</pre>
     a[i] = i *0.5;
#pragma acc exit data copyout(a[0:N])
```

```
printf("I am process %d, I have initialized a vector of size %ld bytes on
the GPU. Sending acknowledgment to process 1.", rank, N);
    ack = 1;
    MPI_Send(&ack, 1, MPI_INT, 1, 0, MPI_COMM_WORLD);
    } else if(rank == 1) {
        MPI_Recv(&ack, 1, MPI_INT, 0, 0, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
        printf("I am process %d, I have received the acknowledgment from process 0
that data in the GPU has been initialized.\n", rank, N);
        fflush(stdout);
    }
    // do some more work
MPI_Finalize();
    return 0;
```

#### We compile the program with:

\$ mpicc -acc -o error\_handling\_mpi error\_handling\_mpi.c

If we run this program with two MPI processes, the output will look like the following:

Process 0 failed while allocating memory on the GPU and terminated unexpectedly with an error. In this case **mpirun** was able to identify that one of the processes failed, so it shut down the remaining process and terminated the application. A simple two-process program like this is straightforward to debug. In a real world application though, with hundreds or thousands of processes, having a process exit prematurely may cause the application to hang indefinitely. Therefore it would be ideal to catch the failure of a process, control the termination of the other processes, and provide a useful error message.

We can use the OpenACC error handling feature to improve the previous program and correctly terminate the application in case of failure of an MPI process.

In the following sample code, we have added an error handling callback routine that will shut down the other processes if a process encounters an error while executing on the GPU. Process 0 tries to allocate a large array into the GPU and, if the operation is successful, process 0 will send an acknowledgment to process 1. Process 0 calls the OpenACC function acc\_set\_error\_routine to set the function handle\_gpu\_errors as an error handling callback routine. This routine prints a message and calls MPI\_Abort to shut down all the MPI processes. If process 0 successfully allocates the array on the GPU, process 1 will receive the acknowledgment. Otherwise, if process 0 fails, it will

terminate itself and trigger the call to **handle\_gpu\_errors**. Process 1 is then terminated by the code executed in the callback routine.

```
#include <stdio.h>
#include <stdlib.h>
#include "mpi.h"
#define N 2147483648
typedef void (*exitroutinetype)(char *err msg);
extern void acc set error routine (exitroutinetype callback routine);
void handle_gpu_errors(char *err_msg) {
 printf("GPU Error: %s", err_msg);
 printf("Exiting...\n\n");
 MPI_Abort(MPI_COMM_WORLD, 1);
 exit(-1);
int main(int argc, char **argv)
 int rank, size;
 MPI Init(&argc, &argv);
 MPI Comm rank(MPI COMM WORLD, &rank);
 MPI Comm size (MPI COMM WORLD, &size);
 int ack;
 if(rank == 0) {
    float *a = (float*) malloc(sizeof(float) * N);
   acc set error routine (&handle gpu errors);
#pragma acc enter data create(a[0:N])
#pragma acc parallel loop independent
   for(int i = 0; i < N; i++) {</pre>
     a[i] = i *0.5;
#pragma acc exit data copyout(a[0:N])
   printf("I am process %d, I have initialized a vector of size %ld bytes on
 the GPU. Sending acknowledgment to process 1.", rank, N);
   fflush(stdout);
   ack = 1;
   MPI Send(&ack, 1, MPI INT, 1, 0, MPI COMM WORLD);
 } else if(rank == 1) {
   MPI Recv(&ack, 1, MPI INT, 0, 0, MPI COMM WORLD, MPI STATUS IGNORE);
   printf("I am process %d, I have received the acknowledgment from process 0
 that data in the GPU has been initialized.\n", rank, N);
   fflush(stdout);
  1
 // more work
 MPI Finalize();
 return 0;
```

#### Again, we compile the program with:

\$ mpicc -acc -o error\_handling\_mpi error\_handling\_mpi.c

We run the program with two MPI processes and obtain the output below:

```
$ mpirun -n 2 ./error_handling_mpi
Out of memory allocating -8589934592 bytes of device memory
total/free CUDA memory: 11995578368/11919294464
Present table dump for device[1]:
NVIDIA Tesla GPU 0, compute capability 3.7, threadid=1
...empty...
GPU Error: call to cuMemAlloc returned error 2: Out of memory
Exiting...
```

MPI\_ABORT was invoked on rank 0 in communicator MPI\_COMM\_WORLD with errorcode 1.

This time the error on the GPU was intercepted by the application which managed it with the error handling callback routine. In this case the routine printed some information about the problem and called **MPI\_Abort** to terminate the remaining processes and avoid any unexpected behavior from the application.

### 2.11. C Examples

The simplest C example of OpenACC is a vector addition on the GPU:

```
#include <stdio.h>
#include <stdlib.h>
void vecaddgpu( float *restrict r, float *a, float *b, int n ){
    #pragma acc kernels loop copyin(a[0:n],b[0:n]) copyout(r[0:n])
    for( int i = 0; i < n; ++i ) r[i] = a[i] + b[i];</pre>
}
int main( int argc, char* argv[] ){
    int n; /* vector length */
    float * a; /* input vector 1 */
float * b; /* input vector 2 */
    float * r; /* output vector */
    float * e; /* expected output values */
    int i, errs;
    if ( argc > 1 ) n = atoi ( argv[1] );
    else n = 100000; /* default vector length */
    if( n <= 0 ) n = 100000;
    a = (float*)malloc( n*sizeof(float) );
    b = (float*)malloc( n*sizeof(float) );
    r = (float*)malloc( n*sizeof(float) );
e = (float*)malloc( n*sizeof(float) );
    for( i = 0; i < n; ++i ) {</pre>
         a[i] = (float)(i+1);
         b[i] = (float) (1000*i);
    /* compute on the GPU */
    vecaddgpu( r, a, b, n );
    /* compute on the host to compare */
    for( i = 0; i < n; ++i ) e[i] = a[i] + b[i];</pre>
    /* compare results */
    errs = 0;
    for( i = 0; i < n; ++i ) {</pre>
        if( r[i] != e[i] ) {
            ++errs;
   }
   printf( "%d errors found\n", errs );
   return errs;
```

The important part of this example is the routine vecaddgpu, which includes one OpenACC directive for the loop. This (#pragma acc) directive tells the compiler to generate a kernel for the following loop (kernels loop), to allocate and copy from the host memory into the GPU memory n elements for the vectors a and b before executing on the GPU, starting at a[0] and b[0] (copyin(a[0:n],b[0:n])), and to allocate n elements for the vector r before executing on the GPU, and copy from the GPU memory out to the host memory those n elements, starting at r[0] (copyout(r[0:n])).

If you type this example into a file a1.c, you can build it using the command nvc - acc a1.c. The -acc flag enables recognition of the OpenACC pragmas and includes the OpenACC runtime library. This command generates the usual a.out executable file, and you run the program by running a.out as normal. You should see the output:

0 errors found

If instead you get the following output, then there is something wrong with your hardware installation or your GPU driver.

libcuda.so not found, exiting Please check that the CUDA driver is installed and the shared object is in the install directory or on your LD LIBRARY PATH.

You can enable additional output by setting environment variables. If you set the environment variable NVCOMPILER\_ACC\_NOTIFY to 1, then the runtime prints a line of output each time you run a kernel on the GPU. For this program, you might get output that looks like:

```
launch CUDA kernel file=/user/guest/al.c function=vecaddgpu
line=5 device=0 threadid=1 num_gangs=782 num_workers=1
vector_length=128 grid=782 block=128
0 errors found
```

The extra output tells you that the program launched a kernel for the loop at line 5, with a CUDA grid of size 782, and a thread block of size 128.

If you set the environment variable NVCOMPILER\_ACC\_NOTIFY to 3, the output will include information about the data transfers as well:

```
upload CUDA data file=/user/guest/al.c function=vecaddgpu
line=4 device=0 threadid=1 variable=a bytes=400000
upload CUDA data file=/user/guest/al.c function=vecaddgpu
line=4 device=0 threadid=1 variable=b bytes=400000
launch CUDA kernel file=/user/guest/al.c function=vecaddgpu
line=5 device=0 threadid=1 num_gangs=782 num_workers=1 vector_length=128
grid=782 block=128
download CUDA data file=/user/guest/al.c function=vecaddgpu
line=6 device=0 threadid=1 variable=r bytes=400000
0 errors found
```

If you set the environment variable NVCOMPILER\_ACC\_TIME to 1, the runtime summarizes the time taken for data movement between the host and GPU, and computation on the GPU. On Linux, you may need to set the LD\_LIBRARY\_PATH environment variable to include the /opt/nvidia/hpc\_sdk/Linux\_x86\_64/23.9/ compilers/lib directory, or the corresponding directory for OpenPOWER or Arm Server targets. An OpenACC executable dynamically loads a shared object to implement this profiling feature, and the path to the library must be available.

For this program, you might get output similar to this:

0 errors found

This tells you that the program entered one accelerator region and spent a total of about 167 microseconds in that region. It copied two arrays to the device, launched one kernel, and brought one array back to the host.

You might also find it useful to enable the compiler feedback when you are writing your own OpenACC programs. This is enabled with the -Minfo flag. If you compile this program with the command nvc -acc -fast -Minfo al.c, you get the output:

```
vecaddqpu:
      4, Generating copyin(a[:n])
        Generating copyout(r[:n])
        Generating copyin(b[:n])
     5, Loop is parallelizable
         Accelerator kernel generated
         Generating Tesla code
          5, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
      5, Loop not fused: no successor loop
        Generated 2 alternate versions of the loop
        Generated vector simd code for the loop
        Generated 2 prefetch instructions for the loop
        Generated vector simd code for the loop
        Generated 2 prefetch instructions for the loop
        Generated vector simd code for the loop
        Generated 2 prefetch instructions for the loop
main:
    21, Loop not fused: function call before adjacent loop
        Loop not vectorized: data dependency
        Loop unrolled 16 times
        Generated 1 prefetches in scalar loop
    28, Loop not fused: dependence chain to sibling loop
        Generated 2 alternate versions of the loop
        Generated vector and scalar versions of the loop; pointer conflict
tests determine which is executed
        Generated 2 prefetch instructions for the loop
        Generated vector and scalar versions of the loop; pointer conflict
tests determine which is executed
        Generated 2 prefetch instructions for the loop
        Generated vector and scalar versions of the loop; pointer conflict
tests determine which is executed
        Generated 2 prefetch instructions for the loop
        Loop unrolled 16 times
        Generated 1 prefetches in scalar loop
    31, Loop not fused: function call before adjacent loop
```

This output gives the *schedule* used for the loop; in this case, the schedule is gang, vector(128). This means the iterations of the loop are broken into vectors of 128, and the vectors executed in parallel by SMs or compute units of the GPU.

This output is important because it tells you when you are going to get parallel execution or sequential execution. If you remove the restrict keyword from the

declaration of the dummy argument r to the routine vecaddgpu, the -Minfo output tells you that there may be dependences between the stores through the pointer r and the fetches through the pointers a and b:

```
5, Complex loop carried dependence of b->,a-> prevents
parallelization
Loop carried dependence of r-> prevents parallelization
Loop carried backward dependence of r-> prevents vectorization
Accelerator serial kernel generated
Accelerator kernel generated
Generating Tesla code
5, #pragma acc loop seq
5, Complex loop carried dependence of b->,a-> prevents parallelization
Loop carried dependence of r-> prevents parallelization
Loop carried backward dependence of r-> prevents vectorization
Loop carried backward dependence of r-> prevents vectorization
Loop not fused: no successor loop
Generated 2 alternate versions of the loop; pointer conflict
tests determine which is executed
```

A scalar kernel runs on one thread of one thread block, which runs about 1000 times slower than the same parallel kernel. For this simple program, the total time is dominated by GPU initialization, so you might not notice the difference in times, but in production mode you need parallel kernel execution to get acceptable performance.

For our second example, we modify the program slightly by replacing the data clauses on the kernels pragma with a present clause, and add a data construct surrounding the call to the vecaddgpu routine. The data construct moves the data across to the GPU in the main program. The present clause in the vecaddgpu routine tells the compiler to use the GPU copy of the data that has already been allocated on the GPU. If you run this program on the GPU with NVCOMPILER\_ACC\_TIME set, you see that the kernel region now has no data movement associated with it. Instead, the data movement is all associated with the data construct in the main program.

```
#include <stdio.h>
#include <stdlib.h>
void vecaddgpu( float *restrict r, float *a, float *b, int n ){
       #pragma acc kernels loop present(r,a,b)
       for( int i = 0; i < n; ++i ) r[i] = a[i] + b[i];</pre>
}
int main( int argc, char* argv[] ){
       int n; /* vector length */
       float * a; /* input vector 1 */
       float * b; /* input vector 2 */
       float * r; /* output vector */
       float * e; /* expected output values */
       int i, errs;
       if( argc > 1 ) n = atoi( argv[1] ); else n = 100000; /* default vector length */
       if (n \le 0) n = 100000;
       a = (float*)malloc( n*sizeof(float) );
       b = (float*)malloc( n*sizeof(float) );
       r = (float*)malloc( n*sizeof(float) );
       e = (float*)malloc( n*sizeof(float) );
       for( i = 0; i < n; ++i ) {</pre>
           a[i] = (float)(i+1);
           b[i] = (float) (1000*i);
       /* compute on the GPU */
```

```
#pragma acc data copyin(a[0:n],b[0:n]) copyout(r[0:n])
{
    vecaddgpu( r, a, b, n );
}
/* compute on the host to compare */
for( i = 0; i < n; ++i ) e[i] = a[i] + b[i];
/* compare results */
errs = 0;
for( i = 0; i < n; ++i ) {
    if( r[i] != e[i] ) {
      ++errs;
      }
    printf( ``%d errors found\n", errs );
return errs;</pre>
```

## 2.12. Fortran Examples

}

The simplest Fortan example of OpenACC is a vector addition on the GPU.

### 2.12.1. Vector Addition on the GPU

The section contains two Fortan examples of vector addition on the GPU:

```
module vecaddmod
 implicit none
 contains
 subroutine vecaddgpu( r, a, b, n )
  real, dimension(:) :: r, a, b
  integer :: n
  integer :: i
!$acc kernels loop copyin(a(1:n),b(1:n)) copyout(r(1:n))
   do i = 1, n
   r(i) = a(i) + b(i)
   enddo
  end subroutine
end module
program main
 use vecaddmod
 implicit none
 integer :: n, i, errs, argcount
 real, dimension(:), allocatable :: a, b, r, e
  character*10 :: arg1
 argcount = command_argument_count()
  n = 1000000 ! default value
 if( argcount >= 1 )then
  call get_command_argument( 1, arg1 )
read( arg1, '(i)' ) n
if( n <= 0 ) n = 100000</pre>
  endif
  allocate(a(n), b(n), r(n), e(n))
  do i = 1, n
  a(i) = i
  b(i) = 1000*i
  enddo
  ! compute on the GPU
  call vecaddgpu( r, a, b, n )
  ! compute on the host to compare
  do i = 1, n
  e(i) = a(i) + b(i)
  enddo
 ! compare results
```

```
errs = 0
do i = 1, n
if( r(i) /= e(i) )then
errs = errs + 1
endif
enddo
print *, errs, ' errors found'
if( errs ) call exit(errs)
end program
```

The important part of this example is the subroutine vecaddgpu, which includes one OpenACC directive for the loop. This (!\$acc) directive tells the compiler to generate a kernel for the following loop (kernels loop), to allocate and copy from the host memory into the GPU memory n elements for the vectors a and b before executing on the GPU, starting at a(1) and b(1) (copyin(a(1:n),b(1:n)), and to allocate n elements for the vector r before executing on the GPU, and copy from the GPU memory out to the host memory those n elements, starting at r(1) (copyout (r(1:n)).

If you type this example into a file f1.f90, you can build it using the command nvfortran -acc f1.f90. The -acc flag enables recognition of the OpenACC pragmas and includes the OpenACC runtime library. This command generates the usual a.out executable file, and you run the program by running a.out as normal. You should see the output:

0 errors found

If instead you get the following output, then there is something wrong with your hardware installation or your CUDA driver.

```
libcuda.so not found, exiting
Please check that the CUDA driver is installed and the shared object
is in the install directory or on your LD LIBRARY PATH.
```

You can enable additional output by setting environment variables. If you set the environment variable NVCOMPILER\_ACC\_NOTIFY to 1, then the runtime prints a line of output each time you run a kernel on the GPU. For this program, you might get output that looks like:

The extra output tells you that the program launched a kernel for the loop at line 9, with a CUDA grid of size 7813, and a thread block of size 128. If you set the environment variable NVCOMPILER\_ACC\_NOTIFY to 3, the output will include information about the data transfers as well:

```
upload CUDA data file=/user/guest/f1.f90 function=vecaddgpu
line=8 device=0 threadid=1 variable=a bytes=4000000
upload CUDA data file=/user/guest/f1.f90 function=vecaddgpu
line=8 device=0 threadid=1 variable=b bytes=4000000
launch CUDA kernel file=/user/guest/f1.f90 function=vecaddgpu
line=9 device=0 threadid=1 num_gangs=7813 num_workers=1 vector_length=128
grid=7813 block=128
download CUDA data file=/user/guest/f1.f90 function=vecaddgpu
line=12 device=0 threadid=1 variable=r bytes=4000000
0 errors found
```

If you set the environment variable NVCOMPILER\_ACC\_TIME to 1, the runtime summarizes the time taken for data movement between the host and GPU, and computation on the GPU. For this program, you might get output similar to this:

```
0 errors found
Accelerator Kernel Timing data
/home/ams/tat/example-f/f1.f90
vecaddgpu NVIDIA devicenum=0
time(us): 1,040
8: compute region reached 1 time
9: kernel launched 1 time
grid: [7813] block: [128]
device time(us): total=19 max=19 min=19 avg=19
elapsed time(us): total=738 max=738 min=738 avg=738
8: data region reached 2 times
8: data copyin transfers: 2
device time(us): total=689 max=353 min=336 avg=344
12: data copyout transfers: 1
device time(us): total=332 max=332 min=332 avg=332
```

This tells you that the program entered one accelerator region and spent a total of about 1 millisecond in that region. It copied two arrays to the device, launched one kernel and brought one array back to the host.

You might also find it useful to enable the compiler feedback when you are writing your own OpenACC programs. This is enabled with the -Minfo flag.

If you compile this program with the command nvfortran -acc -fast -Minfo f1.f90, you get the output: vecaddqpu: 8, Generating copyin(a(:n)) Generating copyout(r(:n)) Generating copyin(b(:n)) 9, Loop is parallelizable Accelerator kernel generated Generating Tesla code 9, !\$acc loop gang, vector(128) ! blockidx%x threadidx%x 9, Loop not fused: no successor loop Generated 2 alternate versions of the loop Generated vector simd code for the loop Generated 2 prefetch instructions for the loop Generated vector simd code for the loop Generated 2 prefetch instructions for the loop Generated vector simd code for the loop Generated 2 prefetch instructions for the loop

```
main:
29, Loop not fused: function call before adjacent loop
Loop not vectorized: may not be beneficial
Unrolled inner loop 8 times
36, Loop not fused: function call before adjacent loop
2 loops fused
```

This output gives the schedule used for the loop; in this case, the schedule is gang, vector (128). This means the iterations of the loop are broken into vectors of 128, and the vectors are executed in parallel by SMs of the GPU. This output is important because it tells you when you are going to get parallel execution or sequential execution.

For our second example, we modify the program slightly by replacing the data clauses on the kernels pragma with a present clause, and add a data construct surrounding the call to the vecaddgpu subroutine. The data construct moves the data across to the GPU in the main program. The present clause in the vecaddgpu subroutine tells the compiler to use the GPU copy of the data that has already been allocated on the GPU. If you run this program on the GPU with NVCOMPILER\_ACC\_TIME set, you see that the kernel region now has no data movement associated with it. Instead, the data movement is all associated with the data construct in the main program.

In Fortran programs, you don't have to specify the array bounds in data clauses if the compiler can figure out the bounds from the declaration, or if the arrays are assumed-shape dummy arguments or allocatable arrays.

```
module vecaddmod
 implicit none
contains
 subroutine vecaddgpu( r, a, b, n )
  real, dimension(:) :: r, a, b
  integer :: n
  integer :: i
!$acc kernels loop present(r,a,b)
  do i = 1, n
   r(i) = a(i) + b(i)
  enddo
 end subroutine
end module
program main
 use vecaddmod
 implicit none
 integer :: n, i, errs, argcount
 real, dimension(:), allocatable :: a, b, r, e
 character*10 :: arg1
 argcount = command argument count()
 n = 1000000 ! default value
 if ( argcount >= 1 ) then
 call get command argument( 1, arg1 )
  read( arg1, '(i)' ) n
  if(n \le 0) n = 100000
  endif
 allocate(a(n), b(n), r(n), e(n))
 do i = 1, n
  a(i) = i
  b(i) = 1000*i
 enddo
  ! compute on the GPU
!$acc data copyin(a,b) copyout(r)
 call vecaddgpu( r, a, b, n )
!$acc end data
  ! compute on the host to compare
 do i = 1, n
  e(i) = a(i) + b(i)
 enddo
  ! compare results
  errs = 0
 do i = 1, n
  if (r(i) /= e(i)) then
    errs = errs + 1
  endif
  enddo
 print *, errs, ' errors found'
 if( errs ) call exit(errs)
end program
```

### 2.12.2. Multi-Threaded Program Utilizing Multiple Devices

This simple example shows how to run a multi-threaded host program that utilizes multiple devices.

```
program tdot
! Compile with "nvfortran -mp -acc tman.f90 -lblas
! Set OMP NUM THREADS environment variable to run with
! up to 2 threads, currently.
use openacc
use omp lib
integer, parameter :: N = 10000
real*8 x(N), y(N), z
integer, allocatable :: offs(:)
real*8, allocatable :: zs(:)
real*8 ddot
! Max at 2 threads for now
nthr = omp get max threads()
if (nthr .gt. 2) nthr = 2
call omp_set_num_threads(nthr)
! Run on host
call random number(x)
call random number(y)
z = ddot(N, x, 1, y, 1)
print *, "Host Serial", z
! Attach each thread to a device
!$omp PARALLEL private(i)
     i = omp get thread num()
     call acc_set_device_num(i, acc_device_nvidia)
!$omp end parallel
! Break up the array into sections
nsec = N / nthr
allocate (offs (nthr), zs (nthr))
offs = (/ (i*nsec, i=0, nthr-1) /)
zs = 0.0d0
! Decompose the problem across devices
!$omp PARALLEL private(i,j,z)
     i = omp_get_thread_num() + 1
     z = 0.0\overline{d}0
     !$acc kernels loop &
        copyin(x(offs(i)+1:offs(i)+nsec),y(offs(i)+1:offs(i)+nsec))
     do j = offs(i)+1, offs(i)+nsec
    z = z + x(j) * y(j)
     end do
     zs(i) = z
!$omp end parallel
z = sum(zs)
print *, "Multi-Device Parallel", z
end
```

The program starts by having each thread call acc\_set\_device\_num so each thread will use a different GPU. Within the computational OpenMP parallel region, each thread copies the data it needs to its GPU and proceeds.

# 2.13. Troubleshooting Tips and Known Limitations

This release of the NVIDIA HPC SDK compilers implements most features of the OpenACC 2.7 specification. For an explanation of what features are not yet implemented, refer to Chapter 3, Implemented Features.

The Linux CUDA driver will power down an idle GPU. This means if you are using a GPU with no attached display, or an NVIDIA compute-only GPU, and there are no open CUDA contexts, the GPU will power down until it is needed. Since it may take up to a second to power the GPU back up, you may experience noticeable delays when you start your program. When you run your program with the environment variable NVCOMPILER\_ACC\_TIME set to 1, this time will appear as initialization time. If you are running many tests, or want to isolate the actual time from the initialization time, you can run the NVIDIA utility nvcudainit in the background. This utility opens a CUDA context and holds it open until you kill it or let it complete.

The NVIDIA OpenACC compilers support the async clause and wait directive. When you use asynchronous computation or data movement, you are responsible for ensuring that the program has enough synchronization to resolve any data races between the host and the GPU. If your program uses the async clause and wrong answers are generated, you can test whether the async clause is causing problems by setting the environment variable NVCOMPILER\_ACC\_SYNCHRONOUS to 1 before running your program. This action causes the OpenACC runtime to ignore the async clauses and run the program in synchronous mode.

# Chapter 3. IMPLEMENTED FEATURES

This section outlines the OpenACC features currently implemented in the NVIDIA HPC SDK compilers and lists known limitations.

# 3.1. OpenACC specification compliance

The NVIDIA HPC SDK compilers include support for most features of the OpenACC 2.7 specification. The following OpenACC 2.7 features are not supported:

- Declare link
- Nested parallelism
- Restricting **cache** clause variable refs to variables within a cached region.
- Subarrays and composite variables in **reduction** clauses
- The self clause
- The default clause on data constructs

### 3.2. Defaults

The default ACC\_DEVICE\_TYPE is acc\_device\_nvidia, just as the -acc compiler option targets an NVIDIA GPU by default. The device types acc\_device\_default and acc\_device\_not\_host behave the same as acc\_device\_nvidia. The device type can be changed using the environment variable or by a call to acc\_set\_device\_type().

The default ACC\_DEVICE\_NUM is 0 for the acc\_device\_nvidia type, which is consistent with the CUDA device numbering system. For more information, refer to the nvaccelinfo output in Prepare Your System. The device number can be changed using the environment variable or by a call to acc\_set\_device\_num.

# 3.3. Environment Variables

This section summarizes the environment variables that NVIDIA OpenACC supports. These environment variables are user-setable environment variables that control behavior of accelerator-enabled programs at execution. These environment variables must comply with these rules:

- The names of the environment variables must be upper case.
- The values of environment variables are case insensitive and may have leading and trailing white space.
- The behavior is implementation-defined if the values of the environment variables change after the program has started, even if the program itself modifies the values.

The following table contains the environment variables that are currently supported and provides a brief description of each.

Use this environment variable	To do this
NVCOMPILER_ACC_CUDA_PROFS	Set to 1 (or any positive value) to tell the runtime environment to insert an 'atexit(cuProfilerStop)' call upon exit. This behavior may be desired in the case where a profile is incomplete or where a message is issued to call cudaProfilerStop().
NVCOMPILER_ACC_DEVICE_NUM	Sets the default device number to use. NVCOMPILER_ACC_DEVICE_NUM. Specifies the default device number to use when executing accelerator regions. The value of this environment variable must be a nonnegative integer between zero and the number of devices attached to the host.
ACC_DEVICE_NUM	Legacy name. Superseded by NVCOMPILER_ACC_DEVICE_NUM.
NVCOMPILER_ACC_DEVICE_TYPE	Sets the default device type to use for OpenACC regions. NVCOMPILER_ACC_DEVICE_TYPE. Specifies which accelerator device to use when executing accelerator regions when the program has been compiled to use more than one different type of device. The value of this environment variable is implementation-defined, and in the NVIDIA OpenACC implementation may be the strings NVIDIA, MULTICORE or HOST
ACC_DEVICE_TYPE	Legacy name. Superseded by NVCOMPILER_ACC_DEVICE_TYPE.
NVCOMPILER_ACC_GANGLIMIT	For NVIDIA CUDA devices, this defines the maximum number of gangs (CUDA thread blocks) that will be launched by a kernel.
NVCOMPILER_ACC_NOTIFY	With no argument, a debug message will be written to stderr for each kernel launch and/or data transfer. When set to an integer value, the value is used as a bit mask to print information about:
	1: kernel launches
	2: data transfers
	4: region entry/exit
	8: wait operations or synchronizations with the device

 Table 1
 Supported Environment Variables

Use this environment variable	To do this
	16: device memory allocates and deallocates
NVCOMPILER_ACC_PROFLIB	Enables 3rd party tools interface using the new profiler dynamic library interface.
NVCOMPILER_ACC_SYNCHRONOU	Disables asynchronous launches and data movement.
NVCOMPILER_ACC_TIME	Enables a lightweight profiler to measure data movement and accelerator kernel execution time and print a summary at the end of program execution.

### 3.4. OpenACC Fortran API Extensions

This section summarizes the OpenACC API extensions implemented in the NVIDIA Fortran compiler.

### 3.4.1. acc\_malloc

The acc\_malloc function returns a device pointer, in a variable of type(c\_devptr), to newly allocated memory on the device. If the data can not be allocated, this function returns C\_NULL\_DEVPTR.

There is one supported call format in NVIDIA Fortran:

```
type(c_devptr) function acc_malloc (bytes)
```

where *bytes* is an integer which specifies the number of bytes requested.

### 3.4.2. acc\_free

The acc\_free subroutine frees memory previously allocated by acc\_malloc. It takes as an argument either a device pointer contained in an instance of derived type(c\_devptr), or for convenience, a CUDA Fortran device array. In NVIDIA Fortran, calling acc\_free (or cudaFree) with a CUDA Fortran device array that was allocated using the F90 allocate statement results in undefined behavior.

There are two supported call formats in NVIDIA Fortran:

```
subroutine acc_free ( devptr )
```

where *devptr* is an instance of derived type(c\_devptr)

```
subroutine acc free ( dev )
```

where *dev* is a CUDA Fortran device array

### 3.4.3. acc\_map\_data

The acc\_map\_data routine associates (maps) host data to device data. The first argument is a host array, contiguous host array section, or address contained in a type(c\_ptr). The second argument must be a device address contained in a type(c\_devptr), such as would be returned from acc\_malloc or acc\_deviceptr, or a CUDA Fortran device array.

There are four supported call formats in NVIDIA Fortran:

subroutine acc\_map\_data ( host, dev, bytes )

where *host* is a host variable, array or starting array element *dev* is a CUDA Fortran device variable, array, or starting array element *bytes* is an integer which specifies the mapping length in bytes)

```
subroutine acc_map_data ( host, dev )
```

where *host* is a host array or contiguous host array section *dev* is a CUDA Fortran device array or array section which conforms to host

```
subroutine acc_map_data ( host, devptr, bytes )
```

where *host* is a host variable, array or starting array element *devptr* is an instance of derived type(c\_devptr) *bytes* is an integer which specifies the mapping length in bytes)

subroutine acc\_map\_data ( ptr, devptr, bytes )

where *ptr* is an instance of derived type(c\_ptr) *devptr* is an instance of derived type(c\_devptr) *bytes* is an integer which specifies the mapping length in bytes)

### 3.4.4. acc\_unmap\_data

The acc\_unmap\_data routine unmaps (or disassociates) the device data from the specified host data.

There is one supported call format in NVIDIA Fortran:

subroutine acc\_unmap\_data ( host )

where *host* is a host variable that was mapped to device data in a previous call to acc\_map\_data.

### 3.4.5. acc\_deviceptr

The acc\_deviceptr function returns the device pointer, in a variable of type(c\_devptr), mapped to a host address. The input argument is a host variable or array element that has an active lifetime on the current device. If the data is not present, this function returns C\_NULL\_DEVPTR.

There is one supported call format in NVIDIA Fortran: type(c devptr) function acc deviceptr ( host )

where *host* is a host variable or array element of any type, kind and rank.

### 3.4.6. acc\_hostptr

The acc\_hostptr function returns the host pointer, in a variable of type(c\_ptr), mapped to a device address. The input argument is a device address, such as would be returned from acc\_malloc or acc\_deviceptr, or a CUDA Fortran device array.

#### There are two supported call formats in NVIDIA Fortran:

type(c\_ptr) function acc\_hostptr ( dev )

#### where *dev* is a CUDA Fortran device array

type(c\_ptr) function acc\_hostptr ( devptr )

where *devptr* is an instance of derived type(c\_devptr)

#### 3.4.7. acc\_is\_present

The acc\_is\_present function returns .true. or .false. depending on whether a host variable or array region is present on the device.

There are two supported call formats in NVIDIA Fortran:

logical function acc\_is\_present ( host )

where *host* is a contiguous array section of intrinsic type.

logical function acc\_is\_present ( host, bytes )

where *host* is a host variable of any type, kind, and rank. *bytes* is an integer which specifies the length of the data to check.

### 3.4.8. acc\_memcpy\_to\_device

The acc\_memcpy\_to\_device routine copies data from local memory to device memory. The source address is a host array, contiguous array section, or address contained in a type(c\_ptr). The destination address must be a device address, such as would be returned from acc\_malloc or acc\_deviceptr, or a CUDA Fortran device array.

There are four supported call formats in NVIDIA Fortran:

subroutine acc\_memcpy\_to\_device ( dev, src, bytes )

where *dev* is a CUDA Fortran device variable, array or starting array element. *src* is a host variable, array, or starting array element.

*bytes* is an integer which specifies the length of the copy in bytes.

subroutine acc\_memcpy\_to\_device ( dev, src )

where *dev* is a CUDA Fortran device array or contiguous array section. *src* is a host array or array section which conforms to dev.

subroutine acc\_memcpy\_to\_device ( devptr, src, bytes )

where *devptr* is an instance of derived type(c\_devptr).

*src* is a host variable, array, or starting array element.

*bytes* is an integer which specifies the length of the copy in bytes.

subroutine acc\_memcpy\_to\_device ( devptr, ptr, bytes )

where *devptr* is an instance of derived type(c\_devptr).

*ptr* is an instance of derived type(c\_ptr).

*bytes* is an integer which specifies the length of the copy in bytes.

### 3.4.9. acc\_memcpy\_from\_device

The acc\_memcpy\_from\_device routine copies data from device memory to local memory. The source address must be a device address, such as would be returned from acc\_malloc, acc\_deviceptr, or a CUDA Fortran device array. The source address is a host array, contiguous array section, or address contained in a type(c\_ptr).

There are four supported call formats in NVIDIA Fortran:

```
subroutine acc_memcpy_from_device ( dest, dev, bytes )
```

where *dest* is a host variable, array, or starting array element. *dev* is a CUDA Fortran device variable, array or starting array element. *bytes* is an integer which specifies the length of the copy in bytes)

```
subroutine acc_memcpy_from_device ( dest, dev )
```

where *dest* is a host array or contiguous array section. *dev* is a CUDA Fortran device array or array section which conforms to dest subroutine.

subroutine acc\_memcpy\_from\_device ( dest, devptr, bytes )

where *dest* is a host variable, array, or starting array element. *devptr* is an instance of derived type(c\_devptr). *bytes* is an integer which specifies the length of the copy in bytes)

```
subroutine acc_memcpy_from_device ( ptr, devptr, bytes )
```

where *ptr* is an instance of derived type(c\_ptr). *devptr* is an instance of derived type(c\_devptr). *bytes* is an integer which specifies the length of the copy in bytes)

### 3.4.10. acc\_get\_cuda\_stream

The acc\_get\_cuda\_stream function returns the CUDA stream value which corresponds to an OpenACC async queue. The input argument is an async number or a pre-defined value such as acc\_async\_sync. This call is only supported on NVIDIA platforms.

There is one supported call format in NVIDIA Fortran: integer(acc\_handle\_kind) function acc\_get\_cuda\_stream ( async )

where *async* is a user-defined or pre-defined async value.

### 3.4.11. acc\_set\_cuda\_stream

The acc\_set\_cuda\_stream subroutine sets the CUDA stream value for an OpenACC async queue on the current device. The input arguments are an async number and a stream. This call is only supported on NVIDIA platforms.

There is one supported call format in NVIDIA Fortran:

```
subroutine acc_set_cuda_stream ( async, stream )
```

where *async* and *stream* are integers of acc\_handle\_kind.

## 3.5. Known Limitations

This section includes the known limitations in the NVIDIA HPC SDK compilers implementations of the OpenACC API.

### 3.5.1. ACC routine directive Limitations

- Extern variables may not be used with acc routine procedures.
- Reductions in procedures with acc routine are only supported for NVIDIA GPUs supporting compute capability 3.0 or higher.
- Fortran assumed-shape arguments are not yet supported.

### 3.5.2. C++ and OpenACC Limitations

There are limitations to the data that can appear in OpenACC data constructs and compute regions:

- Variable-length arrays are not supported in OpenACC data clauses; VLAs are not part of the C++ standard.
- Variables of class type that require constructors and destructors do not behave properly when they appear in data clauses.
- Exceptions are not handled in compute regions.
- Member variables are not fully supported in the use\_device clause of a host\_data construct; this placement may result in an error at runtime.

### 3.5.3. Other Limitations

 Targeting another accelerator device after acc\_shutdown has been called is not supported.

### 3.6. Interactions with Optimizations

This section discusses interactions with compiler optimizations that programmers should be aware of.

### 3.6.1. Interactions with Inlining

Procedure inlining may be enabled in several ways. User-controlled inlining is enabled using the -Minline flag, or with -Mextract=lib: and -Minline=lib: flags. For C and C++, compiler-controlled inlining is enabled using the -Mautoinline or - fast flags. Interprocedural analysis can also control inlining using the -Mipa=inline option. Inlining is a performance optimization by removing the overhead of the procedure call, and by specializing and optimizing the code of the inlined procedure at the point of the call site.

When a procedure containing a compute construct (acc parallel or acc kernels) is inlined into an acc data construct, the compiler will use the data construct clauses to optimize data movement between the host and device. In some cases, this can produce different answers, when the host and device copies of some variable are different. For instance, the data construct may specify a data clause for a scalar variable or a Fortran common block that contains a scalar variable. The compute construct in the inlined procedure will now see that the scalar variable is present on the device, and will use the device copy of that variable. Before inlining, the compute construct may have used the default firstprivate behavior for that scalar variable, which would use the host value for the variable.

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