



# NVIDIA<sup>®</sup>

## HPC Compilers

OPENACC GETTING STARTED GUIDE

# TABLE OF CONTENTS

Chapter 1. Overview.....	1
1.1. System Prerequisites.....	1
1.2. Prepare Your System.....	1
1.3. Supporting Documentation and Examples.....	2
Chapter 2. Using OpenACC with the NVIDIA HPC Compilers.....	3
2.1. CUDA Versions.....	3
2.2. Compute Capability.....	5
2.3. C Structs in OpenACC.....	6
2.4. C++ Classes in OpenACC.....	7
2.5. Fortran Derived Types in OpenACC.....	11
2.6. Fortran I/O.....	12
2.6.1. OpenACC PRINT Example.....	13
2.7. OpenACC Atomic Support.....	13
2.8. OpenACC Declare Data Directive for Global and Fortran Module Variables.....	13
2.9. OpenACC Error Handling.....	16
2.10. C Examples.....	19
2.11. Fortran Examples.....	23
2.11.1. Vector Addition on the GPU.....	23
2.11.2. Multi-Threaded Program Utilizing Multiple Devices.....	27
2.12. Troubleshooting Tips and Known Limitations.....	28
Chapter 3. Implemented Features.....	29
3.1. OpenACC specification compliance.....	29
3.2. Defaults.....	29
3.3. Environment Variables.....	30
3.4. OpenACC Fortran API Extensions.....	31
3.4.1. acc_malloc.....	31
3.4.2. acc_free.....	31
3.4.3. acc_map_data.....	31
3.4.4. acc_unmap_data.....	32
3.4.5. acc_deviceptr.....	32
3.4.6. acc_hostptr.....	33
3.4.7. acc_is_present.....	33
3.4.8. acc_memcpy_to_device.....	33
3.4.9. acc_memcpy_from_device.....	34
3.4.10. acc_get_cuda_stream.....	34
3.4.11. acc_set_cuda_stream.....	35
3.5. Known Limitations.....	35
3.5.1. ACC routine directive Limitations.....	35
3.5.2. C++ and OpenACC Limitations.....	35
3.5.3. Other Limitations.....	35

3.6. Interactions with Optimizations.....	35
3.6.1. Interactions with Inlining.....	36

## LIST OF TABLES

Table 1 Supported Environment Variables .....	30
---	----

# 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](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](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 20.9 packages from the [NVIDIA download webpage](https://developer.nvidia.com/nvidia-downloads) at [nvcompilers.com/downloads](https://developer.nvidia.com/nvidia-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/20.9/compilers/bin` directory to your path, where *target* is one of `Linux_x86_64`, `Linux_ppc64` 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:

```
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: Yes
Total Constant Memory:         65536
Total Shared Memory per Block: 49152
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
NVIDIA Default Target:         cc70
```

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](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 installation package installs bundled CUDA Toolkit components into an HPC SDK installation sub-directory, and typically supports the last 3 released versions of the CUDA Toolkit.

An NVIDIA CUDA driver must be installed on a system with a GPU before you can run a program compiled for the GPU on that system. NVIDIA HPC SDK products do not contain CUDA device drivers. You must download and install the appropriate [CUDA Driver from NVIDIA](#). The CUDA Driver version must be at least as new as the CUDA version with which you compile your code.

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 20.9 includes components from the following versions of the CUDA Toolkit:

- ▶ CUDA 10.1
- ▶ CUDA 10.2
- ▶ CUDA 11.0

You can let the compiler choose which version of CUDA to use based on the configuration of your system, or you can force it to use a particular version using the `-gpu` command-line option.

If you do not specify a version of CUDA on the command line, the compiler uses the version of the CUDA Driver installed on the system on which you are compiling to determine which CUDA version to use. In the absence of any other information, the compiler will look for a CUDA toolchain version in the `/opt/nvidia/hpc_sdk/target/cuda` directory that matches the version of the CUDA Driver installed on the system. If a match is not found, the compiler searches for the newest CUDA toolchain version that is not newer than the CUDA Driver version. If there is no CUDA Driver installed, the compilers fall back to the default of CUDA 10.1.

You can change the compiler's default selection of CUDA version using one of the following methods:

- ▶ Use 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 toolchain version for one invocation of the compiler. For example, to compile a C file with the CUDA 11.0 toolchain you would use:

```
nvc -acc -gpu=cuda11.0
```

- ▶ Use an rcfile variable. Add a line defining `DEFCUDAVERSION` to the `siterc` file in the installation `bin` directory or to a file named `.mynvrc` in your home directory. For example, to specify the CUDA 10.2 toolchain as the default, add the following line to one of these files:

```
set DEFCUDAVERSION=10.2;
```

Using an rcfile variable changes the CUDA toolchain version for all invocations of the compilers reading the rcfile.

When you specify a CUDA version, you can additionally instruct the compiler to use a CUDA Toolkit installation separate from the defaults bundled with the current installation of the HPC SDK compilers. While most users do not need to use any other CUDA toolchain version than those provided with the HPC SDK, situations do arise where this capability is needed. Developers working with pre-release CUDA software may occasionally need to test with a CUDA Toolkit version not formally supported in an HPC SDK release. Conversely, some developers might find a need to compile with a CUDA toolchain older than the oldest CUDA toolchain bundled with a given HPC SDK release. For these users, the NVIDIA HPC compilers can interoperate with components from a CUDA Toolkit installed outside of the HPC SDK installation directories.

NVIDIA tests extensively using the bundled versions of the CUDA components and fully supports their use. Use of CUDA Toolkit components not included with an NVIDIA install is done with your understanding that functionality differences may exist.



The ability to compile with CUDA toolchain components other than the versions installed with the HPC SDK compilers is supported on all platforms.

To use a CUDA toolkit that is not installed with an NVIDIA release, there are three options:

- ▶ Use the rcfile variable `DEFAULT_CUDA_HOME` to override the base default

```
set DEFAULT_CUDA_HOME = /opt/cuda-10.0;
```

- ▶ Set the environment variable `CUDA_HOME`

```
export CUDA_HOME=/opt/cuda-10.0
```

- ▶ Use the compiler command-line assignment `CUDA_HOME=`

```
nvfortran CUDA_HOME=/opt/cuda-10.0
```

The HPC SDK compilers use the following order of precedence when determining which version of the CUDA toolchain to use.

1. If you do not specify which CUDA version to use, the compiler picks the CUDA version from the HPC SDK installation directory that matches the version of the CUDA Driver installed on your system. If the HPC SDK installation directory does not contain a direct match, the newest version in that directory which is not newer than the CUDA driver version is used. If there is no CUDA driver installed on your system, the compiler falls back on an internal default.
2. The rcfile variable `DEFAULT_CUDA_HOME` will override the base default.
3. The environment variable `CUDA_HOME` will override all of the above defaults.
4. The environment variable `NVCOMPILER_CUDA_HOME` overrides all of the above; it is available for advanced users in case they need to override an already-defined `CUDA_HOME`.
5. A user-specified `cudaX.Y` sub-option to `-gpu` will override all of the above defaults and the corresponding version of the CUDA toolchain located in the HPC SDK installation directory will be used.
6. The compiler command-line assignment `CUDA_HOME=` will override all of the above defaults (including the `cudaX.Y` sub-option).

## 2.2. Compute Capability

The compilers can generate code for NVIDIA GPU compute capabilities 3.0 through 8.0. 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 select `cc35`, `cc50`, `cc60`, and `cc70`.

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 blank-separated 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. 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;
    }
}
```

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;
    }
}
```

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->x[i] = base[i];
        A->y[i] = sqrtf( base[i] );
        A->z[i] = 0;
    }
}

```

## 2.4. 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 elementype> 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];

```

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:

```

T1 &dupvector<T1>::operator [](int) const [with T1=float]:
    35, Generating implicit acc routine seq

```

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 inc1( int i, elemtype y ){
        data[i] += y;
    }
}
...
#pragma acc parallel loop present(v,x)
    for( int i = 0; i < n; ++i ) v.inc1( i, x[i] );
```

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 );
```

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 );
```

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.

## 2.5. 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 vecaddgpu()
    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
```

## 2.6. 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.



## 2.6.1. 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
```

## 2.7. 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)
  {
    #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);
  }
```

## 2.8. 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);
}
```

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 **modx**, which refers to the global **x** pointer and **coef** struct. When called on the host, this routine will access the global **x** 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 **modx** 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], yy[0: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;
        }
        ...
    }
}
```

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 :: max1 = 100000
  real, dimension(max1) :: 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
```

## 2.9. 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++) {
            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:

```
$ 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...
call to cuMemAlloc returned error 2: Out of memory

-----
Primary job terminated normally, but 1 process returned
a non-zero exit code.. Per user-direction, the job has been aborted.
```

```
-----
mpirun detected that one or more processes exited with non-zero status,
thus causing the job to be terminated.
```

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++) {
        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);
}

// 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.

## 2.10. 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];
}

```

```

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 ){
        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];
    /* compare results */
    errs = 0;
    for( i = 0; i < n; ++i ){
        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 `NVIDIA_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/a1.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 `NVIDIA_ACC_NOTIFY` to 3, the output will include information about the data transfers as well:

```
upload CUDA data file=/user/guest/a1.c function=vecaddgpu
line=4 device=0 threadid=1 variable=a bytes=400000
upload CUDA data file=/user/guest/a1.c function=vecaddgpu
line=4 device=0 threadid=1 variable=b bytes=400000
launch CUDA kernel file=/user/guest/a1.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/a1.c function=vecaddgpu
line=6 device=0 threadid=1 variable=r bytes=400000
0 errors found
```

If you set the environment variable `NVIDIA_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_64/20.9/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

Accelerator Kernel Timing data
/user/guest/a1.c
  vecaddgpu NVIDIA devicenum=0
    time(us): 167
      4: compute region reached 1 time
        5: kernel launched 1 time
          grid: [782] block: [128]
          device time(us): total=5 max=5 min=5 avg=5
          elapsed time(us): total=700 max=700 min=700 avg=700
      4: data region reached 2 times
        4: data copyin transfers: 2
          device time(us): total=110 max=67 min=43 avg=55
        6: data copyout transfers: 1
          device time(us): total=52 max=52 min=52 avg=52
```

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 a1.c`, you get the output:

```
vecaddgpu:
  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 not fused: no successor loop
  Generated 2 alternate versions of the loop
  Generated vector and scalar 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 `NVIDIA_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];
}

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 ){
        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;
}
```

## 2.11. Fortran Examples

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

### 2.11.1. Vector Addition on the GPU

The section contains two Fortran 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
  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:

```
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
0 errors found
```

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:

```
vecaddgpu:
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 <= 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

```

## 2.11.2. 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 = 0.0d0
!$acc kernels loop &
    copyin(x(offs(i)+1:offs(i)+nsec),y(offs(i)+1:offs(i)+nsec))
do j = offs(i)+1, offs(i)+nsec
    z = z + x(j) * y(j)
end do
zs(i) = z
!$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.

## 2.12. 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.
- ▶ Arrays, 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.

Table 1 Supported Environment Variables

Use this environment variable...	To do this...
NVCOMPILER_ACC_BUFFERSIZE	For NVIDIA CUDA devices, this defines the size of the pinned buffer used to transfer data between host and device.
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_DEBUG	Set to 1 to instruct the runtime to generate information about device memory allocation, data movement, kernel launches, and more. NVCOMPILER_ACC_DEBUG is designed mostly for use in debugging the runtime itself, but it may be helpful in understanding how the program interacts with the device. Expect copious amounts of output.
NVCOMPILER_ACC_DEVICE_NUM = ACC_DEVICE_NUM	Sets the default device number to use. NVCOMPILER_ACC_DEVICE_NUM overrides ACC_DEVICE_NUM. Controls 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.
NVCOMPILER_ACC_DEVICE_TYPE = ACC_DEVICE_TYPE	Sets the default device type to use. NVCOMPILER_ACC_DEVICE_TYPE overrides ACC_DEVICE_TYPE. Controls which accelerator device to use when executing accelerator regions, if 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 implementation may be the string NVIDIA, MULTICORE or HOST
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	Writes out a line for each kernel launch and/or data movement. When set to an integer value, the value, is used as a bit mask to print information about kernel launches (value 1), data transfers (value 2), region entry/exit (value 4), wait operations or synchronizations with the

Use this environment variable...	To do this...
	device (value 8), and device memory allocates and deallocates (value 16).
NVCOMPILER_ACC_PROFLIB	Enables 3rd party tools interface using the new profiler dynamic library interface.
NVCOMPILER_ACC_SYNCHRONOUS	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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