



OpenACC CUDA Interoperability

JSC OpenACC Course 2022

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Contents

OpenACC is a team player!

OpenACC can interplay with

- CUDA
- GPU-enabled libraries and applications

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Motivation

The Keyword

Tasks

Task 1

Task 2

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Motivation

Usually, three reasons for mixing OpenACC with others

1 Libraries!

- A lot of hard problems have already been solved by others
- Make use of this!

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1 Libraries!

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→ Make use of this!

2 Existing environment

- You build up on other's work
- Part of code is already ported (e.g. with CUDA), the rest should follow
- OpenACC is a good first step in porting, CUDA a possible next

Motivation

Usually, three reasons for mixing OpenACC with others

1 Libraries!

- A lot of hard problems have already been solved by others
→ Make use of this!

2 Existing environment

- You build up on other's work
- Part of code is already ported (e.g. with CUDA), the rest should follow
- OpenACC is a good first step in porting, CUDA a possible next

3 OpenACC coverage

- Sometimes, OpenACC does not support specific *part* needed (very well)
- Sometimes, more fine-grained manipulation needed

The Keyword

OpenACC's Rosetta Stone

```
host_data use_device
```

The Keyword

OpenACC's Rosetta Stone

host_data use_device

- Background
 - GPU and CPU are different devices, have different memory
 - Distinct address spaces
- OpenACC hides handling of addresses from user
 - For every chunk of accelerated data, **two** addresses exist
 - One for CPU data, one for GPU data
 - OpenACC uses appropriate address in accelerated kernel
- **But:** Automatic handling not working when out of OpenACC (OpenACC will default to host address)
 - **host_data use_device** uses the address of the GPU device data for scope

The host_data Construct

C

C

- Usage:

```
double* foo = new double[N];           // foo on Host
#pragma acc data copyin(foo[0:N])      // foo on Device
{
    ...
    #pragma acc host_data use_device(foo)
    some_lfunc(foo);                   // Device: OK!
    ...
}
```

- Directive can be used for structured block as well

The `host_data` Construct

Fortran

- Usage example

```
real(8) :: foo(N)           ! foo on Host
!$acc data copyin(foo)      ! foo on Device
...
!$acc host_data use_device(foo)
call some_func(foo);      ! Device: OK!
!$acc end host_data
...
!$acc end data
```

The Inverse: `deviceptr`

When CUDA is involved

- For the inverse case:
 - Data has been copied by CUDA or a CUDA-using library
 - Pointer to data residing on devices is returned
 - Use this data in OpenACC context
- `deviceptr` clause declares data to be on device

The Inverse: `deviceptr`

When CUDA is involved

- For the inverse case:
 - Data has been copied by CUDA or a CUDA-using library
 - Pointer to data residing on devices is returned→ Use this data in OpenACC context
- `deviceptr` clause declares data to be on device
- Usage (C):

```
float * n;  
int n = 4223;  
cudaMalloc((void**)&x, (size_t)n*sizeof(float));  
// ...  
#pragma acc kernels deviceptr(x)  
for (int i = 0; i < n; i++) {  
    x[i] = i;  
}
```

The Inverse: `deviceptr`

When CUDA is involved

- For the inverse case:
 - Data has been copied by CUDA or a CUDA-using library
 - Pointer to data residing on devices is returned→ Use this data in OpenACC context
- `deviceptr` clause declares data to be on device
- Usage (Fortran):

```
integer, parameter :: n = 4223
real, device, dimension(N) :: x ! automatically on device
integer :: i
! ...
!$acc kernels deviceptr(x)
do i=1, n
    x(i) = i
end do
!$acc end kernels
```

Tasks

Tasks

Task 1

Task 1

Introduction to BLAS

- Use case: Anything linear algebra
- **BLAS**: Basic Linear Algebra Subprograms
 - Vector-vector, vector-matrix, matrix-matrix operations
 - Specification of routines
 - Examples: SAXPY, DGEMV, ZGEMM→ <http://www.netlib.org/blas/>
- **cuBLAS**: NVIDIA's linear algebra routines with BLAS interface, readily accelerated
→ <http://docs.nvidia.com/cuda/cublas/>
- **Task 1**: Use cuBLAS for vector addition, everything else with OpenACC

Task 1

cuBLAS OpenACC Interaction

- cuBLAS routine used:

```
cublasDaxpy(cublasHandle_t handle, int n,  
            const double *alpha,  
            const double *x, int incx,  
            double *y, int incy)
```

- handle capsules GPU auxiliary data, needs to be created and destroyed with cublasCreate and cublasDestroy
- x and y point to addresses on **device**!
- cuBLAS library needs to be linked with -lcublas

Task 1

cuBLAS on Fortran

- Nvidia offers bindings to cuBLAS out of the box

```
integer(4) function cublasdaxpy_v2(h, n, a, x, incx, y, incy)
type(cublasHandle) :: h
integer :: n
real(8) :: a
real(8), device, dimension(*) :: x, y
integer :: incx, incy
```

- Usage: **use** cublas in code; add -Mcuda -Lcublas during compilation

- Notes

- Legacy (v1) cuBLAS bindings (no handle) also available, i.e. cublasdaxpy()
- nvfortran allows to omit host_data use_device, but not recommended
- Module openacc_cublas exists, specifically designed for usage with OpenACC (no need for host_data use_device)

⇒ Both not part of training

→ <https://docs.nvidia.com/hpc-sdk/compiler/pdf/hpc209cudaint.pdf>

Task 1

Vector Addition with cuBLAS

TASK

C

FORTRAN

- Use cuBLAS for vector addition

Task 1: OpenACC+cuBLAS

- Location of code:
5- Interoperability/Tasks/{C,Fortran}/Tasks/Task1
- Work on TODOs in `vecAddRed.c`
 - Use `host_data use_device` to provide correct pointer
 - Check [cuBLAS documentation](#) for details on `cublasDaxpy()`
- Compile: `make`
- Submit to the batch system: `make run`

Tasks

Task 2

Task 2

CUDA Need-to-Know

- Use case:
 - Working on legacy code
 - Need the *raw* power (/flexibility) of CUDA
- CUDA need-to-knows:
 - Thread → Block → Grid
Total number of threads should map to your problem; threads are always given per block
 - A kernel is called from every thread on GPU device
Number of kernel threads: *triple chevron syntax*
`kernel<<<nBlocks, nThreads>>>(arg1, arg2, ...)`
 - Kernel: Function with `__global__` prefix
Aware of its index by global variables, e.g. `threadIdx.x`
→ <http://docs.nvidia.com/cuda/>

Task 2

TASK

C

Vector Addition with CUDA Kernel: C

- CUDA kernel for vector addition, rest OpenACC
- Marrying CUDA C and OpenACC:
 - No need to use wrappers! OpenACC and CUDA directly supported by nvc++

Task 2: OpenACC+CUDA

- Change to 5-Interoperability/Tasks/C/Tasks/Task2 directory
- Work on TODOs in `vecAddRed.c`
 - Use `host_data use_device` to provide correct pointer
 - Implement computation in kernel, implement call of kernel
- Compile: `make`; Submit to the batch system: `make run`

Task 2

TASK

FORTRAN

Vector Addition with CUDA Kernel: Fortran

- CUDA kernel for vector addition, rest OpenACC
- Marrying CUDA **Fortran** and OpenACC:
 - No need to use wrappers! OpenACC and CUDA Fortran directly supported in same source
 - Having a dedicated module file could make sense anyway

Task 2: OpenACC+CUDA

- Change to 5-Interoperability/Tasks/Fortran/Tasks/Task2 directory
- Work on TODOs in `vecAddRed.F03`
 - Use `host_data use_device` to provide correct pointer
 - Implement computation in kernel, implement call of kernel
- Compile: `make`; Submit to the batch system: `make run`

Tasks

Task 3

Thrust

Iterators! Iterators everywhere! 

- $\frac{\text{Thrust}}{\text{CUDA}} = \frac{\text{STL}}{\text{C++}}$
- Template library
- Based on iterators, but also works with plain C
- Data-parallel primitives (`scan()`, `sort()`, `reduce()`, ...); algorithms

→ <http://thrust.github.io/>
<http://docs.nvidia.com/cuda/thrust/>

Thrust

Code example

```
int a = 42;
int n = 10;
thrust::host_vector<float> x(n), y(n);
// fill x, y

thrust::device_vector d_x = x, d_y = y;

using namespace thrust::placeholders;
thrust::transform(d_x.begin(), d_x.end(), d_y.begin(), d_y.begin(), a * _1 + _2);

x = d_x;
```

Task 3

Vector Addition with Thrust: C

TASK

C

- Use Thrust for reduction, everything else of vector addition with OpenACC

Task 3: OpenACC+Thrust

- Change to directory 5-Interoperability/Tasks/C/Tasks/Task3
- Work on TODOs in `vecAddRed.c`
 - Use `host_data use_device` to provide correct pointer
 - Implement call to `thrust::reduce` using `c_ptr`
- Compile: `make`
- Submit to the batch system: `make run`

Task 3

Vector Addition with Thrust: Fortran

TASK

FORTRAN

- Use Thrust for reduction, everything else of vector addition with OpenACC
- Thrust used via ISO_C_BINDING (*one more wrapper*)

Task 3: OpenACC+Thrust

- Change to directory
5-Interoperability/Tasks/Fortran/Tasks/Task3
- Work on TODOs in `vecAddRed.F03`, `thrustWrapper.cu` and `fortranthrust.F03`
 - Familiarize yourself with setup of Thrust called via ISO_C_BINDING
 - Use `host_data use_device` to provide correct pointer
 - Implement call to `thrust::reduce` using `c_ptr`
- Compile: `make`
- Submit to the batch system: `make run`

Tasks

Task 4

Task 4

Stating the Problem

- We want to solve the Poisson equation

$$\Delta\Phi(x,y) = -\rho(x,y)$$

with periodic boundary conditions in x and y

- Needed, e.g., for finding electrostatic potential Φ for a given charge distribution ρ
- Model problem

$$\begin{aligned}\rho(x,y) &= \cos(4\pi x) \sin(2\pi y) \\ (x,y) &\in [0,1)^2\end{aligned}$$

- Analytically known: $\Phi(x,y) = \Phi_0 \cos(4\pi x) \sin(2\pi y)$
- Let's solve the Poisson equation with a Fourier Transform!

Task 4

Introduction to Fourier Transforms

- Discrete Fourier Transform and Re-Transform:

$$\hat{f}_k = \sum_{j=0}^{N-1} f_j e^{-\frac{2\pi i k j}{N}} \Leftrightarrow f_j = \sum_{k=0}^{N-1} \hat{f}_k e^{\frac{2\pi i j k}{N}}$$

- Time for all \hat{f}_k : $\mathcal{O}(N^2)$
- Fast Fourier Transform: Recursively splitting $\rightarrow \mathcal{O}(N \log(N))$
- Find derivatives in Fourier space:

$$f'_j = \sum_{k=0}^{N-1} i k \hat{f}_k e^{\frac{2\pi i j k}{N}}$$

It's just multiplying by ik !

Task 4

Plan for FFT Poisson Solution

Start with charge density ρ

- 1 Fourier-transform ρ

$$\hat{\rho} \leftarrow \mathcal{F}(\rho)$$

- 2 *Integrate* ρ in Fourier space twice

$$\hat{\phi} \leftarrow -\hat{\rho} / (k_x^2 + k_y^2)$$

- 3 Inverse Fourier-transform $\hat{\phi}$

$$\phi \leftarrow \mathcal{F}^{-1}(\hat{\phi})$$

Task 4

Plan for FFT Poisson Solution

Start with charge density ρ

- 1 Fourier-transform ρ
 $\hat{\rho} \leftarrow \mathcal{F}(\rho)$
- 2 *Integrate* ρ in Fourier space twice
 $\hat{\phi} \leftarrow -\hat{\rho} / (k_x^2 + k_y^2)$
- 3 Inverse Fourier-transform $\hat{\phi}$
 $\phi \leftarrow \mathcal{F}^{-1}(\hat{\phi})$

cuFFT

OpenACC

cuFFT

Task 4

cuFFT: C

- cuFFT: NVIDIA's (Fast) Fourier Transform library
 - 1D, 2D, 3D transforms; complex and real data types
 - Asynchronous execution
 - Modeled after FFTW library (API)
 - Part of CUDA Toolkit
 - Fortran: NVIDIA offers bindings with **use** cufft

→ <https://developer.nvidia.com/cufft>

```
cufftDoubleComplex *src, *tgt;           // Device data!
cufftHandle plan;
// Setup 2d complex-complex trafo w/ dimensions (Nx, Ny)
cufftCreatePlan(plan, Nx, Ny, CUFFT_Z2Z);
cufftExecZ2Z(plan, src, tgt, CUFFT_FORWARD); // FFT
cufftExecZ2Z(plan, tgt, tgt, CUFFT_INVERSE); // iFFT
// Inplace trafo ^----^
cufftDestroy(plan);                      // Clean-up
```

Task 4

cuFFT: Fortran

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 - Asynchronous execution
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 - Part of CUDA Toolkit
 - Fortran: NVIDIA offers bindings with **use** cufft

→ <https://developer.nvidia.com/cufft>

```
double complex, allocatable :: src(:, :), tgt(:, :) ! Device
integer :: plan, ierr
```

```
! Setup 2d complex-complex trafo w/ dimensions (Nx, Ny)
```

```
ierr = cufftCreatePlan(plan, Nx, Ny, CUFFT_Z2Z)
```

```
ierr = cufftExecZ2Z(plan, src, tgt, CUFFT_FORWARD) ! FFT
```

```
ierr = cufftExecZ2Z(plan, tgt, tgt, CUFFT_INVERSE) ! iFFT
```

```
! Inplace trafo ^-----^
```

```
ierr = cufftDestroy(plan) ! Clean-up
```

Task 4

Synchronizing cuFFT: C

- CUDA Streams enable interleaving of computational tasks
- cuFFT uses streams for asynchronous execution
- cuFFT runs in default CUDA stream;
OpenACC does not → trouble

⇒ Force cuFFT on OpenACC stream

```
#include <openacc.h>  
// Obtain the OpenACC default stream id  
cudaStream_t accStream = (cudaStream_t) acc_get_cuda_stream(acc_async_sync);  
// Execute all cufft calls on this stream  
cufftSetStream(accStream);
```

Task 4

Synchronizing cuFFT: Fortran

- CUDA Streams enable interleaving of computational tasks
- cuFFT uses streams for asynchronous execution
- cuFFT runs in default CUDA stream;
OpenACC does not → trouble

⇒ Force cuFFT on OpenACC stream

```
use openacc
integer :: stream
! Obtain the OpenACC default stream id
stream = acc_get_cuda_stream(acc_async_sync)
! Execute all cufft calls on this stream
ierr = cufftSetStream(plan, stream)
```

Task 4

OpenACC and cuFFT

TASK

C

FORTRAN

- Use case: Fourier transforms
- Use cuFFT and OpenACC to solve Poisson's Equation

Task 4: OpenACC+cuFFT

- Change to Interoperability/Tasks/{C,Fortran}/Tasks/Task4 directory
- Work on TODOs in `poisson.{c,F03}`
 - `solveRSpace` Force cuFFT on correct stream; implement data handling with
`host_data use_device`
 - `solveKSpace` Implement data handling and parallelism
- Compile: `make`
- Submit to the batch system: `make run`

Summary & Conclusion

- If needed, OpenACC can play team with
 - GPU-accelerated libraries
 - Plain CUDA code
- For Fortran, ISO_C_BINDING might be needed

Summary & Conclusion

- If needed, OpenACC can play team with
 - GPU-accelerated libraries
 - Plain CUDA code
- For Fortran, ISO_C_BINDING might be needed

*Thank you
for your attention!*



Appendix
Glossary
References

List of Tasks

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Glossary I

CUDA Computing platform for GPUs from NVIDIA. Provides, among others, CUDA C/C++. 2, 3, 4, 5, 6, 11, 12, 13, 21, 22, 23, 34, 35, 36, 37, 39, 40, 42

NVIDIA US technology company creating GPUs. 16, 34, 35, 43

OpenACC Directive-based programming, primarily for many-core machines. 1, 2, 3, 4, 5, 6, 7, 8, 11, 12, 13, 16, 17, 18, 19, 22, 23, 27, 28, 32, 33, 36, 37, 38, 39, 40, 42

Thrust A parallel algorithms library for (among others) GPUs. See <https://thrust.github.io/>. 25, 26, 27, 28, 42

References: Images, Graphics I

- [1] Chester Alvarez. *Untitled*. Freely available at Unsplash. URL: <https://unsplash.com/photos/bphc6kyobMg>.