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PRACE

NVIDIA | DEEP LEARNING INSTITUTE

PRACE Workshop: Deep Learning and GPU programming workshop

15 – 18 June 2020

VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

MODULE FOUR: GPU PROGRAMMING

Dr. Volker Weinberg | LRZ | 16.06.2020

OpenACC
More Science, Less Programming

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MODULE OVERVIEW

OpenACC Directives

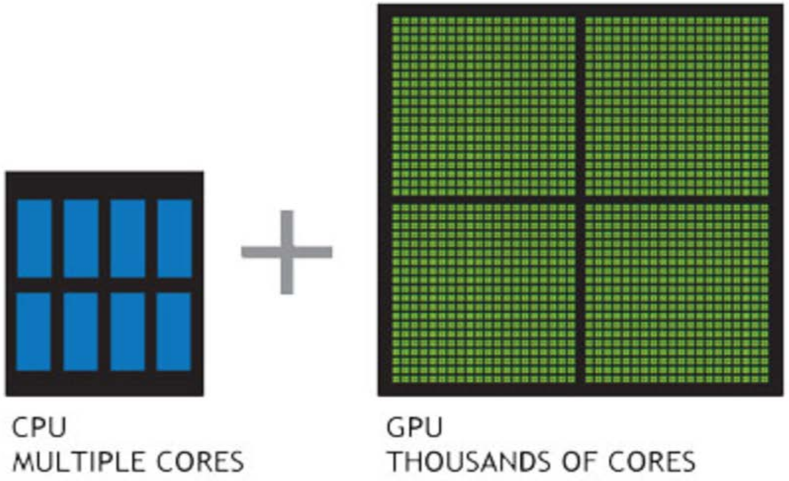
- Multicore CPU vs GPU
- Introduction to GPU Data Management
- CUDA Managed Memory
- GPU Profiling with PGProf

CPU VS GPU

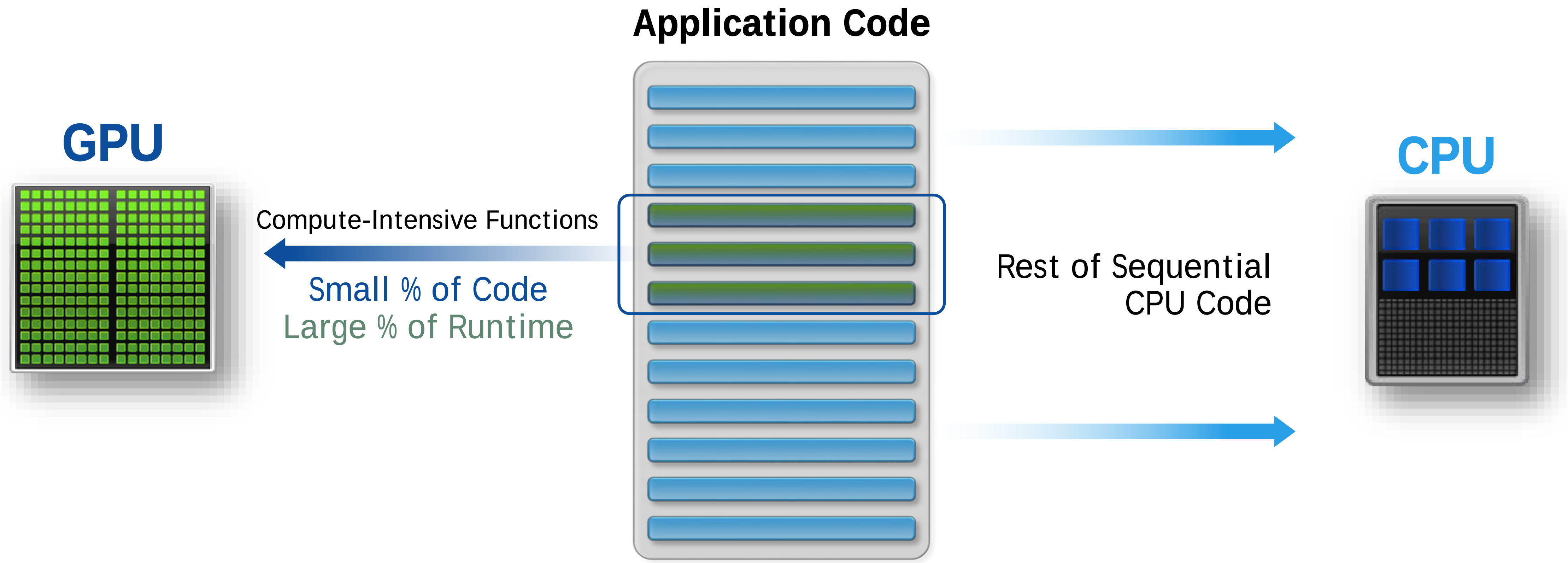
CPU VS GPU

Number of cores and parallelism

- Both are extremely popular parallel processors, but with different degrees of parallelism
- CPUs generally have a small number of very fast physical cores
- GPUs have thousands of simple cores able to achieve high performance in aggregate
- Both require parallelism to be fully utilized, but GPUs require much more

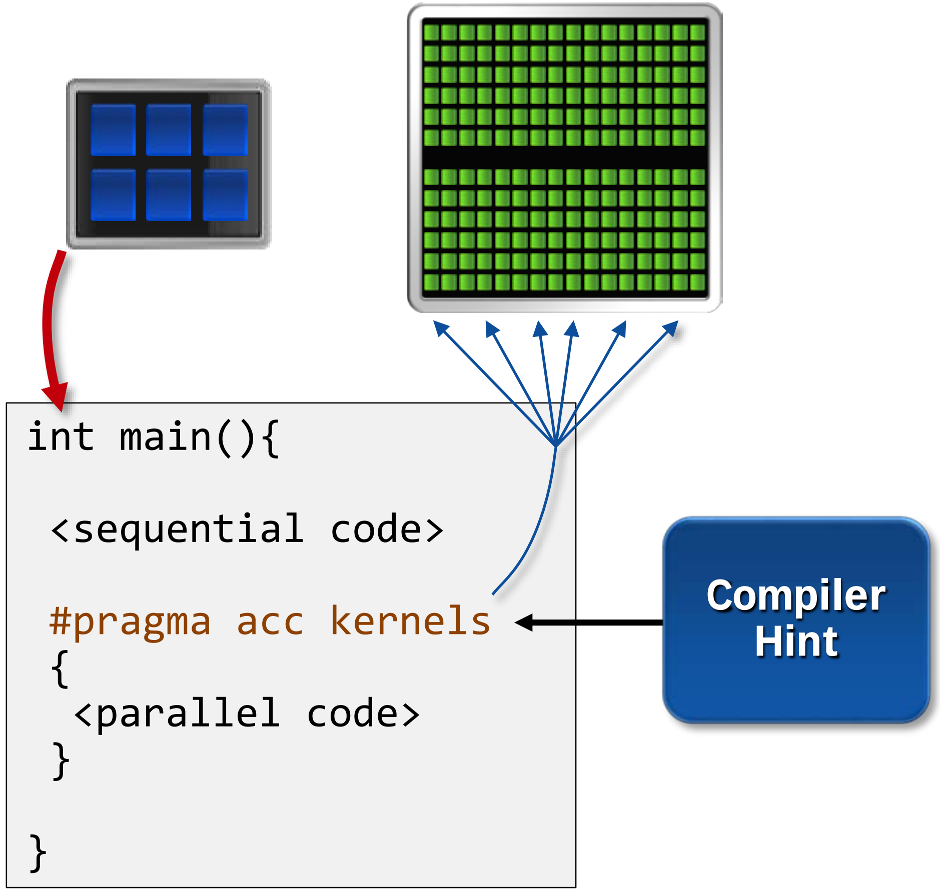


CPU + GPU WORKFLOW



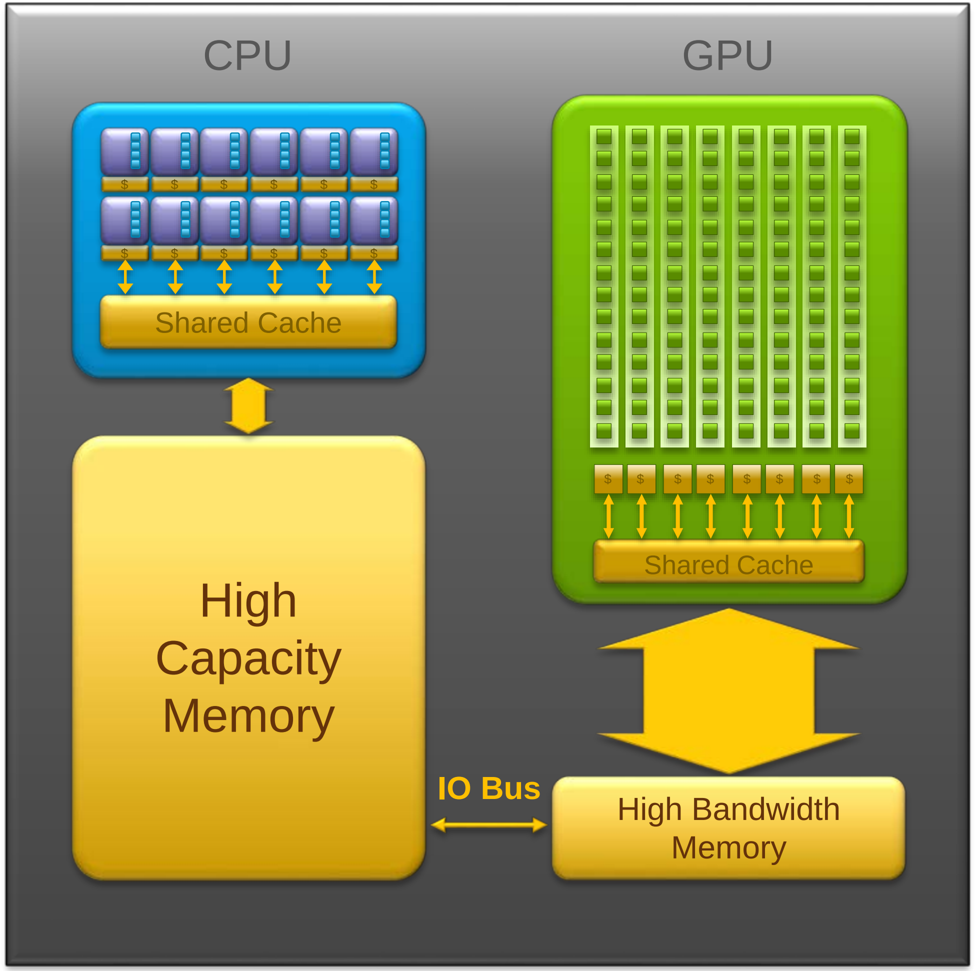
GPU PROGRAMMING IN OPENACC

- Execution always begins and ends on the *host* CPU
- Compute-intensive loops are offloaded to the GPU using directives
- Offloading may or may not require data movement between the *host* and *device*.



CPU + GPU
Physical Diagram

- CPU memory is larger, GPU memory has more bandwidth
- CPU and GPU memory are usually separate, connected by an I/O bus (traditionally PCI-e)
- Any data transferred between the CPU and GPU will be handled by the I/O Bus
- The I/O Bus is relatively slow compared to memory bandwidth
- The GPU cannot perform computation until the data is within its memory

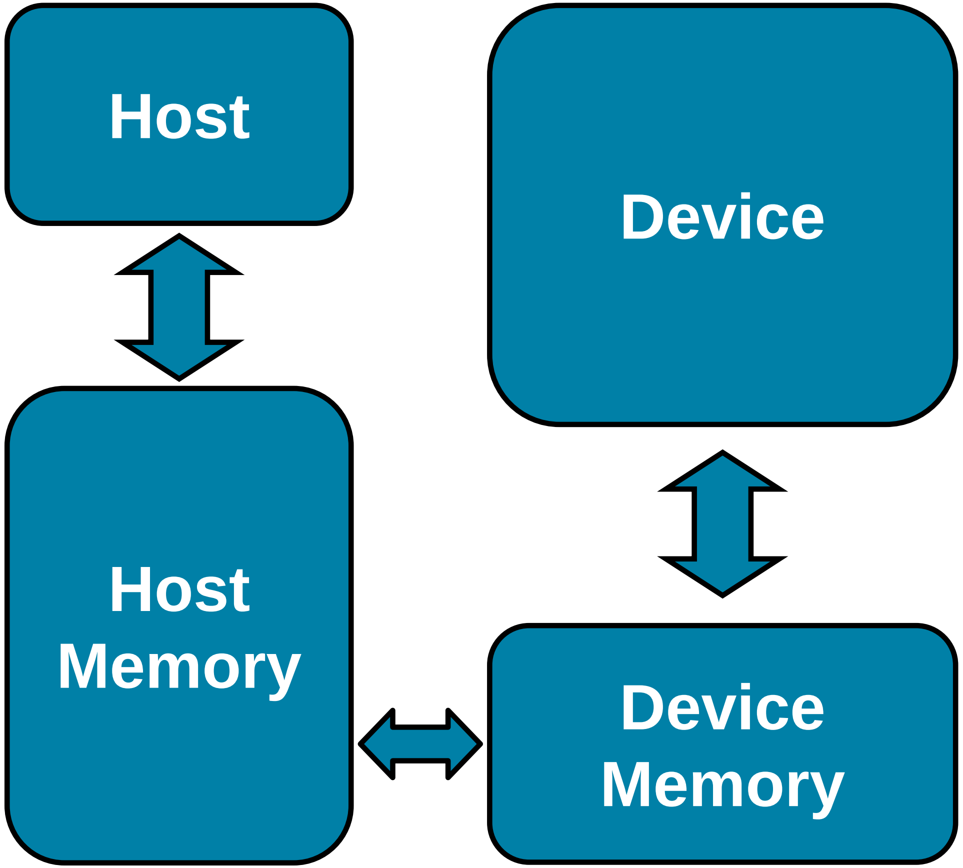


BASIC DATA MANAGEMENT

BASIC DATA MANAGEMENT

Between the host and device

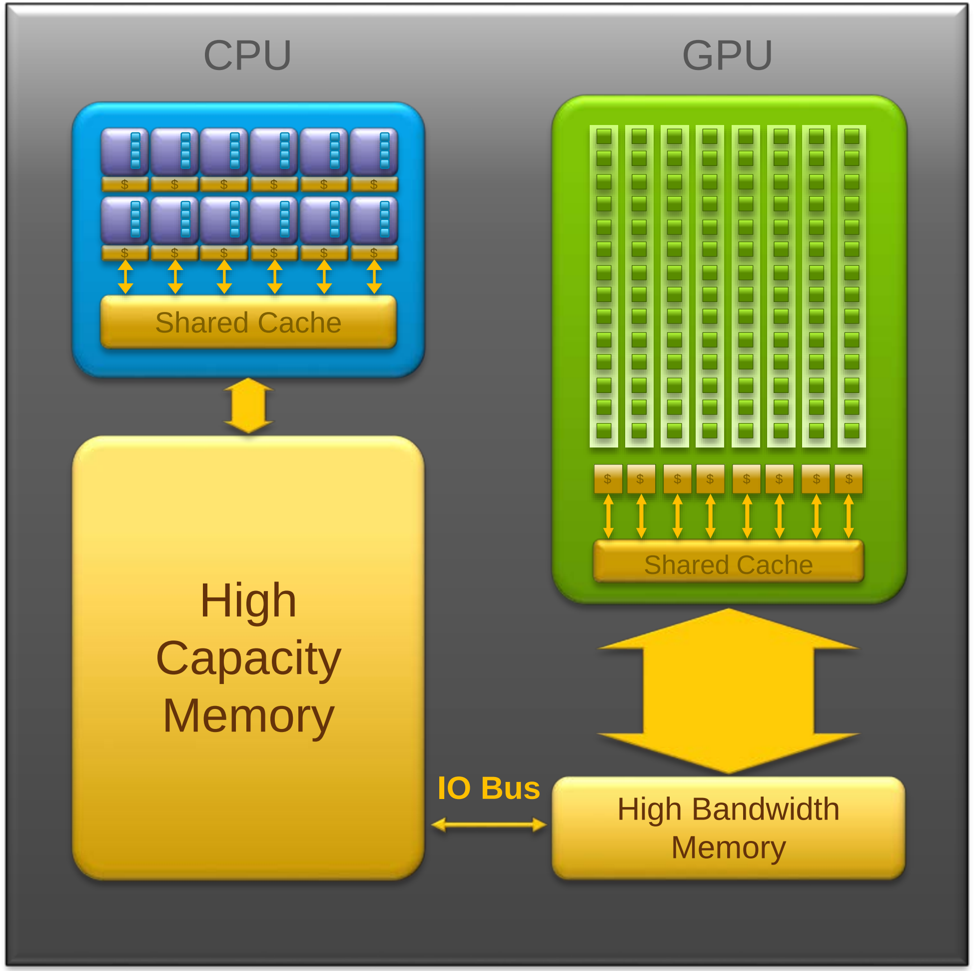
- The **host** is traditionally a CPU
- The **device** is some parallel accelerator
- When our target hardware is multicore, the host and device are the same, meaning that their memory is also the same
- There is no need to explicitly manage data when using a shared memory accelerator, such as the multicore target



BASIC DATA MANAGEMENT

Between the host and device

- When the target hardware is a GPU data will usually need to migrate between CPU and GPU memory
- The next lecture will discuss OpenACC data management, for now we'll assume a unified Host/Accelerator memory



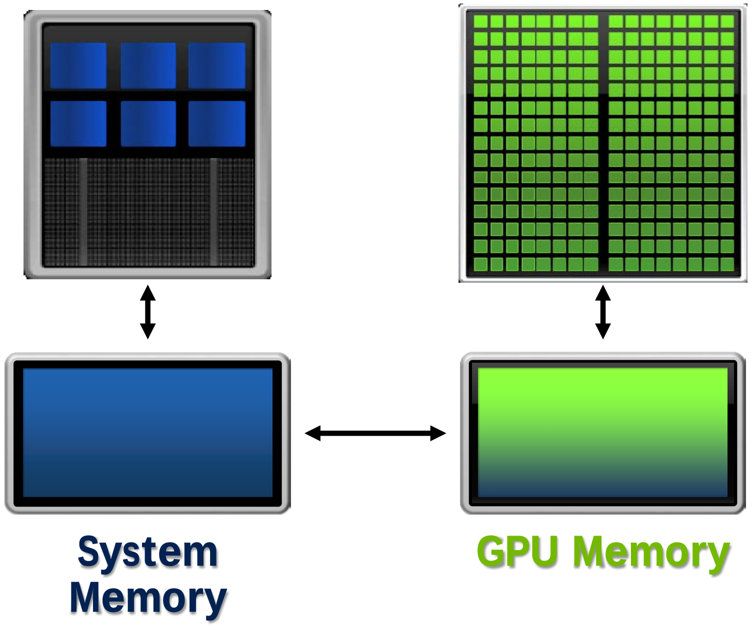
CUDA MANAGED MEMORY

CUDA MANAGED MEMORY

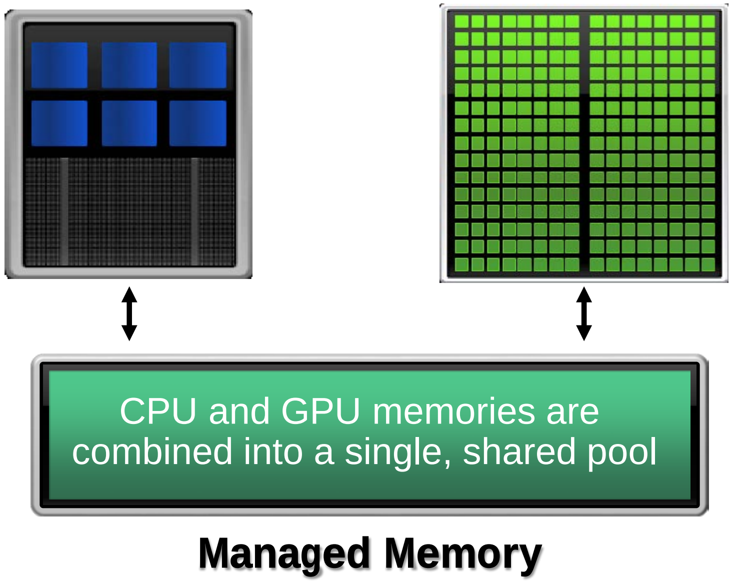
Simplified Developer Effort

Commonly referred to as "unified memory."

Without Managed Memory



With Managed Memory



CUDA MANAGED MEMORY

Usefulness

- Handling explicit data transfers between the host and device (CPU and GPU) can be difficult
- The PGI compiler can utilize CUDA Managed Memory to defer data management
- This allows the developer to concentrate on parallelism and think about data movement as an optimization

```
$ pgcc -fast -acc -ta=tesla:managed -Minfo=accel main.c
```

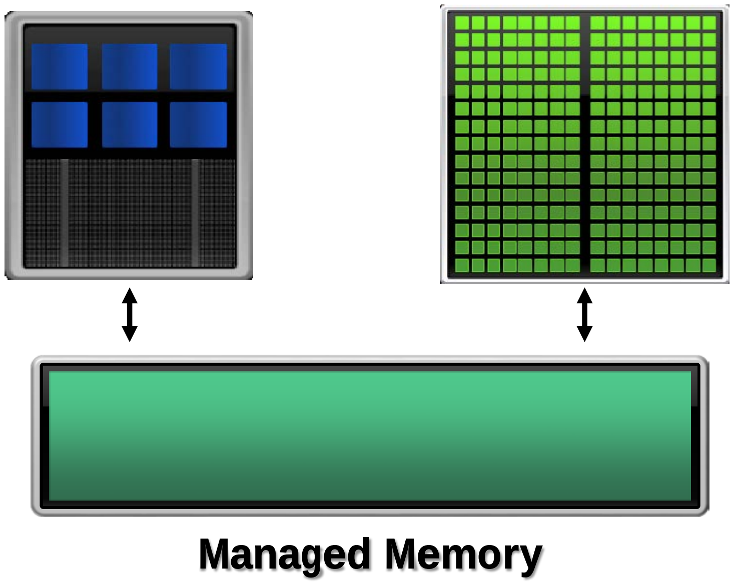
```
$ pgfortran -fast -acc -ta=tesla:managed -Minfo=accel main.f90
```

MANAGED MEMORY

Limitations

- The programmer will almost always be able to get better performance by manually handling data transfers
- Memory allocation/deallocation takes longer with managed memory
- Cannot transfer data asynchronously
- Currently only available from PGI on NVIDIA GPUs.

With Managed Memory



OPENACC WITH MANAGED MEMORY

An Example from the Lab Code

```
while ( error > tol && iter < iter_max )
{
  error = 0.0;
#pragma acc kernels
  {
    for( int j = 1; j < n-1; j++)
    {
      for( int i = 1; i < m-1; i++ )
      {
        Anew[j][i] = 0.25 * ( A[j][i+1] + A[j][i-1]
                            + A[j-1][i] + A[j+1][i]);
        error = fmax( error, fabs(Anew[j][i] - A[j][i]));
      }
    }

    for( int j = 1; j < n-1; j++)
    {
      for( int i = 1; i < m-1; i++ )
      {
        A[j][i] = Anew[j][i];
      }
    }
  }
}
```

Without Managed Memory the compiler must determine the size of A and Anew and copy their data to and from the GPU each iteration to ensure correctness

With Managed Memory the underlying runtime will move the data only when needed

INTRODUCTION TO DATA CLAUSES

BASIC DATA MANAGEMENT

Moving data between the Host and Device using copy

- Data clauses allow the programmer to tell the compiler which data to move and when
- Data clauses may be added to **kernels** or **parallel** regions, but also **data**, **enter data**, and **exit data**, which will discussed shortly

C/C++

```
#pragma acc kernels
for(int i = 0; i < N; i++){
 a[i] = 0;
}
```

BASIC DATA MANAGEMENT

Moving data between the Host and Device using copy

- Data clauses allow the programmer to tell the compiler which data to move and when
- Data clauses may be added to **kernels** or **parallel** regions, but also **data**, **enter data**, and **exit data**, which will discussed shortly

C/C++

```
#pragma acc parallel loop copyout(a[0:n])
for(int i = 0; i < N; i++){
 a[i] = 0;
}
```

I don't need the initial value of a, so I'll only copy it out of the region at the end.

BASIC DATA MANAGEMENT

Moving data between the Host and Device using copy

1. Allocate ‘a’ on GPU
2. Copy ‘a’ from CPU to GPU
3. Execute Kernels
4. Copy ‘a’ from GPU to CPU
5. Deallocate ‘a’ from GPU

```
#pragma acc parallel loop copy(a[0:N])
for(int i = 0; i < N; i++){
 a[i] = 2 * a[i];
}
```

BASIC DATA MANAGEMENT

Moving data between the Host and Device using copy

Allocate ‘a’ on GPU → Copy ‘a’ from CPU to GPU → Execute Kernels → Copy ‘a’ from GPU to CPU → Deallocate ‘a’ from GPU

CPU MEMORY

A’

GPU MEMORY

A’

DATA CLAUSES

`copy( list )` **Allocates memory on GPU and copies data from host to GPU when entering region and copies data to the host when exiting region.**

Principal use: For many important data structures in your code, this is a logical default to input, modify and return the data.

`copyin( list )` **Allocates memory on GPU and copies data from host to GPU when entering region.**

Principal use: Think of this like an array that you would use as just an input to a subroutine.

`copyout( list )` **Allocates memory on GPU and copies data to the host when exiting region.**

Principal use: A result that isn't overwriting the input data structure.

`create( list )` **Allocates memory on GPU but does not copy.**

Principal use: Temporary arrays.

ARRAY SHAPING

- Sometimes the compiler needs help understanding the *shape* of an array
- The first number is the start index of the array
- In C/C++, the second number is how much data is to be transferred
- In Fortran, the second number is the ending index

```
copy(array[starting_index:length])
```

C/C++

```
copy(array(starting_index:ending_index))
```

Fortran

BASIC DATA MANAGEMENT

Multi-dimensional Array shaping

```
copy(array[0:N][0:M])
```

C/C++

```
copy(array(1:N, 1:M))
```

Fortran

PLEASE START LAB NOW!

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PROFILING GPU CODE

PROFILING GPU CODE (PGI)

Obtaining information about your GPU

- Using the **pgaccelinfo** command will display information about available accelerators

Terminal Window

```
$ pgaccelinfo
  Device Number: 0
  Device Name: Tesla P100-PCIE-16GB
  ...
  Managed Memory: Yes
  PGI Compiler Option: -ta=tesla:cc60
```

PROFILING GPU CODE

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PROFILING GPU CODE

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PROFILING GPU CODE

Obtaining information about your GPU

- Using the **pgaccelinfo** command will display information about available accelerators
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- The Device Name identifies the type of accelerator
- Can Managed Memory be used?

Terminal Window

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```

PROFILING GPU CODE

Obtaining information about your GPU

- Using the **pgaccelinfo** command will display information about available accelerators
- Each device is numbered starting with 0
- The Device Name identifies the type of accelerator
- Can Managed Memory be used?
- What compiler options should be used to target this device?

Terminal Window

```
$ pgaccelinfo
  Device Number: 0
  Device Name: Tesla P100-PCIE-16GB
  ...
  Managed Memory: Yes
  PGI Compiler Option: -ta=tesla:cc60
```

Without Manage Memory

```
$ pgcc –ta=tesla:cc60 main.c
```

With Manage Memory

```
$ pgcc –ta=tesla:cc60,managed main.c
```

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COMPILING GPU CODE

Terminal Window

```
$ pgcc -fast -ta=tesla:cc60 -Minfo=accel jacobi.c laplace2d.c
  calcNext:
        37, Generating copy(Anew[:m*n],A[:m*n])
            Accelerator kernel generated
            Generating Tesla code
            37, Generating reduction(max:error)
            38, #pragma acc loop gang /* blockIdx.x */
            41, #pragma acc loop vector(128) /* threadIdx.x */
        41, Loop is parallelizable
  swap:
        56, Generating copy(Anew[:m*n],A[:m*n])
            Accelerator kernel generated
            Generating Tesla code
            57, #pragma acc loop gang /* blockIdx.x */
            60, #pragma acc loop vector(128) /* threadIdx.x */
        60, Loop is parallelizable
```

We can see that our data copies are being applied by the compiler

COMPILING GPU CODE

Terminal Window

```
$ pgcc -fast -ta=tesla:cc60 -Minfo=accel jacobi.c laplace2d.c
  calcNext:
        37, Generating copy(Anew[:m*n],A[:m*n])
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            Generating Tesla code
            57, #pragma acc loop gang /* blockIdx.x */
            60, #pragma acc loop vector(128) /* threadIdx.x */
        60, Loop is parallelizable
```

We also see that the compiler is generating code for our GPU

COMPILING GPU CODE

Terminal Window

```
$ pgcc -fast -ta=tesla:cc60 -Minfo=accel jacobi.c laplace2d.c
  calcNext:
        37, Generating copy(Anew[:m*n],A[:m*n])
            Accelerator kernel generated
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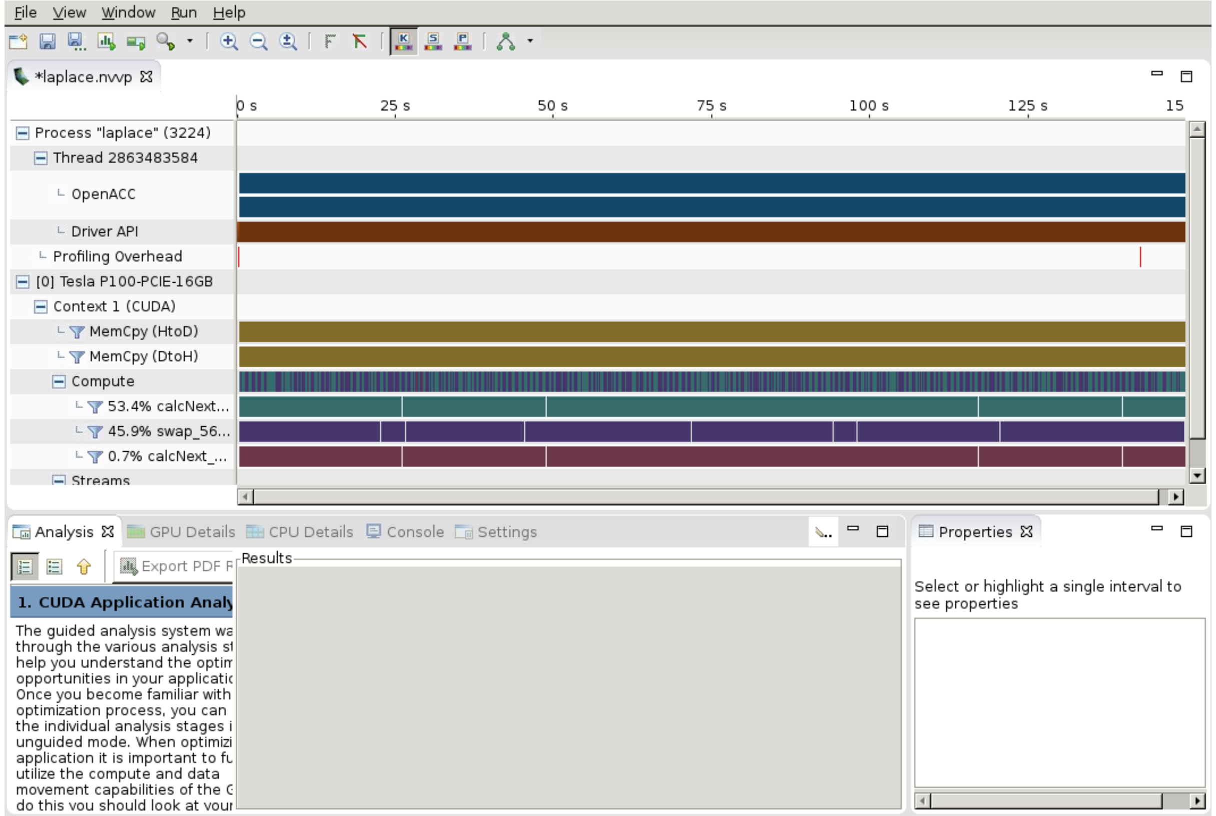
            57, #pragma acc loop gang /* blockIdx.x */
            60, #pragma acc loop vector(128) /* threadIdx.x */
        60, Loop is parallelizable
```

This is the parallelization of the **outer loop**

PROFILING GPU CODE (PGPROF)

Using PGPROF to profile GPU code

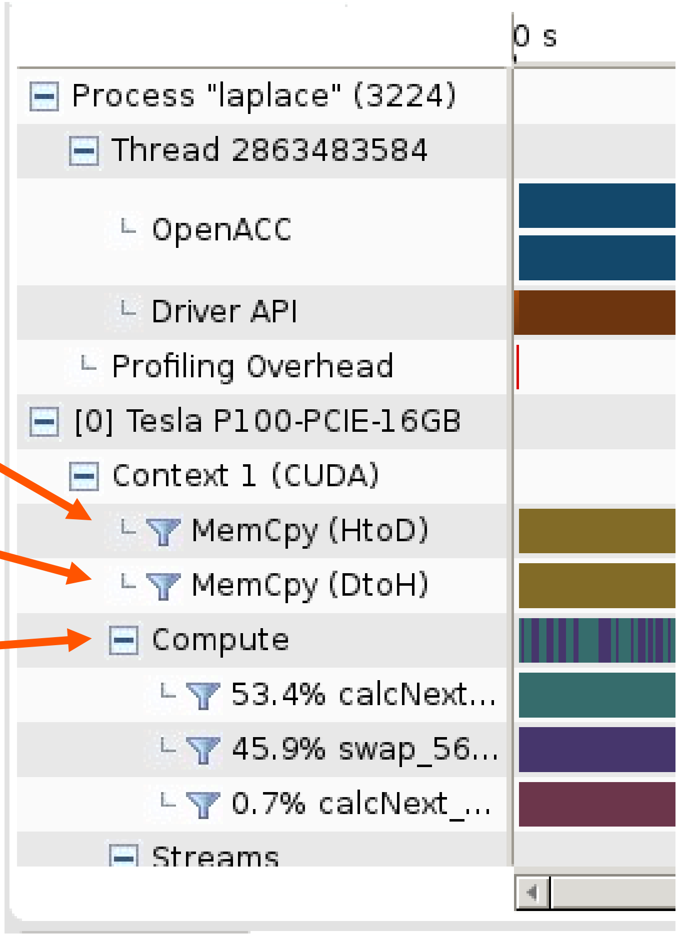
- PGPROF presents far more information when running on a GPU
- We can view CPU Details, GPU Details, a Timeline, and even do Analysis of the performance



PROFILING GPU CODE (PGPROF)

Using PGPROF to profile GPU code

- **MemCpy(HtoD):** This includes data transfers from the Host to the Device (CPU to GPU)
- **MemCpy(DtoH):** These are data transfers from the Device to the Host (GPU to CPU)
- **Compute:** These are our computational functions. We can see our calcNext and swap function



PROFILING GPU CODE

Receiving unexpected code results

- Here we can see the runtime of our application: 151 seconds
- The program is now performing over 3 times **worse** than the sequential version
- A profiler can help us understand why this performance is worse

Terminal Window

```
$ pgcc –ta=tesla:cc60 jacobi.c laplace2d.c
$ ./a.out
    0, 0.250000
  100, 0.002397
  200, 0.001204
  300, 0.000804
  400, 0.000603
  500, 0.000483
  600, 0.000403
  700, 0.000345
  800, 0.000302
  900, 0.000269
  total: 151.772627 s
```

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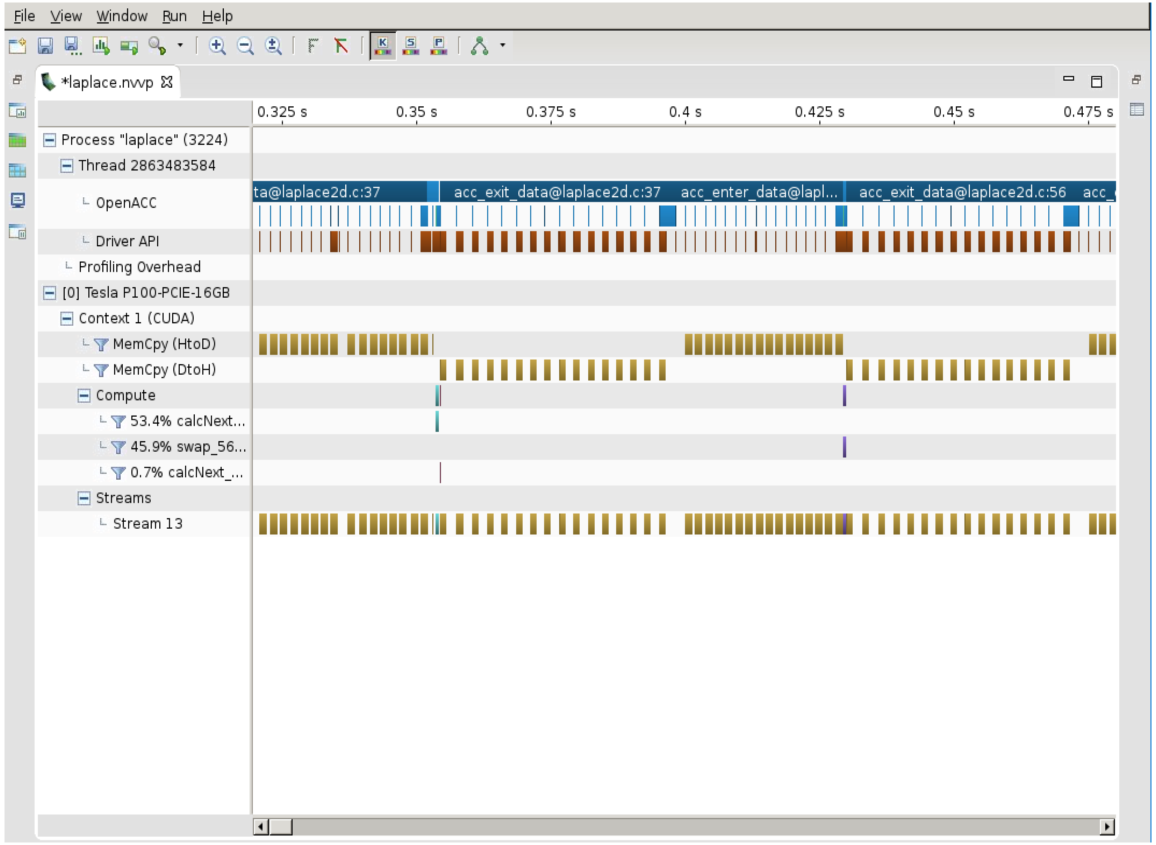
PROFILING GPU CODE

Inspecting the PGPROF timeline

- Zooming in gives us a better view of the timeline
- At a first glance, it looks like our program is spending a significant amount of time transferring data between the host and device
- We also see that the compute regions are very small and spread out
- What if we try Managed Memory?



PROFILING GPU CODE

Using managed memory

- Using managed memory drastically improves performance
- This managed memory version is performing over 20x better than the sequential code
- What does the profiler tell us about this?

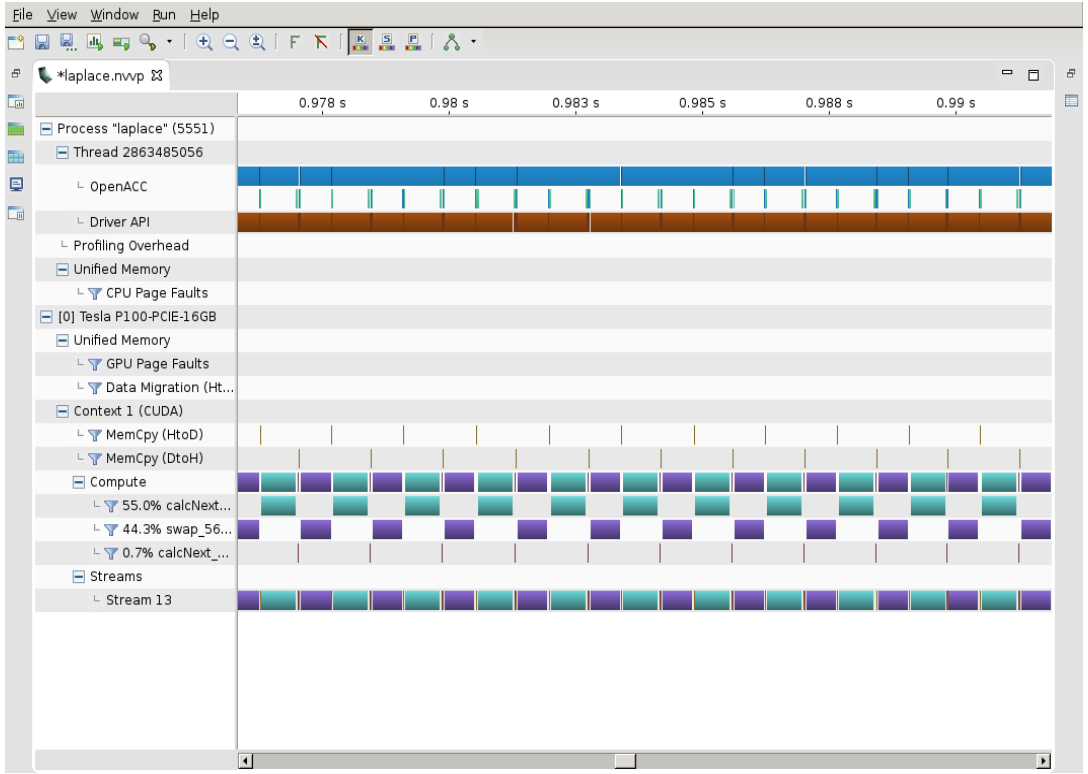
Terminal Window

```
$ pgcc -ta=tesla:cc60,managed jacobi.c
  laplace2d.c
$ ./a.out
    0, 0.250000
  100, 0.002397
  200, 0.001204
  300, 0.000804
  400, 0.000603
  500, 0.000483
  600, 0.000403
  700, 0.000345
  800, 0.000302
  900, 0.000269
  total: 1.474951 s
```

PROFILING GPU CODE

Using managed memory

- The data no longer needs to transfer between each kernel
- The data is only moved when it's first accessed on the GPU or CPU
- During the timestepping data remains on the device
- Now a higher percentage of time is spent computing



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KEY CONCEPTS

In this module we discussed…

- The fundamental differences between CPUs and GPUs
- Assisting the compiler by providing information about array sizes for data management
- Managed memory

THANK YOU

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