MODULE FOUR: GPU PROGRAMMING

Speaker, Date
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

Application Code

GPU

Small % of Code
Large % of Runtime

Compute-Intensive Functions

Rest of Sequential CPU Code

CPU
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

Without Managed Memory

With Managed Memory

Commonly referred to as “unified memory.”

CPU and GPU memories are combined into a single, shared pool.
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

```bash
$ 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.
An Example from the Lab Code

```c
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
#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 be discussed shortly

C/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

- 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

```fortran
!$acc parallel loop copyout(a(1:N))
do i = 1, N
   a(i) = 0
end do
```

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

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

```c
#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’
<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
<th>Principal use</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>copy(list)</code></td>
<td>Allocates memory on GPU and copies data from host to GPU when entering region and copies data to the host when exiting region.</td>
<td>For many important data structures in your code, this is a logical default to input, modify and return the data.</td>
</tr>
<tr>
<td><code>copyin(list)</code></td>
<td>Allocates memory on GPU and copies data from host to GPU when entering region.</td>
<td>Think of this like an array that you would use as just an input to a subroutine.</td>
</tr>
<tr>
<td><code>copyout(list)</code></td>
<td>Allocates memory on GPU and copies data to the host when exiting region.</td>
<td>A result that isn’t overwriting the input data structure.</td>
</tr>
<tr>
<td><code>create(list)</code></td>
<td>Allocates memory on GPU but does not copy.</td>
<td>Temporary arrays.</td>
</tr>
</tbody>
</table>
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.

- C/C++: `copy(array[starting_index:length])`
- Fortran: `copy(array(starting_index:ending_index))`
BASIC DATA MANAGEMENT
Multi-dimensional Array shaping

\[ \text{copy(array}[0:N][0:M]) \]  \hspace{1cm} \text{C/C++}

\[ \text{copy(array}(1:N, 1:M)) \]  \hspace{1cm} \text{Fortran}
PROFILING GPU CODE
PROFILING GPU CODE (PGI)

Obtaining information about your GPU

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

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

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.

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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?

**Terminal Window**

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PGI Compiler Option: -ta=tesla:cc60
```
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
```
$ pgcc -fast -ta=tesla:cc60 -Minfo=accel jacobiac.c laplace2dc.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

Terminal Window

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])
   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 */
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   Accelerator kernel generated
   Generating Tesla code
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60, #pragma acc loop vector(128) /* threadIdx.x */
60, Loop is parallelizable

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

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
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
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?

```
$ 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
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
ADDITIONAL RESOURCES

YouTube OpenACC Introduction Series by Michael Wolfe

Introduction to Parallel Programming with OpenACC – Part 3
Introduction to Parallel Programming with OpenACC – Part 4

Follow along by downloading the code here!