Introduction to Graphical Processing Units as Tools for Scientific Computing

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Introduction to Graphical Processing Units as Tools for Scientific Computing

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Hopefully this talk will (partially) answer...

- What is a GPU?
- Why would I use a GPU for scientific computing?
- When should I consider using GPUs to solve my problem?
- What are the main hardware features available to the GPU programmer?
- How do I use the GPU to solve my problem really fast?
What is a graphical processing unit (GPU)?

- A processor you add to your computer to accelerate graphical applications, e.g. computer games
- Most desktops and laptop computers already contain a GPU of some kind

http://www.nvnews.net/previews/geforce_8800_gtx/images/geforce_8800_gts.jpg
Why do we want to use GPUs for scientific computing?

- They are inexpensive
- They are readily available, and possibly already present in your desktop workstation
- They are fast for floating point math
- The operations involved in game software are similar to those in scientific applications

<table>
<thead>
<tr>
<th>Processor</th>
<th>Cost</th>
<th>Floating Point Performance</th>
<th>Memory Bandwidth</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quad-Core Intel Xeon E5506 @2.13GHz</td>
<td>$1500</td>
<td>68 Gflop/s</td>
<td>19 GB/s</td>
</tr>
<tr>
<td>NVidia GTX 275</td>
<td>+$300</td>
<td>304 Gflop/s</td>
<td>127 GB/s</td>
</tr>
</tbody>
</table>

GPUs outperform CPUs on a per dollar basis
How is a game similar to a physics simulation?

- Games are physics simulations
- Graphical manipulations are linear algebra

Physics and games both require fast floating point math
How fast?


Thanks to Axel Kohlmeyer and David LeBard
How fast?

- Radial Distribution Functions
Density functional calculation - A single water molecule in a 15 Å periodic box, Pade functional
GPU Acceleration Strategies

- Link to Libraries
- Hand-code Performance-Critical Subroutines
  - More Work to Code
  - Faster Performance
- Rewrite Whole Code From Scratch
  - CP2K (2-3x speedup)
  - HOOMD (30x speedup)
  - Radial Distribution Functions (10-100x speedup)
NVidia GPU Architecture

- Parallelism
- Memory Hierarchy

- Multiprocessor (processes 32 threads)
  - 8192 32-bit Registers
  - Shared Memory (16 kB / Multiproc.)
  - Constant Cache (8 kB / Multiproc.)

- Multiprocessor (processes 32 threads)
  - 8192 32-bit Registers

- Up to 32 Multi-processors
- Device Memory (up to 4 GB)
  - Constant Memory (up to 64 kB)

- To PCI-E bus
  - 76.8 GB/s
  - 8.0 GB/s
**NVidia GPU Architecture**

- Applies the same instruction to 32 pieces of data simultaneously (SIMD)

Multiprocessor (processes 32 threads)

```
1 + 8 =  9
4 + 8 = 12
9 + 0 =  9
3 + 4 =  7
3 + 5 =  8
7 + 7 = 14
...
1 * 8 =  8
4 + 8 = 12
9 - 0 =  9
3 + 4 =  7
3 * 5 = 15
7 / 7 =  1
...
```
NVidia GPU Architecture

- Double precision floating point math is 7x slower than single (next generation “Fermi” will be only 2x slower)
- Fused multiply-add

Multiprocessor (processes 32 threads)

1 * 2 + 8 = 10
4 * 3 + 8 = 20
9 * 1 + 0 = 9
3 * 8 + 4 = 28
3 * 3 + 5 = 14
7 * 4 + 7 = 35
...
A GPU chip contains between 1 and 32 multiprocessors.

32 multiprocessors * 32 threads / multiprocessor * 2 FLOPs per cycle = 2048 FLOPS at one time!

The key to successful GPU programming is keeping all multiprocessors busy as much as is possible.
NVidia GPU Architecture

On-Chip

- Multiprocessor (processes 32 threads)
- 8192 32-bit Registers
- Shared Memory (16 kB / Multiproc.)
- Constant Cache (8 kB / Multiproc.)

Off-Chip/On-Card

- Constant Memory (up to 64 kB)
- Device Memory (up to 4 GB)

- To PCI-E bus

- 8.0 GB/s
- 76.8 GB/s

- 32-bit load / thread / 4 cycles
- Slow off-chip memory
NVidia GPU Architecture

- Slow off-chip memory
- Fast on-chip memory
NVidia GPU Architecture

Device (Global) Memory
- Slow
- Large
- Analogous to main memory in a desktop computer
- Typically not cached
- Accessible from all threads on GPU and from the CPU

- Multiprocessor (processes 32 threads)
  - 8192 32-bit Registers
  - 32-bit load / thread / 4 cycles

- Shared Memory (16 kB / Multiproc.)
- Constant Cache (8 kB / Multiproc.)

- Device Memory (up to 4 GB)
- Constant Memory (up to 64 kB)

- To PCI-E bus
  - 76.8 GB/s
  - 8.0 GB/s
NVidia GPU Architecture

Registers
- Loads very fast
- Limited supply (~25/thread for good performance)
- Each thread has its own
- Analogous to registers in a computer
- Can be accessed only from the GPU
NVidia GPU Architecture

Shared memory
- *Can* be as fast as registers
- Limited supply
- Like a cache, but user controlled
- Shared by several threads
- Can only be accessed by the GPU

- Multiprocessor (processes 32 threads)
  - 32-bit load / thread / 4 cycles
  - 8192 32-bit Registers

- Shared Memory (16 kB / Multiproc.)

- Constant Cache (8 kB / Multiproc.)

- Device Memory (up to 4 GB)
  - To PCI-E bus
  - 76.8 GB/s

- Constant Memory (up to 64 kB)
  - 8.0 GB/s
NVidia GPU Architecture

Constant Memory
- Device memory which is associated with an on-chip cache
- As fast as registers if you are accessing cached data
- Limited supply
- Read-only from GPU
- Read-write from CPU
Memory Hierarchy Summary

Layers of memory differ in:

- size
- speed
- whether they shared between among several threads
- whether they can be written to from the GPU or only read
- whether they are associated with a cache

The programmer has almost complete control over the location of data in this hierarchy!
What we’ve learned so far...

- GPUs are fast
- GPUs are relatively inexpensive
- The more time you put into programming, the faster your GPU code can be
- GPUs are highly parallel processors
- GPU memory is broken down into a large amount of slow memory, and several small chunks of fast memory

But what do we do if we want to use it?
First, stop and **THINK**

- How much time do I have to code? – A lot of coding is needed to gain a large speedup in most cases.
- Which parts of my code are performance critical? – Perhaps optimizing a single routine could give a substantial speedup.
- Will my problem map well to the GPU?
Will my problem map well to the GPU?

Those which involve:
- performing the same operations on a lot of data
- lots of floating point math
- regular memory access pattern
- problem which can be solved (mostly) in single precision

Examples
- algorithms based on linear algebra
- parallel random number generation (MC with multiple walkers)
Compute Unified Device Architecture (CUDA)

- Created by NVidia to allow their GPUs to be used for general high-performance computing applications
- An extension to the C programming language
- To learn more about applications and find online tutorials: [http://www.nvidia.com/object/cuda_education.html](http://www.nvidia.com/object/cuda_education.html)
Installing CUDA

- Download and install three things
  - CUDA driver – tells your computer how to access the GPU hardware
  - CUDA toolkit – contains the NVCC compiler and libraries needed to compile GPU accelerated code
  - CUDA standard developers kit (SDK) – contains example codes which are useful in learning CUDA
- Easiest to install with one of the supported Linux distributions (Redhat Enter., Fedora, SUSE Enter., OpenSUSE, Ubuntu)
Compiling CUDA Code

- Include the cuda_runtime header file at the beginning of your source file
  ```
  #include <cuda_runtime.h>
  ```
- Use nvcc just like any other compiler
  ```
  nvcc -o xyz.exe xyz.cu
  ```
- Preprocessing is the same as for C
- IMPORTANT – simply adding the above `#include` statement and compiling with `nvcc` does not result in any portion of your code being run on the GPU!
Emulation Mode

- Emulation mode executables run GPU code on the CPU only
- Emulation mode is particularly useful for debugging because input/output (e.g. `printf`) is not available on the GPU
- To compile in emulation mode:
  
  ```
  nvcc -o xyz.e -deviceemu -D__DEVICEEMU xyz.cu
  ```
- Then, to print
  
  ```
  #ifdef __DEVICEEMU
  printf("debugging info");
  #endif
  ```
Math Libraries

- **CUBLAS – Linear Algebra**
  - Single and Double Precision BLAS Routines
  - Helper functions
    - `cublasInit` and `cublasShutdown` must be run before and after any calls
    - Routines to allocate and free device memory
    - Routines to move data between main memory and device
  - [http://developer.download.nvidia.com/compute/cuda/2.0/docs/CUBLAS_Library_2.0.pdf](http://developer.download.nvidia.com/compute/cuda/2.0/docs/CUBLAS_Library_2.0.pdf)

- **CUFFFT – Fast Fourier Transforms**
  - Interface similar to FFTW
Linking to the Math Libraries

- To link to the CUBLAS or CUFFT libraries include the appropriate header file in your source code
  ```
  #include <cublas.h>
  #include <cufft.h>
  ```
- Pass the option to link to the appropriate library to nvcc
  ```
  nvcc -o xyz.exe -lcublas xyz.cu
  nvcc -o xyz.exe -lcufft xyz.cu
  ```
Terminology

- Host = the non-GPU part of your machine
  - Host memory = main memory
  - Host processor = CPU
- Device = the graphics card
  - Device memory = the off-chip memory on the device (global memory)
The following code squares each element of a vector $A_{host}$ on the CPU.

```c
void square_vec(float* A_host, int n) {
    for (int i=0; i<n; i++) {
        A_host[i] = A_host[i] * A_host[i];
    }
}
```
What Does CUDA Code Look Like?

- The main routine looks almost like standard C
- It is called from and executed on the CPU

```c
void square_vec(float* A_host, int n) {
    float* A_dev;
    cudaMalloc((void**)&A_dev, n * sizeof(float));
    cudaMemcpy(A_dev, A_host, n * sizeof(float), cudaMemcpyHostToDevice);
    gpu_kernel<<<1,n>>>(A_dev);
    cudaMemcpy(A_host, A_dev, n * sizeof(float), cudaMemcpyDeviceToHost);
    cudaMemcpyHostToDevice);
    cudaMemcpy(A_host, A_dev, n * sizeof(float), cudaMemcpyDeviceToHost);
    cudaFree(A_dev);
}
```
What Does CUDA Code Look Like?

`A_host` is a vector of length `n` stored in the host (main) memory.

This code will calculate:

\[ A_{host}[i] = A_{host}[i]^2 \]

for all elements of `A_host` in parallel on the GPU.

```c
void square_vec(float* A_host, int n) {
    float* A_dev;
    cudaMalloc((void**)&A_dev, n * sizeof(float));
    cudaMemcpy(A_dev, A_host, n * sizeof(float), cudaMemcpyHostToDevice);
    gpu_kernel<<<1,n>>>(A_dev);
    cudaMemcpy(A_host, A_dev, n * sizeof(float), cudaMemcpyDeviceToHost);
    cudaFree(A_dev);
}
```
What Does CUDA Code Look Like?

Enough global memory to store the array on the device is dynamically allocated using the `cudaMalloc` library routine.

```c
void square_vec(float* A_host, int n) {
    float* A_dev;
    cudaMalloc((void**)&A_dev, n * sizeof(float));
    cudaMemcpy(A_dev, A_host, n * sizeof(float), cudaMemcpyHostToDevice);
    gpu_kernel<<<1,n>>>(A_dev);
    cudaMemcpy(A_host, A_dev, n * sizeof(float), cudaMemcpyDeviceToHost);
    cudaFree(A_dev);
}
```
What Does CUDA Code Look Like?

The contents of \texttt{A\_host} (in main memory) are copied to \texttt{A\_dev} (in device memory) using the \texttt{cudaMemcpy} library routine.

```c
void square_vec(float* A_host, 
               int n) {
    float* A_dev; 
    cudaMalloc((void**)&A_dev, 
               n * sizeof(float));
    cudaMemcpy(A_dev, A_host, 
               n * sizeof(float),
               cudaMemcpyHostToDevice);
    gpu_kernel<<<1,n>>>(A_dev);
    cudaMemcpy(A_host, A_dev, 
               n * sizeof(float),
               cudaMemcpyDeviceToHost);
    cudaFree(A_dev);
}
```
What Does CUDA Code Look Like?

`gpu_kernel` is a user written routine which runs on the GPU.

The bracketed numbers `<<<1,n>>>` denote that 1 block of n threads will be spawned.

Blocks of threads share shared memory and can be synchronized with barriers; threads in different blocks cannot share memory or be synchronized.

```c
void square_vec(float* A_host, int n) {
    float* A_dev;
    cudaMalloc((void**)&A_dev, n * sizeof(float));
    cudaMemcpy(A_dev, A_host, n * sizeof(float), cudaMemcpyHostToDevice);
    gpu_kernel<<<1,n>>>(A_dev);
    cudaMemcpy(A_host, A_dev, n * sizeof(float), cudaMemcpyDeviceToHost);
    cudaFree(A_dev);
}
```
What Does CUDA Code Look Like?

After `gpu_kernel` completes, the contents of `A_dev` (in device memory) are copied to `A_host` (in main memory) using the `cudaMemcpy` library routine.
What Does CUDA Code Look Like?

```c
void square_vec(float* A_host,
    int n) {
    float* A_dev;
    cudaMalloc((void**) &A_dev,
               n * sizeof(float));
    cudaMemcpy(A_dev, A_host,
               n * sizeof(float),
               cudaMemcpyHostToDevice);
    gpu_kernel<<<1,n>>>(A_dev);
    cudaMemcpyHostToDevice);
    cudaMemcpy(A_dev, A_host,
               n * sizeof(float),
               cudaMemcpyDeviceToHost);
    cudaFree(A_dev);
}
```

The dynamically allocated device memory pointed to by `A_dev` is freed.
What Does CUDA Code Look Like?

```c
void square_vec(float* A_host, 
    int n) {

    float* A_dev;
    cudaMemcpy((void**)&A_dev, 
        n * sizeof(float));
    cudaMemcpy(A_dev, A_host, 
        n * sizeof(float),
        cudaMemcpyHostToDevice);
    gpu_kernel<<<1,n>>>(A_dev);
    cudaMemcpy(A_host, A_dev, 
        n * sizeof(float),
        cudaMemcpyDeviceToHost);
    cudaFree(A_dev);
}
```
Define the function with the `__global__` function type qualifier to tell the compiler that this function will be called from the host, but run on the device.

```c
__global__ void gpu_kernel(float* A_dev) {
    float tmp;
    tmp = A_dev[threadIdx.x];
    tmp = tmp * tmp;
    A_dev[threadIdx.x] = tmp;
}
```
What Does CUDA Code Look Like?

Declaring `tmp` without a variable type qualifier indicates that we want the compiler to store `tmp` in a register if possible.

If the compiler determines that it does not want to use a register for this variable it will be placed in global memory.

```c
__global__ void gpu_kernel(float* A_dev) {
    float tmp;
    tmp = A_dev[threadIdx.x];
    tmp = tmp * tmp;
    A_dev[threadIdx.x] = tmp;
}
```
What Does CUDA Code Look Like?

We load an element of the \texttt{A\_dev} into the register (\texttt{tmp})

\texttt{threadIdx.x} is a unique identifier for each thread of the block, starting at 0 and counting up to \texttt{blockDim.x-1}, thus we load a unique element of \texttt{A\_dev} for each thread.
What Does CUDA Code Look Like?

Just multiplication, nothing special

```c
__global__ void gpu_kernel(float* A_dev) {
    float tmp;
    tmp = A_dev[threadIdx.x];
    tmp = tmp * tmp;
    A_dev[threadIdx.x] = tmp;
}
```
What Does CUDA Code Look Like?

__global__ void gpu_kernel(
    float* A_dev) {
    float tmp;
    tmp = A_dev[threadIdx.x];
    tmp = tmp * tmp;
    A_dev[threadIdx.x] = tmp;
}
What Does CUDA Code Look Like?

If we want we can create `__device__` functions which are callable from the GPU and run on the GPU.

```c
__global__ void gpu_kernel(float* A_dev) {
    float tmp;
    tmp = A_dev[threadIdx.x];
    tmp = square(tmp);
    A_dev[threadIdx.x] = tmp;
}

__device__ float square(float x) {
    float y
    y = x * x;
    return y;
}
```
Summary of CUDA extensions to standard C

- Memory Management
  - `cudaMalloc` – Allocates global memory on the device
  - `cudaMemcpy` – Copies memory from host to device and from device to host
  - `cudaFree` – Frees dynamically allocated global memory
Summary of CUDA extensions to standard C

- Function type qualifiers
  - __host__ or no type qualifier – runs on the host and is callable only from the host
  - __global__ – runs on the device but is callable only from the host
  - __device__ – runs on the device and is callable only from the device
Summary of CUDA extensions to standard C

- Variable type qualifiers
  - No type qualifier – a scalar variable will usually be stored as a register, an array will go to slow device memory. In both cases the variable is accessible only from a single thread.
  - __shared__ – store variable in fast shared memory. Variable is accessible from all threads in the thread block.