Introduction to GPU Computing

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Goals for this tutorial

- Understand the architectural differences between GPUs and CPUs and the associated trade-offs
- Recognize several GPU programming models and how/when to use each
- Understand how to analyze GPU performance
- Recognize very basic GPU optimizations

This tutorial is not...

- A deep-dive on GPU programming
- The be all and end all on GPU optimization
- A recipe for getting 10, 100, 1000X speed-ups for your application

GPU ARCHITECTURE BASICS

Section Goals

- Recognize the differences between CPU/GPU architectures
- Identify when one architecture may be better suited than the other.

CPU/GPU Architectures



CPU/GPU Architectures

CPU

- Large memory, directly accessible
- Each core has own, independent control logic
 - Allows independent execution
- Coherent caches between cores
 - Can share & synchronize

GPU

- Relatively small memory, must be managed by CPU
- Groups of compute cores share control logic
 - Saves space, power, ...
- Shared cache & synchronization within groups
 - None between groups

Play to your strengths

CPU

- Tuned for serial execution with short vectors
- Multiple independent threads of execution
- Branch-prediction
- Memory latency hidden by cache & prefetching
 - Requires regular data access patterns

GPU

- Tuned for highly parallel execution
- Threads work in lockstep within groups
 - Much like vectors
- Serializes branchy code
- Memory latency hidden by swapping away stalled threads
 - Requires 1000s of concurrent threads

GPU Glossary

Hardware	Software
(CUDA) Core	Thread/Work Unit
Streaming Multiprocessor (SM)	Thread Block/Work Group

- A *Grid* is a group of related *Thread Blocks* running the same kernel
- A Warp is Nvidia's term for 32 Threads running in lock-step
- *Warp Diversion* is what happens when some threads within a warp stall due to a branch
- Shared Memory is a user-managed cache within a Thread Block
- Occupancy is the degree to which all of the GPU hardware can be used in a Kernel
 - Heavily influenced by registers/thread and threads/block
- *Stream* is a series of data transfers and kernel launches that happen in series

GPU PROGRAMMING MODELS

Section Goals

- Introduce several GPU programming models
- Discuss why someone may choose one programming paradigm over the others.

Explicit/Implicit GPU Programming

Explicit

- Bottom-up approach
- Explicit Kernel written from threads' perspective
- Memory management controlled by programmer
- Thread Blocks & Grid defined by programmer
- GPU code usually distinct from CPU code

Implicit

- Traditional Top-down programming
 - Big Picture
- Compiler handles memory and thread management
 - May be guided by programmer
- CPU & GPU may use the same code
 - Easier code maintenance

GPU Programming Models

- Explicit
 - CUDA C (Free from Nvidia)
 - CUDA Fortran (Commercial from PGI)
 - OpenCL (Free from Multiple Vendors)
- Implicit
 - Proposed OpenMP Directives (Multiple Vendors)
 - PGI Directives (Commercial from PGI)
 - HMPP Directives (Commercial from CAPS)
 - Libraries (CUBLAS, MAGMA, etc.)

Multi-node Programming

- GPU papers & tutorials usually focus on 1 node, what about the rest of the machine?
- High-level MPI parallelism between nodes
 - You're probably already doing this
- Loose, on-node parallelism via threads
 - Most codes today are using MPI, but threading is becoming more important
- Tight, on-node, vector parallelism
 - SSE/AVX on CPUs
 - GPU threaded parallelism

Programmers need to expose the same parallelism with/without GPUs

Using the Machine Efficiently

MPI MPI CPU0 GPU0 GPU0 GPU1 GPU1 MPI MPI MPI MPI CPU1 CPU1

• Neglects the CPU

So-So Hybridization

• Suffers from Amdahl's Law

Better Hybridization



- Overlap CPU/GPU work and data movement.
- Even better if you can overlap communication too!

Original S3D

RHS – Called 6 times for each time step – Runge Kutta iterations

Calculate Primary Variable – point wise Mesh loops within 5 different routines

Perform Derivative computation – High order differencing

Calculate Diffusion – 3 different routines with some derivative computation

Perform Derivative computation for forming rhs – lots of communication

Perform point-wise chemistry computation

All major loops are at low level of the Call tree Green – major computation – point-wise Yellow – major computation – Halos 5 zones thick

Restructured S3D for multi-core systems





Explicit: CUDA C/Fortran & OpenCL

- Programmer writes a kernel in C/Fortran that will be run on the GPU
 - This is essentially the loop body from original CPU code
- GPU memory must be explicitly allocated, freed, and filled from CPU memory over PCIe
 - Generally results in 2 variables referring to every pertinent array, one in each memory domain (hostA, devA)
- Programmer declares how to decompose into thread blocks and grid
 - Must understand limits of thread block size and how to maximize occupancy
- CPU code launches kernel on device.
 - May continue to work while GPU executes kernel(s)

CUDA C Example



CUDA Fortran Example



Implicit: Directives

- Programmer adds directives to existing CPU code
- Compiler determines
 - Memory management
 - Thread management
- Programmer adds directives to guide compiler
 - Higher-level data regions
 - Partial array updates
 - Improved thread blocking

Proposed OpenMP Directives Example



Implicit: Libraries

- Calls to existing Math libraries replaced with accelerated libraries
 - BLAS, LAPACK
 - FFT
 - Sparse kernels
- Unless application spends very high % of runtime in library calls, this will need to be combined with other methods

Libraries Example

info = cublas_set_matrix(Ida, na, sizeof_Z, a, Ida, devA, Ida)

info = cula_device_zgetrf(m,m,devA+idx2f(ioff+1,ioff+1,Ida)*sizeof_Z,Ida,devIPVT) info = cula_device_zgetrs('n',m,ioff,devA+idx2f(ioff+1,ioff+1,Ida)*sizeof_Z,Ida,devIPVT,

& devA+idx2f(ioff+1,1,lda)*sizeof_Z,lda)

call cublas_zgemm('n','n',n,ioff-k+1,na-ioff,cmone,devA+idx2f(joff+1,ioff+1,lda)*sizeof_Z,lda,

& devA+idx2f(ioff+1,k,lda)*sizeof_Z,lda,cone,devA+idx2f(joff+1,k,lda)*sizeof_Z,lda) call cublas_zgemm('n','n',blk_sz(1),blk_sz(1)-k+1,na-blk_sz(1),

& cmone,devA+idx2f(1,blk_sz(1)+1,lda)*sizeof_Z,lda,

& devA+idx2f(blk_sz(1)+1,k,lda)*sizeof_Z,lda,cone,devA,lda)

info = cublas_get_matrix(lda, na, sizeof_Z, devA, lda, a, lda)

info = cublas_get_matrix(lda, na, sizeof_Z, devA, lda, a, lda)

PERFORMANCE ANALYSIS

Section Goals

 Understand multiple options for gathering GPU performance metrics

- Increasing number of tools available, I'll cover
 3 methods
 - Explicit event instrumentation
 - CUDA Profiler
 - CrayPAT Preview

CUDA Event API

- Most CUDA API calls are asynchronous: explicit CPU timers won't work
- CUDA allows inserting events into the stream
 - Insert an event before and after what needs to be timed
 - Synchronize with events
 - Calculate time between events
- Introduces small driver overhead and may synchronize asynchronous calls
 - Don't use in production

CUDA Event Example



```
ierr = cudaEventRecord(st0,0)
allocate(d a(n))
ierr = cudaEventRecord(st1,0)
da = a
ierr = cudaEventRecord(st2,0)
call &
    scaleit kernel<<<grd,blk>>>&
    (d a, n)
ierr = cudaEventRecord(st3,0)
a = d a
ierr = cudaEventRecord(st4,0)
deallocate(d a)
ierr = cudaEventRecord(st5,0)
ierr = cudaEventSynchronize(st2)
ierr = cudaEventSynchronize(st3)
ierr = cudaEventElapsedTime &
       (et, st2, st3)
write(*,*) 'Kernel Time',et
```

CUDA Profiler

- Silently built-in to CUDA driver and enabled via environment variable
 - Works with both CUDA and Directives programs
- Returns time of memory copies and kernel launches by default
 - Also reports kernel occupancy
 - Can be configured to report many other metrics
- All metrics are recorded at driver level and high resolution
 - May add small kernel overhead and synchronize asynchronous operations.

CUDA Profiler Example

Enable Profiler

\$ export CUDA PROFILE=1

\$ aprun ./a.out

```
$ cat cuda_profile_0.log
```

```
# CUDA_PROFILE_LOG_VERSION 2.0
# CUDA_DEVICE 0 Tesla M2090
# TIMESTAMPFACTOR fffff6f3e9b1f6c0
method,gputime,cputime,occupancy
method=[ memcpyHtoD ] gputime=[ 2.304 ] cputime=[ 23.000 ]
method=[ _Z14scaleit_kernelPdi ] gputime=[ 4.096 ] cputime=[
        15.000 ] occupancy=[ 0.667 ]
method=[ memcpyDtoH ] gputime=[ 3.072 ] cputime=[ 34.000 ]
```

CUDA Profiler Example

```
# Customize Experiment
$ cat exp.txt
11 global load miss
11 global load hit
$ export CUDA PROFILE CONFIG=exp.txt
$ aprun ./a.out
$ cat cuda profile 0.log
# CUDA PROFILE LOG VERSION 2.0
# CUDA DEVICE 0 Tesla M2090
# TIMESTAMPFACTOR fffff6f4318519c8
method, gputime, cputime, occupancy, 11 global load miss, 11 global load hit
method=[ memcpyHtoD ] gputime=[ 2.240 ] cputime=[ 23.000 ]
method=[ Z14scaleit kernelPdi ] gputime=[ 4.000 ] cputime=[ 36.000 ]
   occupancy=[ 0.667 ] 11 global load miss=[ 63 ] 11_global_load_hit=[
   0 1
method=[ memcpyDtoH ] gputime=[ 3.008 ] cputime=[ 33.000 ]
```

method=[memcpyDtoH] gputime=[3.008] cputime=[33.000]

CrayPAT Prototype

- Luiz DeRose is giving a tutorial on CrayPAT future work at CUG (you're missing it right now)
- The goal of the CrayPAT team is to make instrumenting applications and understanding the results as simple as possible
 - No code modification
 - Derived metrics
 - Optimization suggestions

 Several new tools are being developed that will help with accelerator development

CrayPAT Preview: Performance Stats

21111	1.3% 2	21.836221	21.630958	6760.318	6	/60.318	3	3201	collisionb_
6	1.1%	18.888240	18.708450	0.000	(6507.596	1	1400	collisionb_(exclusive)
-									
7	0.4%	7.306387	7.291820	0.000	Т	0.000	Ι	200	collisionbASYNC_KERNEL@li.599
7	0.4%	7.158172	7.156827	0.000	Τ	0.000	Ι	200	collisionb .ASYNC KERNEL@li.568
7	0.2%	3.799065	3.799065	0.000	1	6507.596	1	200	collisionb .SYNC COPY@li.593
7	0.0%	0.527203	0.376397	0.000	1	0.000	Т	200	lbm3d2p d .ASYNC COPY@li.129
7	0.0%	0.073654	0.064766	0.000	1	0.000	1	200	collisionb .ASYNC COPY@li.703
7	0.0%	0.013917	0.011082	0.000	1	0.000	1	199	grad exchange .ASYNC COPY@li.428
7	0.0%	0.009707	0.008366	0.000	Т	0.000	T	200	collisionb .ASYNC KERNEL@li.581
711111	0.0%	0.000134	0.000127	0.000	Ť.	0.000	Ť.	1	collisionb .ASYNC COPY@li.566
6	0.2%	2.947981	2.922508	6760.318	Ĺ	252.722	i .	1801	grad exchange
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7 7 7	0.1% 0.0% 0.0% 0.0%	2.485119 0.107396 0.103009 0.065731	2.485119 0.107396 0.103009 0.065731	6507.596 0.000 126.361 0.000	 	0.000 126.361 0.000 126.361	 	200 200 200 200 200	<pre> collisionbSYNC_COPY@li.596 grad_exchangeSYNC_COPY@li.472 grad_exchangeSYNC_COPY@li.452 grad_exchangeSYNC_COPY@li.439</pre>
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This example is taken from a real user application and "ported" using proposed OpenMP extensions.

CrayPAT Preview: Data Transfer Stats

```
Host | Host Time | Acc Time | Acc Copy | Acc Copy | Calls | Group='ACCELERATOR'
Time % | | In (MB) | Out (MB) | PE
100.0% | 42.763019 | 42.720514 | 21877.192 | 20076.420 | 703 | Total
|------
| 100.0% | 42.763019 | 42.720514 | 21877.192 | 20076.420 | 703 | ACCELERATOR
||-----
5|||| 4.6% | 31.319188 | 31.318755 | 19425.659 | 19425.659 | 140 |recolor
|||||||
6||||| 4.5% | 30.661050 | 30.660616 | 18454.376 | 19425.659 | 139 | recolor (exclusive)
7||||| 2.4% | 16.761967 | 16.761967 | 0.000 | 19425.659 | 20 | recolor .SYNC COPY@li.790
7||||| 1.9% | 13.227889 | 13.227889 | 18454.376 | 0.000 | 19 |recolor .SYNC COPY@li.793
7||||| 0.1% 0.668515 0.668480 0.000 0.000 20 recolor .ASYNC KERNEL@li.781
   ||| 0.0% | 0.002122 | 0.002059 | 0.000 | 0.000 | 20 |lbm3d2p d .ASYNC COPY@li.118
   |||| 0.0% | 0.000332 | 0.000105 | 0.000 | 0.000 | 20 |recolor .ASYNC COPY@li.794
7||||| 0.0% 0.000116 0.000057 0.000 0.000 20 recolor .ASYNC COPY@li.789
7||||| 0.0% 0.000110 0.000060 0.000
                                    0.000 | 20 | recolor .ASYNC COPY@li.781
   6||||| 0.1% | 0.658138 | 0.658138 | 971.283 | 0.000 | 1 | streaming exchange
7||||| |
           | recolor .SYNC COPY@li.793
```

Full PCIe data transfer information without any code modifications.

Cray Tools: More Information

• Cray is developing a lot of tools that deserve more time than this tutorial allows, so...

- Go to "Cray GPU Programming Tools" BOF at 4:15 on Wednesday (Track 15B)
- Talk to Luiz DeRose and/or Heidi Poxon while you're here.

BASIC OPTIMIZATIONS

Basic Optimizations

OCCUPANCY

Calculating Occupancy

- Occupancy is the degree to which the hardware is saturated by your kernel
 - Generally higher occupancy results in higher performance
- Heavily affected by
 - Thread decomposition
 - Register usage
 - Shared memory use
- Nvidia provides an "occupancy calculator" spreadsheet as part of the SDK
 - Live example to follow

Calculating Occupancy

- 1. Get the register count
 ptxas info : Compiling entry function
 'laplace_sphere_wk_kernel3' for 'sm_20'
 ptxas info : Used 36 registers, 7808+0 bytes
 smem, 88 bytes cmem[0], 768 bytes cmem[2]
 2. Get the thread decomposition
 blockdim = dim3(4, 4, 26)
 griddim = dim3(101, 16, 1)
- 3. Enter into occupancy calculator

Result: 54%

Improving the Results



Reducing Registers/Thread



- Maximum number of registers/thread can be set via compiler flag
- Reducing the number of registers/thread to 18 increases occupancy to 81%
- Time Before: 924us
- Time After: 837us
- Improvement: ~10%
- Occupancy isn't a silver bullet

Occupancy Case Study

- Results from a Finite Difference Kernel, provided by Paulius Micikevicius of Nvidia
- Default compilation
 - 46 registers, no spills to Imem
 - runs a single 32x16 threadblock per SM concurrently
 - Occupancy: 33%
 - 3,395 MCells/s throughput (39.54ms)

Occupancy Case Study cont.

- Reducing Maximum Registers to 32
 - Set maximum register count via compiler flag
 - 32 registers, 44 bytes spilled to Imem
 - runs two 32x16 threadblocks per SM concurrently
 - Occupancy: 67%
 - 4,275 MCells/s (31.40ms)

• Improvement: ~26%

Basic Optimizations

ASYNCHRONICITY

Asynchronous Execution

 Most GPU Operations are Asynchronous from the CPU code

- Hint: The CPU can be busy doing other things

- Current Hardware can handle 1 Copy-in, 1 Kernel, and 1 Copy-out simultaneous, if in separate streams
 - Hint: Data transfer costs can be hidden by running multiple streams and asynchronous tranfers

Asynchronous Execution with Streams

• Synchronous Execution (1 Stream):



• If data cannot remain resident on device, streaming may allow GPU to offset transfer costs

Asynchronous Execution: Example

- Add some number of streams to existing code
- Use Asynchronous memory copies to copy part of data to/from device
 - GOTCHA: Host arrays must be "pinned" in order to use Async copies
- Add stream parameter to kernel launch
- Sync Time: 0.6987200
- Async Time: 0.2472000

```
integer :: streams(3)
integer :: ierr, j, mystream
do j=1,3
 ierr = cudaStreamCreate(streams(j))
enddo
do j=1,m
 mystream = mod(j,3)
 ierr = cudaMemcpyAsync&
    (d_a(:,j),a(:,j),size(a(:,j)),streams(mystream))
 call
     scaleit kernel<<<grd,blk,0,streams(mystrea
     m)>>>(d_a(:,j),n)
 ierr = cudaMemcpyAsync&
    (a(:,j),d_a(:,j),size(a(:,j)),streams(mystream))
enddo
ierr = cudaStreamSynchronize(streams(1))
ierr = cudaStreamSynchronize(streams(2))
ierr = cudaStreamSynchronize(streams(3))
```

ierr = cudaStreamSynchronize(streams(3))

Asynchronous Case Study

Euler Step Comparisons



CAVEAT: The above kernel over-emphasizes data transfer, thus necessitating streaming.

Basic Optimizations

SHARED MEMORY

Shared Memory

- Much like CPU cache, shared memory is much faster than global memory (up to 100X lower latency)
 - Staging Area
 - Scratch Pad
- 64KB Shared Memory sits on each SM
 - With Fermi, this is split between User-Manager and L1: 48/16 or 16/48
 - Split can be determined kernel to kernel
- If data is shared between threads in a thread block or reused well, staging it into shared memory may be beneficial
 - Think: Cache Prefetching

Simple Matrix Multiply

```
attributes (global) &
  subroutine mm1 kernel(C,A,B,N)
    integer, value, intent(in) :: N
    real(8), intent(in) ::
A(N,N), B(N,N)
    real(8), intent(inout) :: C(N,N)
    integer i,j,k
    real(8) :: val
    i = (blockIdx - 1) * blockDim x
+ threadIdx%x
    j = (blockIdx%y - 1) * blockDim%y
+ threadIdx%y
    val = C(i,j)
    do k=1,N
      val = val + A(i,k) * B(k,j)
    enddo
    C(i,j) = val
end
```

```
enddo
C(i,j) = val
end
```

ptxas info : Compiling entry
 function 'mm1_kernel' for
 'sm_20'
ptxas info : Used 22
 registers, 60 bytes cmem[0]

 No shared memory use, totally relies on hardware L1

Kernel	Time (ms)	Occupancy
Simple	269.0917	67%

Tiled Matrix Multiply

```
integer,parameter :: M = 32
real(8),shared :: AS(M,M),BS(M,M)
real(8) :: val
```

val = C(i,j)

```
do blk=1,N,M
AS(threadIdx%x,threadIdx%y) = &
A(blk+threadIdx%x-1,blk+threadIdx%y-1)
BS(threadIdx%x,threadIdx%y) = &
B(blk+threadIdx%x-1,blk+threadIdx%y-1)
call syncthreads()
```

```
call syncthreads()
enddo
C(i,j) = val
endif
```

ptxas info : Compiling entry
function 'mm2_kernel' for
'sm_20'

- ptxas info : Used 18 registers, 16384+0 bytes smem, 60 bytes cmem[0], 4 bytes cmem[16]
- Now uses 16K of shared memory

Kernel	Time (ms)	Occupancy
Simple	269.0917	67%
Tiled	213.7160	67%

```
enddo
C(i,j) = val
endif
```

What if we increase the occupancy?

- With 32x32 blocks, we'll never get above 67%
- Reduce block size from 32x32 to 16x16?

Kernel	Time (ms)	Occupancy
Simple (32x32)	269.0917	67%
Tiled (32x32)	213.7160	67%
Simple (16x16)	371.7050	83%
Tiled (16x16)	209.8233	83%

• Reduce Max Registers to 18?

Kernel	Time (ms)	Occupancy
Simple (16x16)	371.7050	83%
Tiled (16x16)	209.8233	83%
Simple (16x16) 18 registers	345.7340	100%
Tiled (16x16) 18 registers	212.2826	100%

• Turns out the 16 is even worse.

Basic Optimizations

MEMORY COALESCING

Coalescing Memory Accesses

- The GPU will try to load needed memory in as few memory transactions as possible.
 - 128 B if possible
 - If not, 2 X 64 B
 - If not, 64 B may be split to 32 B
 - Continue until every thread has needed data
- Coalescing is possible if:
 - 128B aligned
 - All threads access elements in same segment

Why is coalescing important?

- Issuing 1 128B transaction reduces memory latency and better utilizes memory bandwidth
- L1/Shared Memory cache lines are 128B
 Not using all fetched addresses wastes bandwidth
- Nvidia Guide: "Because of this possible performance degradation, memory coalescing is the most critical aspect of performance optimization of device memory."

Coalescing Examples

Simple, Stride-1:



Every thread accesses memory within same 128B-aligned memory segment, so the hardware will coalesce into 1 transaction.

Will This Coalesce?



Yes! Every thread is still accessing memory within a single 128B segment and segment is 128B aligned.



No. Although this is stride-1, it is misaligned, accessing 2 128B segments. 2 64B transactions will result.

Will This Coalesce?

Stride-2, half warp:



Yes, but..

- Half of the memory transaction is wasted.
- Poor utilization of the memory bus.

Striding

 Striding results in more memory transactions and wastes cache line entries

```
attributes(global)&
subroutine stride_kernel(datin,
datout, st)
integer,value :: st
real(8) :: datin(n), datout(n)
integer i

i = (blockIdx%x * blockDim%x ) &
+ (threadIdx%x * st)
datout(i) = datin(i)
end subroutine stride kernel
```

Striding: Relative Bandwidth



datout(i) = datin(i)
end subroutine stride kernel

Offsets (Not 128B-aligned)

 Memory offsets result in more memory transactions by crossing segment boundaries

```
attributes(global)&
subroutine offset_kernel(datin,
datout, st)
integer,value :: st
real(8) :: datin(n), datout(n)
integer i

i = (blockIdx%x * blockDim%x ) &
+ threadIdx%x + st
datout(i) = datin(i)
end subroutine offset_kernel
```

Offset: Relative Bandwidth



datout(i) = datin(i)
end subroutine offset kernel

ADDITIONAL RESOURCES

On The Web

- GTC 2010 Tutorials: <u>http://www.nvidia.com/object/gtc2010-</u> <u>presentation-archive.html</u>
- Nvidia CUDA online resources: <u>http://developer.nvidia.com/cuda-education-</u> <u>training</u>
- PGI CUDA Fortran: <u>http://www.pgroup.com/resources/cudafortra</u> <u>n.htm</u>