HIGH-PERFORMANCE COMPUTING WITH CUDA AND TESLA GPUS

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WHAT IS GPU COMPUTING?

What is GPU Computing?





Computing with CPU + GPU Heterogeneous Computing

Low Latency or High Throughput?



CPU

- Optimised for low-latency access to cached data sets
- Control logic for out-of-order and speculative execution



GPU

- Optimised for data-parallel, throughput computation
- Architecture tolerant of memory latency
- More transistors dedicated to computation



Fermi: The Computational GPU

Performance

Flexibility

- 13× Double Precision of CPUs
 IEEE 754-2008 SP & DP Floating Point
- Increased Shared Memory from 16 KB to 64 KB
- Added L1 and L2 Caches
- ECC on all Internal and External Memories
- Enable up to 1 TeraByte of GPU Memories
- High Speed GDDR5 Memory Interface
- Multiple Simultaneous Tasks on GPU
- 10× Faster Atomic Operations
- C++ Support
- System Calls, printf support





Usability

Streaming Multiprocessor Architecture

- 32 CUDA cores per SM (512 total)
- 2:1 ratio SP:DP floating-point performance
 - **Dual Thread Scheduler**
 - 64 KB of RAM for shared memory and L1 cache (configurable)





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Tesla C-Series Workstation GPUs



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CUDA ARCHITECTURE



CUDA Parallel Computing Architecture

- Parallel computing architecture and programming model
- Includes a CUDA C compiler, support for OpenCL and DirectCompute
- Architected to natively support multiple computational interfaces (standard languages and APIs)



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NVIDIA CUDA C and OpenCL







CUDA PROGRAMMING MODEL

Processing Flow





DRAM

3. Copy results from GPU memory to CPU memory

CUDA Kernels



Parallel portion of application: execute as a kernel

Entire GPU executes kernel, many threads

CUDA threads:

- Lightweight
- Fast switching
- 1000s execute simultaneously

CPU	Host	Executes functions
GPU	Device	Executes kernels

CUDA Kernels: Parallel Threads



- A kernel is an array of threads, executed in parallel
 - All threads execute the same code
 - Each thread has an ID Select input/output data Control decisions











Threads are grouped into blocks





Threads are grouped into blocks
Blocks are grouped into a grid





- Threads are grouped into blocks
- Blocks are grouped into a grid
- A kernel is executed as a grid of blocks of threads

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- Threads are grouped into blocks
- Blocks are grouped into a grid
- A kernel is executed as a grid of blocks of threads

Communication Within a Block



Threads may need to cooperate

- Memory accesses
- Share results

Cooperate using shared memory

Accessible by all threads within a block

Restriction to "within a block" permits scalability

Fast communication between N threads is not feasible when N large

Transparent Scalability – G84





Transparent Scalability – G80









Transparent Scalability – GT200







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CUDA Programming Model - Summary



A block is a batch of threads

Communicate through shared memory

Each block has a block ID

Each thread has a thread ID







MEMORY MODEL

- Thread:
 - Registers



- Thread:
 - Registers
 - Thread:

Private memory



- Thread:
 - Registers
- Thread:
 - Private memory
- Block of threads (work group):
 - Local memory



- Thread:
 - Registers
- Thread:
 - Private memory
- Block of threads (work group):
 - Local memory



- Thread:
 - Registers
 - Thread:

- Private memory
- Block of threads (work group):
 - Local memory
 - All blocks:
 - Global memory



- Thread:
 - Registers
 - Thread:

- Private memory
- Block of threads (work group):
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- All blocks:
 - Global memory





Memory Spaces



Memory	Location	Cached	Access	Scope	Lifetime
Register	On-chip	N/A	R/W	One thread	Thread
Local	Off-chip	No	R/W	One thread	Thread
Shared	On-chip	N/A	R/W	All threads in a block	Block
Global	Off-chip	No	R/W	All threads + host	Application
Constant	Off-chip	Yes	R	All threads + host	Application
Texture	Off-chip	Yes	R	All threads + host	Application



COMPILATION

Visual Studio

Separate file types

- .c/.cpp for host code
- .cu for device/mixed code

Compilation rules: cuda.rules

- Syntax highlighting
- Intellisense

Integrated debugger and profiler: Nsight



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Linux

Separate file types

- .c/.cpp for host code
- .cu for device/mixed code

Typically makefile driven

cuda-gdb, Allinea DDT, TotalView for debugging

CUDA Visual Profiler



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Compilation Commands



nvcc <filename>.cu [-o <executable>]

Builds release mode

nvcc -g <filename>.cu

- Builds debug (device) mode
- Can debug host code but not device code (runs on GPU)

nvcc –deviceemu <filename>.cu

- Builds device emulation mode
- All code runs on CPU, but no debug symbols

nvcc –deviceemu –g <filename>.cu

- Builds debug device emulation mode
- All code runs on CPU, with debug symbols
- Debug using gdb or other linux debugger
Exercise 0: Run a Simple Program



- Log on to test system
- Compile and run pre-written CUDA program — deviceQuery

CUPArDeyice Queive (SuppireiAglouversion (CUDART static linking) There are 2 devices supporting CUDA

Device 0: "Quadro FX 570M"	
₽₽₽₩ਫ਼₽o₽∶rë₹₽₽₽₽nChQhQër:	1
MURArCapapilitynMager:revision number:	1
fupalcanabality yippalrawasion number:	2 68107776 bytes
NonBeranountlefpglebslopsnory:	4 294705152 bytes
Number of multiprocessors:	32
Nomberanduserse:constant memory:	8∮936 bytes
Fotal amount of snastantemeryryer block:	15384 bytes
Total august of segisdersmay i pariblesk: block:	ۇ ∮§§4 bytes
Watalsnumber of registers available per block:	36 384
MaxPm&m ^z fumber of threads per block:	§22
Maximum sumbsropfethreadmensiohlofka block:	512 x 512 x 64
Maximum sizes of each dimension of a block:	64335 x 1855364x 1
Maximum memory of each dimension of a grid:	262344xb66835 x 1
Maximum menganenitch:	268164tbytes
Texture aelignment:	₿5 6 5bgĦgs
Constrfete:copy and execution:	⊉e∯4 GHz
Concurrent copy and execution:	Yes
TeBunp t ġmeDlimit on kernels:	No
Integrated:	No
Pr&yppentekoet page-locked memory mapping:	Yes
Compute mode:	Exclusive (only
one host thread at a time can use this device)	



CUDA C PROGRAMMING LANGUAGE

CUDA C — C with Runtime Extensions



Device management: cudaGetDeviceCount(), cudaGetDeviceProperties()

Device memory management: cudaMalloc(), cudaFree(), cudaMemcpy()

Texture management: cudaBindTexture(), cudaBindTextureToArray()

Graphics interoperability: cudaGLMapBufferObject(), cudaD3D9MapVertexBuffer()

CUDA C — C with Language Extensions



Function qualifiers

global	<pre>void MyKernel() {}</pre>	// call from host, execute on GP	U
device	<pre>float MyDeviceFunc() {}</pre>	// call from GPU, execute on GPU	
host	<pre>int HostFunc() {}</pre>	// call from host, execute on ho	st

Variable qualifiers

device	<pre>float MyGPUArray[32];</pre>	//	in GPU memory space
constant	<pre>float MyConstArray[32];</pre>	11	write by host; read by GPU
shared	<pre>float MySharedArray[32];</pre>	11	shared within thread block

Built-in vector types

int1, int2, int3, int4
float1, float2, float3, float4
double1, double2
etc.

CUDA C — C with Language Extensions



Execution configuration

dim3 dimGrid(100, 50); // 5000 thread blocks
dim3 dimBlock(4, 8, 8); // 256 threads per block
MyKernel <<< dimGrid, dimBlock >>> (...); // Launch kernel

Built-in variables and functions valid in device code:

dim3	gridDim;	//	Grid dimension
dim3	blockDim;	//	Block dimension
dim3	blockIdx;	11	Block index
dim3	threadIdx;	//	Thread index
void		11	Thread synchronization



SAXPY: Host Code



```
// Allocate two N-vectors h_x and h_y
int size = N * sizeof(float);
float* h_x = (float*)malloc(size);
float* h y = (float*)malloc(size);
```

// Initialize them...

// Allocate device memory
float* d_x; float* d_y;
cudaMalloc((void**)&d_x, size));
cudaMalloc((void**)&d_y, size));

```
// Copy host memory to device memory
cudaMemcpy(d_x, h_x, size, cudaMemcpyHostToDevice);
cudaMemcpy(d_y, h_y, size, cudaMemcpyHostToDevice);
```

```
// Invoke parallel SAXPY kernel with 256 threads/block
int nblocks = (N + 255) / 256;
saxpy_parallel<<<nblocks, 256>>>(N, 2.0, d_x, d_y);
```

```
// Copy result back from device memory to host memory
cudaMemcpy(h_y, d_y, size, cudaMemcpyDeviceToHost);
```

Exercise 1: Move Data between Host and GPU



- Start from the "cudaMallocAndMemcpy" template.
- Part 1: Allocate memory for pointers d_a and d_b on the device.
- Part 2: Copy h_a on the host to d_a on the device.
- Part 3: Do a device to device copy from d_a to d_b.
- Part 4: Copy d_b on the device back to h_a on the host.
- Part 5: Free d_a and d_b on the host.
- Bonus: Experiment with *cudaMallocHost* in place of *malloc* for allocating *h_a*.

Launching a Kernel



Call a kernel with

Func <<<Dg,Db,Ns,S>>> (params); dim3 Dg(mx,my,1); // grid spec dim3 Db(nx,ny,nz); // block spec size_t Ns; // shared memory cudaStream_t S; // CUDA stream

- Execution configuration is passed to kernel with built-in variables dim3 gridDim, blockDim, blockIdx, threadIdx;
- Extract components with threadIdx.x, threadIdx.y, threadIdx.z, etc.



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Exercise 2: Launching Kernels



- Start from the "myFirstKernel" template.
- Part1: Allocate device memory for the result of the kernel using pointer d_a.
- Part2: Configure and launch the kernel using a 1-D grid of 1-D thread blocks.
- Part3: Have each thread set an element of d_a as follows: idx = blockIdx.x*blockDim.x + threadIdx.x d_a[idx] = 1000*blockIdx.x + threadIdx.x
- Part4: Copy the result in *d_a* back to the host pointer *h_a*.
 Part5: Verify that the result is correct.

Exercise 3: Reverse Array, Single Block



- Given an input array $\{a_0, a_1, ..., a_{n-1}\}$ in pointer d_a , store the reversed array $\{a_{n-1}, a_{n-2}, ..., a_0\}$ in pointer d_b
- Start from the "reverseArray_singleblock" template
 - Only one thread block launched, to reverse an array of size N = numThreads = 256 elements
- Part 1 (of 1): All you have to do is implement the body of the kernel "reverseArrayBlock()"
 - Each thread moves a single element to reversed position
 - Read input from d_a pointer
 - Store output in reversed location in d_b pointer

Exercise 4: Reverse Array, Multi-Block



- Given an input array $\{a_0, a_1, ..., a_{n-1}\}$ in pointer d_a , store the reversed array $\{a_{n-1}, a_{n-2}, ..., a_0\}$ in pointer d_b
- Start from the "reverseArray_multiblock" template
 - Multiple 256-thread blocks launched
 - To reverse an array of size N, N/256 blocks
- Part 1: Compute the number of blocks to launch
- Part 2: Implement the kernel reverseArrayBlock()
- Note that now you must compute both
 - The reversed location within the block
 - The reversed offset to the start of the block



PERFORMANCE CONSIDERATIONS

Single-Instruction, Multiple-Thread Execution





- Warp: set of 32 parallel threads that execute together in single-instruction, multiple-thread mode (SIMT) on a streaming multiprocessor (SM)
- SM hardware implements zero-overhead warp and thread scheduling
- Threads can execute independently
- SIMT warp diverges and converges when threads branch independently
- Best efficiency and performance when threads of a warp execute together, so no penalty if all threads in a warp take same path of execution
- Each SM executes up to 1024 concurrent threads, as 32
 SIMT warps of 32 threads

Global Memory





Efficient Access to Global Memory



Single memory transaction (coalescing) for some memory addressing patterns



- Linear pattern
- Not all need participate
- Anywhere in block OK

Shared Memory





- More than 1 Tbyte/sec aggregate memory bandwidth
- Use it
 - As a cache
 - To reorganize global memory accesses into coalesced pattern
 - To share data between threads
 - 16 kbytes per SM

Shared Memory Bank Conflicts





- Successive 32-bit words assigned to different banks
- Simultaneous access to the same bank by threads in a halfwarp causes conflict and serializes access
- Linear access pattern
- Permutation
- Broadcast (from one address)
- Conflict, stride 8

Exercise 5: Optimize Reverse Array



Array reversal has a performance problem

Use the CUDA visual profiler to run the code

Take a note of GPU Time

Exercise 5: Optimize Reverse Array



\er

- Goal: Get rid of incoherent loads/stores and improve performance
 - Up and red for ory an verse er in a ck art 1: compute the num er of l /tes of har an One er int putt ead
 - F rt 2: i .pl mer .th ke nel
 - Comments should help
 - Don't forget to compute the correct block offset!
- **Part 3: Profile the working code**
 - Compare value of GLD/GST_INCOHERENT to previous
 - Compare GPU Time to previous

Reverse in Shared Memory





Matrix Transpose



- Access columns of a tile in shared memory to write contiguous data to global memory
- Requires _____syncthreads() since threads write data read by other threads
- Pad shared memory array to avoid bank conflicts



Matrix Transpose



There are further optimisations: see the New Matrix Transpose SDK example.



OTHER GPU MEMORIES

Texture Memory





- Texture is an object for reading data
- Data is cached
- Host actions
 - Allocate memory on GPU
 - Create a texture memory reference object
 - Bind the texture object to memory
 - Clean up after use
 - **GPU** actions
 - Fetch using texture references text1Dfetch(), tex1D(), tex2D(), tex3D()

Constant Memory





- Write by host, read by GPU
- Data is cached
- Useful for tables of constants



EXECUTION CONFIGURATION

Execution Configuration



vectorAdd <<< BLOCKS, THREADS_PER_BLOCK >>> (N, 2.0, d_x, d_y);

- How many blocks?
 - At least one block per SM to keep every SM occupied
 - At least two blocks per SM so something can run if block is waiting for a synchronization to complete
 - Many blocks for scalability to larger and future GPUs
- How many threads?
 - At least 192 threads per SM to hide read after write latency of 11 cycles (not necessarily in same block)
 - Use many threads to hide global memory latency
 - Too many threads exhausts registers and shared memory
 - Thread count a multiple of warp size
 - Typically, between 64 and 256 threads per block

Occupancy Calculator





 $occupancy = \frac{blocks \text{ per SM} \times threads \text{ per block}}{maximum threads \text{ per SM}}$

- Occupancy calculator shows trade-offs between thread count, register use, shared memory use
- Low occupancy is bad
- Increasing occupancy doesn't always help



DEBUGGING AND PROFILING

Debugging



 nvcc flags

 -debug (-g) Generate debug information for host code
 --device-debug <level> (-G <level>) Generate debug information for device code, plus also specify the optimisation level for the device code in order to control its 'debuggability'. Allowed values for this option: 0,1,2,3

 Debug with cuda-gdb a.out
 Usual gdb commands available

Debugging



Additional commands in cuda-gdb

- thread Display the current host and CUDA thread of focus.
- thread <<<(TX,TY,TZ)>>> Switch to the CUDA thread at specified coordinates
- thread <<<(BX,BY),(TX,TY,TZ)>>> Switch to the CUDA block and thread at specified coordinates
- info cuda threads Display a summary of all CUDA threads that are currently resident on the GPU
- info cuda threads all Display a list of each CUDA thread that is currently resident on the GPU
 - info cuda state Display information about the current CUDA state.
- next and step advance all threads in a warp, except at _syncthreads() where all warps continue to an implicit barrier following sync

Parallel Nsight 1.0

Nsight Parallel Debugger

GPU source code debugging Variable & memory inspection

Nsight Analyzer

Platform-level Analysis For the CPU and GPU Nsight Graphics Inspector

Visualize and debug graphics content



Allinea DDT



Blinea scale to new heights

GPU Debugging Making it easy Allinea DDT — CUDA Enabled

TotalView for CUDA





CUDA Visual Profiler



- cudaprof
- Documentation in \$CUDA/cudaprof/doc/cudaprof.html


CUDA Visual Profiler



- Open a new project
- Select session settings through dialogue
- **Execute CUDA program by clicking Start button**
- Various views of collected data available
- Results of different runs stored in sessions for easy comparison
- Project can be saved



MISCELLANEOUS TOPICS

Expensive Operations



- 32-bit multiply; ___mul24() and ___umul24() are fast 24-bit multiplies
- sin(), exp() etc.; faster, less accurate versions are ___sin(), ___exp() etc.
- Integer division and modulo; avoid if possible; replace with bit shift operations for powers of 2
- Branching where threads of warp take differing paths of control flow

Host to GPU Data Transfers



- PCI Express Gen2, 8 Gbytes/sec peak
- Use page-locked (pinned) memory for maximum bandwidth between GPU and host
- Data transfer host-GPU and GPU-host can overlap with computation both on host and GPU

Application Software (written in C)



CUDA Libraries			
cuFFT	cuBLAS	cuDf	р
CPU Hardware	CUDA Compiler		CUDA Tools
1U PCI-E Switch	C Fort	ran	Debugger Profiler



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On-line Course



- Programming Massively Parallel Processors, Wen-Mei Hwu, University of Illinois at Urbana-Champaign <u>http://courses.ece.illinois.edu/ece498/al/</u>
- PowerPoint slides, MP3 recordings of lectures, draft of textbook by Wen-Mei Hwu and David Kirk (NVIDIA)

GPU Programming Text Book



David Kirk (NVIDIA) Wen-mei Hwu (UIUC)

Chapter 1: Introduction Chapter 2: History of GPU Computing Chapter 3: Introduction to CUDA Chapter 4: CUDA Threads Chapter 5: CUDA Memories Chapter 6: Performance Considerations Chapter 7: Floating-Point Considerations Chapter 8: Application Case Study I - Advanced MRI Reconstruction Chapter 9: Application Case Study II – Molecular Visualization and Analysis **Chapter 10: Parallel Programming and Computational Thinking Chapter 11: A Brief Introduction to OpenCL Chapter 12: Conclusion and Future Outlook Appendix A: Matrix Multiplication Example Code** Appendix B: Speeds and feeds of current generation CUDA devices



CUDA Zone: www.nvidia.com/CUDA



- CUDA Toolkit
 - Compiler
 - Libraries
- CUDA SDK Code samples
- **CUDA** Profiler
- Forums
- Resources for CUDA developers

