GPU Architecture and CUDA Programming

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Logistics

Reading

GPU parallel program development using CUDA by Tolga Soyata

- Ch 6 start GPU Coverage
- ► UMN Library Link

A2 Out

- Take a quick tour
- Arriving soon: testing files for Problems 2/3 + optional Problem 4
- ▶ Note on SSH + MPI stalls

Poll on Final Exam

Will poll on Final Exam options over the next 5 days

- Option A: Mini-exam 4 (10%) + Final Exam (10%)
- Option B: Final Exam Last Day of class (20%)

Today

Continue GPU Discussions

GPUs will Feel Different

Distributed / Threaded Programming

- Most effective strategies looked for ways to assign lots of work to limited number of procs/threads
- $lackbox{ Poo-pooed the idea of "Assume length N array and N processors", too impractical$

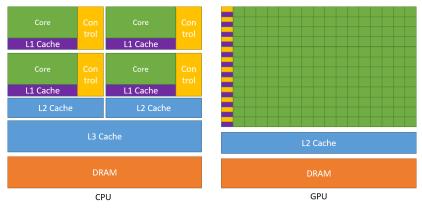
GPU Programming

- Threads are essentially cost-free, close to theoretical models so...
 - Assume length N array and N processors. It's actually practical and beneficial.
- Will require some mental adjustment

GPUs are a Co-Processor or Accelerator

- CPU is still in charge, has access to main memory
- GPU is a partner chip, has a distinct set of memory
- Sections of code will feel like Distributed architecture
 - ► CPU / GPU memory transfers
 - Barriers / synchronization as CPU waits for GPU to finish
- GPU itself is like a multicore system on steroids

CPU vs GPU



Source: NVidia Docs "CUDA C++ Programming Guide"

- GPU cores are simpler, slower, but there are TONs of them
- GPU has its own memory hierarchy: cache and DRAM
- Requires explicit transfers to/from CPU

5

Why do GPUs Look like this?

140 ■ GPU Parallel Program Development Using CUDA

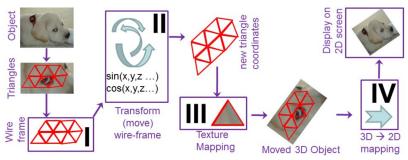


FIGURE 6.2 Steps to move triangulated 3D objects. Triangles contain two attributes: their *location* and their *texture*. Objects are moved by performing mathematical operations only on their coordinates. A final texture mapping places the texture back on the moved object coordinates, while a 3D-to-2D transformation allows the resulting image to be displayed on a regular 2D computer monitor.

Source: GPU parallel program development using CUDA by Tolga Soyata, 2018. (UMN Library Link)

CUDA: NVidia's General Purpose GPU Technology

- Games exploit GPU capabilities for parallelism via specialized graphics libraries like OpenGL
 - Oriented specifically towards graphics operations
 - Vendor like NVidia provides their OpenGL library which accelerates graphics processing
- Researchers wanted to exploit the massively parallel FP operations in GPUs to speed simulations (circa year 2000)
 - Started reverse engineering physics simulations to present them as Graphics problems
 - Achieved tremendous speedup but it was a pain to code
- NVidia recognized the new market for their chips, began exposing GPU capabilities for other applications: GPGPU is a General Purpose GPU
 - CUDA version 1 released 2007
 - Provides GPU capabilities through Threads
 - Provides a C/C++ code interface to run "kernel" functions on the GPU with many threads

CUDA Terminology

- Thread A set of operations; can be as small as a single addition; each thread has identifying information (index, # of other threads)
- Kernel A function which expresses what a thread should do.

 Many Threads execute the same Kernel code but can
 operate on different data based on their Thread
 index.
- Block A group of executing threads which can share some local memory
- Execution Context Parameters for a Kernel run indicating number of Blocks, Threads per Block, and amount of shared memory
 - Host The CPU, sets Execution Context, launches Kernels on GPU, waits for results.
 - Device The GPU which runs Kernels on tons of threads

Hello CUDA

```
// hello.cu: C code demonstrating basics of cuda
2
    #include <stdio.h>
3
4
    __global__ void hello_gpu() { // __global__ => called from CPU/GPU,
5
      printf("Block %02d Thread %02d: Hello World\n", // runs on GPU
6
7
             blockIdx.x, // ever-present structs which gives
             threadIdx.x); // each GPU thread indexing info
8
    }
9
10
    int main (int argc, char *argv[]){
11
12
      printf("CPU: Running 1 block w/ 16 threads\n");
      hello_gpu<<<1,16>>>(); // executes in 1 block, 16 threads per block
13
      cudaDeviceSynchronize();  // ensures GPU completes operations
14
15
      printf("\n");
16
17
      int nblocks = argc < 2 ? 3 : atoi(argv[1]); // default 3 blocks</pre>
18
      int nthreads = argc < 3 ? 4 : atoi(argv[2]); // default 4 threads/block</pre>
19
      printf("CPU: Running %d blocks w/ %d threads\n",
20
             nblocks, nthreads);
21
22
      hello_gpu<<<nblocks, nthreads>>>();
23
      cudaDeviceSynchronize();
24
25
      return 0:
    }
26
```

Compiling and Running Code

```
# log into the veggie cluster for access to an NVidia GPU
val [~]% ssh csel-broccoli.cselabs.umn.edu
# check for presence of nvidia hardware
csel-broccoli [~]% lspci | grep -i nvidia
3b:00.0 3D controller: NVIDIA Corporation TU104GL [Tesla T4] (rev a1)
csel-broccoli [~]% cd 14-gpu-cuda-code
# load CUDA tools on CSE Labs
csel-broccoli [14-gpu-cuda-code]% module load soft/cuda
# nvcc is the CUDA compiler - C++ syntax, gcc-like behavior
csel-broccoli [14-gpu-cuda-code]% nvcc hello.cu
# run with defaults
csel-broccoli [14-gpu-cuda-code]% ./a.out
CPU: Running 1 block w/ 16 threads
Block 00 Thread 00: Hello World
Block 00 Thread 01: Hello World
. . .
Block 00 Thread 15: Hello World
CPU: Running 3 blocks w/ 4 threads
Block 00 Thread 00: Hello World
Block 00 Thread 01: Hello World
Block 00 Thread 02: Hello World
Block 00 Thread 03: Hello World
Block 02 Thread 00: Hello World
. . .
```

Low-level Contents of CUDA Executables

```
>> module load soft/cuda
                               # load tools
>> nvcc hello.cu
                                  # ncompile code
>> file a.out
                                  # show file type of executable
a.out: ELF 64-bit LSB shared object, x86-64, version 1 (SYSV),
dynamically linked, interpreter /lib64/ld-linux-x86-64.so.2,
... for GNU/Linux 3.2.0, not stripped
>> readelf -S a.out | grep -i nv  # search for special ELF sections
  [17] .nv_fatbin
                   PROGRITS
                                        000000000007f4f0 0007f4f0
  [18] nv module id PROGBITS
                                        00000000000805c8 000805c8
  [29] .nvFatBinSegment PROGBITS
                                        000000000009e058 0009d058
```

- Compiled CUDA programs are ELF format executable
- Standard sections present like .text with host instructions (x86-64) and global data .data, .bss etc.
- Additional sections contain a nested ELF file with GPU code in PTX, the Assembly language used in NVidia GPUs

PTX: CUDA Assembly Language

- ▶ PTX: Parallel Thread Execution, VM instructions for the GPU
- Converted on the fly to GPU execution, can use inline PTX

```
# disassemble CUDA portion of exec
>> cuobjdump a.out -sass -ptx
                                    # show GPU PTX assembly instructions
Fatbin elf code:
_____
arch = sm 52
code version = [1,7]
producer = <unknown>
host = linux
compile size = 64bit
code for sm 52
       Function : _Z9hello_gpuv
.headerflags
               Q"EF CUDA SM52 EF CUDA PTX SM(EF CUDA SM52)"
                                                         /* 0x001c4400fe0007f6 */
/*0008*/
                           MOV R1. c[0x0][0x20]:
                                                         /* 0x4c98078000870001 */
/*0010*/
                           IADD32I R1, R1, -0x8;
                                                         /* 0x1c0ffffffff870101 */
/*0018*/
                           S2R R3. SR TID.X
                                                         /* 0xf0c8000002170003 */
                                                         /* 0x001fd000e22007f0 */
/*0028*/
                           MOV32I R4. 0x0 :
                                                         /* 0x010000000007f004 */
/*0030*/
                           S2R R2, SR CTAID.X
. . .
```

Link: cuobjdump Documentation

I'm Not Fat, I'm Just full of Code

CUDA Executable are "Fat" binaries - may contain multiple embedded ELF files to support several GPU versions

```
>> nvcc hello.cu
                               # compile with defaults
>> cuobjdump a.out -lelf
                               # list embedded ELF files
ELF file 1: a.1.sm 52.cubin
ELF file 2: a.2.sm 52.cubin
# compile with specific CUDA version support embedded
>> nvcc hello.cu -gencode arch=compute_52,code=sm_52 \
                -gencode arch=compute_70,code=sm_70
# list embedded ELF files pertaining to CUDA
>> cuobjdump a.out -lelf
ELF file 1: a.1.sm_52.cubin
ELF file 2: a.2.sm 70.cubin
ELF file 3: a.3.sm_52.cubin
ELF file 4: a.4.sm_70.cubin
```

Fat executables are not novel, have been used by Apple in transition periods every time they change their mind about processor architecture

CUDA is Advancing 1 / 2

CUDA is a **rapidly** advancing in technology with frequent changes.



Note the mention of **Compute Capability** which refers to the version of CUDA supported by GPU hardware; version reported via

- Utilities like nvidia-smi or
- Programmatically within CUDA (see device query example)

CUDA is Advancing 2 / 2

5.4.1. Arithmetic Instructions

Table 3 gives the throughputs of the arithmetic instructions that are natively supported in hardware for devices of various compute capabilities.

Table 3. Throughput of Native Arithmetic Instructions. (Number of Results per Clock Cycle per Multiprocessor)

	Compute Capability								
	3.5, 3.7	5.0, 5.2	5.3	6.0	6.1	6.2	7.x	8.0	8.6
16-bit floating- point add, multiply, multiply-add	N/A 256		256	128	2	256	128 256 ³		6 ³
32-bit floating- point add, multiply, multiply-add	192 128		28	64	128		64		128
64-bit floating- point add, multiply, multiply-add	64 ⁴	4		32	4		32 ⁵	32	2
32-bit floating- point reciprocal, reciprocal square root, base-2 logarithm (_log2f), base 2 exponential (exp2f), sine (_sinf), cosine (_cosf)	32			16	32		16		
32-bit integer add, extended- precision add, subtract, extended- precision subtract	160	128		64	128		64		
32-bit integer multiply, multiply-add, extended- precision multiply-add	32	2 Multiple instruct.					64 [©]		

Source: NVidia CUDA Toolkit Documentation, v11.5

Doing Work in CUDA

- 1. Transfer data from CPU (host) to GPU (device)
- 2. Launch Kernels to compute results on GPU in parallel
- 3. Transfer results from GPU (device) back to CPU (host)
- #2 above can be "looped"

vecadd_cuda.cu Demo

- Demonstrates transfer to/from GPU
- Simple kernel to do element-wise addition in an array

Device Memory Allocation / De-Allocation

```
// vecadd_cuda.cu
int main(){
    ...;
    // allocate device (GPU) memory
    float *dev_x, *dev_y, *dev_z;
    cudaMalloc((void**) &dev_x, length * sizeof(float));
    cudaMalloc((void**) &dev_y, length * sizeof(float));
    cudaMalloc((void**) &dev_z, length * sizeof(float));
    ...;
    // free device memory
    cudaFree(dev_x); cudaFree(dev_y); cudaFree(dev_z);
    ...
}
```

- Similar semantics to malloc() / free()
- cudaMalloc() returns int with success as CUDA_SUCCESS

Data Transfer Between Host / Device

```
// vecadd_cuda.cu
int main(){
    ...;
    // copy host memory to device
    cudaMemcpy(dev_x, host_x, length*sizeof(float), cudaMemcpyHostToDevice);
    cudaMemcpy(dev_y, host_y, length*sizeof(float), cudaMemcpyHostToDevice);
    ...;

// do some work here

// copy device memory to host
    cudaMemcpy(host_z, dev_z, length*sizeof(float), cudaMemcpyDeviceToHost);
    ...;
}
```

- Like distributed memory send / receive
- lacktriangle Copying memory GPU ightarrow CPU always blocks CPU
 - ► GPU / CPU work independently (asynchronously)
 - Memory transfer induces a sync point: CPU waits for launched kernels to complete, transfer of data
- ▶ It is possible to create memory maps between host/device to automate this, may discuss later

Kernel Launch

- ▶ Algorithm assumes 1 thread per array element
- ► Threads always launched in blocks w/ identical # of threads
- lacktriangle Must ensure enough blocks imes threads created to cover array
- ► May lead to "extra" threads : handle this in kernel

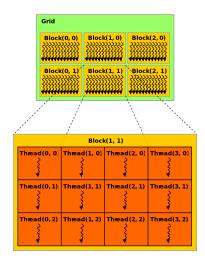
Kernel Code

- ► Each thread handles 1 addition
- Index calculated using variables threadIdx, blockDim; several pre-defined variables like this in CUDA

```
threadIdx.x // x-index of thread within block
blockDim.x // x-dim (width) of thread's block
blockIdx.x // x-index of thread's block within grid
gridDim.x // x-dim (width) of the thread's grid
// x/y/z fields available for all of these
```

Note conditional which excludes "excess" threads

Threads in Blocks in Grids



Source: Wikip "Threaded Block (CUDA)"

CUDA grouping is

- Thread (threadIdx) in Block (blockDim)
- Block (blockIdx) in Grid (gridDim)

Memory

- Threads in the same Block can Share local/fast Memory (cache)
- All threads can access Global GPU Memory

Likely we will only deal with Threads + Blocks as they are enough trouble

Repeated Kernel Invocation has Overhead 1 / 2

GPU threads perfectly capable of iteration, often better to launch a single Kernel that loops than repeatedly launching a kernel

```
// vecloop cuda.cu
// KERNEL: each thread performs one pair-wise addition
__global__ void vector_add(long length, float* x, float* y, float* z) {
 long idx = threadIdx.x + blockDim.x * blockIdx.x;
 if(idx < length){
   z[idx] = x[idx] + y[idx];
// KERNEL: each thread performs a loop of additions
global void vector loopadd(long iters, long length, float* x, float* y, float* z) {
  int idx = threadIdx.x + blockDim.x * blockIdx.x:
  if(idx < length){
   for(long i=0; i<iters; i++){</pre>
      z[idx] = x[idx] + v[idx]:
int main(int argc, char *argv[]){
  . . . :
  for(long i=0; i<iterations; i++){</pre>
    vector_add<<<nblocks, nthreads>>>(length, dev_x, dev_y, dev_z);
  . . . ;
  vector_loopadd<<<nblocks, nthreads>>>(iterations, length, dev_x, dev_y, dev_z);
```

Repeated Kernel Invocation has Overhead 2 / 2

Lesson: if computation allows for iteration, do so on GPU

Exercise: Array Summing

- Consider summing an array stored on the CPU
- Describe basic steps to do execute this on the GPU
- How is this problem different from the vector_add() version
- What makes it trickier?

Answers: Array Summing

- Same basic steps
 - Transfer data to GPU
 - Execute summing kernel
 - ► Transfer answer back to CPU
- Each thread has little work
- Primary work is a **Reduction** which requires synchronization between thread and blocks

Array Sum: Naive vs Synchronization

```
// arraysum_cuda.cu
// all threads hit the same global sum; no syncronization on global
// memory so results are not computed correctly
__global__ void array_sum_1(int length, float* data, float *sum)
 int i = threadIdx.x + blockDim.x * blockIdx.x;
 if(i < length){</pre>
   float myelem = data[i];
   *sum += mylelem;
                              // unsynced add to sum
// all threads hit the same global sum with atomic operations
__global__ void array_sum_2(int length, float* data, float *sum)
 int i = threadIdx.x + blockDim.x * blockIdx.x;
 if(i < length){
   float myelem = data[i];
   atomicAdd(sum, myelem); // safe add to sum
```

- array_sum_1() is incorrect due to race conditions
- array_sum_2() is correct but slow

CUDA Atomic Operations

- All threads can access GPU global memory but it is NOT synchronized
- CUDA Atomic Operations¹ like atomicAdd() are guaranteed to avoid race conditions between threads
- Variety of ops provided including arithmetic, bitwise ops, and compare + exchange operations

 $^{^{1} \}verb| https://docs.nvidia.com/cuda/cuda-c-programming-guide/index.html #atomic-functions| \\$

Speeding up Reductions

- ▶ NVIDIA has its own presentation² on fast reductions
- ► It's a tricky business as GPU is better at embarrassingly parallel execution and CUDA is tailored to this
- ► We will touch on a few aspects but to demonstrate different aspects CUDA techniques but won't strive for perfection

 $^{^{2}}_{\tt https://developer.download.nvidia.com/assets/cuda/files/reduction.pdf}$

Block Shared Memory

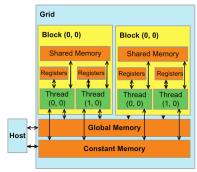


FIGURE 5.2

Overview of the CUDA device memory model.

Source: Programming Massively Parallel Processors by

Kirk and Hwu

CUDA allows explicit control over cache memory shared among threads in block via shared keyword

```
__global__ void some_kernel(...){
{
    __shared__ float blockvals[256];
    // stored in cache, all threads in
    // block can access the array
    ...;
```

By default must use compile-time constant sizes for shared arrays

Synchronizing Threads

- ▶ Blocks of Threads will not all run in parallel
- Usually a Warp of 32 threads is run together
- Means some threads in a block may execute before others
- Presents a problem for shared memory
- __syncthreads(); used as a Barrier for threads, guarantees all complete one set of operations

```
// example
__global__ void some_kernel(...){
 shared int blockvals[256]; // shared data in cache
 int tid = threadIdx.x;
 blockvals[tid] = tid;
                                // all threads assign to blockvals
 __syncthreads();
                                // barrier to ensure all threads assign
                                // to blockvals before proceeding to...
 if(tid < 256-2){
    int mvsum =
      blockvals[tid+0]+
                                // depends on blockvals[] being filled
      blockvals[tid+1]+
                                // by all threads
      blockvals[tid+2];
    . . . ;
```

Dynamically Allocating Shared Memory

When using shared memory, often want size dependent on number of threads

Statically Allocated

```
// static allocation of shared block
#define NTHREADS 64
__global__ void some_kern(...){
    __shared__ int blockvals[NTHREADS];
    ...
}
int main(...){

some_kern<<<nblocks, NTHREADS>>>(..);
    ...;
}
```

Can use static size for shared memory + pre-defined number of threads

Dynamically Allocated

```
// dynamic allocation of shared block
__global__ void some_kern(...){
    {
        extern __shared__ int blockvals[];
        ...
}
int main(...){
        int nthreads = ...;
        size_t shared_size = nthreads*sizeof(float);
        some_kern<<<nblocks, nthreads, shared_size>>>(..);
        ...;
}
```

Kernel Invocation can include size of shared memory, kernel declares with extern keyword

Exercise: Compare Kernels

30

```
global void array sum 3(int length, float* data, float *sum) {
      if(threadIdx.x == 0){
        float blocksum = 0.0;
        int idx = threadIdx.x + blockDim.x * blockIdx.x:
        for(int i=0: i < blockDim.x: i++){</pre>
          if(idx+i >= length){
6
            break:
                                                            Describe the differences
          blocksum += data[i+idx];
                                                            between these two kernels.
10
                                                            Predict which is speedier.
11
        atomicAdd(sum. blocksum):
     }
13
14
15
     global void array sum 4(int length, float* data, float *sum) {
16
      extern __shared__ float blockvals[];
17
      blockvals[threadIdx.x] = 0.0;
      int idx = threadIdx.x + blockDim.x * blockIdx.x;
18
      if(idx < length){
        blockvals[threadIdx.x] = data[idx];
      syncthreads();
      if(threadIdx.x == 0){
        float blocksum = 0.0:
25
        for(int i=0; i < blockDim.x; i++){</pre>
          blocksum += blockvals[i]:
        atomicAdd(sum, blocksum);
```

Answers: Compare Kernels

- array_sum_3() simply has Thread 0 sum some array elements in a local variable (register) and then atomicAdd() to the global sum
- array_sum_4() has all threads load elements into a shared
 array
- Leads to cached data
- MUST synchronize threads prior to moving ahead to ensure all elements loaded into the array
- ► Thread 0 then iterates through this array summing and doing a final atomicAdd()

SPEED

```
broccoli>> ./a.out 10000000 128 3
Kernel 3 nblocks 78125 nthreads 128 sum: 10000000.0 gpu_millis: 0.9872
broccoli>> ./a.out 10000000 128 4
Kernel 4 nblocks 78125 nthreads 128 sum: 10000000.0 gpu_millis: 0.6389 ***
```

Exercise: A True Reduction

```
// Perform a true multi-thread reduction using shared memory
     __global__ void array_sum_5(int length, float* data, float *sum)
 3
 4
       extern __shared__ float blockvals[];
       blockvals[threadIdx.x] = 0.0:
 5
 6
 7
       int idx = threadIdx.x + blockDim.x * blockIdx.x:
 8
       if(idx < length){
         blockvals[threadIdx.x] = data[idx];
9
10
11
       syncthreads();
12
                                      // WHY IS THIS NEEDED
                                      // WHAT DOES THIS LOOP DO
13
       for(int i=blockDim.x/2; i > 0; i \neq 2){
14
15
         int partner = threadIdx.x + i:
         if(threadIdx.x < i){
16
17
           blockvals[threadIdx.x] += blockvals[partner];
18
         __syncthreads();
19
                                      // WHY IS THIS NEEDED
20
21
       if(threadIdx.x == 0){
22
23
         atomicAdd(sum. blockvals[0]):
24
25
     }
```

Answers: A True Reduction

- First syncthreads() ensures all threads have populated their part of the block-shared array
- ► Loop performs reduction: each iteration has half remaining threads add on a partner value
- Number of active threads is reduced each time
- MUST __syncthreads() after each iteration to ensure adds complete
- Thread 0 ends with final sum and atomically adds

SPEED

See arraysum-timing.txt for all times

```
Kernel 3 nblocks 78125 nthreads 128 sum: 10000000.0 gpu_millis: 0.9872
Kernel 4 nblocks 78125 nthreads 128 sum: 10000000.0 gpu_millis: 0.6389 ***
Kernel 5 nblocks 78125 nthreads 128 sum: 10000000.0 gpu_millis: 0.8909
```

Well that was sort of a wasted effort...

Timing in arraysum_cuda.cu

- CUDA provides its own timing for GPU-specific events
- Standard clock() functions measure CPU while timeofday() funcs are in CPU which is running asynchronously from GPU
- Typical timing pattern is

cuBLAS for the Win

- Reduction is tricky to get right and at the point you want to do it, look around for a library
- CUDA provides the cuBLAS with predefined routines for many linear algebra operations (matrix multiply, matrix vector multiply, norms, etc.)
- Example in arraysum_cublas.cu

SPFFD

```
Kernel 3 nblocks 78125 nthreads 128 sum: 10000000.0 gpu_millis: 0.9872
Kernel 4 nblocks 78125 nthreads 128 sum: 10000000.0 gpu_millis: 0.6389 ***
Kernel 5 nblocks 78125 nthreads 128 sum: 10000000.0 gpu_millis: 0.8909
cudablasSdot sum: 10000000.0 gpu_millis: 0.2590 !!!
```

Somebody at NVidia knows their chip well. Stand on their shoulders.

Next Time

- Wrap up CUDA by discussing 2D and 3D indexing
- ▶ Possible further discussion of architecture and effects
- ▶ Possible discussion of sorting in CUDA