Nvidia G80 Architecture and CUDA Programming

CUDA Programming Model: A Highly Multithreaded Coprocessor

- The GPU is viewed as a compute device that:
  - Is a coprocessor to the CPU or host
  - Has its own DRAM (device memory)
  - Runs many threads in parallel
- Data-parallel portions of an application are executed on the device as kernels which run in parallel on many threads
- Differences between GPU and CPU threads
  - GPU threads are extremely lightweight
    - Very little creation overhead
  - GPU needs 1000s of threads for full efficiency
    - Multi-core CPU needs only a few

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Thread Batching: Grids and Blocks

- A kernel is executed as a grid of thread blocks
  - All threads share data memory space
- A thread block is a batch of threads that can cooperate with each other by:
  - Synchronizing their execution
    - For hazard-free shared memory accesses
  - Efficiently sharing data through a low latency shared memory
- Two threads from two different blocks cannot cooperate

Block and Thread IDs

- Threads and blocks have IDs
  - So each thread can decide what data to work on
  - Block ID: 1D or 2D
  - Thread ID: 1D, 2D, or 3D
- Simplifies memory addressing when processing multidimensional data
  - Image processing
  - Solving PDEs on volumes
  - …
CUDA Device Memory Space Overview

- Each thread can:
  - R/W per-thread registers
  - R/W per-thread local memory
  - R/W per-block shared memory
  - R/W per-grid global memory
  - Read only per-grid constant memory
  - Read only per-grid texture memory

- The host can R/W global, constant, and texture memories

Global, Constant, and Texture Memories (Long Latency Accesses)

- Global memory
  - Main means of communicating R/W Data between host and device
  - Contents visible to all threads

- Texture and Constant Memories
  - Constants initialized by host
  - Contents visible to all threads

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CUDA Processor Terminology

- **SPA**
  - Streaming Processor Array (variable across GeForce 8-series, 8 in GeForce8800)
- **TPC**
  - Texture Processor Cluster (2 SM + TEX)
- **SM**
  - Streaming Multiprocessor (8 SP)
  - Multi-threaded processor core
  - Fundamental processing unit for CUDA thread block
- **SP**
  - Streaming Processor
  - Scalar ALU for a single CUDA thread

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Streaming Multiprocessor (SM)

- Streaming Multiprocessor (SM)
  - 8 Streaming Processors (SP)
  - 2 Super Function Units (SFU)
- Multi-threaded instruction dispatch
  - 1 to 768 threads active
  - Shared instruction fetch per 32 threads
  - Cover latency of texture/memory loads
- 20+ GFLOPS
- 16 KB shared memory
- DRAM texture and memory access

G80 Thread Computing Pipeline

- The future of GPUs is programmable processing
- So build the architecture around the processor
Thread Life Cycle in HW

- Grid is launched on the SPA
- Thread Blocks are serially distributed to all the SM’s
  - Potentially >1 Thread Block per SM
- Each SM launches Warps of Threads
  - 2 levels of parallelism
- SM schedules and executes Warps that are ready to run
- As Warps and Thread Blocks complete, resources are freed
  - SPA can distribute more Thread Blocks

SM Executes Blocks

- Threads are assigned to SMs in Block granularity
  - Up to 8 Blocks to each SM as resource allows
  - SM in G80 can take up to 768 threads
    - Could be 256 (threads/block) * 3 blocks
    - Or 128 (threads/block) * 6 blocks, etc.
- Threads run concurrently
  - SM assigns/maintains thread id #s
  - SM manages/schedules thread execution
Thread Scheduling/Execution

- Each Thread Blocks is divided in 32-thread Warps
  - This is an implementation decision, not part of the CUDA programming model
- Warps are scheduling units in SM
- **Warps use the SIMD execution model**
- If 3 blocks are assigned to an SM and each Block has 256 threads, how many Warps are there in an SM?
  - Each Block is divided into 256/32 = 8 Warps
  - There are 8 * 3 = 24 Warps
  - At any point in time, only one of the 24 Warps will be selected for instruction fetch and execution.

SM Warp Scheduling

- SM hardware implements zero-overhead Warp scheduling
  - Warps whose next instruction has its operands ready for consumption are eligible for execution
  - Eligible Warps are selected for execution on a prioritized scheduling policy
  - All threads in a Warp execute the same instruction when selected
  - 4 clock cycles needed to dispatch the same instruction for all threads in a Warp in G80
    - If one global memory access is needed for every 4 instructions
    - A minimal of 13 Warps are needed to fully tolerate 200-cycle memory latency
A Simple Running Example
Matrix Multiplication

- A straightforward matrix multiplication example that illustrates the basic features of memory and thread management in CUDA programs
  - Leave shared memory usage until later
  - Local, register usage
  - Thread ID usage
  - Memory data transfer API between host and device

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An Example: Matrix Multiplication $P = M \times N$

- Simple code in C
  ```c
  void MatrixMulOnHost(const Matrix M, const Matrix N, Matrix P)
  {
    for (int i = 0; i < M.height; ++i)
      for (int j = 0; j < N.width; ++j) {
        double sum = 0;
        for (int k = 0; k < M.width; ++k) {
          double a = M.elements[i * M.width + k];
          double b = N.elements[k * N.width + j];
          sum += a * b;
        }
        P.elements[i * N.width + j] = sum;
      }
  }
  
  Optimizing the CPU code lays a solid foundation to optimize GPU code.
  ```

Data Structure
```
typedef struct {
  int width;
  int height;
  int pitch;
  float* elements;
} Matrix;
```

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Analyzing the matrix multiplication (CPU) code

• # of instructions to be executed
  – # of memory access instructions (i.e., loads) to be executed
    • 2 * M.height * N.Width * M.width
    • Loading each element in M for N.Width times
    • Loading each element in N for M.Height times
  – The ratio of computation over memory access instructions
    • For every two loads, one multiply and one add

• For CPU, cache locality (spatial and temporal) help to reduce the load latencies. For large M and N, temporal locality is low.

• Optimization?
  – Unroll and Jam.

CUDA Device Memory Allocation

• cudaMalloc()
  – Allocates object in the device Global Memory
  – Requires two parameters
    • Address of a pointer to the allocated object
    • Size of allocated object
• cudaFree()
  – Frees object from device Global Memory
  – Pointer to freed object

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CUDA Device Memory Allocation (cont.)

- Code example:
  - Allocate a 64 * 64 single precision float array
  - Attach the allocated storage to Md.elements
  - “d” is often used to indicate a device data structure

```c
BLOCK_SIZE = 64;
Matrix Md
int size = BLOCK_SIZE * BLOCK_SIZE * sizeof(float);

cudaMalloc((void**)&Md.elements, size);
cudaFree(Md.elements);
```

CUDA Host-Device Data Transfer

- cudaMemcpy()
  - memory data transfer
  - Requires four parameters
    - Pointer to source
    - Pointer to destination
    - Number of bytes copied
    - Type of transfer
      - Host to Host
      - Host to Device
      - Device to Host
      - Device to Device
  - Asynchronous in CUDA 1.0

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CUDA Host-Device Data Transfer (cont.)

- Code example:
  - Transfer a 64 * 64 single precision float array
  - M is in host memory and Md is in device memory
  - cudaMemcpyHostToDevice and cudaMemcpyDeviceToHost are symbolic constants

\[
\text{cudaMemcpy(Md.elements, M.elements, size, cudaMemcpyHostToDevice);}\\
\text{cudaMemcpy(M.elements, Md.elements, size, cudaMemcpyDeviceToHost);}
\]

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CUDA Function Declarations

<table>
<thead>
<tr>
<th>Function Declaration</th>
<th>Executed on the:</th>
<th>Only callable from the:</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>device</strong> float DeviceFunc()</td>
<td>device</td>
<td>device</td>
</tr>
<tr>
<td><strong>global</strong> void KernelFunc()</td>
<td>device</td>
<td>host</td>
</tr>
<tr>
<td><strong>host</strong> float HostFunc()</td>
<td>host</td>
<td>host</td>
</tr>
</tbody>
</table>

- __global__ defines a kernel function
  - Must return void
- __device__ and __host__ can be used together

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CUDA Function Declarations (cont.)

- `__device__` functions cannot have their address taken
- For functions executed on the device:
  - No recursion
  - No static variable declarations inside the function
  - No variable number of arguments

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Calling a Kernel Function – Thread Creation

- A kernel function must be called with an execution configuration:

```c
__global__ void KernelFunc(...);
dim3 DimGrid(100, 50);  // 5000 thread blocks
dim3 DimBlock(4, 8, 8);  // 256 threads per block
size_t SharedMemBytes = 64;  // 64 bytes of shared memory
KernelFunc<<< DimGrid, DimBlock, SharedMemBytes >>>(...);
```

- Any call to a kernel function is asynchronous from CUDA 1.0 on, explicit synch needed for blocking

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Programming Model: Parallelizing Matrix Multiplication

- \( P = M \times N \) of size \( WIDTH \times WIDTH \)
- Without tiling:
  - One thread handles one element of \( P \)
  - \( M \) and \( N \) are loaded \( WIDTH \) times from global memory

Step 1: Matrix Data Transfers

```c
// Allocate the device memory where we will copy \( M \) to Matrix Md;
Md.width = WIDTH;
Md.height = WIDTH;
Md.pitch = WIDTH;
int size = WIDTH * WIDTH * sizeof(float);
cudaMalloc((void**)&Md.elements, size);

// Copy \( M \) from the host to the device
cudaMemcpy(Md.elements, M.elements, size, cudaMemcpyHostToDevice);

// Read \( M \) from the device to the host into \( P \)
cudaMemcpy(P.elements, Md.elements, size, cudaMemcpyDeviceToHost);
...

// Free device memory
cudaFree(Md.elements);
```

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**Step 2: Matrix Multiplication**

A Simple Host Code in C

// Matrix multiplication on the (CPU) host in double precision
// for simplicity, we will assume that all dimensions are equal

```c
void MatrixMulOnHost(const Matrix M, const Matrix N, Matrix P) {
    for (int i = 0; i < M.height; ++i) {
        for (int j = 0; j < N.width; ++j) {
            double sum = 0;
            for (int k = 0; k < M.width; ++k) {
                double a = M.elements[i * M.width + k];
                double b = N.elements[k * N.width + j];
                sum += a * b;
            }
            P.elements[i * N.width + j] = sum;
        }
    }
}
```

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**Multiply Using One Thread Block**

- One Block of threads compute matrix P
  - Each thread computes one element of P
- Each thread
  - Loads a row of matrix M
  - Loads a column of matrix N
  - Perform one multiply and addition for each pair of M and N elements
  - Compute to off-chip memory access ratio close to 1:1 (not very high)

- Size of matrix limited by the number of threads allowed in a thread block

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Step 3: Matrix Multiplication Host-side Main Program Code

```c
int main(void) {
    // Allocate and initialize the matrices
    Matrix M = AllocateMatrix(WIDTH, WIDTH, 1);
    Matrix N = AllocateMatrix(WIDTH, WIDTH, 1);
    Matrix P = AllocateMatrix(WIDTH, WIDTH, 0);

    // M * N on the device
    MatrixMulOnDevice(M, N, P);

    // Free matrices
    FreeMatrix(M);
    FreeMatrix(N);
    FreeMatrix(P);
    return 0;
}
```

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Step 3: Matrix Multiplication
Host-side code

```c
// Matrix multiplication on the device
void MatrixMulOnDevice(const Matrix M, const Matrix N, Matrix P) {
    // Load M and N to the device
    Matrix Md = AllocateDeviceMatrix(M);
    CopyToDeviceMatrix(Md, M);
    Matrix Nd = AllocateDeviceMatrix(N);
    CopyToDeviceMatrix(Nd, N);

    // Allocate P on the device
    Matrix Pd = AllocateDeviceMatrix(P);
    CopyToDeviceMatrix(Pd, P); // Clear memory
}
```

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### Step 3: Matrix Multiplication

**Host-side Code (cont.)**

// Setup the execution configuration
dim3 dimBlock(WIDTH, WIDTH);
dim3 dimGrid(1, 1);

// Launch the device computation threads!
MatrixMulKernel<<dimGrid, dimBlock>>>(Md, Nd, Pd);

// Read P from the device
CopyFromDeviceMatrix(P, Pd);

// Free device matrices
FreeDeviceMatrix(Md);
FreeDeviceMatrix(Nd);
FreeDeviceMatrix(Pd);

---

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### Step 4: Matrix Multiplication

**Device-side Kernel Function**

// Matrix multiplication kernel – thread specification
__global__ void MatrixMulKernel(Matrix M, Matrix N, Matrix P)
{
    // 2D Thread ID
    int tx = threadIdx.x;
    int ty = threadIdx.y;

    // P value is used to store the element of the matrix
    // that is computed by the thread
    float Pvalue = 0;

    // ...
Step 4: Matrix Multiplication
Device-Side Kernel Function (cont.)

for (int k = 0; k < M.width; ++k)
{
    float Melement = M.elements[ty * M.pitch + k];
    float Nelement = Nd.elements[k * N.pitch + tx];
    Pvalue += Melement * Nelement;
}

// Write the matrix to device memory;
// each thread writes one element
P.elements[ty * P.pitch + tx] = Pvalue;

Step 5: Some Loose Ends

// Allocate a device matrix of same size as M.
Matrix AllocateDeviceMatrix(const Matrix M)
{
    Matrix Mdevice = M;
    int size = M.width * M.height * sizeof(float);
    cudaMalloc((void**)&Mdevice.elements, size);
    return Mdevice;
}

// Free a device matrix.
void FreeDeviceMatrix(Matrix M) {
    cudaFree(M.elements);
}

void FreeMatrix(Matrix M) {
    free(M.elements);
}

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**Step 5: Some Loose Ends (cont.)**

```c
// Copy a host matrix to a device matrix.
void CopyToDeviceMatrix(Matrix Mdevice, const Matrix Mhost) {
    int size = Mhost.width * Mhost.height * sizeof(float);
    cudaMemcpy(Mdevice.elements, Mhost.elements, size,
                cudaMemcpyHostToDevice);
}

// Copy a device matrix to a host matrix.
void CopyFromDeviceMatrix(Matrix Mhost, const Matrix Mdevice) {
    int size = Mdevice.width * Mdevice.height * sizeof(float);
    cudaMemcpy(Mhost.elements, Mdevice.elements, size,
                cudaMemcpyDeviceToHost);
}
```

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**Step 6: Handling Arbitrary Sized Square Matrices**

- Have each 2D thread block to compute a (BLOCK_WIDTH)^2 sub-matrix (tile) of the result matrix
  - Each has (BLOCK_WIDTH)^2 threads
- Generate a 2D Grid of (WIDTH/BLOCK_WIDTH)^2 blocks

You still need to put a loop around the kernel call for cases where WIDTH is greater than Max grid size!

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How about performance?

- All threads access global memory for their input matrix elements
  - Two memory accesses (8 bytes) per floating point multiply-add
  - 4B/s of memory bandwidth / GFLOPS
  - 86.4 GB/s limits the code at 21.6 GFLOPS
- The actual code should run at about 15 GFLOPS
- Need to drastically cut down memory accesses to get closer to the peak 346.5 GFLOPS

Developing High Performance Multithreaded Programs

- Can be very complex, application dependent

- General Guidelines
  - Improving Parallelism (thread level).
    - \#of thread blocks, \#of threads in a block
  - Optimizing memory usage to achieve high memory bandwidth
    - Memory-level parallelism
    - Memory coalescing
    - Reduce memory accesses
    - Improving the instruction throughput

- Those goals may conflict.
  - E.g., increase number of insns to get higher parallelism
  - Additional hardware constraints due to registers, memory sizes, etc.
Idea # 1: Use Shared Memory to reuse global memory data

- Each input element is read by WIDTH threads.
- If we load each element into Shared Memory and have several threads use the local version, we can drastically reduce the memory bandwidth
  - Tiled algorithms

Tiled Multiply Using Thread Blocks

- One block computes one square sub-matrix $P_{sub}$ of size BLOCK_SIZE
- One thread computes one element of $P_{sub}$
- Assume that the dimensions of $M$ and $N$ are multiples of BLOCK_SIZE and square shape
Shared Memory Usage

- Each SMP has 16KB shared memory
  - Each Thread Block uses $2 \times 256 \times 4B = 2KB$ of shared memory.
  - Can potentially have up to 8 Thread Blocks actively executing
  - For $\text{BLOCK\_SIZE} = 16$, this allows up to $8 \times 512 = 4,096$ pending loads
    - In practice, there will probably be up to half of this due to scheduling to make use of SPs.
  - The next $\text{BLOCK\_SIZE} = 32$ would lead to $2 \times 32 \times 32 \times 4B = 8KB$ shared memory usage per Thread Block, allowing only up to two Thread Blocks active at the same time

First-order Size Considerations

- Each Thread Block should have a minimal of 192 threads
  - $\text{BLOCK\_SIZE}$ of 16 gives $16 \times 16 = 256$ threads

- A minimal of 32 Thread Blocks
  - A 1024$^2$ P Matrix gives $64 \times 64 = 4096$ Thread Blocks

- Each thread block perform $2 \times 256 = 512$ float loads from global memory for $256 \times (2 \times 16) = 8,192$ mul/add operations.
  - Memory bandwidth no longer a limiting factor
CUDA Code – Kernel Execution Configuration

// Setup the execution configuration
dim3 dimBlock(BLOCK_SIZE, BLOCK_SIZE);
dim3 dimGrid(N.width / dimBlock.x,
            M.height / dimBlock.y);

For very large N and M dimensions, one will need to add another level of blocking and execute the second-level blocks sequentially.

CUDA Code – Kernel Overview

// Block index
int bx = blockIdx.x;
int by = blockIdx.y;

// Thread index
int tx = threadIdx.x;
int ty = threadIdx.y;

// Pvalue stores the element of the block sub-matrix that is computed by the thread
float Pvalue = 0;

// Loop over all the sub-matrices of M and N required to compute the block sub-matrix
for (int m = 0; m < M.width/BLOCK_SIZE; ++m) {
    code from the next few slides
}
Multiply Using Several Blocks

- One block computes one square sub-matrix $P_{sub}$ of size $BLOCK_SIZE$
- One thread computes one element of $P_{sub}$
- Assume that the dimensions of $M$ and $N$ are multiples of $BLOCK_SIZE$ and square shape

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CUDA Code - Load Data to Shared Memory

```c
// Get a pointer to the current sub-matrix $M_{sub}$ of $M$
Matrix $M_{sub} = GetSubMatrix(M, m, by);$

// Get a pointer to the current sub-matrix $N_{sub}$ of $N$
Matrix $N_{sub} = GetSubMatrix(N, bx, m);$

__shared__ float $Ms[BLOCK_SIZE][BLOCK_SIZE]$;
__shared__ float $Ns[BLOCK_SIZE][BLOCK_SIZE]$;

// each thread loads one element of the sub-matrix
Ms[ty][tx] = GetMatrixElement($M_{sub}$, tx, ty);

// each thread loads one element of the sub-matrix
Ns[ty][tx] = GetMatrixElement($N_{sub}$, tx, ty);
```

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Multiply Using Several Blocks

- One block computes one square sub-matrix $P_{sub}$ of size BLOCK_SIZE
- One thread computes one element of $P_{sub}$
- Assume that the dimensions of M and N are multiples of BLOCK_SIZE

CUDA Code - Compute Result

```c
// Synchronize to make sure the sub-matrices are loaded
// before starting the computation
__syncthreads();

// each thread computes one element of the block sub-matrix
for (int k = 0; k < BLOCK_SIZE; ++k)
    Pvalue += Ms[ty][k] * Ns[k][tx];

// Synchronize to make sure that the preceding
// computation is done before loading two new
// sub-matrices of M and N in the next iteration
__syncthreads();
```

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Shared Memory Bank Conflicts

- Threads in the same Warp may have bank conflict for Nsub accesses
  - This should be minimal since the warp likely spans the horizontal direction, resulting in broadcast of Msub accesses and no/little conflict for N accesses

CUDA Code - Save Result

```c
// Get a pointer to the block sub-matrix of P
Matrix Psub = GetSubMatrix(P, bx, by);

// Write the block sub-matrix to device memory;
// each thread writes one element
SetMatrixElement(Psub, tx, ty, Pvalue);
```

This code should run at about 45 GFLOPS
Idea # 2: Use unrolling & jam to reuse global memory data

- Each thread processes more than 1 element in P
- Multiple elements end with reusing the global memory data
- Which loop to unroll?
  - Which one does the CPU code favor?
  - Which one does the GPU code favor?
    - Can we take advantage of the cache for const memory?

---

Kernel Code for Unroll and Jam (with a unroll factor of 2 in outer loop)

```c
void MatrixMulOnHost(const Matrix M, const Matrix N, Matrix P) {
    for (int i = 0; i < M.height; i += 2)
        for (int j = 0; j < N.width; ++j) {
            double sum1 = 0;
            double sum2 = 0;
            for (int k = 0; k < M.width; ++k) {
                double a1 = M.elements[i * M.width + k];
                double b = N.elements[k * N.width + j];
                double a2 = M.elements[(i + 1)* M.width + k];
                sum1 += a1 * b;
                sum2 += a2 * b;
            }
            P.elements[i * N.width + j] = sum1;
            P.elements[(i+1) * N.width + j] = sum2;
        }
}
```

---
Kernel Code for Unroll and Jam (with a unroll factor of 2 in inner loop)

```c
void MatrixMulOnHost(const Matrix M, const Matrix N, Matrix P)
{
    for (int i = 0; i < M.height; ++i)
        for (int j = 0; j < N.width; j+=2) {
            double sum1 = 0;
            double sum2 = 0;
            for (int k = 0; k < M.width; ++k) {
                double a = M.elements[i * M.width + k];
                double b1 = N.elements[k * N.width + j];
                double b2 = N.elements[k * N.width + j +1];
                sum1 += a * b1;
                sum2 += a * b2;
            }
            P.elements[i * N.width + j] = sum1;
            P.elements[i * N.width + j + 1] = sum2;
        }
}
```

Tradeoff

- Reduced loads
- High register usage (saving those in shared memory?)
- Reduced parallelism (i.e., number of thread blocks)