

University of Zurich^{UZH}

High Performance Computing Lecture 13

Douglas Potter

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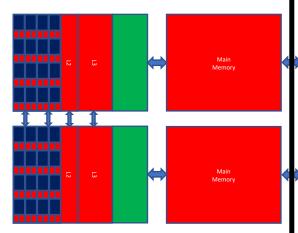
Noah Kubli





- CUDA Architecture
 - Exposes the GPU parallelism for general-purpose computing
 - Retains performance
- CUDA C/C++
 - Based on C/C++
 - Small set of GPU specific extensions
 - API to manage devices, memory, etc.

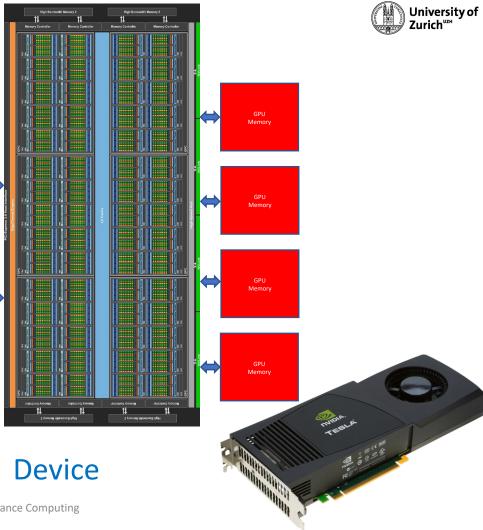
Terminology



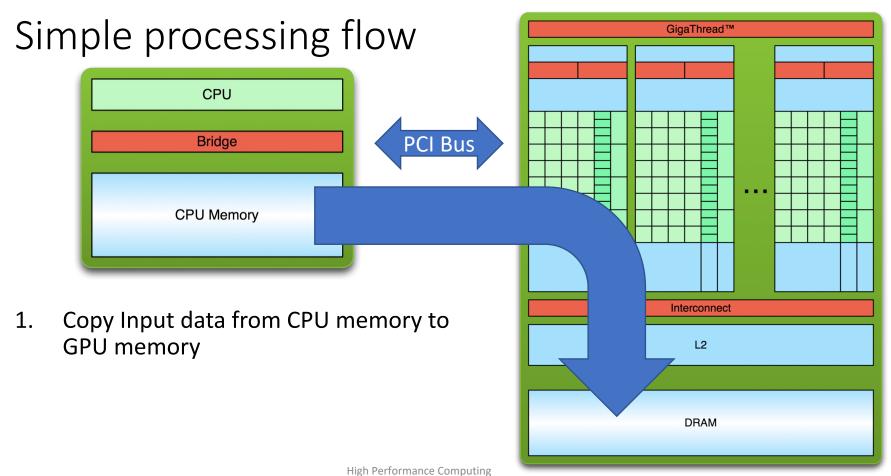




High Performance Computing







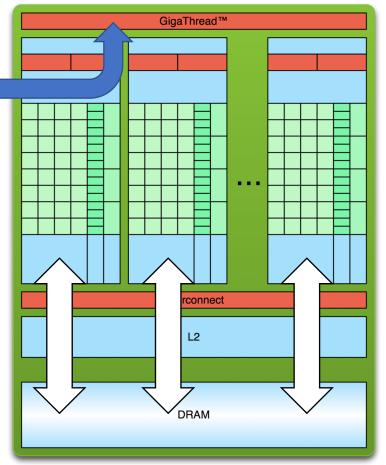


Simple processing flow

CPU PCI Bus

CPU Memory

- 1. Copy Input data from CPU memory to GPU memory
- 2. Load the GPU program and execute it, caching data on chip for performance





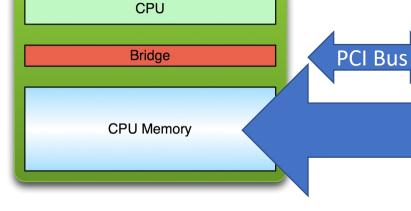
GigaThread™

Interconnect

L2

DRAM





- 1. Copy Input data from CPU memory to GPU memory
- 2. Load the GPU program and execute it, caching data on chip for performance
- 3. Copy the result back to CPU memory

High Performance Computing



Hello World!

```
int main(void) {

    File extension is ".cu"

  printf("Hello world!\n");

    Standard C/C++ code that is run

                                       on the host
  return 0;

    Can compile C/C++ programs

                                       without any device code
 nvcc hello world.cu
$ ./a.out
Hello world!
                                                Compile
                                  Run
                              High Performance Computing
```



Hello world! with device code

```
global void
mykernel(void) {
int main(void) {
  mykernel <<<1,1>>>();
  printf("Hello World!\n");
  return 0:
```

- Two new syntactical elements
- The <u>global</u> keyword is used to indicate that a fuction runs on the **device** and is called from the **host**.
- The nVidia compiler (nvcc) separates host and device code.
 - The device code is processed by the nVidia compiler.
 - The **host** code is passed to **gcc**.



Hello world! with device code

```
global void
mykernel(void) {
int main(void) {
  mykernel <<<1, 1>>>();
  printf("Hello World!\n");
  return 0:
```

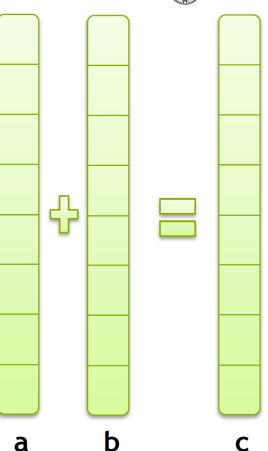
- The triple angle brackets "<<<"
 and ">>>" mark a call from host
 code to device code.
 - Called a "kernel launch"
 - The numbers inside correspond to the number of blocks and threads per block
- This will execute the function "mykernel" on the GPU!
- It doesn't do much yet...



Parallel programming with CUDA

- GPU Programming is about massive parallelism
- Let's start by adding two numbers on the GPU
- Later, we will modify this to add two vectors

This starts to get more complicated





Addition on the device

We copy data to the GPU memory so that's where we will find it!

```
__global__ void add(int *a, int *b, int *c) {
    *c = *a + *b;
}
```

- The __global__ keyword means that the "add" function will be run on the **device** and called from the **host**.
- The kernel "add" will compute: c = a + b
- The variables "a", "b" and "c" are pointers to integers on the device.
 - Of course we have to manage this memory ourselves!



Memory Management

- Host and Device memory are separate entities
 - **Device** pointers point to <u>GPU memory</u>
 - May be passed between **host** functions
 - May NOT be dereferenced in host functions
 - Host pointers point to <u>CPU memory</u>
 - May be passed to/from device code (but why?)
 - May **NOT** be dereferenced in **device** code.
- We will use the CUDA API to manage device memory
 - cudaMalloc(), cudaFree(), cudaMemcpy()
 - Similar to the C functions: malloc(), free(), memcpy()



Back to main() – allocating GPU memory

```
int main(void) {
    int a, b, c; // host copies of a, b, c
   int *a d, *b d, *c d; // device copies
    int size = sizeof(int);
    // Allocate device copies of a, b, c
    cudaMalloc((void **)&a d, size);
    cudaMalloc((void **)&b d, size);
    cudaMalloc((void **)&c d, size);
    // Setup input values
   a = 2;
   b = 7:
```

- We have a copy of the data on the host
 - The variables "a", "b" and "c"
- We need to allocate space on the device
 - The pointers "a_d", "b_d", "c_d"
 - These will point to memory on the device
- We need "size" bytes (one integer)
- Calling cudaMalloc will allocate device memory
 - Allocates "size" bytes
 - Returns the address on the device
 - cudaMalloc is "slow" normall used at startup
- Memory is allocate, but we still need to transfer!



Back to main() – data transfer and kernel

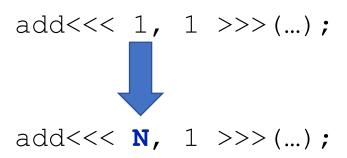
```
// Copy inputs to device
cudaMemcpy(a d,&a,size,cudaMemcpyHostToDevice);
cudaMemcpy(b d,&b,size,cudaMemcpyHostToDevice);
// Launch add() kernel on GPU
add <<<1,1>>> (a d, b d, c d);
// Copy result back to host
cudaMemcpy(&c,c d,size,cudaMemcpyDeviceToHost);
// Print the result
printf("c = %d\n",c);
// Cleanup
cudaFree(a d); cudaFree(b d); cudaFree(c d);
return 0;
```

- We first copy "a" and "b" to the **device**
 - · cudaMemcpy() does this
 - Need to specify the source and destination addresses
 - Also need a direction: HostToDevice
- Now we launch the kernel on the device
- And copy the result "c" back to the host
 - Again with cudaMemcpy()
 - Direction is: DeviceToHost
- Whew! Lots of work to add two numbers!
- Next let's switch to parallel



Parallel "add" kernel

- GPU computing is all about massive parallelism
- To run in parallel we just change the kernel launch parameters



• Instead of executing add() once, it now executes "N" times in parallel



Back to main() – Memory for "N" integers

```
#define N 512
int main(void) {
  int *a, *b, *c; // host copies of a, b, c
  int *a d, *b d, *c d; // device copies
  int size = N * size of (int);
  // Allocate device copies of a, b, c
  cudaMalloc((void **)&a d, size);
  cudaMalloc((void **)&b d, size);
  cudaMalloc((void **)&c d, size);
  // Allocate host copies of a, b, c
  a = (int *)malloc(size); random ints(a, N);
  b = (int *)malloc(size); random ints(b, N);
  c = (int *)malloc(size);
```

- We have a copy of the data on the host
 - The variables "a", "b" and "c"
 - These are now pointers to an array
- · We need to allocate space on the device
 - The pointers "a_d", "b_d", "c_d"
 - · These will point to memory on the device
- We need "size" bytes (N integers)
- Calling cudaMalloc will allocate device memory
 - Allocates "size" bytes
 - · Returns the address on the device
 - cudaMalloc is "slow" normall used at startup



Back to main() – data transfer and kernel

```
// Copy inputs to device
cudaMemcpy(a d,a,size,cudaMemcpyHostToDevice);
cudaMemcpy(b d,b,size,cudaMemcpyHostToDevice);
// Launch add() kernel on GPU
add <<< N, 1>>> (a d, b d, c d);
// Copy result back to host
cudaMemcpy(c,c d,size,cudaMemcpyDeviceToHost);
// Cleanup
free(a); free(b); free(c);
cudaFree(a d); cudaFree(b d); cudaFree(c d);
return 0;
```

- We first copy "a" and "b" to the **device**
 - · cudaMemcpy() does this
 - Need to specify the source and destination addresses
 - Also need a direction: HostToDevice
- Now we launch the kernel on the device
- And copy the result "c" back to the host
 - Again with cudaMemcpy()
 - Direction is: DeviceToHost
- This time we launched "N" threads to process the data in parallel.
- How does the "kernel" change?



Vector addition on the device

We requested that 512 blocks be run on the device

```
#define N 512
add<<<N,1>>>(a_d, b_d, c_d);
```

- Terminology: A set of blocks is called a grid.
- Blocks are numbered sequentially from zero, e.g., 0 to 511
- Each thread can use blockIdx.x to get its block number

```
__global__ void add(int *a, int *b, int *c) {
  c[blockIdx.x] = a[blockIdx.x] + b[blockIdx.x];
}
```

• Using blockIdx.x to index into the array, each block handles a different index.



Vector addition on the device

```
__global__ void add(int *a, int *b, int *c) {
  c[blockIdx.x] = a[blockIdx.x] + b[blockIdx.x];
}
```

• On the device, each block can be executed in parallel

Block 0	Block 1	Block 2	Block 3		
c[0] = a[0] + b[0]	c[1] = a[1] + b[1]	c[2] = a[2] + b[2]	c[3] = a[3] + b[3]		



Summary so far

- Host versus Device
 - Host CPU
 - Device GPU
- Use <u>__global__</u> to declare a function as <u>device</u> code
 - Executes on the device
 - Called from the host
- Passing parameters from host code to a device function.

- Device memory management
 - cudaMalloc()
 - cudaFree()
 - cudaMemcpy()
- Launching parallel kernels
 - Launch N blocks of add() with

Use blockIdx.x for the block index



CUDA Threads

- Terminology: A **block** can be split into parallel **threads**.
- Here is add() using parallel threads instead of blocks

```
__global__ void add(int *a, int *b, int *c) {
  c[threadIdx.x] = a[threadIdx.x] + b[threadIdx.x];
}
```

- We use threadIdx.x instead of blockIdx.x
- We need to make one change to the kernel launch...



Parallel "add" kernel with "N" threads

 Now we run with 1 thread block with N threads instead of N thread blocks with 1 thread each.

```
add<<< N, 1 >>> (...);

add<<< 1, N >>> (...);
```



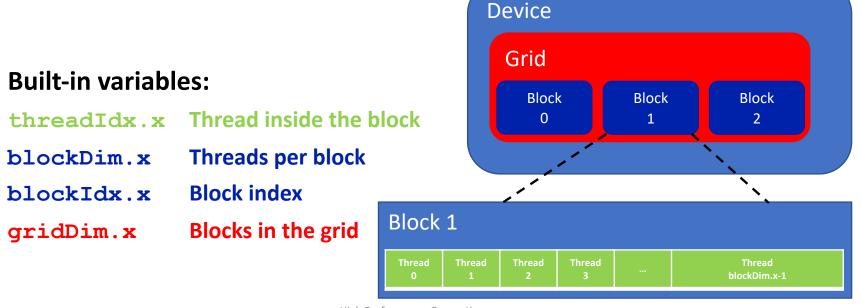
Combining Blocks and Threads

- We've seen parallel vector addition using:
 - Many blocks with one thread each add<<<N, 1>>>
 - One block with many threads
 add<<<1, N>>>
- For optimal performance we need to use both at the same time
 - Threads and blocks have a "hardware" interpretation (more later)
 - Only by using both can you achieve full performance
 - There are hardware limitations that come into play
- Our simple thread indexing (blockldx.x or threadIdx.x) gets complicated
 - We need to use both at the same time.
 - Let's see how...



Indexing

A kernel is launched as a grid of blocks of threads

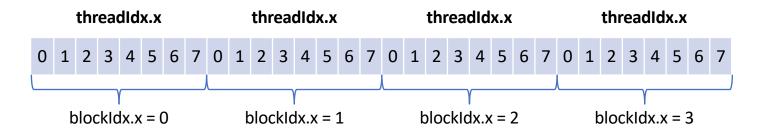


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Indexing arrays

- We can no longer use just blockldx.x or threadldx.x
- Consider 4 blocks with 8 threads per block

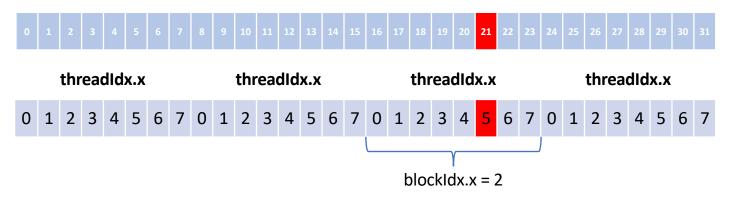


Here gridDim.x == 4 (4 blocks) and blockDim.x == 8 (8 threads), so int index = threadIdx.x + blockIdx.x * blockDim.x



Indexing arrays: Example

Which thread will operate on the red element?



```
int index = threadIdx.x + blockIdx.x * blockDim.x;
= 5 + 2 * 8;
= 21;
```



Vector addition with both threads and blocks

- Here our add() kernel uses both parallel threads and blocks
- We use the formula we just discussed

```
__global___ void add(int *a, int *b, int *c) {
  int index = threadIdx.x + blockIdx.x * blockDim.x;
  c[index] = a[index] + b[index];
}
```

- We use threadIdx.x, blockIdx.x, and blockDim.x
- We need to adjust our main() program again...



Back to main() – Blocks and Threads

```
#define N (2048*2048)
#define BLOCKSIZE 512
int main(void) {
 int *a, *b, *c; // host copies of a, b, c
 int *a d, *b d, *c d; // device copies
 int size = N * sizeof(int);
 // Allocate device copies of a, b, c
  cudaMalloc((void **)&a d, size);
  cudaMalloc((void **)&b d, size);
  cudaMalloc((void **)&c d, size);
 // Allocate host copies of a, b, c
  a = (int *)malloc(size); random ints(a, N);
 b = (int *)malloc(size); random ints(b, N);
  c = (int *)malloc(size);
```

- Increase the total array length
 - N is now $2048^2 = 4'194'304$
- The block size is 512
 - This is the number of threads per block
- How many blocks do we need?
 - N / BLOCKSIZE
 - 8'192



Back to main() – Blocks and Threads

```
// Copy inputs to device
cudaMemcpy(a d,a,size,cudaMemcpyHostToDevice);
cudaMemcpy(b d,b,size,cudaMemcpyHostToDevice);
// Launch add() kernel on GPU
add<<<N/BLOCKSIZE, BLOCKSIZE>>> (a d, b d, c d);
// Copy result back to host
cudaMemcpy(c,c_d,size,cudaMemcpyDeviceToHost);
// Cleanup
free(a); free(b); free(c);
cudaFree(a d); cudaFree(b d); cudaFree(c d);
return 0;
```



How to handle arbitrary vector sizes

- The previous example works if "N" is an exact multiple of BLOCKSIZE
 - What happens if N = 560?
- Change the kernel to avoid accessing beyond the end of the array

```
__global___ void add(int *a, int *b, int *c, int n) {
  int index = threadIdx.x + blockIdx.x * blockDim.x;
  if (index < n) c[index] = a[index] + b[index];
}</pre>
```

• Update the kernel launch – $[N \div BLOCKSIZE]$ (ceiling)

```
add<<<(N+BLOCKSIZE-1)/BLOCKSIZE, BLOCKSIZE>>>(a d, b d, c d, N);
```



Why bother with Threads and Blocks

- Using both seems unnecessarily complicated
 - We have to match our problem to this additional layer
 - Do we really gain anything?
- Threads in a block can communicate through shared memory
 - Threads in different memory can only communicate through global memory
- There is a limit on the number of threads per block
 - The limit is very small usually 1024
- Basically we have to or we won't get good performance



Pascal P100 block diagram





Compute Capability

- Each device has a compute capability level
 - Higher numbers are not necessarily "better".
- You can query
 - the level at runtime, or,
 - · individual device attributes.
- You often don't really care, except:
 - You probably want to specify the correct level when compiling.

NVIDIA Data Center Products

GPU	Compute Capability
NVIDIA A100	8.0
NVIDIA A40	8.6
NVIDIA A30	8.0
NVIDIA A10	8.6
NVIDIA A16	8.6
NVIDIA A2	8.6
NVIDIA T4	7.5
NVIDIA V100	7.0
Tesla P100	6.0
Tesla P40	6.1
Tesla P4	6.1
Tesla M60	5.2
Tesla M40	5.2
Tesla K80	3.7
Tesla K40	3.5
Tesla K20	3.5
Tesla K10	3.0

GeForce and TITAN Products

GPU	Compute Capability
Geforce RTX 3060 Ti	8.6
Geforce RTX 3060	8.6
GeForce RTX 3090	8.6
GeForce RTX 3080	8.6
GeForce RTX 3070	8.6
GeForce GTX 1650 Ti	7.5
NVIDIA TITAN RTX	7.5
Geforce RTX 2080 Ti	7.5
Geforce RTX 2080	7.5
Geforce RTX 2070	7.5
Geforce RTX 2060	7.5
NVIDIA TITAN V	7.0
NVIDIA TITAN Xp	6.1
NVIDIA TITAN X	6.1
GeForce GTX 1080 Ti	6.1
GeForce GTX 1080	6.1
GeForce GTX 1070 Ti	6.1
GeForce GTX 1070	6.1
GeForce GTX 1060	6.1
GeForce GTX 1050	6.1
GeForce GTX TITAN X	5.2
GeForce GTX TITAN Z	3.5

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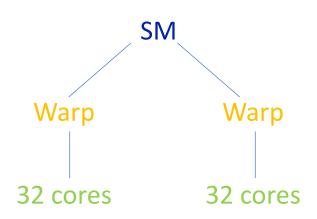


Compute Capability

		Tabl	le 15. Tech	nnical Spe	cifications	per Comp	ute Capat	oility						
	Compute Capability													
Technical Specifications	3.5	3.7	5.0	5.2	5.3	6.0	6.1	6.2	7.0	7.2	7.5	8.0	8.6	8.7
Maximum number of resident grids per device (Concurrent Kernel Execution)	device 32 16 128 32 16 128			16	128									
Maximum dimensionality of grid of thread blocks	3													
Maximum x-dimension of a grid of thread blocks		2 ³¹ -1												
Maximum y- or z-dimension of a grid of thread blocks		65535												
Maximum dimensionality of a thread block	3													
Maximum x- or y-dimension of a block		1024												
Maximum z-dimension of a block		64												
Maximum number of threads per block		1024												
Warp size	32													
Maximum number of resident blocks per SM	16 32 16						6							
Maximum number of resident warps per SM	64 32 64						4	18						
Maximum number of resident threads per SM	2048 1024 2048 1536						36							
Number of 32-bit registers per SM	64 K 128 K 64 K													
Maximum number of 32-bit registers per thread block	64 K 32 K 64 K 32 K 64 K													
Maximum number of 32-bit registers per thread	255													
Maximum amount of shared memory per SM	48 KB 112 KB 64 KB 96 KB 64 KB 96 KB 64 KB 96 KB 64 KB 164 KB 100 K				100 KB	164 KB								
Maximum amount of shared memory per thread block $\frac{33}{}$	48 KB 96 KB 96 KB 64 KB 163 KB 99 KB 16.							163 KB						



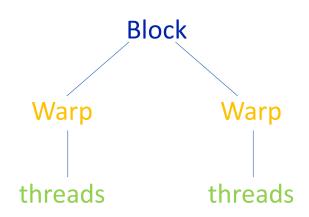
Streaming Multiprocessor (SM)







Streaming Multiprocessor (SM)







Terminology

Concept	Hardware	Description
thread	Core	Each thread is executed by one core. Cores have multiple threads resident at one time. Only one thread is executing at one time.
warp		A warp consists of 32 cores that share register memory and operate on the same instruction currently by construction.
block		Each block is assigned to a SM (streaming multiprocessor), consisting of warps. Each SM shares 64 KB of memory that can be used to share data between threads.
grid		The kernel is run on a grid of blocks.

F=Gmlm2 d2

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$$



Synchonising the Host and Device

- Kernel launches are asynchronous
 - The host can continue processing while the kernel is launched and executed
- The host needs to synchronise (wait) for the results to be ready

cudaMemcpy() Blocks the host until the copy is complete. The copy begins when all

preceding kernels calls have completed.

cudaMemcpyAsync() As above, but does not block the host. Copies occur after all preceding

kernel calls have completed.

cudaDeviceSynchronize() Waits for all transfers and kernel calls to complete.



Detecting Errors

- The CUDA API calls all return an error code (cudaError_t)
 - An error in the API call, or,
 - An error in an earlier asychronous operation (e.g., a kernel launch)
- You can always retrieve the last error with

```
cudaError t cudaGetLastError(void);
```

You can convert the error code into a human friendly string with

```
char *cudaGetErrorString(cudaError_t)
printf("%s\n",cudaGetErrorString(cudaGetLastError()));
```



Multiple Device Management

 A host may have more than one device and this must be managed explicitly with the following API calls

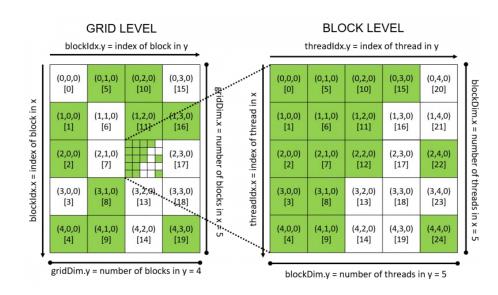
```
cudaGetDeviceCount(int *count)
cudaSetDevice(int device)
cudaGetDevice(int *device)
cudaGetDeviceProperties(cudaDeviceProp *prop, int device)
```

- Multiple host threads can share a device "thread safe"
- A single host thread can access multiple devices cudaSetDevice(i) to select the current device for kernel launches and API calls



3D Indexing

- A kernel is launched as a grid of blocks of threads.
- blockldx and threadIdx are 3D
 - We only used "x"
- Builtin variables have x,y and z
 - threadIdx
 - blockDim
 - blockIdx
 - gridDim
- Some problems map well to 3D
- Total threads: gridDim. $x \times$ gridDim. $y \times$ gridDim. $z \times$ blockDim. $x \times$ blockDim. $y \times$ blockDim. $z \times$





Sharing Data between threads

- Within a block, threads can share data via shared memory.
- Extremely fast on-chip memory, user (you) managed.
- Declare using __shared__, allocated per block.
- Data is not visible to threads in different blocks

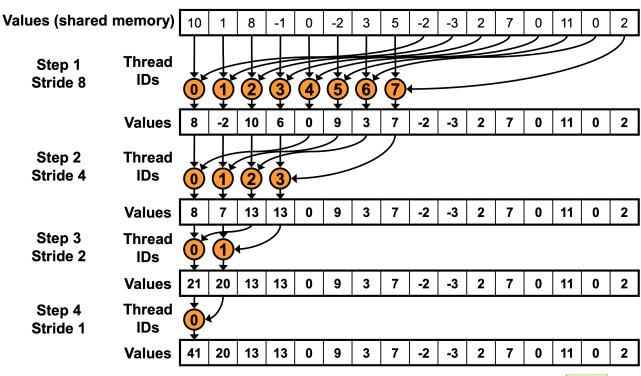
 Threads can execute in any order within a thread block, so to sychronize use

```
void __syncthreads();
```

- This is like a "barrier"; all threads will execute the call before continuing.
- Careful: do not put inside conditional code unless it is uniform across the block.

Shared Memory Reduction

- See <u>Optimizing Parallel</u> <u>Reduction in CUDA</u> by nVidia for details.
- Idea is that you can take 32 (or more!) values and reduce them on the GPU
- Each block must be done separately, and the results sent to the CPU (one result per block).





Importance of Optimising

	Time (2 ²² ints)	Bandwidth	Step Speedup	Cumulative Speedup
Kernel 1: interleaved addressing with divergent branching	8.054 ms	2.083 GB/s		
Kernel 2: interleaved addressing with bank conflicts	3.456 ms	4.854 GB/s	2.33x	2.33x
Kernel 3: sequential addressing	1.722 ms	9.741 GB/s	2.01x	4.68x
Kernel 4: first add during global load	0.965 ms	17.377 GB/s	1.78x	8.34x
Kernel 5: unroll last warp	0.536 ms	31.289 GB/s	1.8x	15.01x
Kernel 6: completely unrolled	0.381 ms	43.996 GB/s	1.41x	21.16x
Kernel 7: multiple elements per thread	0.268 ms	62.671 GB/s	1.42x	30.04x

- Results are from <u>Optimizing</u> Parallel Reduction in CUDA.
- It is "easy" to write a CUDA kernel.
- Hard to write optimal code.
- Kernels can be limited by
 - Compute (number of FLOPS)
 - · Memory bandwidth
- Max for G80: 86.4 GB/s
- Experience and practice!