





# Introduction to GPU and GPU programming

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# Agenda

- Why GPU? (a little bit of history)
- GPU architecture
- How to use/programming GPUs?

## A little bit of history 1: the rising (90s..)

- The CPU has always been slow for Graphics Processing
  - Visualization
  - Games
- Graphics processing is inherently parallel and there is a lot of parallelism – O(pixels)
- GPUs were built to do graphics processing only
- Initially, hardwired logic replicated to provide parallelism
  - Little to no programmability

#### A little bit of history 2: the oo's

- Like CPUs, GPUs benefited from Moore's Law
  - Evolved from fixed-function hardwired logic to flexible, programmable ALUs
- Around 2004, GPUs were programmable "enough" to do some non-graphics computations
  - Severely limited by graphics programming model (shader
  - programming)
- In 2006, GPUs became "fully" programmable
  - NVIDIA releases "CUDA" language to write non-graphics programs that will run on GPUs

#### A little bit of history 3: the 10's (the present)

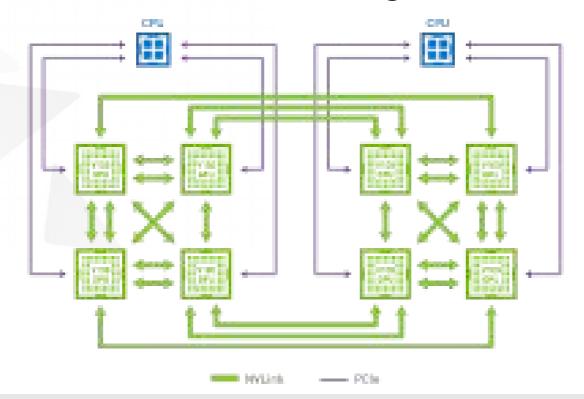
- GPUs are widely deployed as accelerators
- GPUs so successful that other CPU alternatives are dead
  - Sony/IBM Cell BE
  - Clearspeed RSX
  - Intel MIC
- GPU enabled the ML/DL/AI revolution and started the HPC/AI convergence
  - Tensorcore
- There is ONE winner: NVIDIA

#### **Nvlink: avoid PCI- bus contention**

- Direct communication link between two GPUs
- Improves accuracy and convergence of highperformance computing (HPC) and AI

Achieves speeds over an order of magnitude faster than

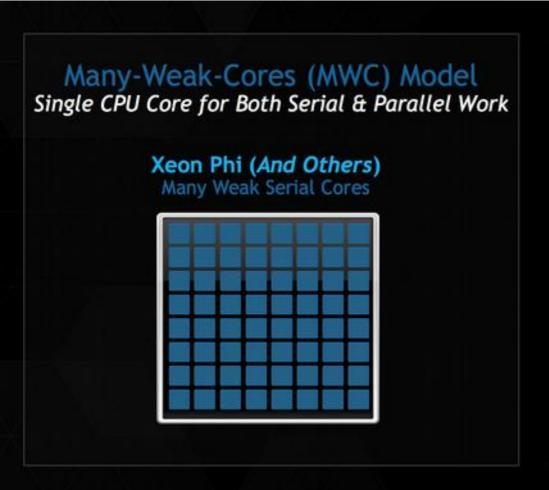
PCIe.

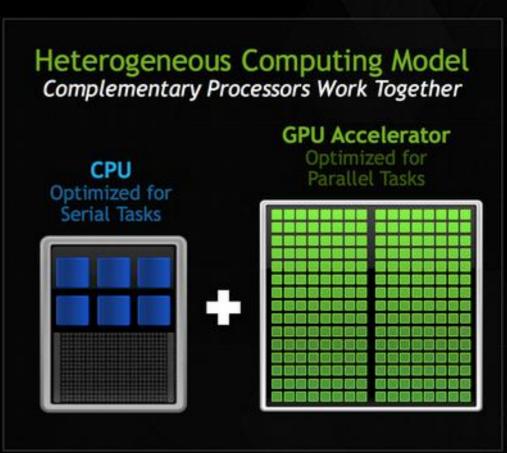


## **Nvdia Cards**

	"Fermi"	"Fermi"	"Kepler"	"Kepler"	"Maxwell"	"Pascal"	"Volta"
Tesla GPU	GF100	GF104	GK104	GK110	GM200	GP100	GV100
Compute Capability	2.0	2.1	3.0	3.5	5.3	6.0	7.0
Streaming Multiprocessors (SMs)	16	16	8	15	24	56	84
FP32 CUDA Cores / SM	32	32	192	192	128	64	64
FP32 CUDA Cores	512	512	1536	2880	3072	3584	5376
FP64 Units	WEN	22	512	960	96	1792	2688
Tensor Core Units							672
Threads / Warp	32	32	32	32	32	32	32
Max Warps / SM	48	48	64	64	64	64	64
Max Threads / SM	1536	1536	2048	2048	2048	2048	2048
Max Thread Blocks / SM	8	8	16	16	32	32	32
32-bit Registers / SM	32768	32768	65536	65536	65536	65536	65536
Max Registers / Thread	63	63	63	255	255	255	255
Max Threads / Thread Block	1024	1024	1024	1024	1024	1024	1024
Shared Memory Size Configs	16 KB	16 KB	16 KB	16 KB	96 KB	64 KB	Config
	48 KB	48 KB	32 KB	32 KB			Up Tp
			48 KB	48 KB			96 KB
Hyper-Q	No	No	No	Yes	Yes	Yes	Yes
Dynamic Parallelism	No	No	No	Yes	Yes	Yes	Yes
Unified Memory	No	No	No	No	No	Yes	Yes
Pre-Emption	No	No	No	No	No	Yes	Yes

#### Nvidia slides: computing mode for accelerator

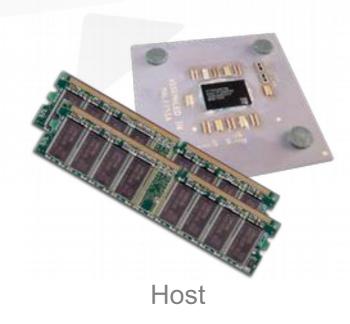






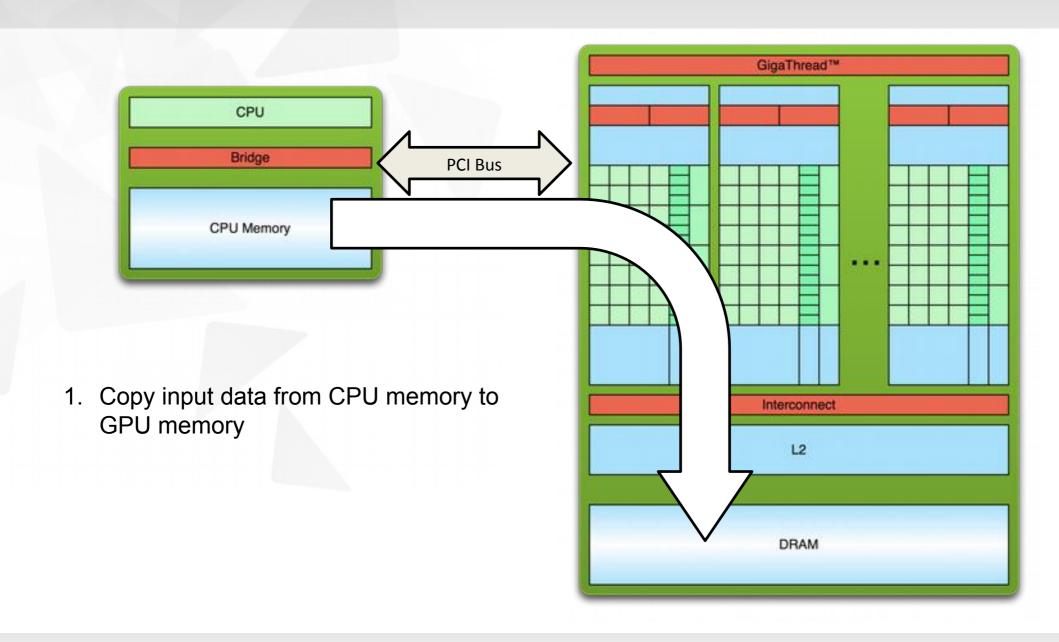
## **Heterogeneous Computing**

- Terminology:
  - Host The CPU and its memory (host memory)
  - Device The GPU and its memory (device memory)

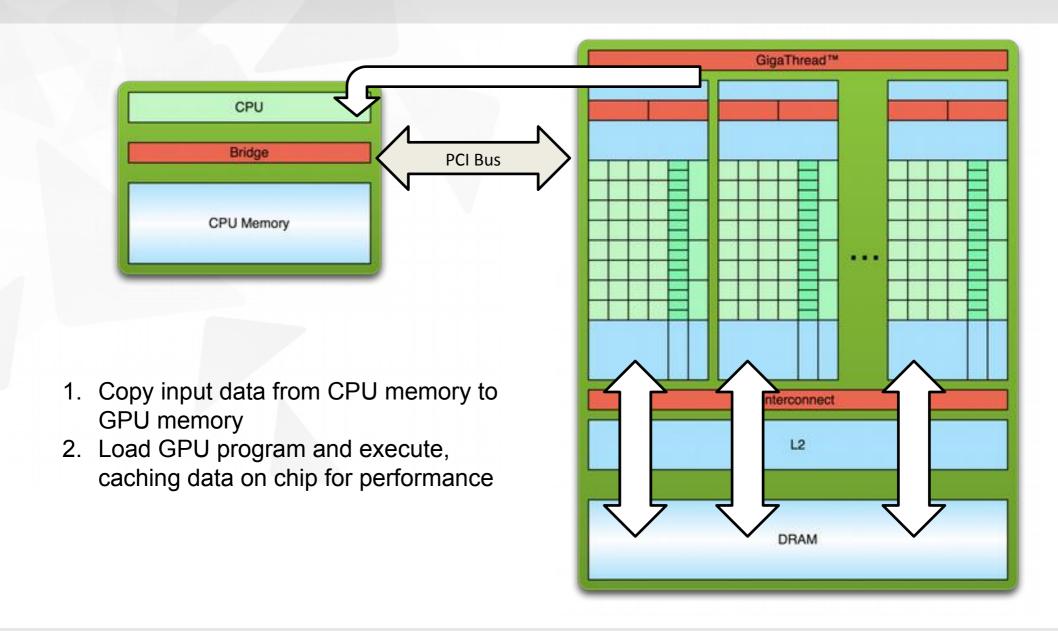




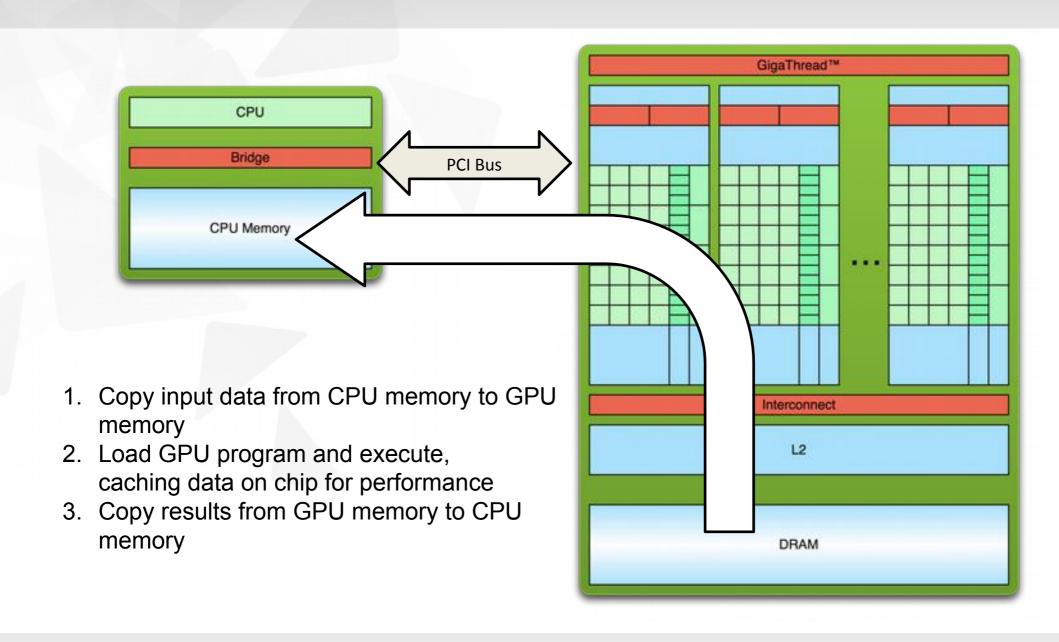
# **Simple Processing Flow**



## **Simple Processing Flow**



## **Simple Processing Flow**



## **CUDA Parallel Computing Platform**

Programming
Approaches

Libraries
OpenACC Directives
Languages

"Drop-in" Acceleration

Easily Accelerate Apps

Maximum Flexibility

Development Environment



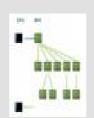
Nsight IDE Linux, Mac and Windows GPU Debugging and Profiling CUDA-GDB debugger NVIDIA Visual Profiler

Hardware Capabilities

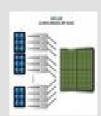


**SMX** 

**Dynamic Parallelism** 



**HyperQ** 



**GPUDirect** 



From: www.nvidia.com/getcuda

#### 3 ways to accelerate applications



Libraries

OpenACC Directives

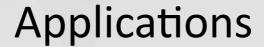
Programming Languages

"Drop-in"
Acceleration

Easily Accelerate Applications

Maximum Flexibility

#### 3 ways to accelerate applications



Libraries

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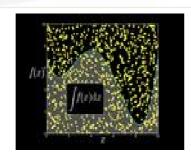
#### Libraries: Easy, High-Quality Acceleration

- Ease of use:
  - Using libraries enables GPU acceleration without in-depth knowledge of GPU programming
- "Drop-in":
  - Many GPU-accelerated libraries follow standard APIs, thus enabling acceleration with minimal code changes
- Quality:
  - Libraries offer high-quality implementations of functions encountered in a broad range of applications
- Performance:
  - NVIDIA libraries are tuned by experts

#### Some GPU-accelerated Libraries



**NVIDIA cuBLAS** 



NVIDIA cuRAND



**NVIDIA cuSPARSE** 



**NVIDIA NPP** 



Vector Signal Image Processing



**GPU** Accelerated Linear Algebra



Matrix Algebra on GPU and Multicore





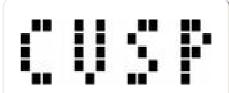
**NVIDIA** cuFFT





ArrayFire Matrix Computations

Building-block Algorithms for CUDA



Sparse Linear Algebra





C++ STL Features for CUDA



#### 3 Steps to CUDA-accelerated application

• Step 1: Substitute library calls with equivalent CUDA library calls

- Step 2: Manage data locality
  - with CUDA: cudaMalloc(), cudaMemcpy(), etc.
  - with CUBLAS: cublasAlloc(), cublasSetVector(), etc.

Step 3: Rebuild and link the CUDA-accelerated library

```
nvcc myobj.o -1 cublas
```

#### **Explore the CUDA (Libraries) Ecosystem**

 CUDA Tools and Ecosystem described in detail on NVIDIA Developer Zone:

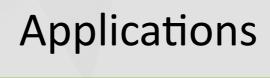
developer.nvidia.com/cuda -tools-ecosystem



# Tutorial: performing DGEMM on CPU and GPU

• See github repo...

#### 3 ways to accelerate applications



Libraries

OpenACC Directives

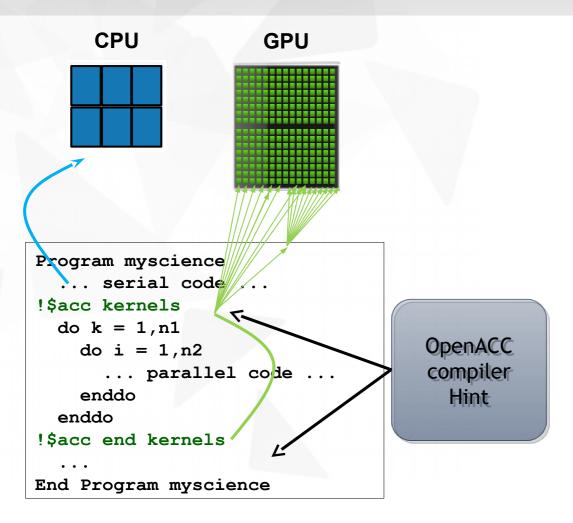
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#### **OpenACC Directives**



- Simple Compiler hints
- Compiler Parallelizes code
- Works on many-core GPUs
   & multicore CPUs

Your original Fortran or C code

#### **OpenACC**



- Easy: Directives are the easy path to accelerate computev intensive applications
- Open: OpenACC is an open GPU directives standard, making GPU programming straightforward and portable across parallel and multi-core processors
- Powerful: GPU Directives allow complete access to the massive parallel power of a GPU

#### Is OpenACC available?

- OpenACC is at version 2.7
- PGI compiler fully implements it
- GCC 9 includes initial support for OpenAcc 2.6

#### OpenACC friendly disclaimer...

OpenACC does not make GPU programming easy. (...)

GPU programming and parallel programming is not easy. It cannot be made easy.

However, GPU programming need not be difficult, and certainly can be made straightforward, once you know how to program and know enough about the GPU architecture to optimize your algorithms and data structures to make effective use of the GPU for computing.

OpenACC is designed to fill that role.

(Michael Wolfe, The Portland Group)

#### **OpenACC – Directive Based Approach**

- Directives are added to serial source code
  - Manage loop parallelization
  - Manage data transfer between CPU and GPU memory
- Works with C, C++, or Fortran
  - Can be combined with explicit CUDA C/Fortran usage
- Directives are formatted as comments
  - They don't interfere with serial execution
- Maintaines portability of original code

#### **Directives: Easy & Powerful**

# Real-Time Object Detection

Global Manufacturer of Navigation Systems



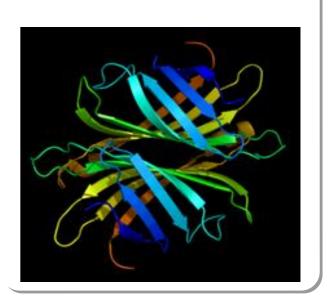
#### Valuation of Stock Portfolios using Monte Carlo

Global Technology Consulting Company



# Interaction of Solvents and Biomolecules

University of Texas at San Antonio



5x in 40 Hours

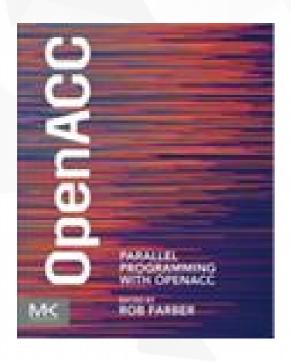
2x in 4 Hours

5x in 8 Hours

www.nvidia.com/gpudirectives

#### **OpenACC** tutorial

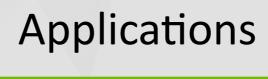
• A section of chapter 1 of this book:



https://www.amazon.com/Parallel-Programming-OpenACC-Rob-Farber/ dp/0124103979

https://github.com/rmfarber/ ParallelProgrammingWithOpenACC

#### 3 ways to accelerate applications



Libraries

OpenACC Directives

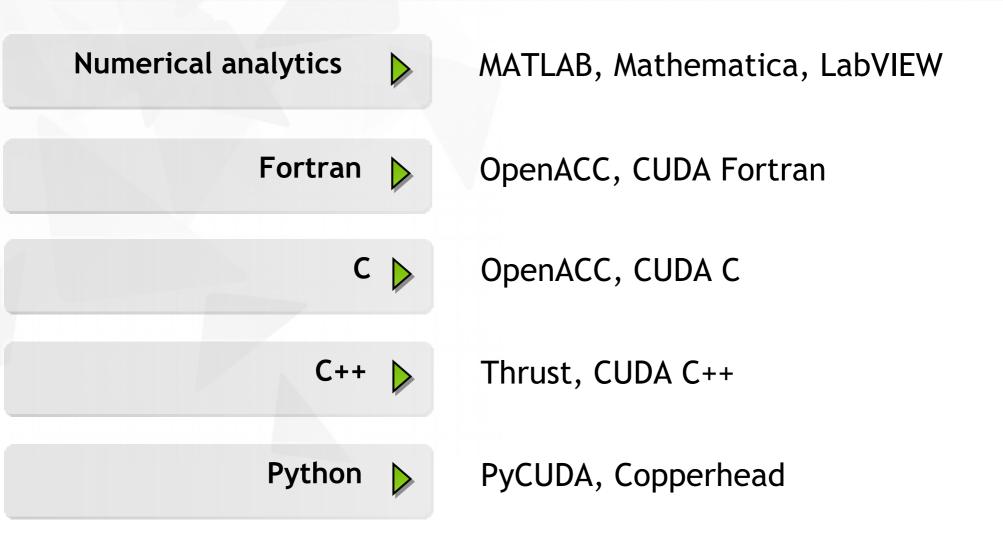
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#### **GPU Programming Languages**



#### **CUDA** programming

- CUDA = Compute Unified Device Architecture
  - Expose general-purpose GPU computing as first-class capability
  - Retain traditional DirectX/OpenGL graphics performance
- CUDA C
  - Based on industry-standard C
  - A handful of language extensions to allow heterogeneous programs
  - Straightforward APIs to manage devices, memory, etc.

#### **CUDA** basic concepts

- The GPU is viewed as a compute device that:
  - has its own RAM (device memory)
  - runs data-parallel portions of an application as kernels by using many threads
- GPU vs. CPU threads
  - GPU threads are extremely lightweight
  - Very little creation overhead
  - GPU needs 1000s of threads for full efficiency
  - A multi-core CPU needs only a few (basically one thread per core)

#### **Hello World!**

```
int main(void) {
    printf("Hello World!\n");
    return 0;
}
>nvcc hello_world.cu
```

- Standard C that runs on the host
- NVIDIA compiler (nvcc) can be used to compile programs with no device code

#### Hello World! with Device Code

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

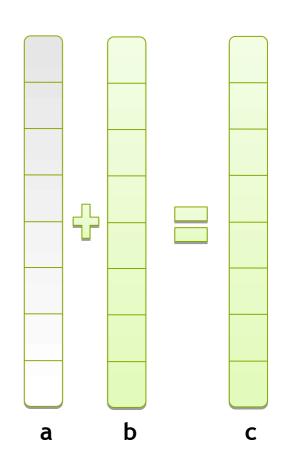
#### Hello World! with Device Code

```
mykernel<<<1,1>>>();
```

- Triple angle brackets mark a call from host code to device code
  - Also called a "kernel launch"
  - We'll return to the parameters (1,1) in a moment
- That's all that is required to execute a function on the GPU

#### Parallel Programming in CUDA C/C++

- But wait... GPU computing is about massive parallelism!
- We need a more interesting example...
- We'll start by adding two integers and build up to vector addition



#### Addition on the Device

A simple kernel to add two integers

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

- As before \_\_global\_ is a CUDA C/C++ keyword meaning
  - add() will execute on the device
  - add() will be called from the host

### **Memory Management**

Host and device memory are separate entities

Device pointers point to GPU memory
 May be passed to/from host code
 May not be dereferenced in host code

Host pointers point to CPU memory
 May be passed to/from device code
 May not be dereferenced in device code

- Simple CUDA API for handling device memory
  - cudaMalloc(), cudaFree(), cudaMemcpy()
  - Similar to the C equivalents malloc(), free(), memcpy()

## Addition on the Device: add()

Returning to our add() kernel

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

Let's take a look at main()...

## Addition on the Device: main()

## **Moving to Parallel**

- GPU computing is about massive parallelism
  - So how do we run code in parallel on the device?

```
Add<<< 1, 1 >>>();

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

 Instead of executing add() once, execute N times in parallel

#### **Vector Addition on the Device**

- With add() running in parallel we can do vector addition
- Terminology: each parallel invocation of add() is referred to as a block
  - The set of blocks is referred to as a grid
  - Each invocation can refer to its block index using blockldx.x

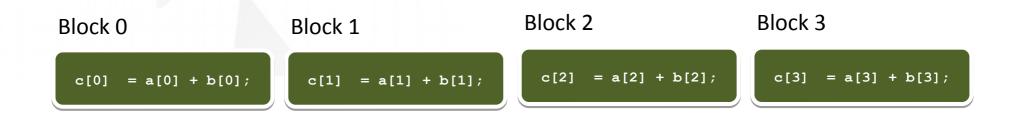
```
__global__ void add(int *a, int *b, int *c) {
c[blockldx.x] = a[blockldx.x] + b[blockldx.x];
}
```

 By using blockldx.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[blockldx.x] = a[blockldx.x] + b[blockldx.x];
}
```

On the device, each block can execute in parallel:



## **Vector Addition on the Device: add()**

Returning to our parallelized add() kernel

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

Let's take a look at main()...

## **Vector Addition on the Device: main() (1)**

```
#define N 512
int main(void) {
  int *a *b *c
                         // host copies of a, b, c
  int *d_a, *d_b, *d_c; // device copies of a, b, c
  int size = N * sizeof(int);
  // Alloc space for device copies of a, b, c
  cudaMalloc((void **)&d_a, size);
  cudaMalloc((void **)&d_b, size);
  cudaMalloc((void **)&d c, size);
  // Alloc space for host copies of a, b, c and setup input values
  a = (int *)malloc(size); random ints(a, N);
  b = (int *)malloc(size); random_ints(b, N);
  c = (int *)malloc(size);
```

## **Vector Addition on the Device: main() (2)**

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

## Review (1 of 2)

- Difference between host and device
  - Host CPU
  - Device GPU
- Using \_\_global\_\_ to declare a function as device code
  - Executes on the device
  - Called from the host
- Passing parameters from host code to a device function

## Review (2 of 2)

- Basic device memory management
  - cudaMalloc()
  - cudaMemcpy()
  - cudaFree()
- Launching parallel kernels
  - Launch и copies of add() with add<<< N,1>>>(...);
  - Use blockldx.x to access block index

#### **CUDA Threads**

Terminology: a block can be split into parallel threads

 Let's change add() to use parallel threads instead of parallel 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

Need to make one change in main()...

# **Vector Addition Using Threads: main() (1)**

```
#define N 512
int main(void) {
  int *a, *b, *c;
                  // host copies of a, b, c
                               // device copies of a, b, c
  int *d_a, *d_b, *d_c;
  int size = N * sizeof(int);
  // Alloc space for device copies of a, b, c
  cudaMalloc((void **)&d a, size);
  cudaMalloc((void **)&d_b, size);
  cudaMalloc((void **)&d c, size);
  // Alloc space for host copies of a, b, c and setup input values
  a = (int *)malloc(size); random ints(a, N);
  b = (int *)malloc(size); random_ints(b, N);
  c = (int *)malloc(size);
```

## **Vector Addition Using Threads: main()**

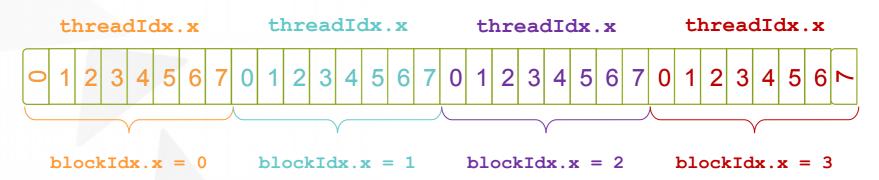
```
// Copy inputs to device
cudaMemcpy(d_a, a, size, cudaMemcpyHostToDevice);
cudaMemcpy(d_b, b, size, cudaMemcpyHostToDevice);
// Launch add() kernel on GPU with N threads
add<<<1,N>>>(d_a, d_b, d_c);
// Copy result back to host
cudaMemcpy(c, d_c, size, cudaMemcpyDeviceToHost);
// Cleanup
free(a);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

### **Combining Blocks and Threads**

- We've seen parallel vector addition using:
  - Many blocks with one thread each
  - One block with many threads
- Let's adapt vector addition to use both blocks and threads
- Why? We'll come to that...
- First let's discuss data indexing...

### **Indexing Arrays with Blocks and Threads**

- No longer as simple as using blockldx.x and threadldx.x
  - Consider indexing an array with one element per thread (8 threads/block)

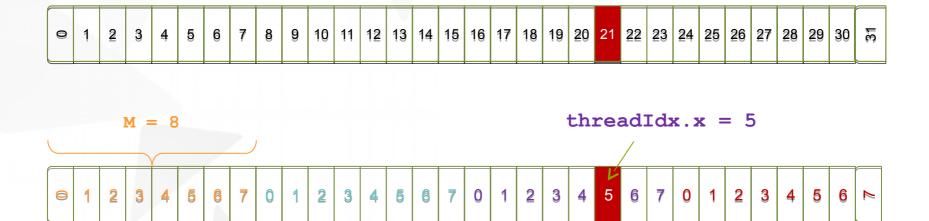


 With M threads/block a unique index for each thread is given by:

```
int index = threadIdx.x + blockIdx.x * M;
```

### **Indexing Arrays: Example**

Which thread will operate on the red element?



blockIdx.x = 2

#### **Addition with Blocks and Threads**

 Use the built-in variable blockDim.x for threads per block

```
int index = threadIdx.x + blockIdx.x * blockDim.x;
```

 Combined version of add() to use parallel threads and parallel blocks

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

What changes need to be made in main()?

## Addition with Blocks and Threads: main()(1)

```
#define N (2048*2048)
#define THREADS PER BLOCK 512
int main(void) {
  int *a, *b, *c; // host copies of a, b, c
  int *d_a, *d_b, *d_c; // device copies of a, b, c
  int size = N * sizeof(int);
  // Alloc space for device copies of a, b, c
  cudaMalloc((void **)&d_a, size);
  cudaMalloc((void **)&d_b, size);
  cudaMalloc((void **)&d c, size);
  // Alloc space for host copies of a, b, c and setup input values
  a = (int *)malloc(size); random ints(a, N);
  b = (int *)malloc(size); random ints(b, N);
  c = (int *)malloc(size);
```

## Addition with Blocks and Threads: main()(2)

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

### **Handling Arbitrary Vector Sizes**

- Typical problems are not friendly multiples of blockDim.x
- Avoid accessing beyond the end of the arrays:

```
__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:

```
add << (N + M-1) / M, M >>> (d_a, d_b, d_c, N);
```

#### Review

- Launching parallel kernels
  - Launch N copies of add() with add<<<N/M,M>>>(...);
  - Use blockIdx.x to access block index
  - Use threadIdx.x to access thread index within block

Allocate elements to threads:

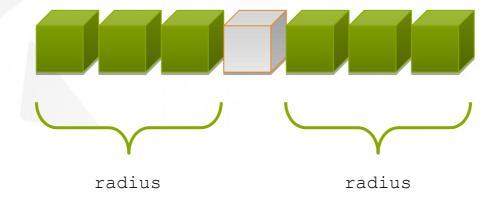
```
int index = threadIdx.x + blockIdx.x * blockDim.x;
```

### Why bother with Threads?

- Threads seem unnecessary
  - They add a level of complexity
  - What do we gain?
- Unlike parallel blocks, threads have mechanisms to:
  - Communicate
  - Synchronize
- To look closer, we need a new example...

#### 1D Stencil

- Consider applying a 1D stencil to a 1D array of elements
  - Each output element is the sum of input elements within a radius
- If radius is 3, then each output element is the sum of 7 input elements:



## Implementing Within a Block

- Each thread processes one output element
  - blockDim.x elements per block
- Input elements are read several times
  - With radius 3, each input element is read seven times





## **Sharing Data Between Threads**

 Terminology: within a block, threads share data via shared memory

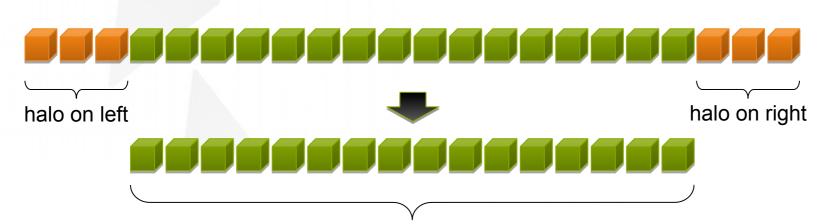
Extremely fast on-chip memory, user-managed

• Declare using shared , allocated per block

Data is not visible to threads in other blocks

### **Implementing With Shared Memory**

- Cache data in shared memory
  - Read (blockDim.x + 2 \* radius) input elements from global memory to shared memory
  - Compute blockDim.x output elements
  - Write blockDim.x output elements to global memory



Each block needs a halo of radius elements at each boundary

#### Stencil kernel

```
global __ void stencil_ld(int *in, int *out) {
    _shared __ int temp[BLOCK_SIZE + 2 * RADIUS];
    int gindex = threadIdx.x + blockIdx.x * blockDim.x;
    int lindex = threadIdx.x + RADIUS;

// Read input elements into shared memory

temp[lindex] = in[gindex];
    if (threadIdx.x < RADIUS) {
     temp[lindex - RADIUS] = in[gindex - RADIUS];
     temp[lindex + BLOCK_SIZE] =
        in[gindex + BLOCK_SIZE];
}</pre>
```

#### Stencil kernel

```
// Apply the stencil
int result = 0;
for (int offset = -RADIUS ; offset <= RADIUS ; offset++)
  result += temp[lindex + offset];

// Store the result
out[gindex] = result;</pre>
```

#### **Data Race!**

- The stencil example will not work...
- Suppose thread 15 reads the halo before thread 0 has fetched it...

Load from temp[19]

# \_\_syncthreads()

• void syncthreads();

- Synchronizes all threads within a block
  - Used to prevent RAW / WAR / WAW hazards

- All threads must reach the barrier
  - In conditional code, the condition must be uniform across the block

#### Stencil kernel

syncthreads();

```
global void stencil 1d(int *in, int *out) {
  shared int temp[BLOCK SIZE + 2 * RADIUS];
int gindex = threadIdx.x + blockIdx.x * blockDim.x;
int lindex = threadIdx.x + RADIUS;
// Read input elements into shared memory
temp[lindex] = in[gindex];
if (threadIdx.x < RADIUS) {</pre>
  temp[lindex - RADIUS] = in[gindex - RADIUS];
  temp[lindex + BLOCK SIZE] =
    in[gindex + BLOCK SIZE];
}
```

// Synchronize (ensure all the data is available)

#### Stencil kernel

```
// Apply the stencil
int result = 0;
for (int offset = -RADIUS ; offset <= RADIUS ; offset++)
  result += temp[lindex + offset];

// Store the result
out[gindex] = result;</pre>
```

### **Coordinating Host & Device**

- Kernel launches are asynchronous
  - Control returns to the CPU immediately

CPU needs to synchronize before consuming the results

cudaMemcpy ()

Blocks the CPU until the copy is complete

Copy begins when all preceding CUDA calls have completed

cudaMemcpyAsync () Asynchronous, does not block the CPU

cudaDeviceSynchronize() Blocks the CPU until all preceding CUDA calls have completed

### **Reporting Errors**

- All CUDA API calls return an error code (cudaError\_t)
  - Error in the API call itself

OR

- Error in an earlier asynchronous operation (e.g. kernel)
- Get the error code for the last error:

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

Get a string to describe the error:

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

### **Device Management**

Application can query and select GPUs

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

- Multiple threads can share a device
- A single thread can manage multiple devices

```
cudaSetDevice(i) to select current device
cudaMemcpy(...) for peer-to-peer copies†
```





End...



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