Software Performance Engineering

LECTURE 19
GPU PROGRAMMING

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November 6, 2025



CSE 822

https://accelerated-computing.github.io/

Spring 2026!

Advanced GPU programming!

Let me know if you're in the waitlist

CSE/CMSE 822: PARALLEL COMPUTING

Instructor: Xuhao Chen

Interested in how GPU works?

Tired of GPU Out-of-memory?

Want to accelerate your training / simulation?

Come learn about...

- Performance modeling & Optimization
- Parallel Algorithms and Theory
- Shared-memory & Multi-core Programming
- Distributed Computing & MPI
- Memory-efficient Programming
- Domain-Specific Languages
- Machine Learning Systems

Syllabus:

https://accelerated-computing.github.io/spring26/syllabus/

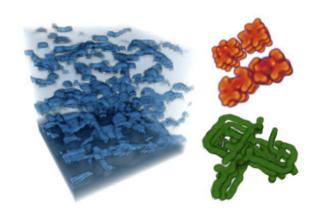
This course aims to teach you how to write fast code for parallel computers & hardware accelerators like GPUs



Outline

- GPU Architecture
 - Three major ideas that make GPU processing cores run fast
 - Closer look at real GPU designs
 - The GPU memory hierarchy: moving data to processors
- General Purpose GPU (GPGPU)
- GPU Programming Model
- Program a GPU with CUDA

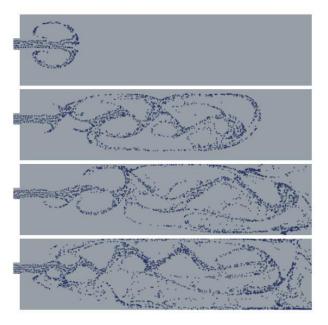
"GPGPU" 2002~2003



Coupled Map Lattice Simulation [Harris 02]



Ray Tracing on Programmable Graphics Hardware [Purcell 02]



Sparse Matrix Solvers [Bolz 03]

Brook stream programming language (2004)

- Stanford graphics lab research project*
- Abstract GPU hardware as data-parallel processor
- Brook compiler translates generic stream program into graphics commands (e.g. drawTriangles) and a set of shader programs

```
kernel void scale(float amount, float a<>, out float b<>) {
       b = amount * a;
float scale amount;
float input stream<1000>; // stream declaration
float output_stream<1000>; // stream declaration
// omitting stream element initialization...
// map kernel function onto streams
scale(scale_amount, input_stream, output_stream);
```

NVIDIA Tesla architecture (2007)

- First alternative, non-graphics-specific ("compute mode") interface to GPU hardware, e.g. GeForce 8800
- Let's say a user wants to run a non-graphics program on the GPU's programmable cores...
 - Application can allocate buffers in GPU memory and copy data to/from buffers
 - Application (via graphics driver) provides GPU a single kernel program binary
 - Application tells GPU to run the kernel in an SPMD fashion ("run N instances of this kernel") e.g. launch(myKernel, N)
- Interestingly, this is a far simpler operation than the graphics operation drawPrimitives()

CUDA programming language

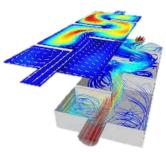
- Introduced in 2007 with NVIDIA Tesla architecture
- "C-like" language to express programs that run on GPUs using the compute-mode hardware interface
- Relatively low-level abstractions: closely match the capabilities/performance characteristics of modern GPUs

Compute Intensive Applications

Bioinformatics



 Computational Fluid **Dynamics**

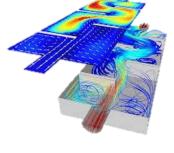


 Computational Chemistry



 Computational Finance

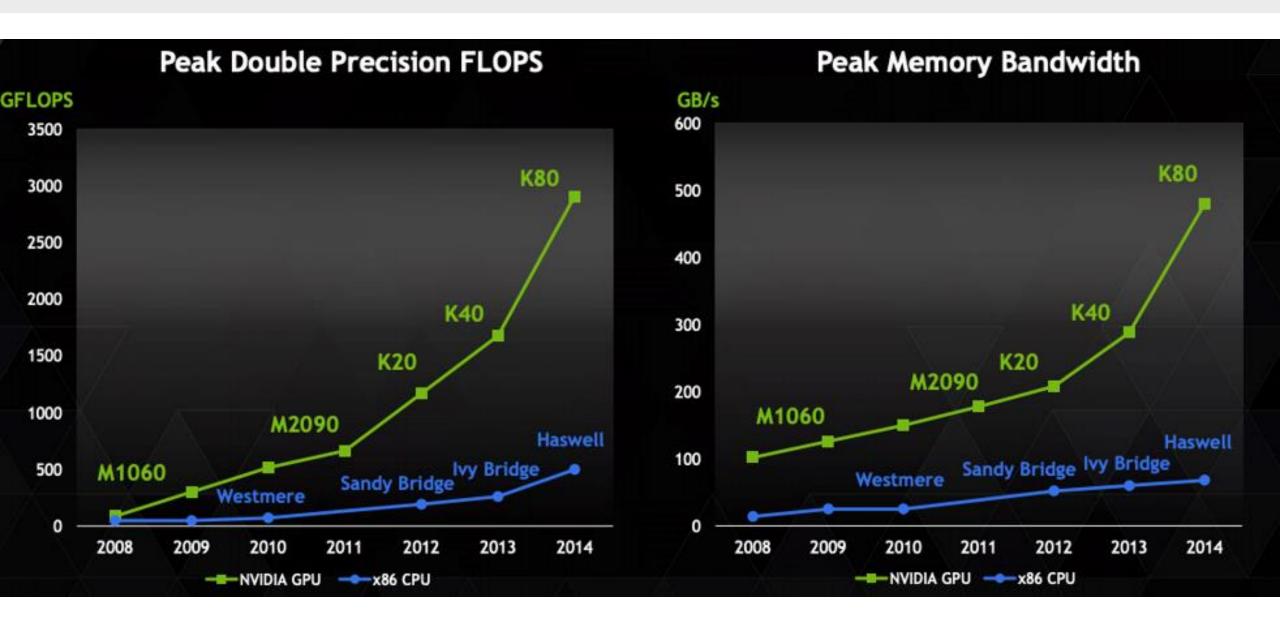




Machine Learning

 Data science, medical imaging,, weather and climate, ...

Why use GPGPU?



Why can't CPUs Scale?

- # cores: Why Not Just Add More?
- SIMD width: Why Not Go Wider?
- Memory bandwidth: Why Not Boost It?

Why GPGPU?

• CPU

- □~10s cores
- Low latency
- Good for serial processing
- Good for interactive tasks
- Task parallelism

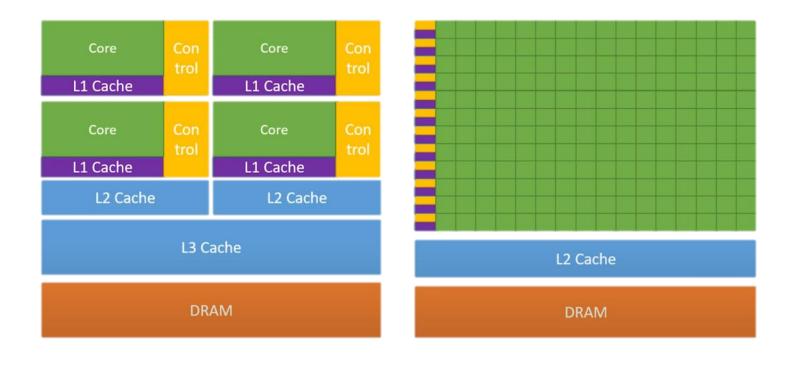


• GPU

- □ 100s ~ 1000s cores
- High throughput
- Good for parallel processing
- Good for big-data tasks
- Data parallelism



Why GPU?



CPU GPU

What's Better?

Scooter



Sport car



What's Better?

Scooter



Deliver many packages within a reasonable timescale

Sport car



Deliver a package as soon as possible

Why can't CPUs Scale?

- # cores: Why Not Just Add More?
- SIMD width: Why Not Go Wider?
- Memory bandwidth: Why Not Boost It?

- The short answer is: they could, but they shouldn't.
- CPUs are latency oriented, GPUs are throughput oriented

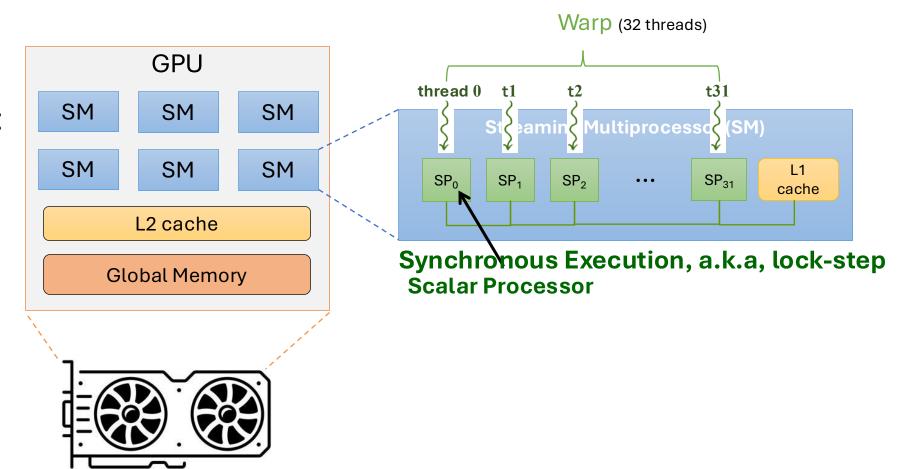
Power, Heat, and Cost Constraints

GPU Architecture

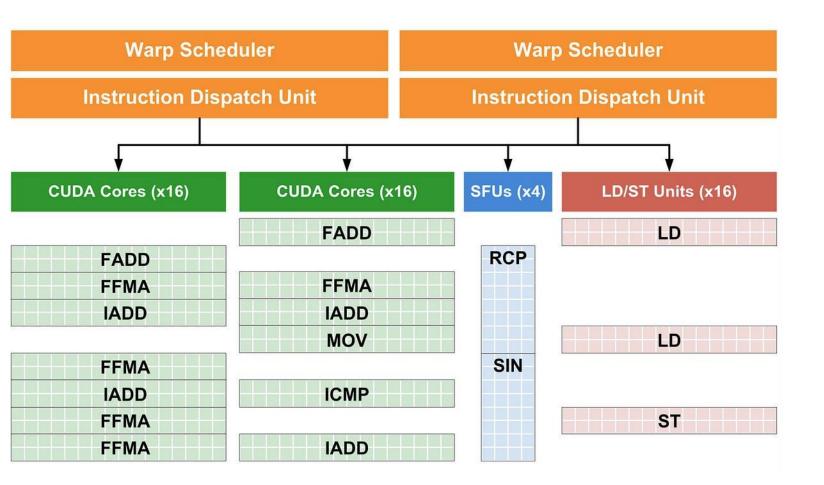
SIMT: single-instruction multiple threads

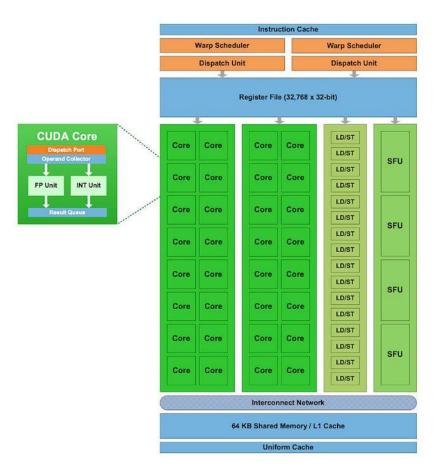
In A100 GPU each SM has:

- 64 FP32 cores
- 32 FP64 cores
- 64 KB registers
- 192 KB L1 + shared mem

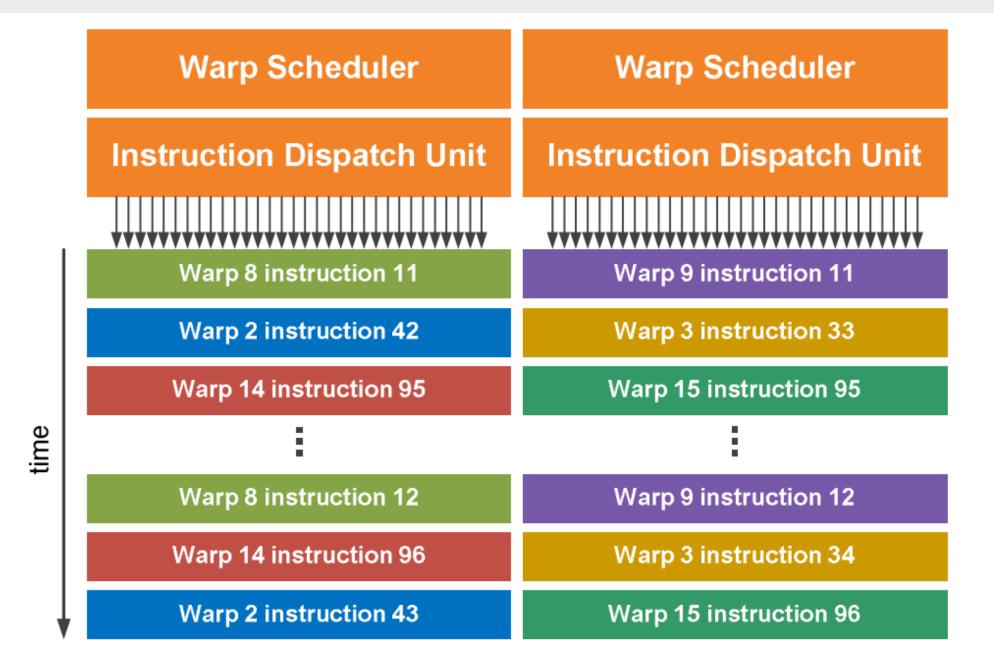


Warp Scheduler

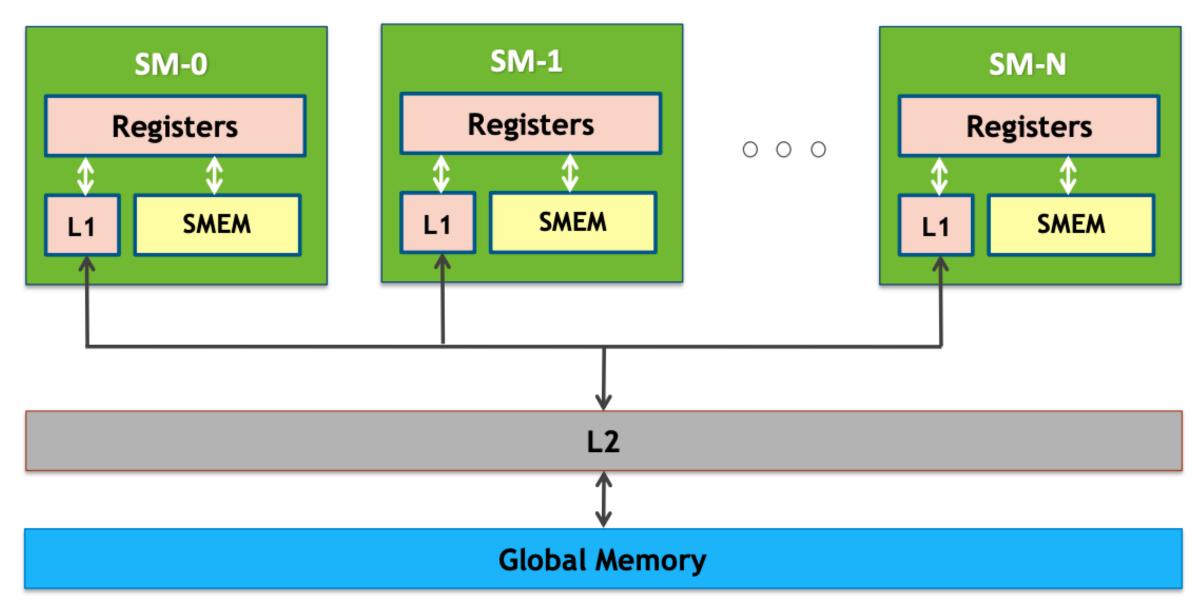




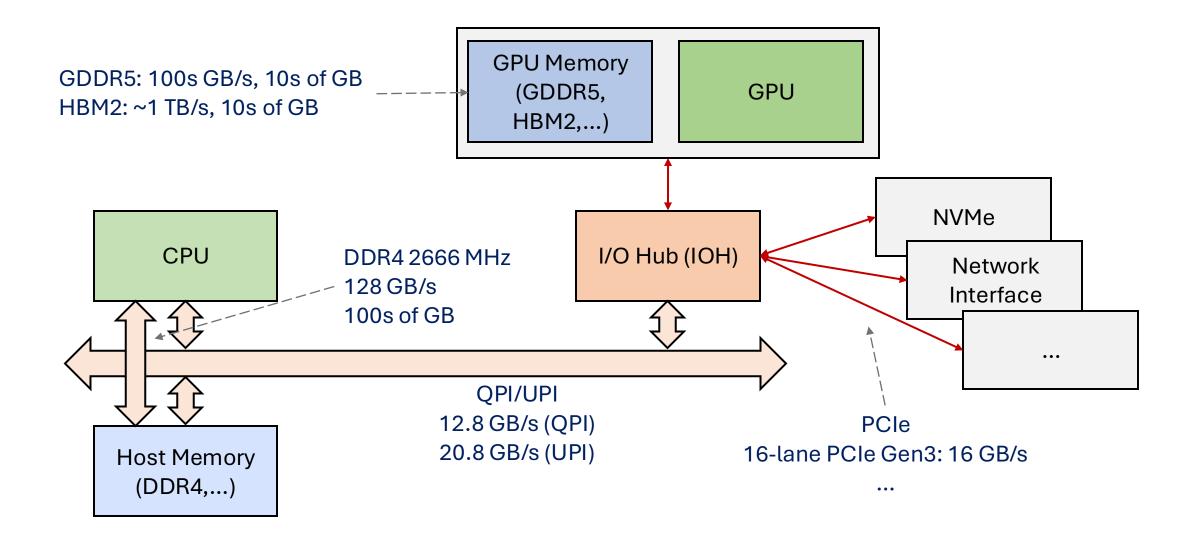
Warp Scheduler



GPU Memory Hierarchy



System Architecture With a GPU (2019)



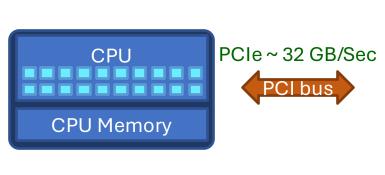
Outline

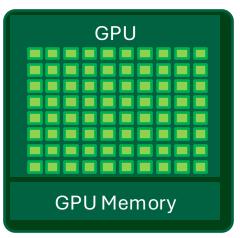
- GPU Architecture
 - Three major ideas that make GPU processing cores run fast
 - Closer look at real GPU designs
 - The GPU memory hierarchy: moving data to processors
- General Purpose GPU (GPGPU)
- GPU Programming Model
- Program a GPU with CUDA

Heterogeneous Programming (CPU+GPU)

- CPU (Milan)
 - □ 64 cores, 2 threads per core
 - 4 NUMA domains per socket
 - 2xAVX2 (256 bit), so 2x4 in double precision
 - ~512 way parallelism (64*2*4)

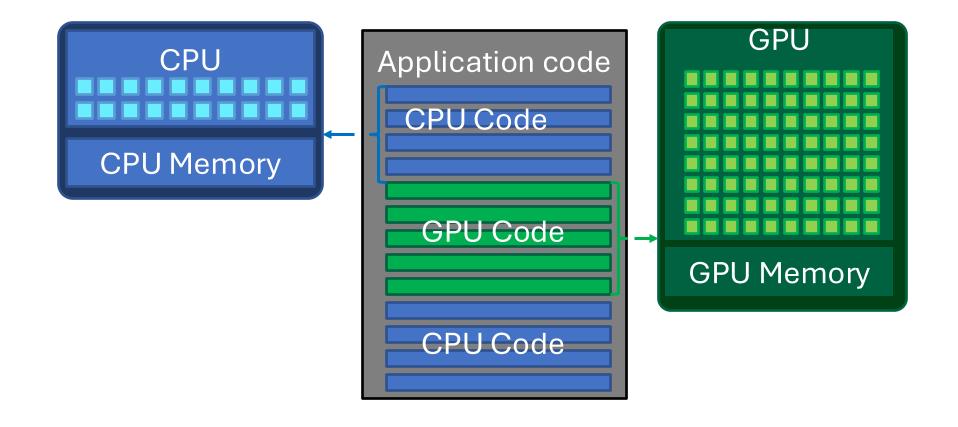
- GPU (A100)
 - □ 108 SM
 - □ 64 warps per SM (32 active at a time)
 - 32 threads per warp in double precision
 - ~200,000+ way parallelism (108*64*32) per GPU



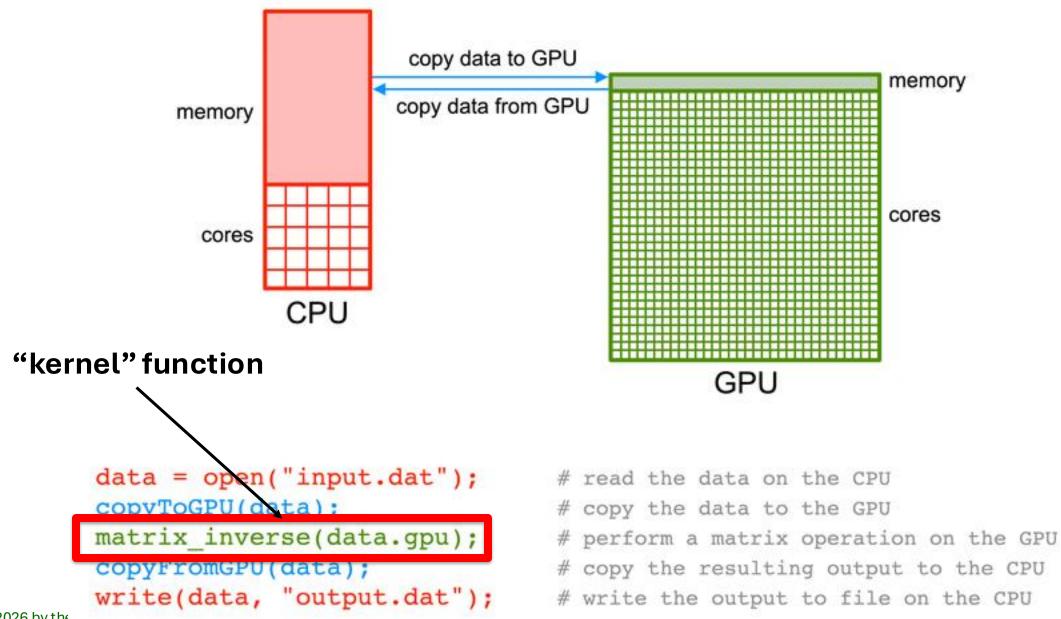


1,500 GB/Sec Memory Bandwidth

Heterogeneous Programming (CPU+GPU)



Data Movement



3 Ways of GPU Acceleration

Applications

GPU-accelerated libraries

OpenACC Directives

Programming Languages

Seamless linking to GPU-enabled libraries.

cuFFT, cuBLAS, Thrust, NPP, IMSL, CULA, cuRAND, etc. Simple directives for easy GPUacceleration of new and existing applications

PGI Accelerator

Most powerful and flexible way to design GPU accelerated applications

C/C++, Fortran, Python, Java, etc.

3 Ways of GPU Acceleration

Applications

Libraries

OpenACC Directives

Programming Languages

"Drop-in"
Acceleration

Easily Accelerate Applications

Maximum Flexibility

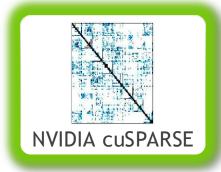
GPU Accelerated Libraries

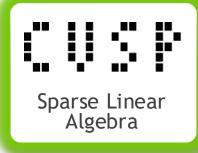




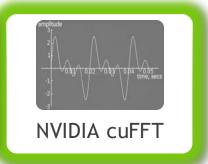












Thrust: Rapid Parallel C++ Development

- Resembles C++ STL
- High-level interface
 - Enhances developer productivity
 - Enables performance portability
 between GPUs and multicore CPUs
- Flexible
 - CUDA, OpenMP, and TBB backends
 - Extensible and customizable
 - Integrates with existing software
- Open source



```
generate 32M random numbers on host
thrust::host vector<int> h vec(32 << 20);</pre>
thrust::generate(h vec.begin(),
                 h vec.end(),
                 rand);
// transfer data to device (GPU)
thrust::device vector<int> d vec = h vec;
// sort data on device
thrust::sort(d vec.begin(), d vec.end());
// transfer data back to host
thrust::copy(d vec.begin(),
             d vec.end(),
             h vec.begin());
```

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

3 Ways of GPU Acceleration

Applications

Libraries

OpenACC Directives

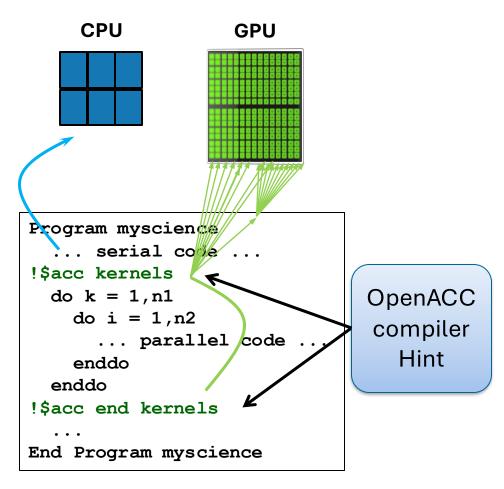
Programming Languages

"Drop-in"
Acceleration

Easily Accelerate Applications

Maximum Flexibility

OpenACC Directives



Your original Fortran or C code

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

Easy

Open

Powerful

3 Ways of GPU Acceleration



Libraries

OpenACC Directives

Programming Languages

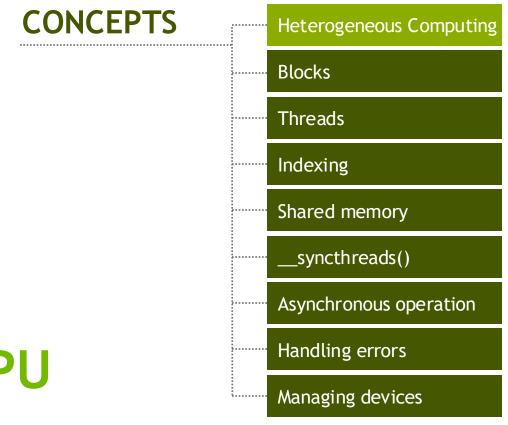
"Drop-in"
Acceleration

Easily Accelerate Applications

Maximum Flexibility

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- Program a GPU with CUDA



PROGRAM A GPU WITH CUDA

Heterogeneous Computing

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

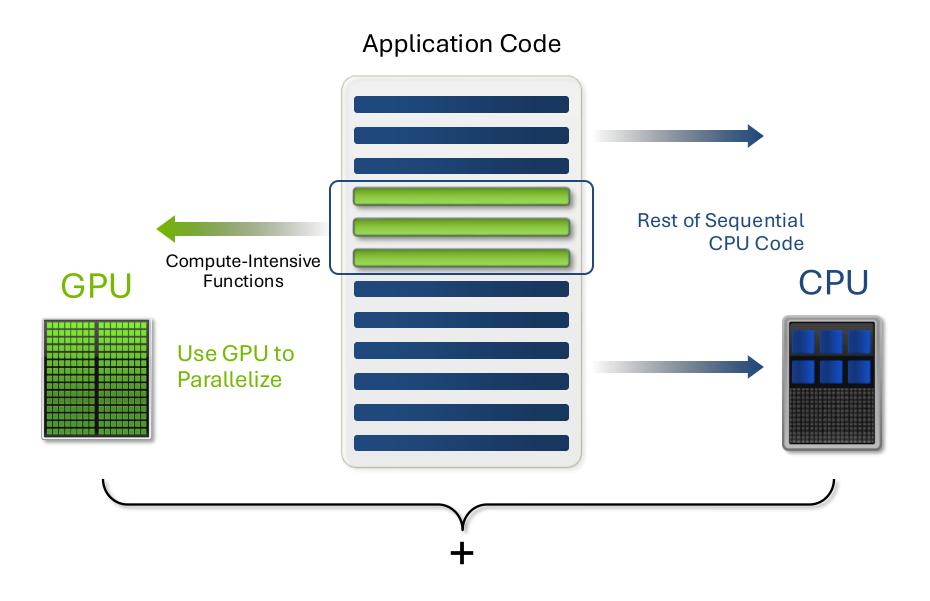




Host: the CPU and its memory

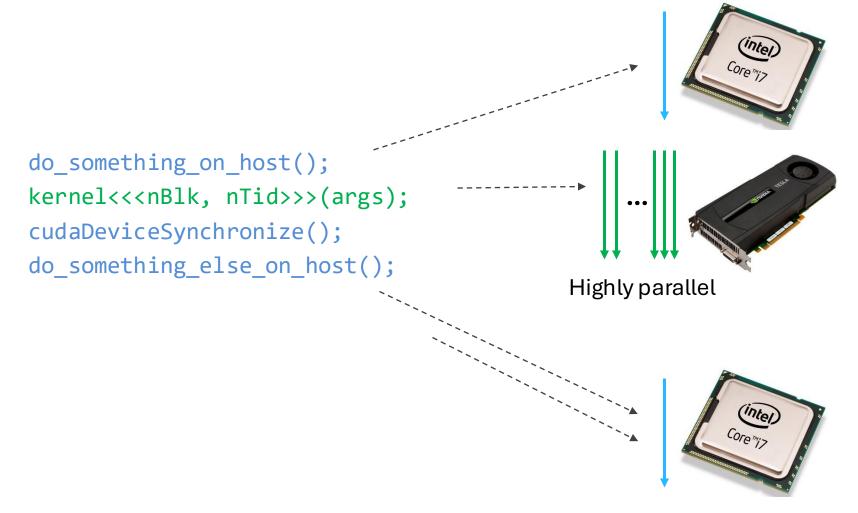
Device: the GPU and its memory

CPU-GPU Heterogeneous Computing

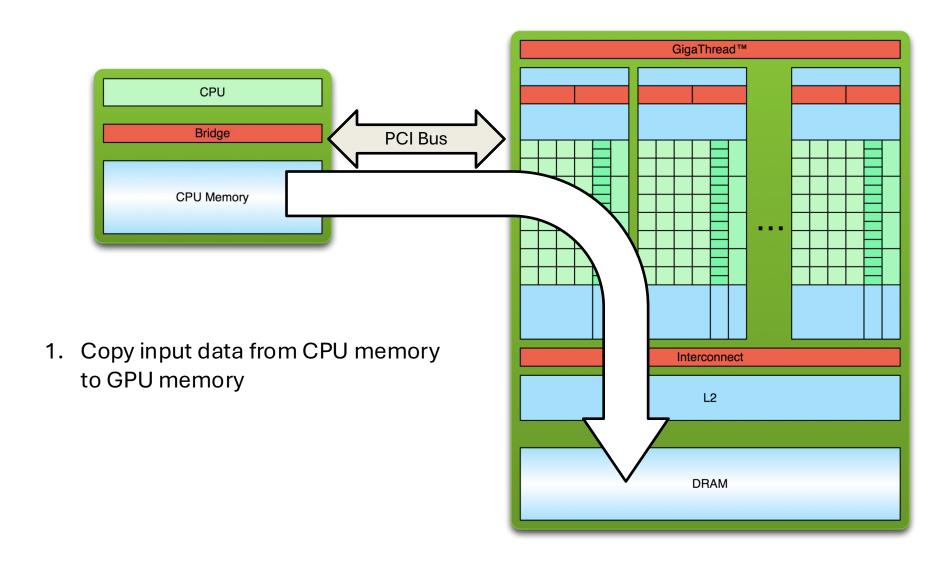


Heterogeneous Computing with CUDA

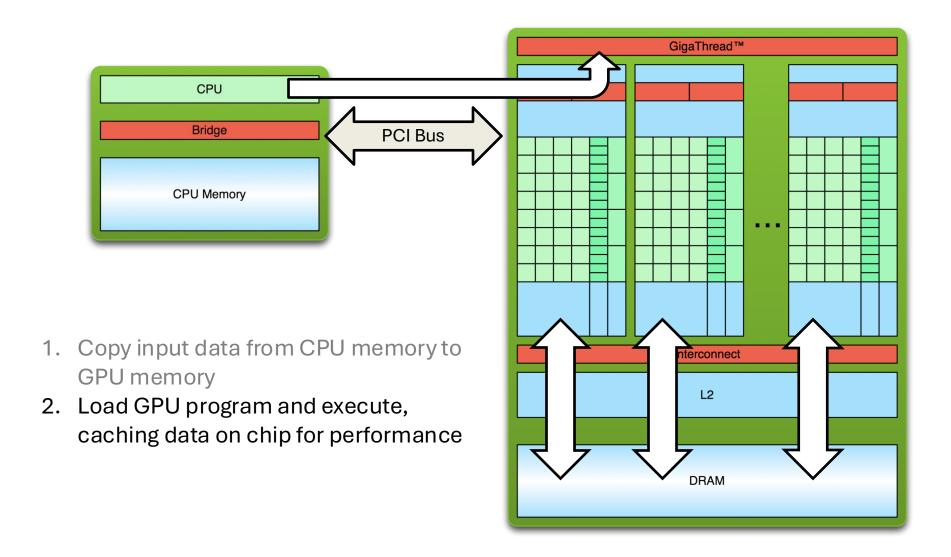
CUDA Compute Unified Device Architecture



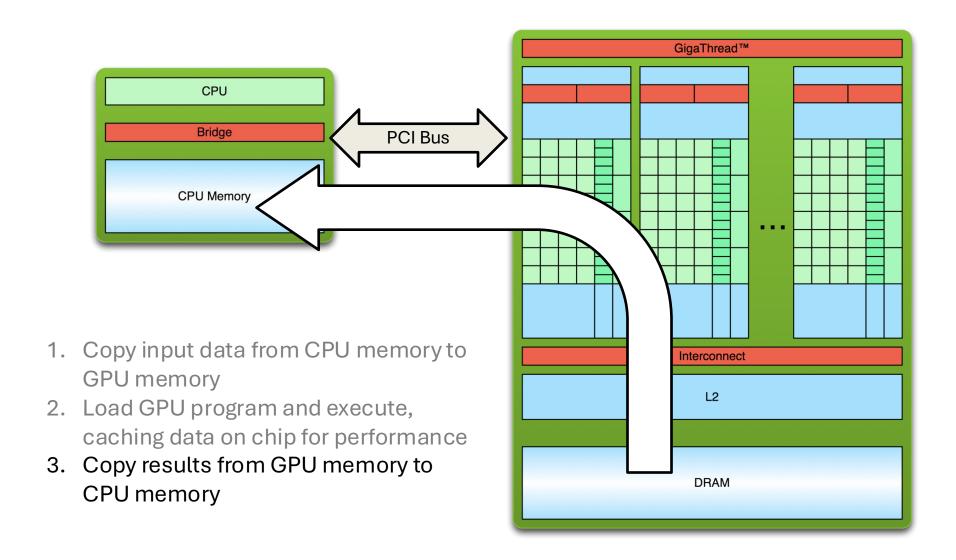
Simple Processing Flow



Simple Processing Flow



Simple Processing Flow



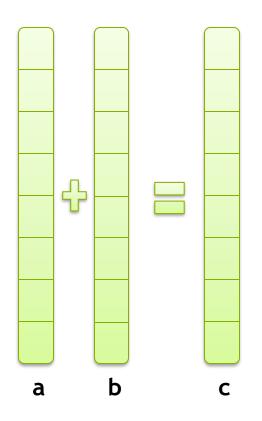
Heterogeneous Computing with CUDA C

Let's start with simply adding two integers

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

- Here __global__ is a CUDA C/C++ keyword meaning
 - □ add () will execute on the device
 - add () will be called from the host

Vector Addition



Addition on the Device

Note that we use pointers for the variables

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

- add () runs on the device, so a, b and c must point to device memory
- We need to allocate memory on the GPU

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: main()

```
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 = sizeof(int);
      // Allocate space for device copies of a, b, c
      cudaMalloc((void **)&d_a, size);
      cudaMalloc((void **)&d b, size);
      cudaMalloc((void **)&d_c, size);
      // Setup input values
      a = 2;
      b = 7;
```

Vector Addition on the Device: main()

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

CONCEPTS

Heterogeneous Computing

Blocks

Threads

Indexing

Shared memory

__syncthreads()

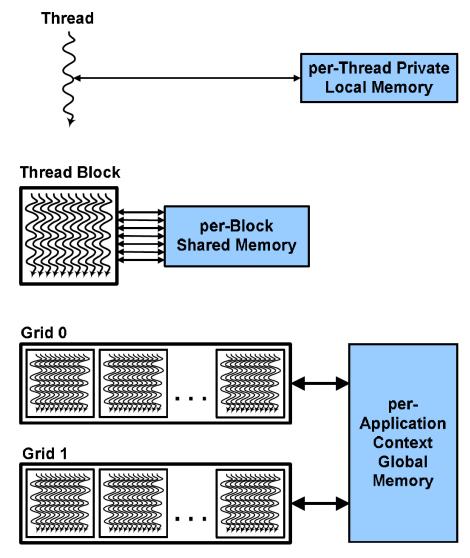
Asynchronous operation

Handling errors

Managing devices

RUNNING IN PARALLEL

Multi-level Threading Model



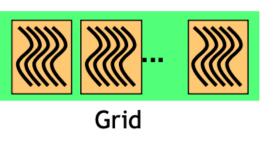
CUDA Hierarchy of threads, blocks, and grids, with corresponding per-thread private, per-block shared, and per-application global memory spaces.

Execution Model

Software

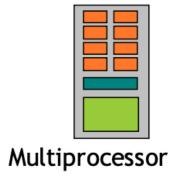


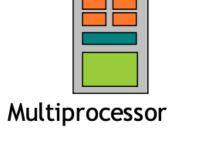


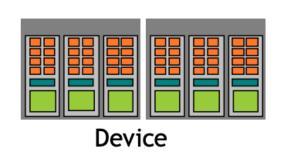


Hardware









Threads are executed by scalar processors

Thread blocks are executed on multiprocessors

Thread blocks do not migrate

Several concurrent thread blocks can reside on one multiprocessor - limited by multiprocessor resources (shared memory and register file)

A kernel is launched as a grid of thread blocks

Moving to Parallel Execution

GPU computing is about massive parallelism

So how do we run code in parallel on the device?

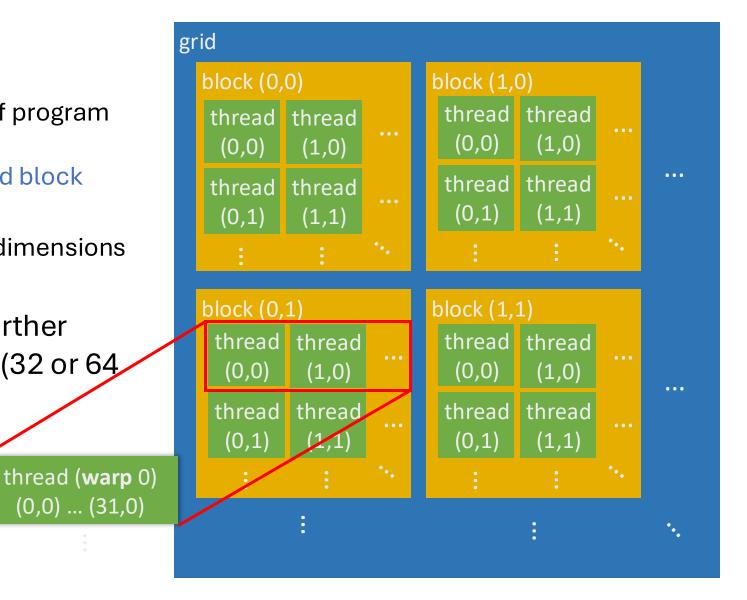
```
add<<< 1, 1 >>>();

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

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

Hierarchical Programming Model

- Multi-level hierarchy
 - □ The thread is the smallest unit of program execution
 - Threads are organized in a thread block
 - Blocks form a grid
 - Block and grid have up to three dimensions
- Threads within a block are further implicitly divided into warps (32 or 64 threads)
- Choose a certain level of granularity given a problem



60

Vector Addition on the Device

- With add() running in parallel we can do vector addition
- 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 blockIdx.x

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

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

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

Vector Addition on the Device: main()

```
#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()

```
// 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 N copies of add() with add<<<N, 1>>>(...);
 - □ Use blockIdx.x to access block index

CONCEPTS

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Threads

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Shared memory

__syncthreads()

Asynchronous operation

Handling errors

Managing devices

INTRODUCING THREADS

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];
}
```

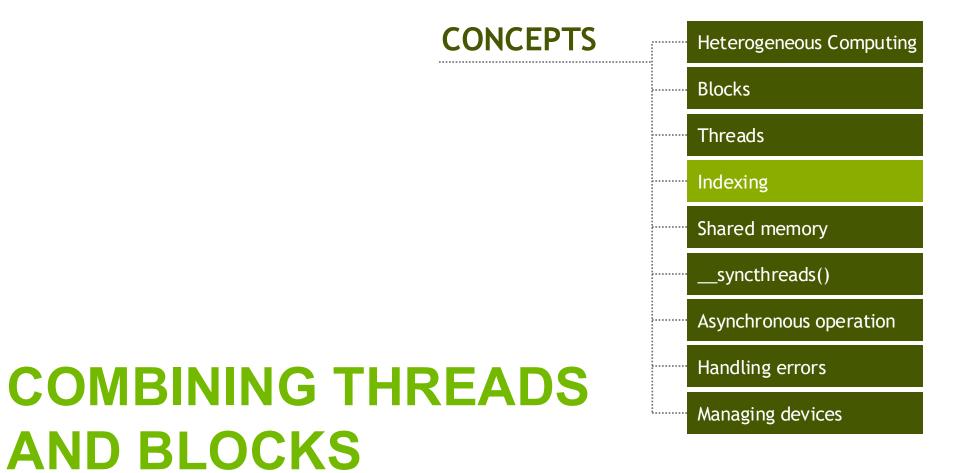
- We use threadIdx.x instead of blockIdx.x
- Need to make one change in main()...

Vector Addition Using Threads: main()

```
#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);
```

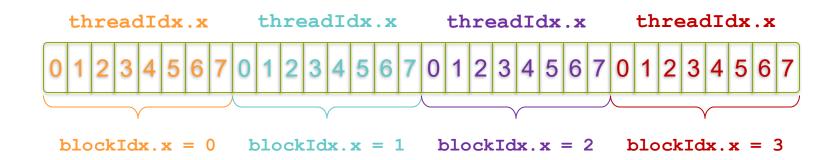
Vector Addition Using Threads: main()

```
// 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
                                                            "kernel" function
       cudaMemcpy(c, d c, size, cudaMemcpyDeviceToHost);
       // Cleanup
       free(a); free(b); free(c);
       cudaFree(d a); cudaFree(d b); cudaFree(d c);
       return 0;
```



Indexing Arrays with Blocks and Threads

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

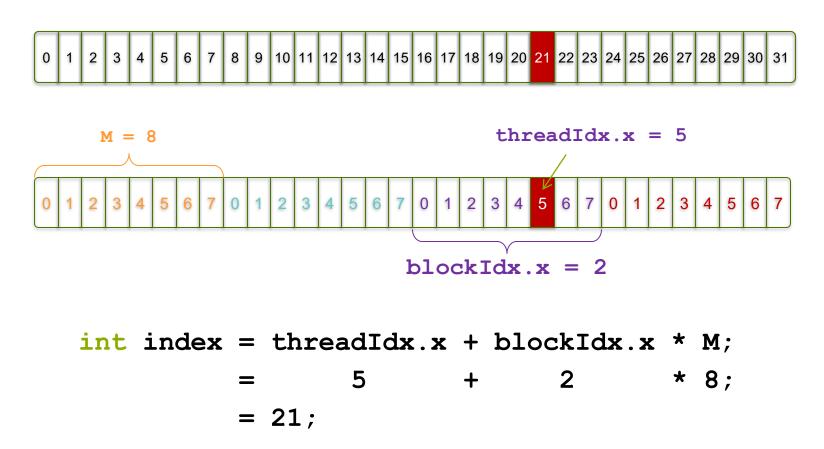


With M threads/block a unique index for each thread is given by

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

Indexing Arrays: Example

Which thread will operate on the red element?



Vector 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()

```
#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()

```
// 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>
Check bound
```

Update the kernel launch:

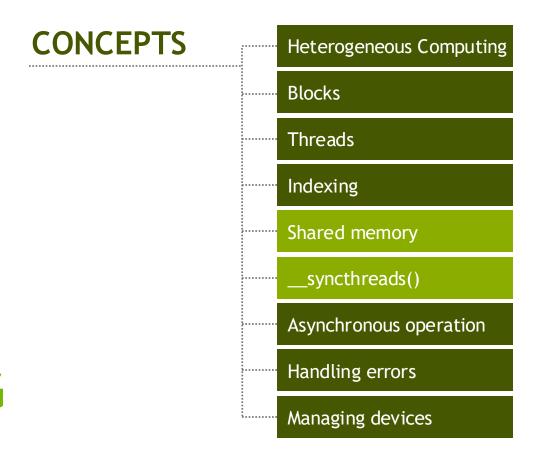
```
add<<<(N-1) / M + 1 M \rightarrow > (d_a, d_b, d_c, N);
```

Why Bother with Threads?

- Threads seem unnecessary
 - They add a level of complexity
 - What do we gain?

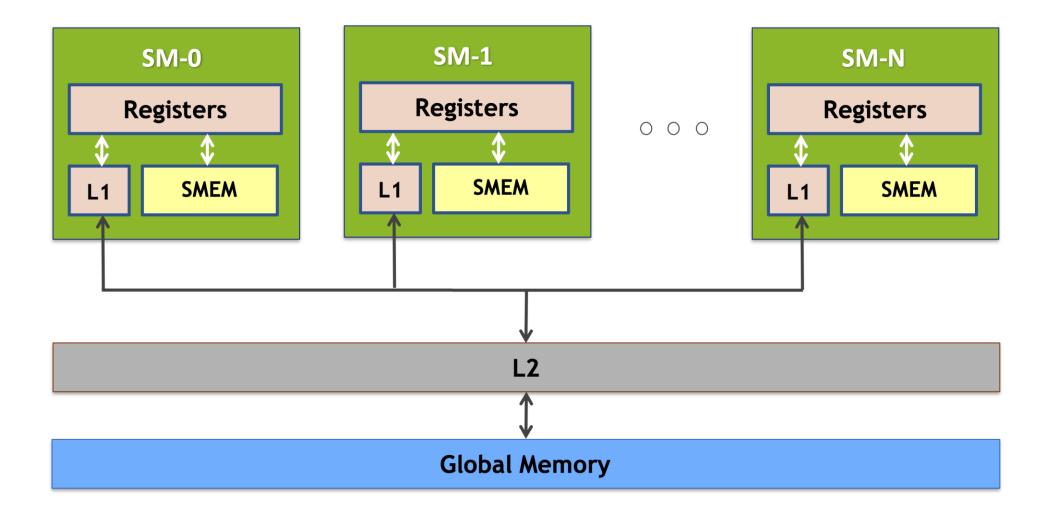
- Unlike parallel blocks, threads have mechanisms to:
 - Communicate
 - Synchronize

To look closer, we need a new example...



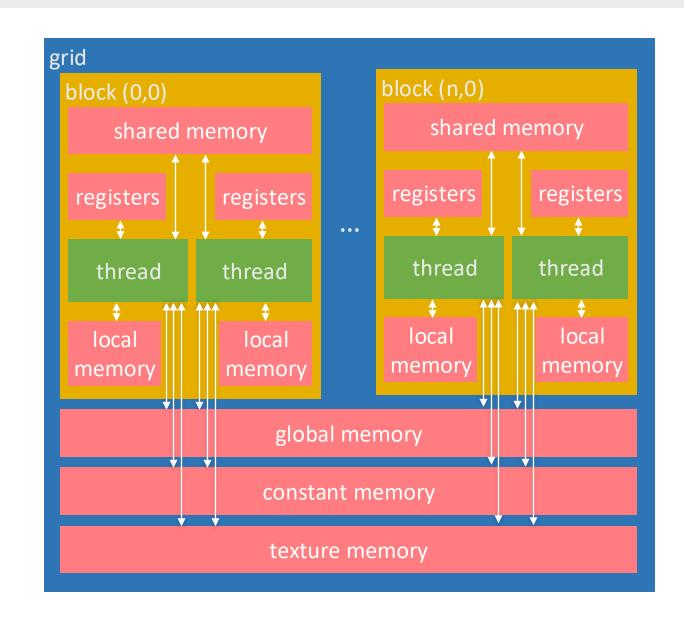
COOPERATING THREADS

GPU memory hierarchy



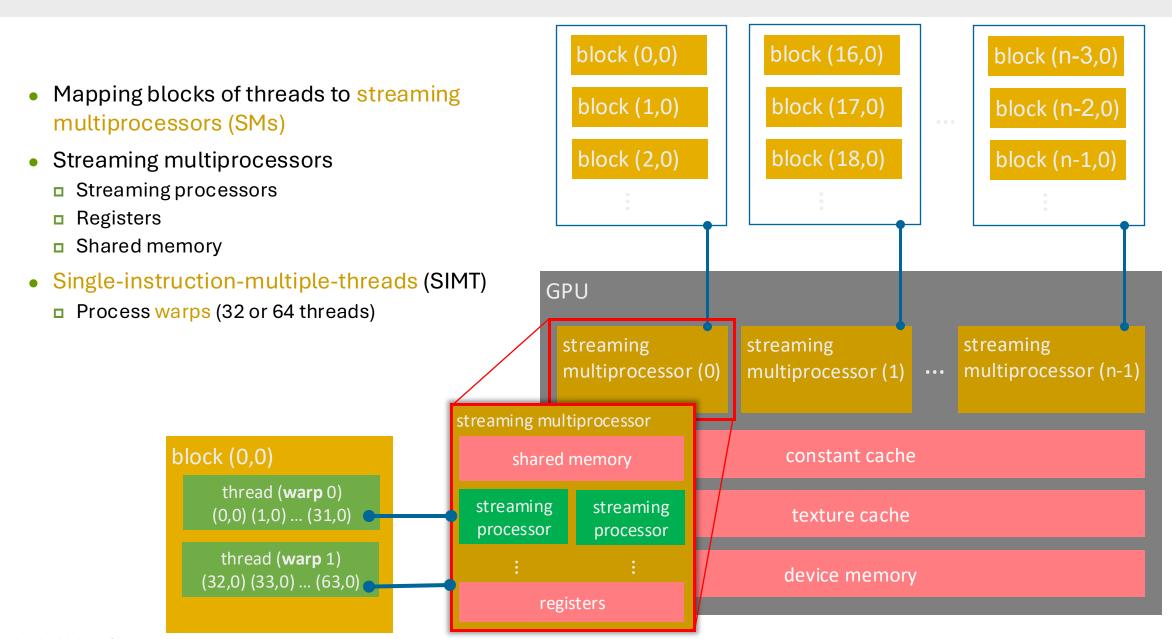
Memory Model

- Define memory hierarchy
- Registers (VGPR, SGPR)
 - Local variables per thread
 - The fastest memory
- Local memory
 - local variables per thread
 - Slow off-chip memory (VRAM)
 - Register spills if not enough registers
- Shared memory (Local data share)
 - Shared between threads in a block
 - Faster on-chip memory
- Global memory
 - Shared with all blocks
 - Largest memory
 - Slow off-chip memory (VRAM)
- Texture and constant memory
 - Cached differently, on off-chip memory



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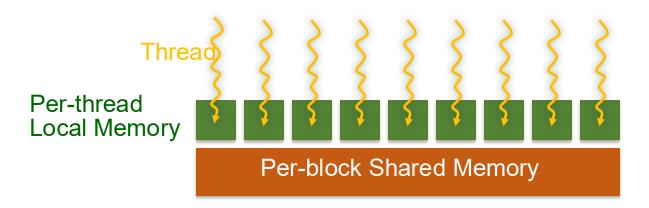
Execution Model



Shared (within a block) Memory

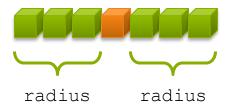
- Declare using __shared__, allocated per block
- Fast on-chip memory, user-managed
- Not visible to threads in other blocks

Thread Block (up to 1024 threads)



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

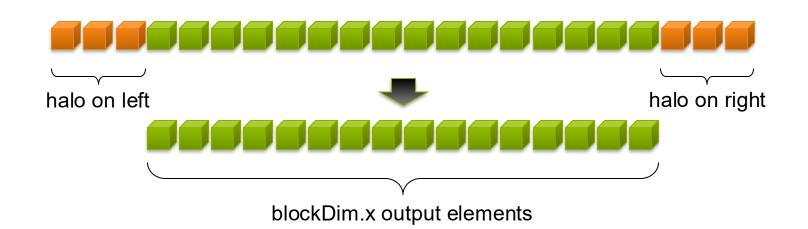
Extremely fast on-chip memory, user-managed

• Declare using shared , allocated per block

Data is not visible to threads in other blocks

Implementing With Shared Memory

- Cache data in shared memory (N = blockDim.x)
 - Read (N + 2 * radius) input elements from global memory to shared memory
 - □ Compute *N* output elements
 - Write N output elements to global memory
 - Each block needs a halo of radius elements at each boundary



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

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

Any problem?

Data Race!

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

__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

```
_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)
   syncthreads();
```

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

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

Review (1 of 2)

- Launching parallel threads
 - □ Launch N blocks with M threads per block with kernel <<< N, M>>> (...);
 - □ Use blockIdx.x to access block index within grid
 - □ Use threadIdx.x to access thread index within block

Allocate elements to threads:

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

Review (2 of 2)

- Use <u>__shared__</u> to declare a variable/array in shared memory
 - Data is shared between threads in a block
 - Not visible to threads in other blocks

- Use syncthreads () as a barrier
 - Use to prevent data hazards

CONCEPTS

Heterogeneous Computing

Blocks

Threads

Indexing

Shared memory

__syncthreads()

Asynchronous operation

Handling errors

Managing devices

MANAGING THE DEVICE

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<sup>†</sup>
```

[†] requires OS and device support

CUDA Summary

- GPU Architecture for Data Parallelism
- GPU Programming Model: SIMT
- Write and launch CUDA C/C++ kernels

```
□ __global__, blockIdx.x, threadIdx.x, <<<>>>
```

- Manage GPU memory
 - cudaMalloc(), cudaMemcpy(), cudaFree()
- Manage communication and synchronization

```
shared__, __syncthreads()
```

- cudaMemcpy() vs.cudaMemcpyAsync()
- cudaDeviceSynchronize()