# **ACES: GPU Programming**

### Introduction to CUDA



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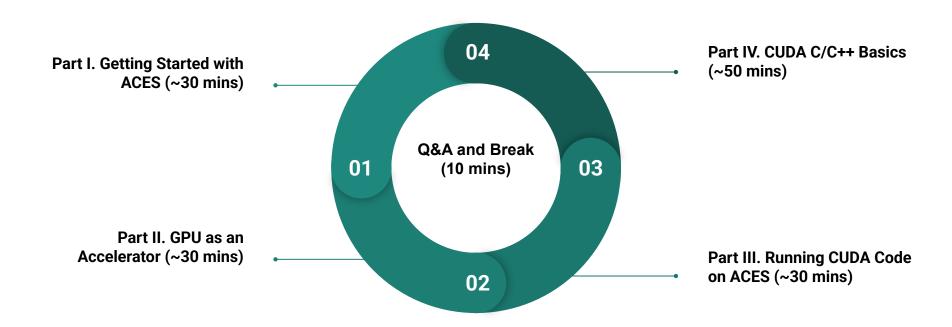








### **Introduction to CUDA Programming**



# Part I. Get Started with ACES



### **NSF ACES**

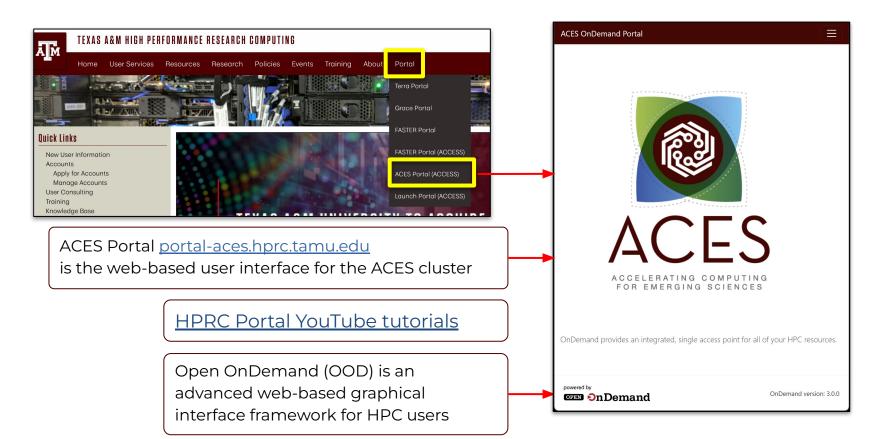
### Accelerating Computing for Emerging Sciences

#### Our Mission:

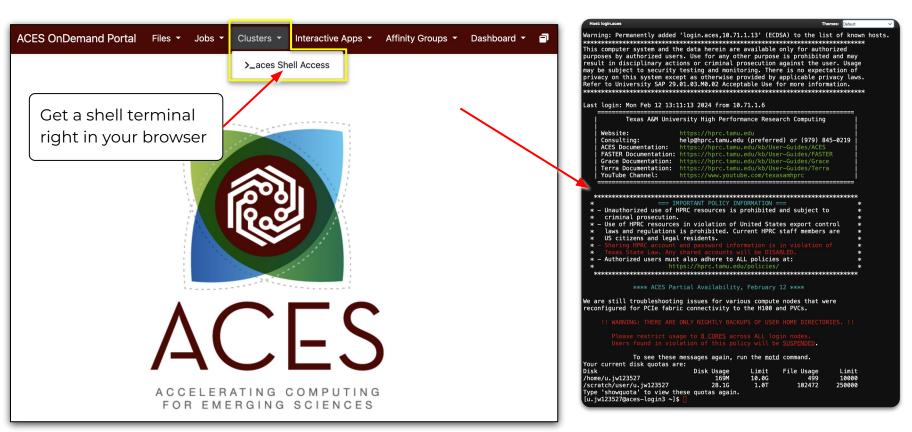
- NSF Advanced Computing Systems & Services (ACSS) CI test-bed
- Offer an accelerator testbed for numerical simulations and AI/ML workloads
- Provide consulting, technical guidance, and training to researchers
- Collaborate on computational and data-enabled research.



### **ACES Portal**

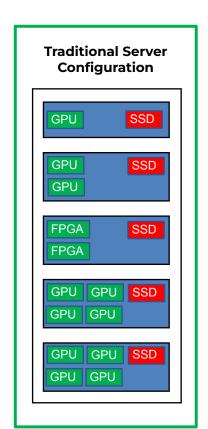


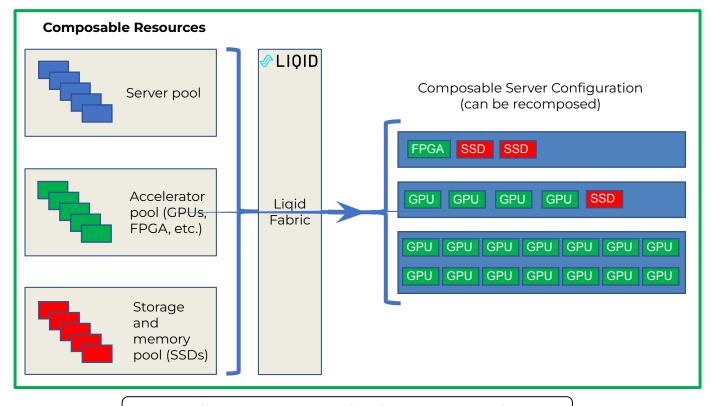
### Shell Access via the Portal





### Composability





https://hprc.tamu.edu/kb/User-Guides/ACES

### **NSF ACES**

### Accelerating Computing for Emerging Sciences

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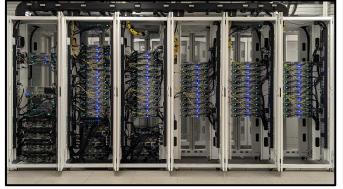


### **ACES In Action**









#### **ACES Configuration NEC VE** Node Ice Lake Nodes (15) Data Management Login Development Transfer Nodes (4) Nodes (3) Hosts Nodes (2) Graphcore Bow POD16 **Lustre System NDR InfiniBand** 2.54 PB usable Graphcore Colossus POD16 **SPR SPR SPR** SPR **SPR SPR** SPR **SPR** Nodes (12) **Nodes (15) Nodes (15)** Nodes (12) **Nodes (13) Nodes (13) Nodes (15) Nodes (15)** Composable Composable Composable Composable Composable Composable Composable Composable PCle Gen4 PCle Gen4 PCle Gen4 PCle Gen4 PCIe Gen5 PCle Gen5 PCle Gen5 PCIe Gen5 **Intel PVC Intel PVC** Intel PVC Intel PVC **Intel PVC** Intel PVC Intel PVC **NVIDIA H100 Optane SSD Optane SSD NVIDIA A30 Optane SSD NVIDIA H100** NextSilicon Intel FPGA BittWare FPGA BittWare FPGA



# **ACES System Description**

Component	Quantity	Description	
Sapphire Rapids Nodes: Compute Nodes Data Transfer Nodes Login & Management Nodes	110 nodes 2 nodes 5 nodes	96 cores per node, dual Intel Xeon 8468 processors 512 GB DDR5 memory 1.6 TB NVMe storage Compute: NVIDIA Mellanox NDR 200 Gbps InfiniBand adapter DTNs & Login & Management nodes: 100 Gbps Ethernet adapter	
Ice Lake Login & Management Nodes	2 nodes	64 cores per node, dual Intel Xeon 8352Y processors 512 GB DDR4 memory 1.6 TB NVMe storage NVIDIA Mellanox NDR 200 Gbps InfiniBand adapter	
PCIe Gen4 Composable Infrastructure	50 SPR nodes	Dynamically reconfigurable infrastructure that allows up to 20 PCIe cards (GPU, FPGA, etc.) per compute node	
PCIe Gen5 Composable Infrastructure	60 SPR nodes	Dynamically reconfigurable infrastructure that allows up to 16 H100s or 14 PVCs per compute node	
NVIDIA InfiniBand (IB) Interconnect	110 nodes	Two leaf and two spine switches in a 2:1 fat tree topology	
DDN Lustre Storage	2.5 PB usable	HDR IB connected flash and disk storage for Lustre file systems	

### **ACES Accelerators**

Component	Quantity	Description	
Graphcore IPU	32	16 Colossus GC200 IPUs, 16 Bow IPUs. Each IPU group hosted with a CPU servel as a POD16 on a 100 GbE RoCE fabric	
FPGAs:			
Intel PAC D5005	2	Accelerator with Intel Stratix 10 GX FPGA and 32 GB DDR4	
BittWare IA-840F	3	Accelerator with Agilex AGF027 FPGA and 64 GB of DDR4	
NextSilicon Coprocessor	2	Reconfigurable accelerator with an optimizer continuously evaluating application behavior.	
NEC Vector Engine	8	Vector computing card (8 cores and HBM2 memory)	
Intel Optane SSD	48	18 TB of SSDs addressable as memory w/ MemVerge Memory Machine.	
NVIDIA GPUs:			
H100	30	For HPC, DL Training, Al Inference	
A30	4	For Al Inference and Mainstream Compute	
Intel PVC GPUs	120	Intel GPUs for HPC, DL Training, Al Inference	

Refer to our Knowledge Base for more:

https://hprc.tamu.edu/kb/User-Guides/ACES/Hardware/



# **Accelerator Access Summary**

Component	Access	node or partition
BittWare IA-840F FPGA	Slurm	partition=bittware
Intel PAC D5005 FPGA	Slurm	partition=d5005
Intel GPU Max 1100 (PVC)	Slurm	partition=pvc
Intel Optane SSD	Slurm	partition=memverge
NextSilicon Coprocessor	Slurm	partition=nextsilicon
NVIDIA A30 GPUs	Slurm	partition=gpu
NVIDIA H100 GPUs	Slurm	partition=gpu
Graphcore Bow IPUs	Interactive	ssh poplar2
Graphcore Colossus IPUs	Interactive	ssh poplar1
NEC Vector Engine	Interactive	ssh dss



## Job Scripts on ACES: Slurm

```
#!/bin/bash
#NECESSARY JOB SPECIFICATIONS
                                          These parameters describe the
#SBATCH --job-name=my job
                                          resources needed for your program
#SBATCH --time=2-00:00:00
                                          to the job scheduler (Slurm)
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=96
                                                   Most of the ACES accelerators will
#SBATCH --mem=488G
                                                   be specified with either a partition
#SBATCH --partition=qpu
                                                   or gres argument
#SBATCH --gres=gpu:h100:2
#SBATCH --output=stdout.%x.%j
#SBATCH --error=stderr.%x.%j
# load required module(s)
module purge
                                          Script to execute
module load GCC/13.1.0
                                          (In this case, set up environment and
                                          launch an executable)
./my program.py
```

# Part II. GPU as an Accelerator



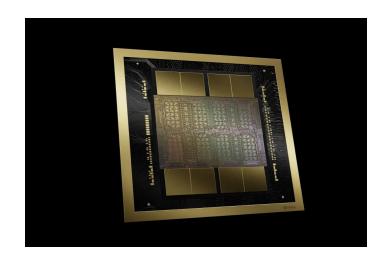
### **CPU**



### **GPU Accelerator**



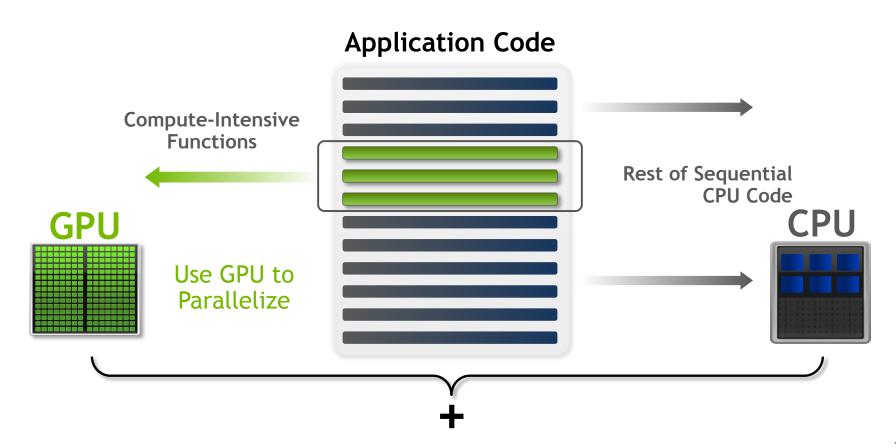
### **NVIDIA** Tesla B200 with 208 Billion Transistors



Announced and released in early 2025 was the Blackwell-based B200 accelerator. Built on TSMC's 4NP process, the B200 features 208 billion transistors and delivers up to 90 teraflops of FP64 performance, 20 petaflops of Al inference with FP4 precision, and incorporates NVIDIA's 6th-generation Tensor Cores. It includes 192GB of HBM3e memory with an impressive 8TB/s memory bandwidth.

17

## Add GPUs: Accelerate Science Applications



# 3 Ways to Accelerate Applications

# **Applications**

Libraries

OpenACC Directives

Programming Languages

"Drop-in"
Acceleration

Easily Accelerate Applications

Maximum Flexibility

# 3 Ways to Accelerate Applications

# **Applications**

Libraries

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Maximum Flexibility

### 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

### **NVIDIA CUDA-X GPU-Accelerated Libraries**

#### **CUDA Math Libraries**

GPU-accelerated math libraries lay the foundation for compute-intensive applications in areas such as molecular dynamics, computational fluid dynamics, computational chemistry, medical imaging, and seismic exploration.



#### cuBLAS

GPU-accelerated basic linear algebra (BLAS) library.

Learn More



#### **cuSOLVER**

GPU-accelerated dense and sparse direct solvers.

Learn More



#### cuDSS

GPU-accelerated direct sparse solver library.

Learn More



#### cuFFT

GPU-accelerated library for Fast Fourier Transform implementations.

Learn More



#### cuRAND

GPU-accelerated random number generation.

Learn More



#### **cuSPARSE**

GPU-accelerated BLAS for sparse matrices.

Learn More >



#### **cuTENSOR**

GPU-accelerated tensor linear algebra library.

Learn More >



#### **CUDA Math API**

GPU-accelerated standard mathematical function APIs.

Learn More >



#### AmgX

GPU-accelerated linear solvers for simulations and implicit unstructured methods.

Learn More

### **CUDA-accelerated Application with Libraries**

• **Step 1:** Substitute library calls with equivalent CUDA library calls saxpy ( ... ) 

■ cublasSaxpy ( ... )

```
• 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 -l cublas
```

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

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



**NVIDIA CUDA Tools & Ecosystem** 

# 3 Ways to Accelerate Applications

# **Applications**

Libraries

OpenACC Directives

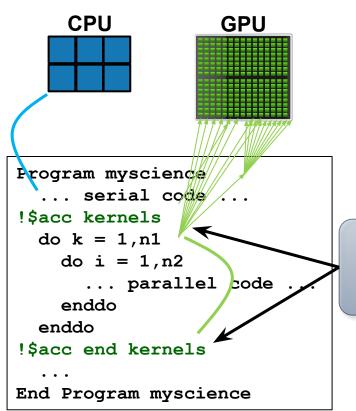
Programming Languages

"Drop-in"
Acceleration

Easily Accelerate Applications

Maximum Flexibility

### **OpenACC Directives**



OpenACC compiler Hint

Simple Compiler hints

Compiler Parallelizes code

Works on many-core GPUs & multicore CPUs

# **OpenACC**



### The Standard for GPU Directives

- **Easy:** Directives are the easy path to accelerate compute 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

# 3 Ways to Accelerate Applications

# **Applications**

Libraries

OpenACC Directives

Programming Languages

"Drop-in"
Acceleration

Easily Accelerate Applications

Maximum Flexibility

### **Learn More**

These languages are supported on all CUDA-capable GPUs. You might already have a CUDA-capable GPU in your laptop or desktop PC!

CUDA C/C++

http://developer.nvidia.com/cuda-toolkit

CuPy (Python)

https://developer.nvidia.com/pycuda

Thrust C++ Template Library

http://developer.nvidia.com/thrust

MATLAB

http://www.mathworks.com/discovery/matlab-gpu.html

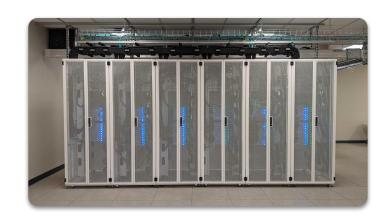
**CUDA Fortran** 

https://developer.nvidia.com/cuda-fortran

Mathematica

http://www.wolfram.com/mathematica/ new-in-8/cuda-and-opencl-support/

# Part III. Running CUDA Code on ACES

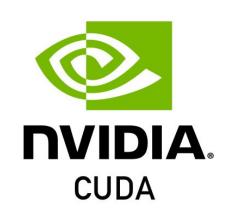




### **Running CUDA Code on ACES**

```
# load CUDA module
$ml CUDA/12.3.2
# copy sample code to your scratch space
$tar -zxvf cuda.exercise.tqz
# compile CUDA code
$cd CUDA
$cd hello world
$nvcc hello world host.cu
$./a.out
# edit job script & submit your GPU job
$sbatch aces cuda run.sh
```

# Part IV. CUDA C/C++ BASICS



### What is CUDA?

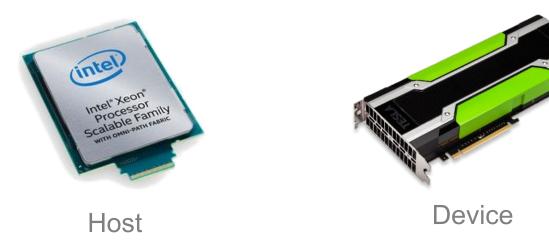
- CUDA Architecture
  - Used to mean "Compute Unified Device Architecture"
  - Expose GPU parallelism for general-purpose computing
  - Retain performance
- CUDA C/C++
  - Based on industry-standard C/C++
  - Small set of extensions to enable heterogeneous programming
  - Straightforward APIs to manage devices, memory etc.

# A Brief History of CUDA

- Researchers used OpenGL APIs for general purpose computing on GPUs before CUDA.
- In 2007, NVIDIA released first generation of Tesla GPU for general computing together their proprietary CUDA development framework.
- Current stable version of CUDA is 12.8 Update 1 (as of Apr 2025).

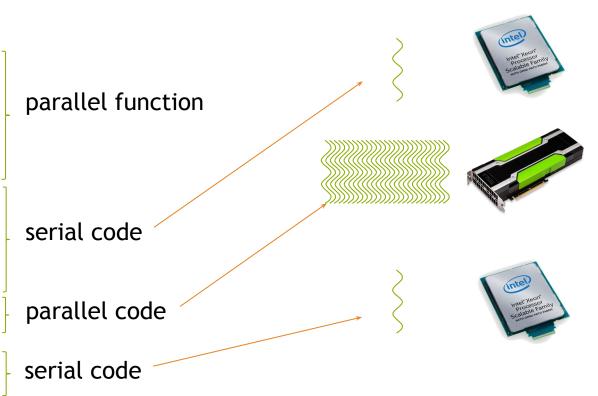
### **Heterogeneous Computing**

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

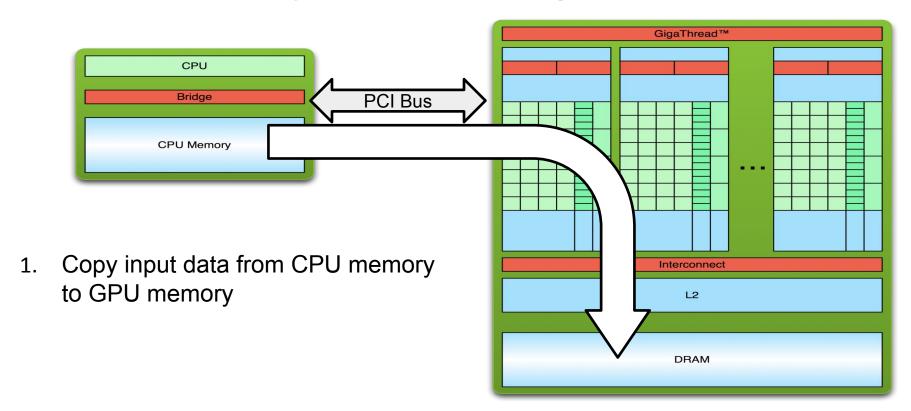


### **Heterogeneous Computing**

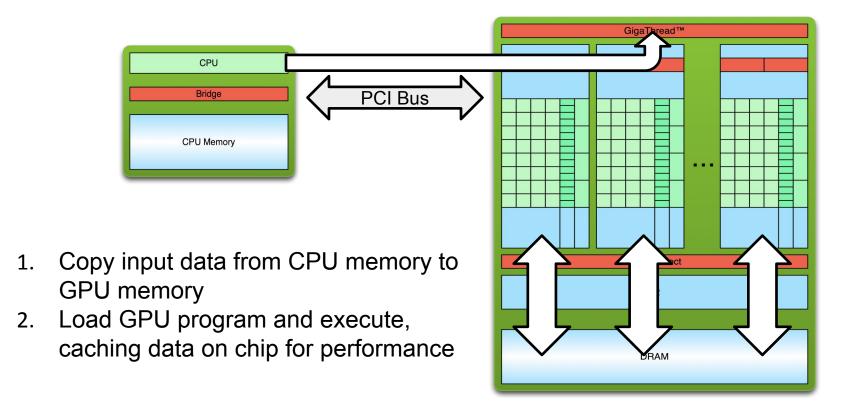
```
#include <iostream>
#include <algorithm>
using namespace std;
#define N 1024
#define RADIUS 3
#define BLOCK SIZE 16
__global__ void stencil_1d(int *in, int *out) {
                       shared__int temp[BLOCK_SIZE + 2 * RADIUS];
                     int gindex = threadIdx.x + blockIdx.x * blockDim.x;
                     int lindex = threadldx.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];
                     // Synchronize (ensure all the data is available)
                     __syncthreads();
                     // Apply the stencil
                     for (int offset = -RADIUS ; offset <= RADIUS ; offset++)
                                          result += temp[lindex + offset];
                     // Store the result
                     out[gindex] = result;
void fill_ints(int *x, int n) {
int main(void) {
                                        // host copies of a, b, c
                     int *d_in, *d_out; // device copies of a, b, c
                     int size = (N + 2*RADIUS) * sizeof(int);
                     // Alloc space for host copies and setup values
                    in = (int *)malloc(size); fill_ints(in, N + 2*RADIUS);
out = (int *)malloc(size); fill_ints(out, N + 2*RADIUS);
                     // Alloc space for device copies
                     cudaMalloc((void **)&d in, size);
                     cudaMalloc((void **)&d_out, size);
                     cudaMemcpy(d_in, in, size, cudaMemcpyHostToDevice);
                     cudaMemcpy(d out, out, size, cudaMemcpyHostToDevice);
                    // Launch stencil_1d() kernel on GPU
stencil_1d<<<N/BLOCK_SIZE,BLOCK_SIZE>>>(d_in + RADIUS, d_out +
RADIUS):
                     cudaMemcpy(out, d_out, size, cudaMemcpyDeviceToHost);
                     free(in); free(out);
                     cudaFree(d_in); cudaFree(d_out);
```



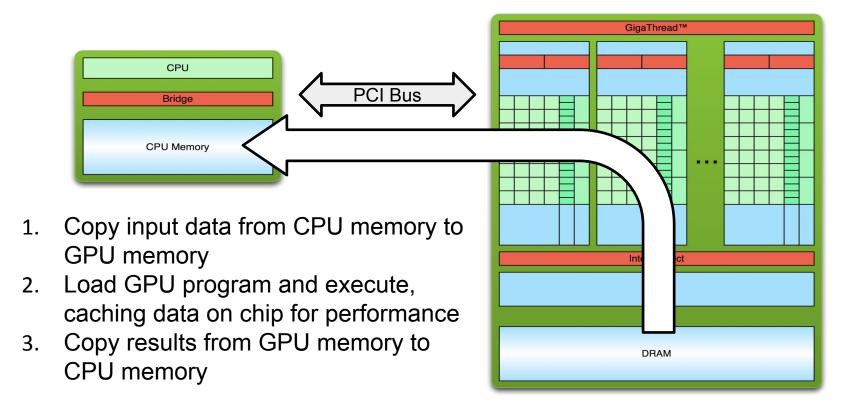
# **Simple Processing Flow**



# **Simple Processing Flow**



# **Simple Processing Flow**



#### **Hello World!**

```
int main(void) {
   printf("Hello World!\n");
   return 0;
}
```

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

#### Output:

```
$ nvcc hello_world.cu
$ ./a.out
$ Hello World!
```

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

Two new syntactic elements...

```
__global__ void mykernel(void) {
}
```

- CUDA C/C++ keyword global indicates a function that:
  - Runs on the device
  - Is called from host code
- nvcc separates source code into host and device components
  - Device functions (e.g. mykernel ()) processed by NVIDIA compiler
  - Host functions (e.g. main ()) processed by standard host compiler
    - gcc, icc, etc.

- 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!

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

#### Output:

```
$nvcc hello.cu
$./a.out
Hello World!
```

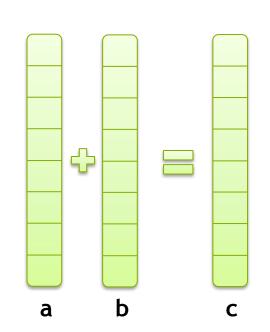
mykernel() does nothing!

# 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

### 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

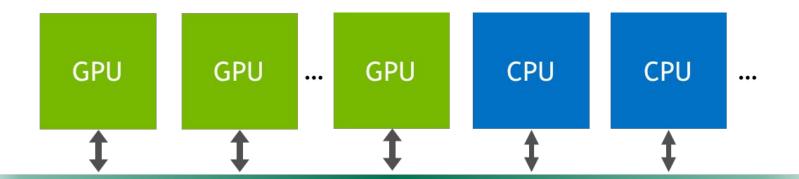
Host pointers point to CPU memory
 May be passed to/from device code
 May not be dereferenced in device code



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

# **Unified Memory**

Software: CUDA 6.0 in 2014 Hardware: Pascal GPU in 2016



**Unified Memory** 

# **Unified Memory**

- A managed memory space where all processors see a single coherent memory image with a common address space.
- Memory allocation with cudaMallocManaged().
- Synchronization with cudaDeviceSynchronize().
- Eliminates the need for cudaMemcpy ().
- Enables simpler code.
- Hardware support since Pascal GPU.

# 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()

```
int main(void) {
                // host copies of a, b, c
    int 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;
```

# 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;
```

# **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 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 element of the array.

#### **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:

```
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];
```

### 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 set up 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;
```

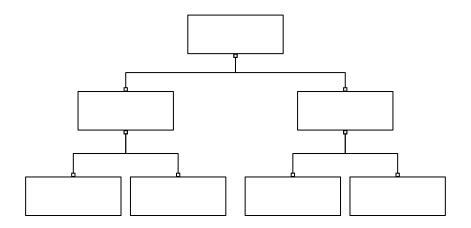
### **Vector Addition with Unified Memory**

```
global void VecAdd(int *ret, int a, int b) {
   ret[blockIdx.x] = a + b + blockIdx.x;
int main() {
    int *ret;
    cudaMallocManaged(&ret, 1000 * sizeof(int));
   VecAdd<<< 1000, 1 >>>(ret, 10, 100);
    cudaDeviceSynchronize();
    for(int i=0; i<1000; i++)
       printf("%d: A+B = %d\n", i, ret[i]);
    cudaFree(ret);
   return 0:
```

# **Vector Addition with Managed Global Memory**

```
device managed int ret[1000];
global void VecAdd(int *ret, int a, int b) {
   ret[blockIdx.x] = a + b + blockIdx.x;
int main() {
   VecAdd<<< 1000, 1 >>>(ret, 10, 100);
   cudaDeviceSynchronize();
    for(int i=0; i<1000; i++)</pre>
       printf("%d: A+B = %d\n", i, ret[i]);
   return 0;
```

# **Hierarchy of Threads**



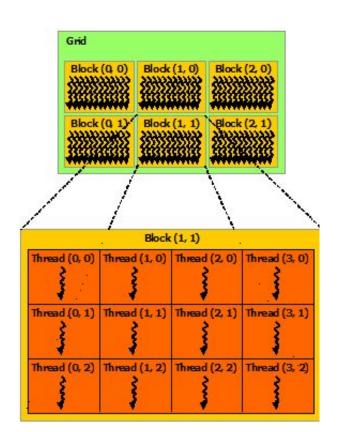
# **Key Programming Abstractions**

Three key abstractions that are exposed to CUDA programmers as a minimal set of language extensions:

- a hierarchy of thread groups
- shared memories
- barrier synchronization

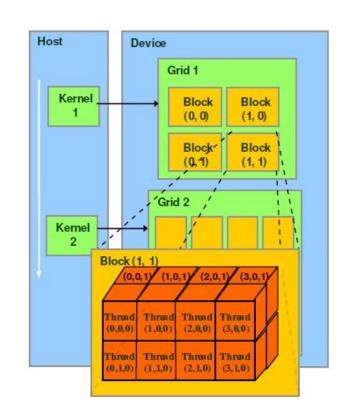
# **Glossary**

- Thread is an abstract entity that represents the execution of the kernel, which is a small program or a function.
- Grid is a collection of Threads. Threads in a Grid execute a Kernel Function and are divided into Thread Blocks.
- Thread Block is a group of threads which execute on the same multiprocessor (SMX). Threads within a Thread Block have access to shared memory and can be explicitly synchronized.



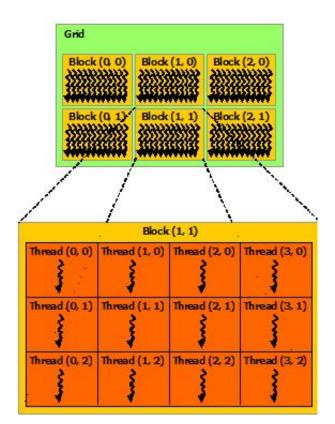
# **Thread Hierarchy - I**

- 1D, 2D, or 3D threads can form 1D,
   2D, or 3D thread blocks.
- 1D, 2D, or 3D blocks can form 1D,
   2D, or 3D grid of thread blocks
- The number of threads per block and the number of blocks per grid are specified in the <<<...>>> syntax.



# **Thread Hierarchy - II**

- Each block within the grid can be identified by an index accessible within the kernel through the built-in 3-component vector blockIdx.
- The dimension of the thread block is accessible within the kernel through the built-in 3-component vector blockDim.



#### Thread Index and Thread ID

• 1D thread ID is the same as the index of a thread

#### • 2D

for a two-dimensional block of size (blockDim.x, blockDim.y), the thread ID of a thread of index (x, y) is (x + y \* blockDim.x)

#### • 3D

```
for a three-dimensional block of size (blockDim.x, blockDim.y, blockDim.z), the thread ID of a thread of index (x, y, z) is (x + y * blockDim.x + z * blockDim.x * blockDim.y)
```

# Indexing Arrays with Blocks and Threads

Consider indexing an array with one element per thread (8 threads/block)

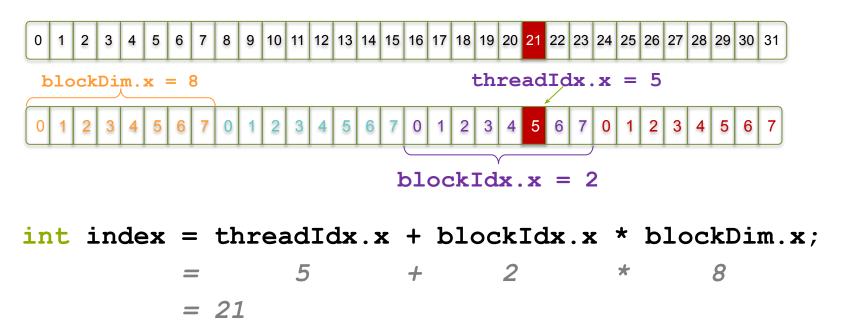
```
threadIdx.x threadIdx.x threadIdx.x threadIdx.x 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6 7 0 1 2 3 4 5 6
```

• With blockDim.x threads/block, the thread is given by:

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

# **Indexing Arrays: Example**

Which thread will operate on the red element?



# **Handling Arbitrary Vector Sizes**

Typical problems are not friendly multiples of

```
blockDim.x
```

Avoid accessing beyond the end of the arrays:

```
__global__ void VecAdd(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];
}
Update the kernel launch: M = blockDim.x
        VecAdd<<<(N + M-1) / M, M>>>(A, B, C, N);
```

# Why Bother with Threads?

- Threads seem unnecessary
  - They add a level of complexity
  - What do we gain?
- Threads within a block can cooperate by sharing data through shared memory
- by synchronizing their execution to coordinate memory accesses with \_\_syncthreads()

# **Managing Devices**



# **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

```
Select current device: cudaSetDevice(i)
For peer-to-peer copies: cudaMemcpy(...)
```

#### **More Resources**

You can learn more about CUDA at

- CUDA Programming Guide (<u>docs.nvidia.com/cuda</u>)
- CUDA Zone tools, training, etc.(developer.nvidia.com/cuda-zone)
- Download CUDA Toolkit & SDK (<u>www.nvidia.com/getcuda</u>)
- Nsight IDE (Eclipse or Visual Studio)(www.nvidia.com/nsight)

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# **HPRC Survey**

https://u.tamu.edu/hprc\_shortcourse\_survey



**HPRC Survey**