Summer School

e-Science with Many-core CPU/GPU Processors

Lecture 2

Introduction to CUDA

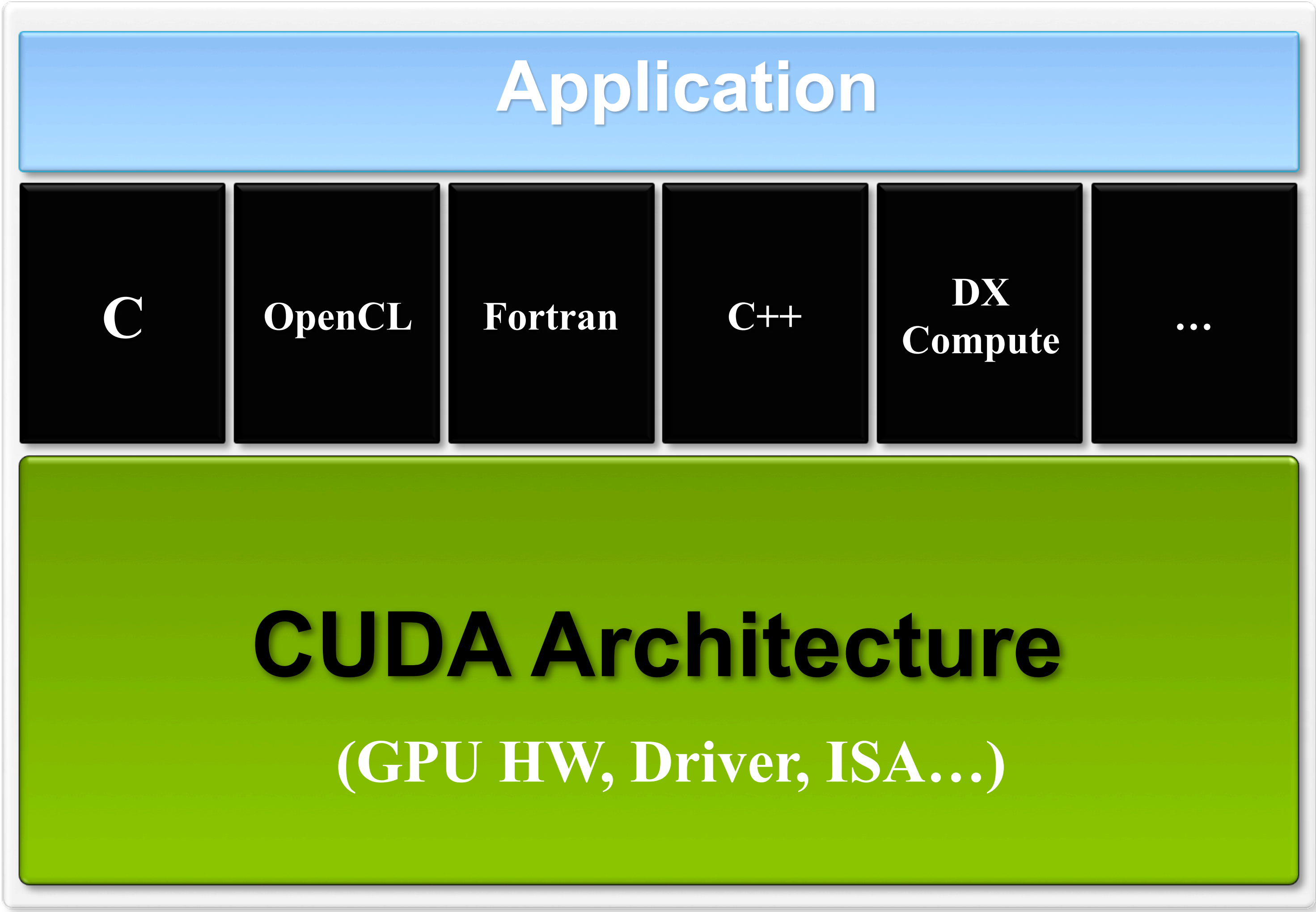
Braga, Portugal, June 14-18, 2010

Overview

- CUDA programming model – basic concepts and data types
- CUDA application programming interface - simple examples to illustrate basic concepts and functionalities
- Performance features will be covered later

Many Language/API Choices

- C/C++
- OpenCL
- DirectX Compute
- Fortran
- Java
- Python
- .Net
- …



CUDA - C with no shader limitations

- Integrated host+device app C program
  - Serial or modestly parallel parts in **host** C code
  - Highly parallel parts in **device** SPMD kernel C code

Serial Code (host)

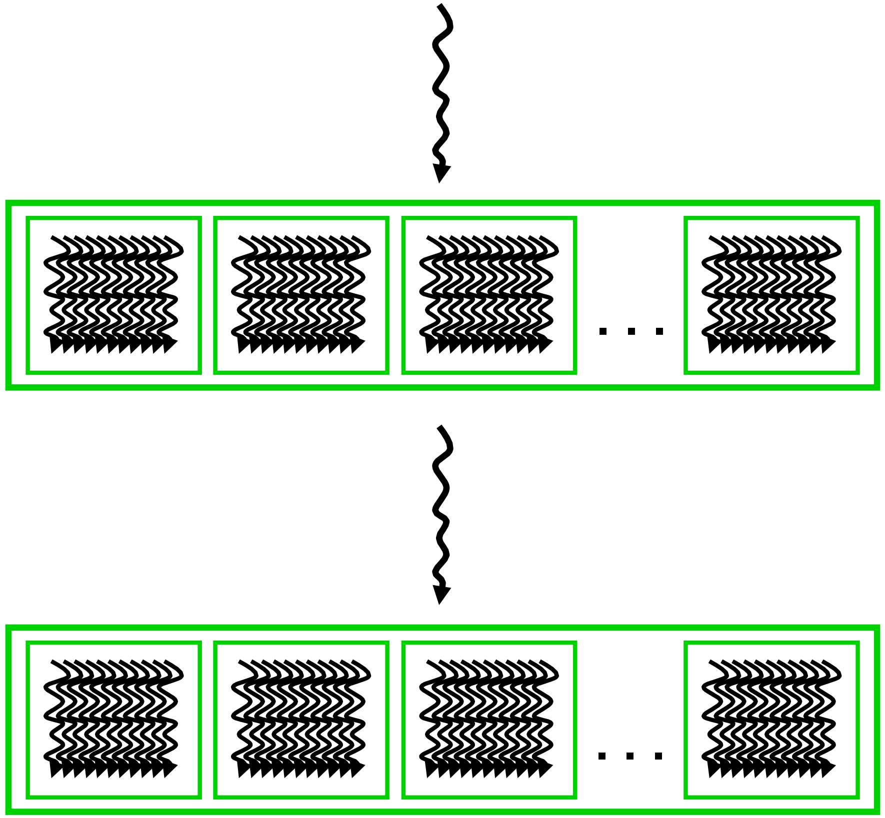
Parallel Kernel (device)

KernelA<<< nBlk, nTid >>>(args);

Serial Code (host)

Parallel Kernel (device)

KernelB<<< nBlk, nTid >>>(args);

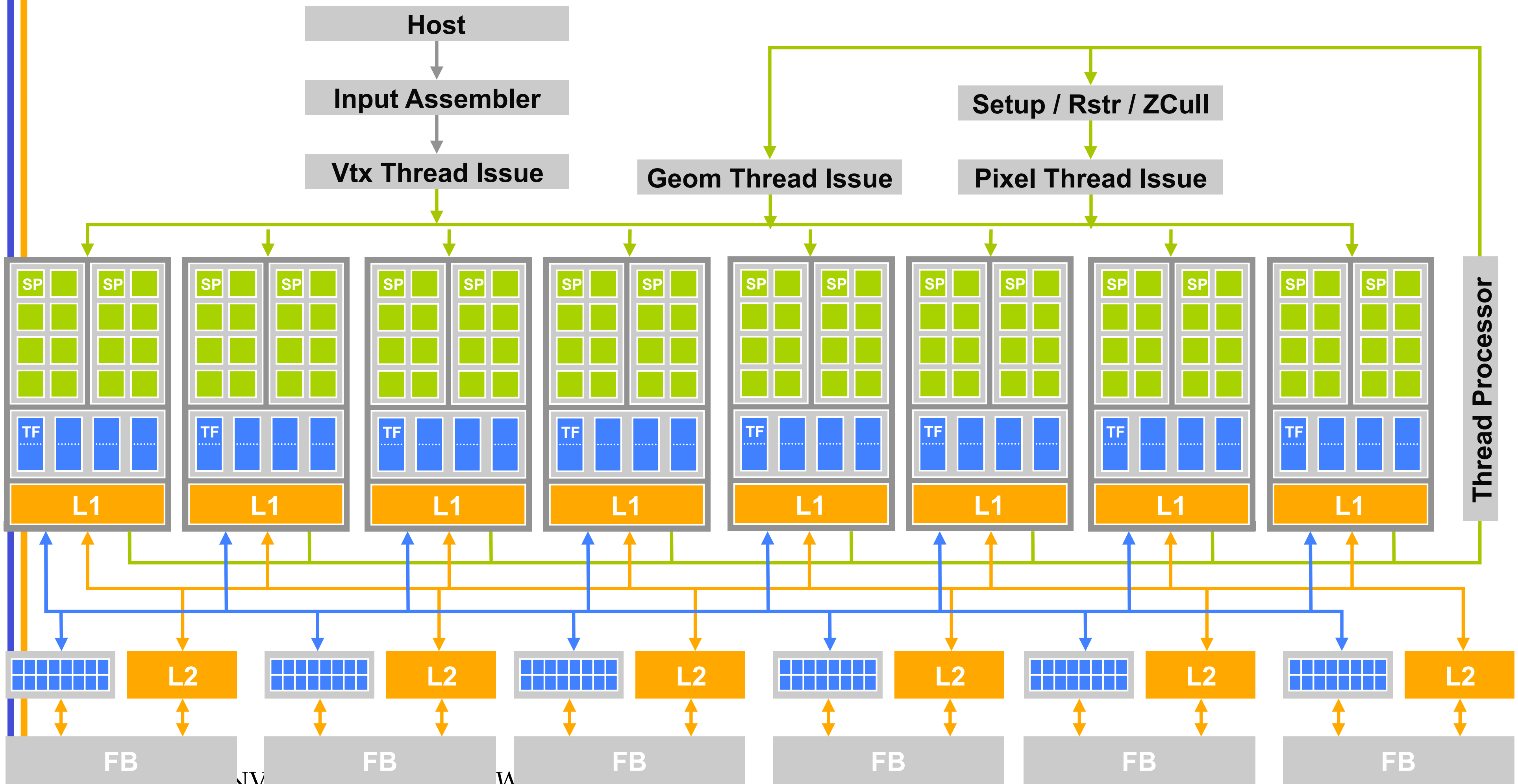


CUDA Devices and Threads

- A compute device
  - Is a coprocessor to the CPU or host
  - Has its own DRAM (device memory)
  - Runs many threads in parallel
  - Is typically a GPU but can also be another type of parallel processing device
- Data-parallel portions of an application are expressed as device kernels which run on many threads
- Differences between GPU and CPU threads
  - GPU threads are extremely lightweight
    - Very little creation overhead
  - GPU needs 1000s of threads for full efficiency
    - Multi-core CPU needs only a few

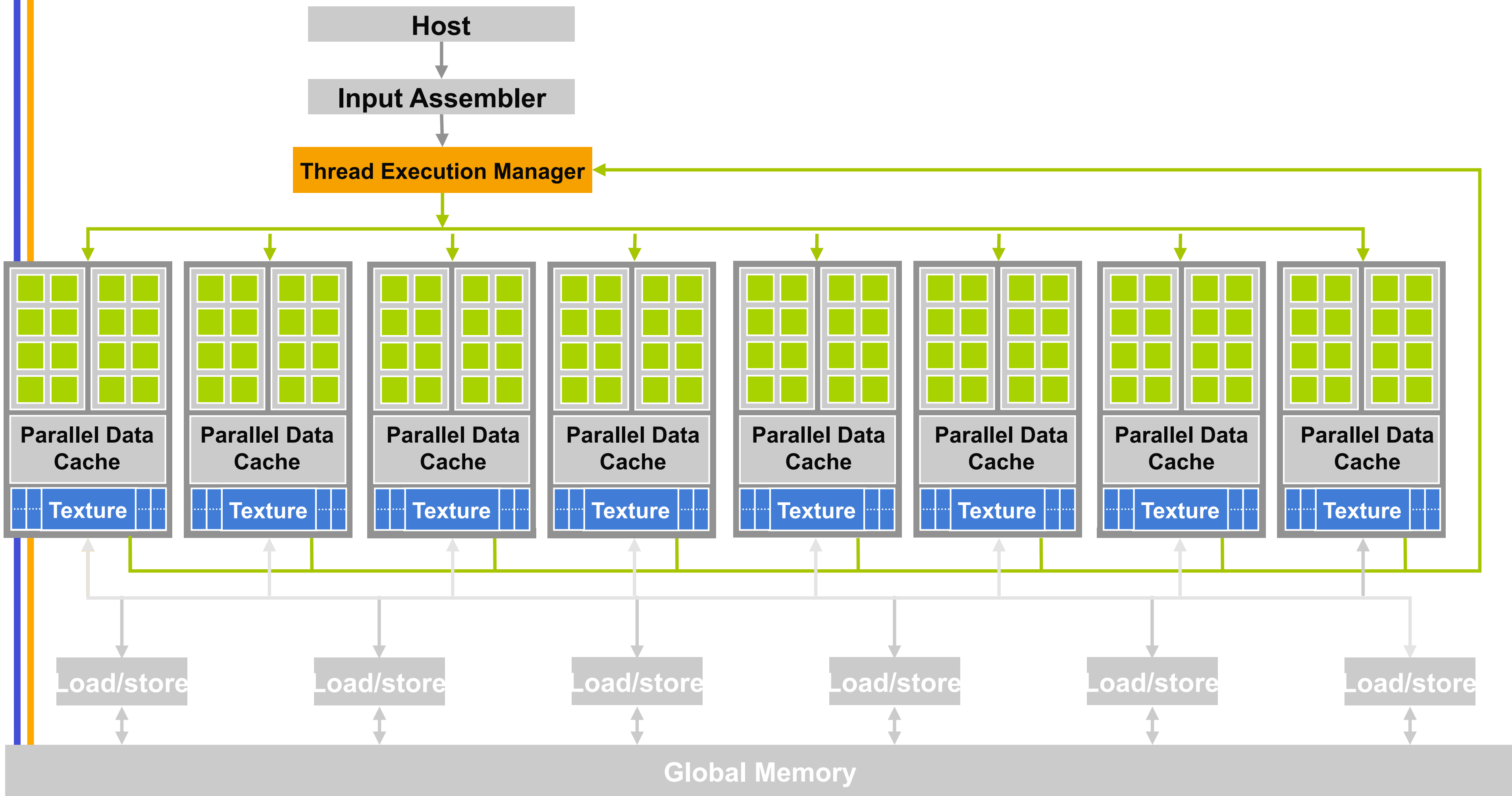
A GPU – Graphics Mode

- The future of GPUs is programmable processing
- So – build the architecture around the processor



CUDA mode – A **Device** Example

- Processors execute computing threads
- New operating mode/HW interface for computing



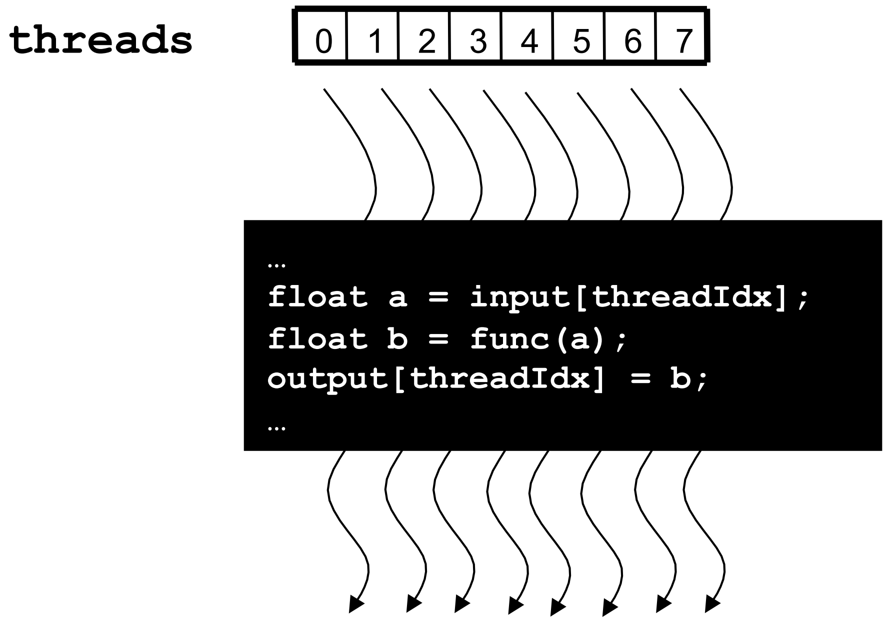
CUDA C - extensions

- **Declspecs**
  - **global, device, shared, local, constant**
- **Keywords**
  - **threadIdx, blockIdx**
- **Intrinsics**
  - **__syncthreads**
- **Runtime API**
  - **Memory, symbol, execution management**
- **Function launch**

```
__device__ float filter[N];

__global__ void convolve (float *image)  {

  __shared__ float region[M];
  ...

  region[threadIdx] = image[i];

  __syncthreads()
  ...

  image[j] = result;
}

// Allocate GPU memory
void *myimage = cudaMalloc(bytes)


// 100 blocks, 10 threads per block
convolve<<<100, 10>>> (myimage);
```

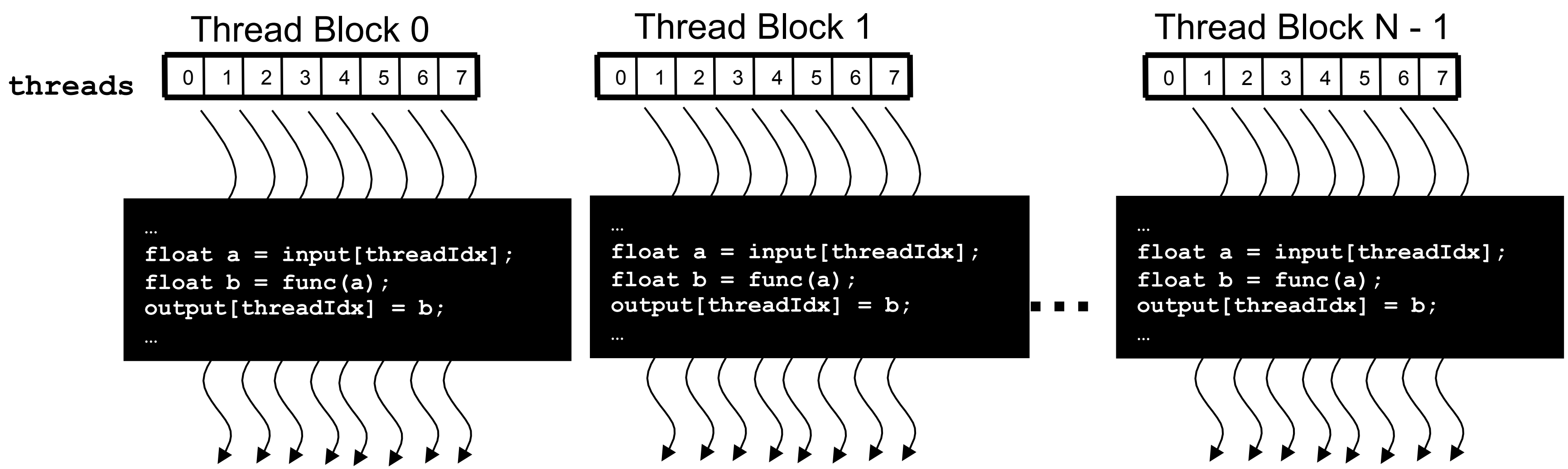
Arrays of Parallel Threads

- A CUDA kernel is executed by an array of threads
  - All threads run the same code (SPMD)
  - Each thread has an index that it uses to compute memory addresses and make control decisions



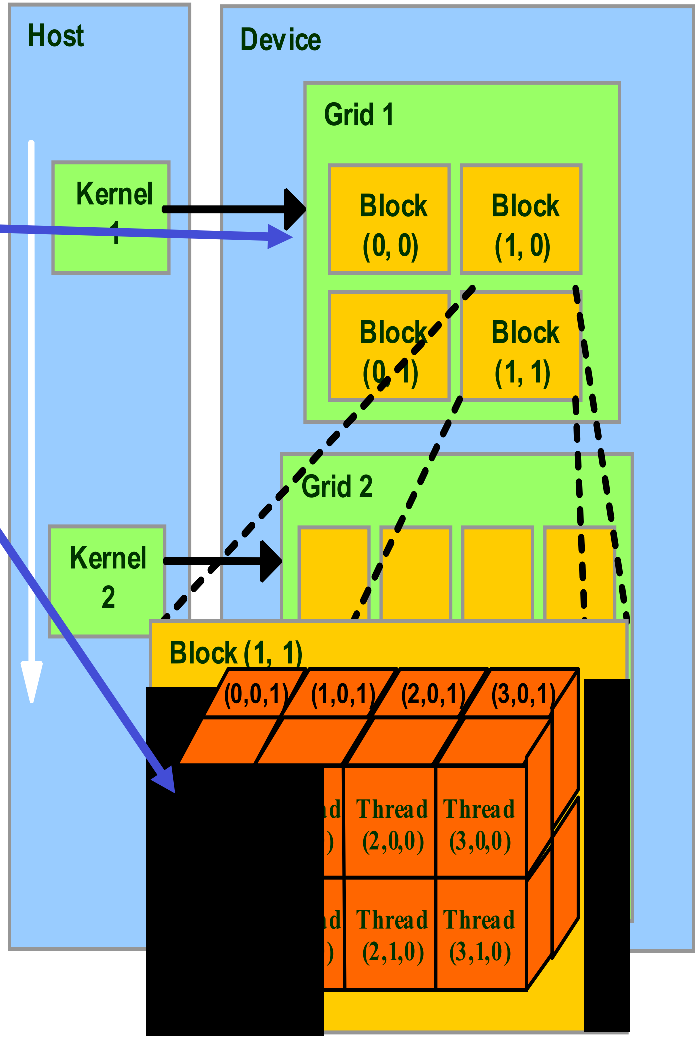
Thread Blocks: Scalable Cooperation

- Divide monolithic thread array into multiple blocks
  - Threads within a block cooperate via **shared memory, atomic operations** and **barrier synchronization**
  - Threads in different blocks cannot cooperate



blockIdx and threadIdx

- Each thread uses indices to decide what data to work on
  - blockIdx: 1D or 2D
  - threadIdx: 1D, 2D, or 3D
- Simplifies memory addressing when processing multidimensional data
  - Image processing
  - Solving PDEs on volumes
  - …



Example: Vector Addition Kernel

Device Code

```
// Compute vector sum C = A+B
// Each thread performs one pair-wise addition
__global__
void vecAdd(float* A, float* B, float* C, int n)
{
    int i = threadIdx.x + blockDim.x * blockIdx.x;
    if(i<n) C[i] = A[i] + B[i];
}

int main()
{
    // Run ceil(N/256) blocks of 256 threads each
    vecAdd<<<ceil(N/256), 256>>>(d_A, d_B, d_C, n);
}
```

Example: Vector Addition Kernel

```
// Compute vector sum C = A+B
// Each thread performs one pair-wise addition
__global__
void vecAdd(float* A, float* B, float* C, int n)
{
    int i = threadIdx.x + blockDim.x * blockIdx.x;
    if(i<n) C[i] = A[i] + B[i];
}
```

Host Code

```
int main()
{
    // Run ceil(N/256) blocks of 256 threads each
    vecAdd<<<ceil(N/256), 256>>>(d_A, d_B, d_C, n);
}
```

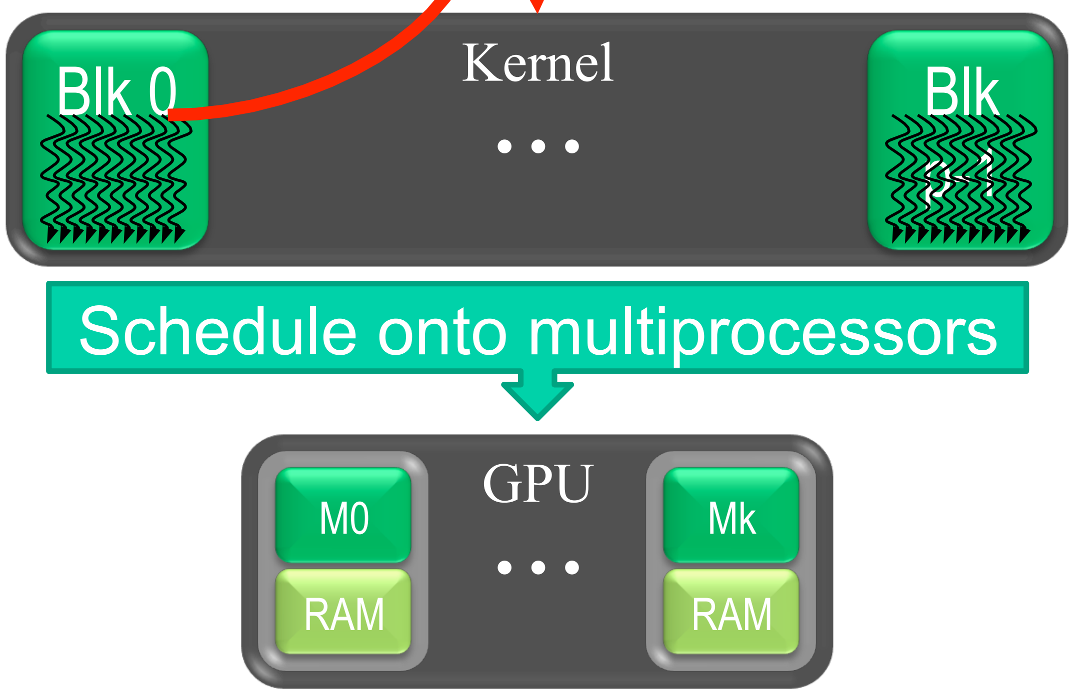
Kernel execution in a nutshell

`__host__`

`__global__`

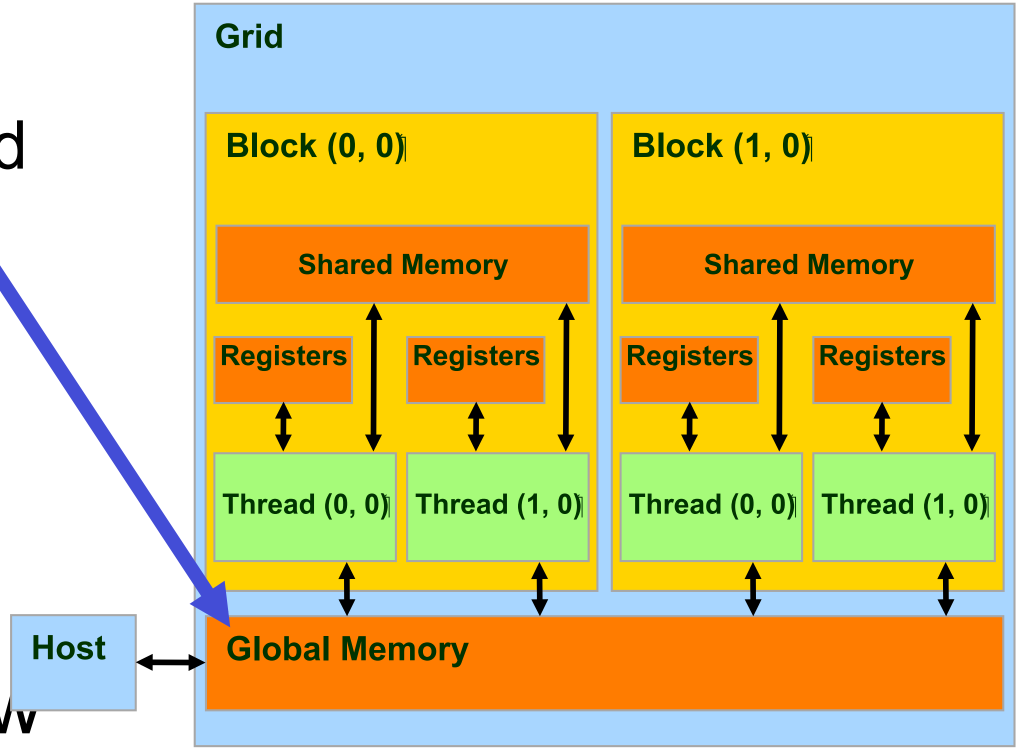
```
saxpy<<<P,B>>>(n, a, x, y);
```

```
blockIdx.x    blockDim.x
     threadIdx.x
```



CUDA Memory Model Overview

- Global memory
  - Main means of communicating R/W Data between host and device
  - Contents visible to all threads
  - Long latency access
- We will focus on global memory for now



CUDA API Highlights: Easy and Lightweight

- The API is an extension to the ANSI C programming language

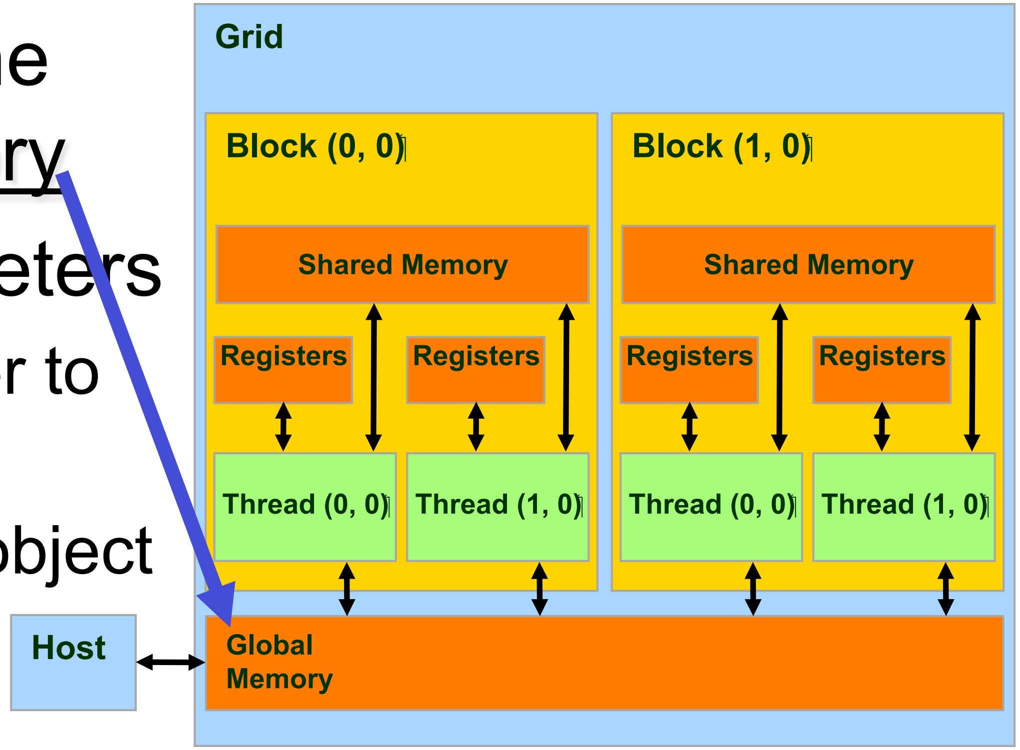
  → Low learning curve

- The hardware is designed to enable lightweight runtime and driver

  → High performance

CUDA Device Memory Allocation

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



CUDA Device Memory Allocation (cont.)

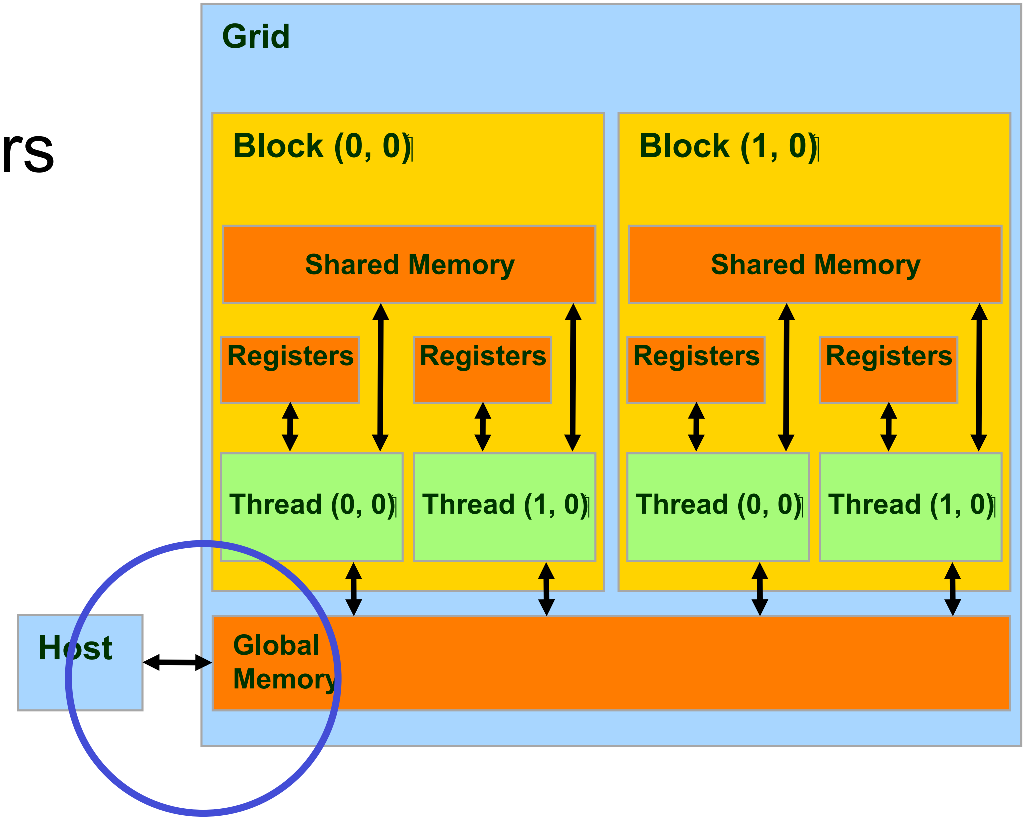
- Code example:
  - Allocate a 64 * 64 single precision float array
  - Attach the allocated storage to Md
  - “d” is often used to indicate a device data structure

```
TILE_WIDTH = 64;
Float* Md
int size = TILE_WIDTH * TILE_WIDTH * sizeof(float);
```

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

CUDA Host-Device Data Transfer

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



CUDA Host-Device Data Transfer (cont.)

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

```
cudaMemcpy(Md, M, size, cudaMemcpyHostToDevice);

cudaMemcpy(M, Md, size, cudaMemcpyDeviceToHost);
```

Example: Host code for `vecAdd`

```
int main()
{
    // allocate and initialize host (CPU) memory
    float *h_A = …,    *h_B = …;

    // allocate device (GPU) memory
    float *d_A, *d_B, *d_C;
    cudaMalloc( (void**) &d_A, N * sizeof(float));
    cudaMalloc( (void**) &d_B, N * sizeof(float));
    cudaMalloc( (void**) &d_C, N * sizeof(float));

    // copy host memory to device
    cudaMemcpy(d_A, h_A, N * sizeof(float), cudaMemcpyHostToDevice) );
    cudaMemcpy(d_B, h_B, N * sizeof(float), cudaMemcpyHostToDevice) );

    // Execute the kernel on ceil(N/256) blocks of 256 threads each
    vecAdd<<<ceil(N/256), 256>>>(d_A, d_B, d_C, n);

    cudaMemcpy(h_C, d_C, N * sizeof(float), cudaMemcpyDeviceToHost) );

    cudaFree(d_A);
    cudaFree(d_B);
    cudaFree(d_C);
}
```

CUDA Keywords

CUDA Function Declarations

	Executed on the:	Only callable from the:
`__device__ float DeviceFunc()`	device	device
`__global__ void KernelFunc()`	device	host
`__host__ float HostFunc()`	host	host

- `__global__` defines a kernel function
  - Each "__" consists of two underscore characters
  - A kernel function must return `void`
- `__device__` and `__host__` can be used together

CUDA Function Declarations (cont.)

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

Calling a Kernel Function – Thread Creation

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

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

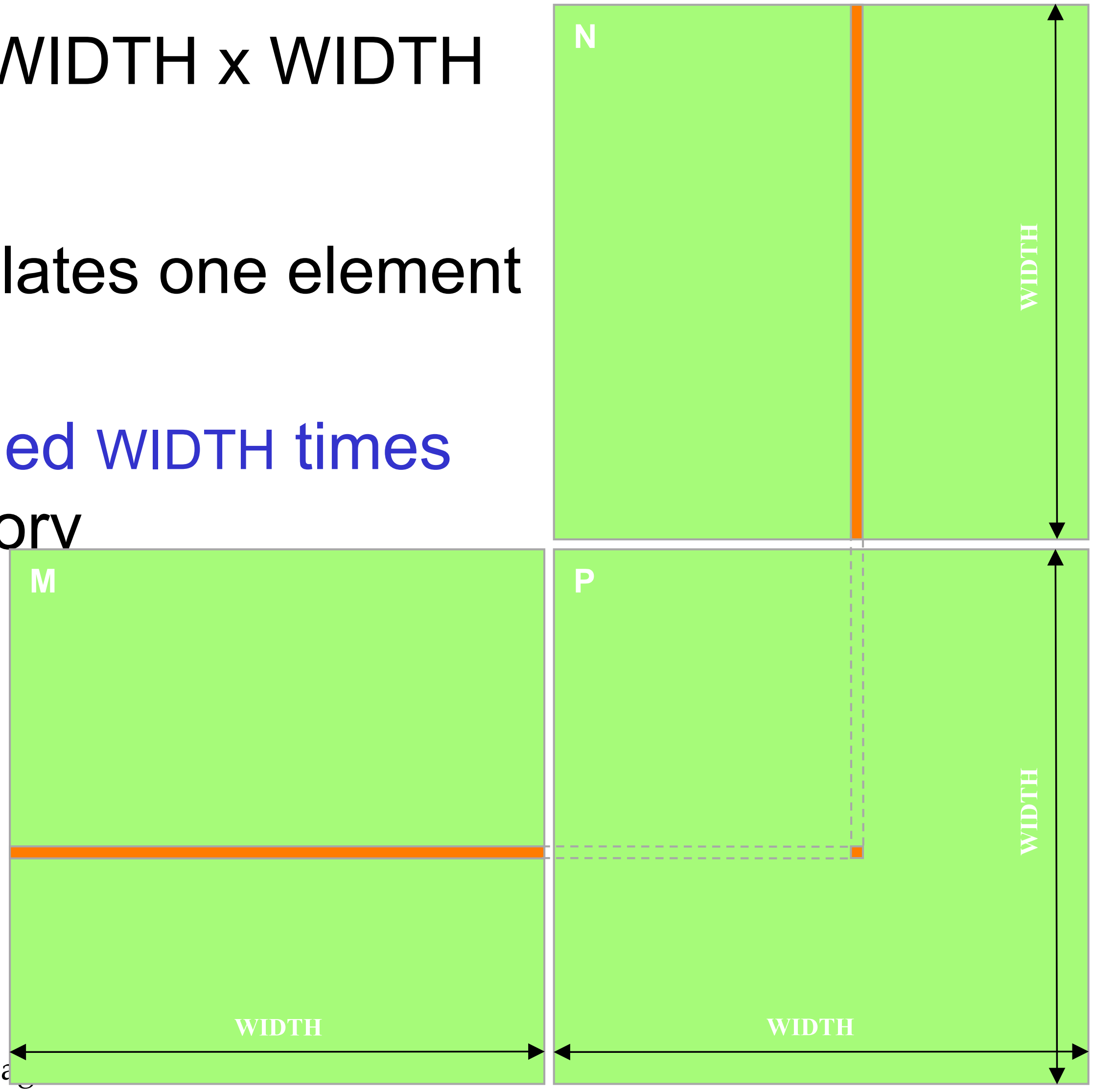
- Any call to a kernel function is asynchronous from CUDA 1.0 on, explicit synch needed for blocking

A Simple Running Example Matrix Multiplication

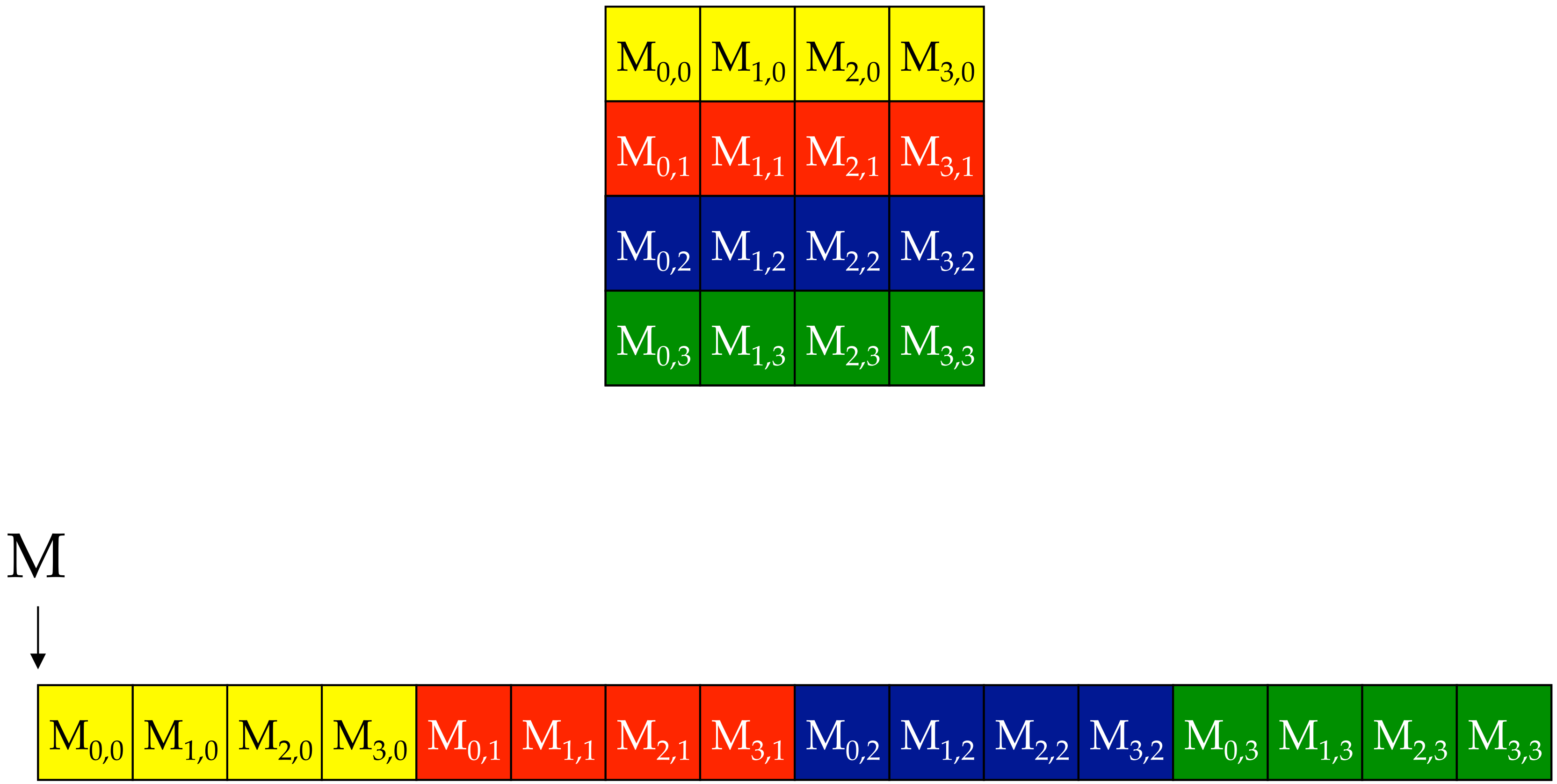
- A simple matrix multiplication example that illustrates the basic features of memory and thread management in CUDA programs
  - Leave shared memory usage until later
  - Local, register usage
  - Thread index usage
  - Memory data transfer API between host and device
  - Assume square matrix for simplicity

Programming Model: Square Matrix-Matrix Multiplication Example

- P = M * N of size WIDTH x WIDTH
- Without tiling:
  - One thread calculates one element of P
  - M and N are loaded WIDTH times from global memory



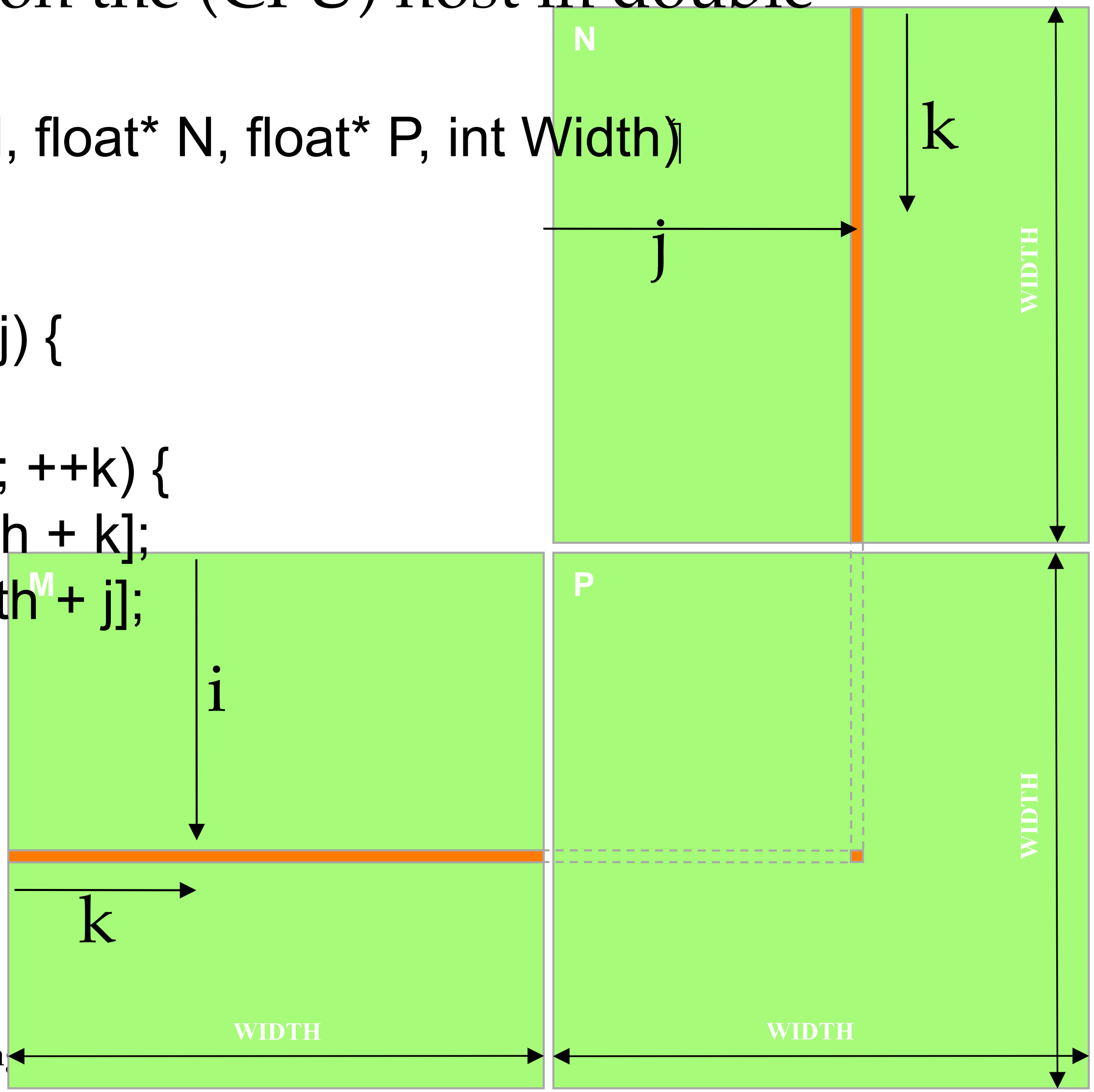
Memory Layout of a Matrix in C



Step 1: Matrix Multiplication
A Simple Host Version in C

// Matrix multiplication on the (CPU) host in double precision

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



Step 2: Input Matrix Data Transfer (Host-side Code)

```
void MatrixMulOnDevice(float* M, float* N, float* P, int Width)
{
   int size = Width * Width * sizeof(float);
   float* Md, Nd, Pd;
   …
1. // Allocate and Load M, N to device memory
   cudaMalloc(&Md, size);
   cudaMemcpy(Md, M, size, cudaMemcpyHostToDevice);

   cudaMalloc(&Nd, size);
   cudaMemcpy(Nd, N, size, cudaMemcpyHostToDevice);

   // Allocate P on the device
   cudaMalloc(&Pd, size);
```

Step 3: Output Matrix Data Transfer (Host-side Code)

2. // Kernel invocation code – to be shown later

…

3. // Read P from the device

cudaMemcpy(P, Pd, size, cudaMemcpyDeviceToHost);

// Free device matrices

cudaFree(Md); cudaFree(Nd); cudaFree (Pd);

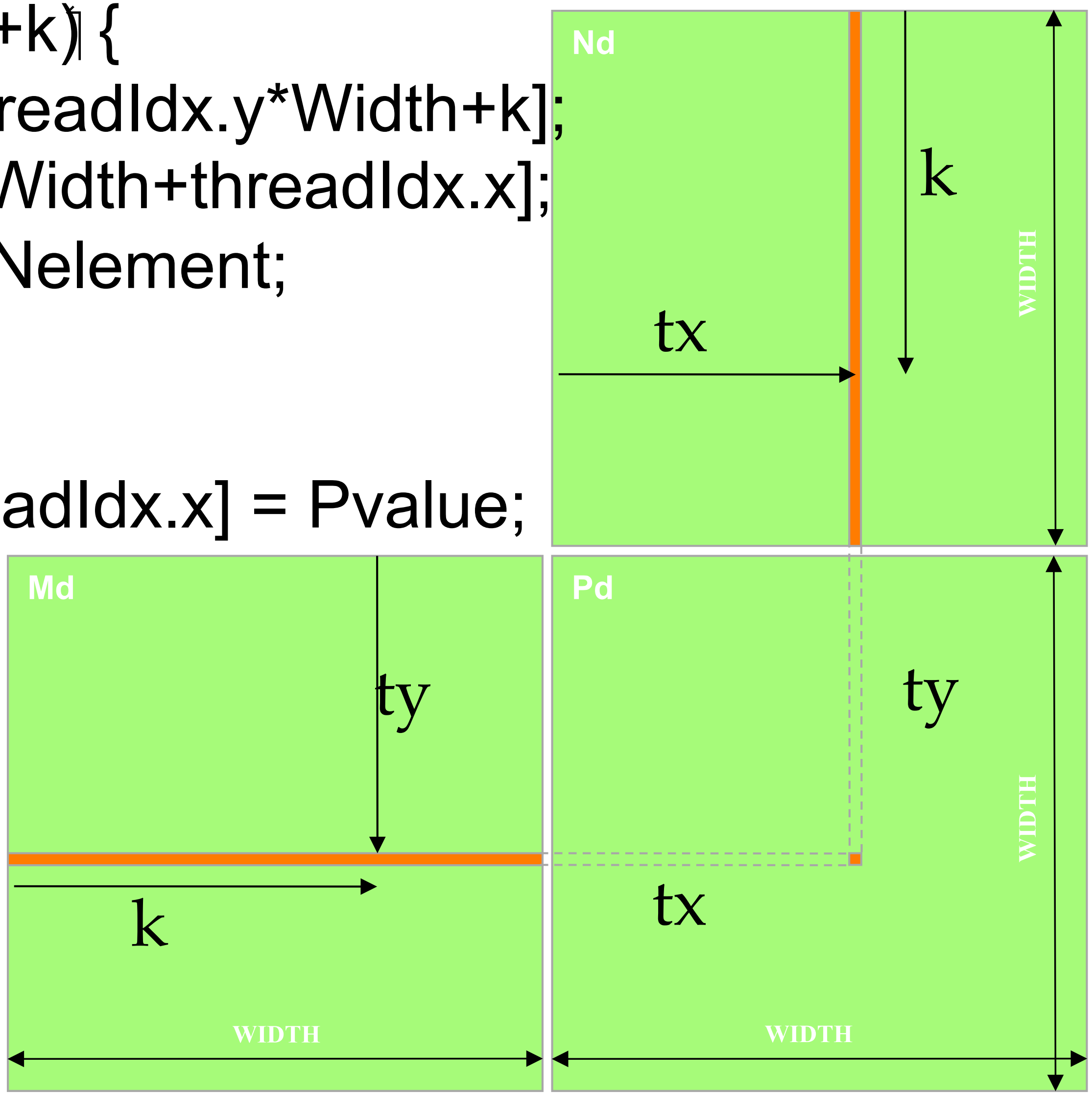
}

Step 4: Kernel Function

```
// Matrix multiplication kernel – per thread code

__global__ void MatrixMulKernel(float* Md, float* Nd, float* Pd, int Width)
{

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

Step 4: Kernel Function (cont.)

```
for (int k = 0; k < Width; ++k) {
    float Melement = Md[threadIdx.y*Width+k];
    float Nelement = Nd[k*Width+threadIdx.x];
    Pvalue += Melement * Nelement;
}

Pd[threadIdx.y*Width+threadIdx.x] = Pvalue;
}
```

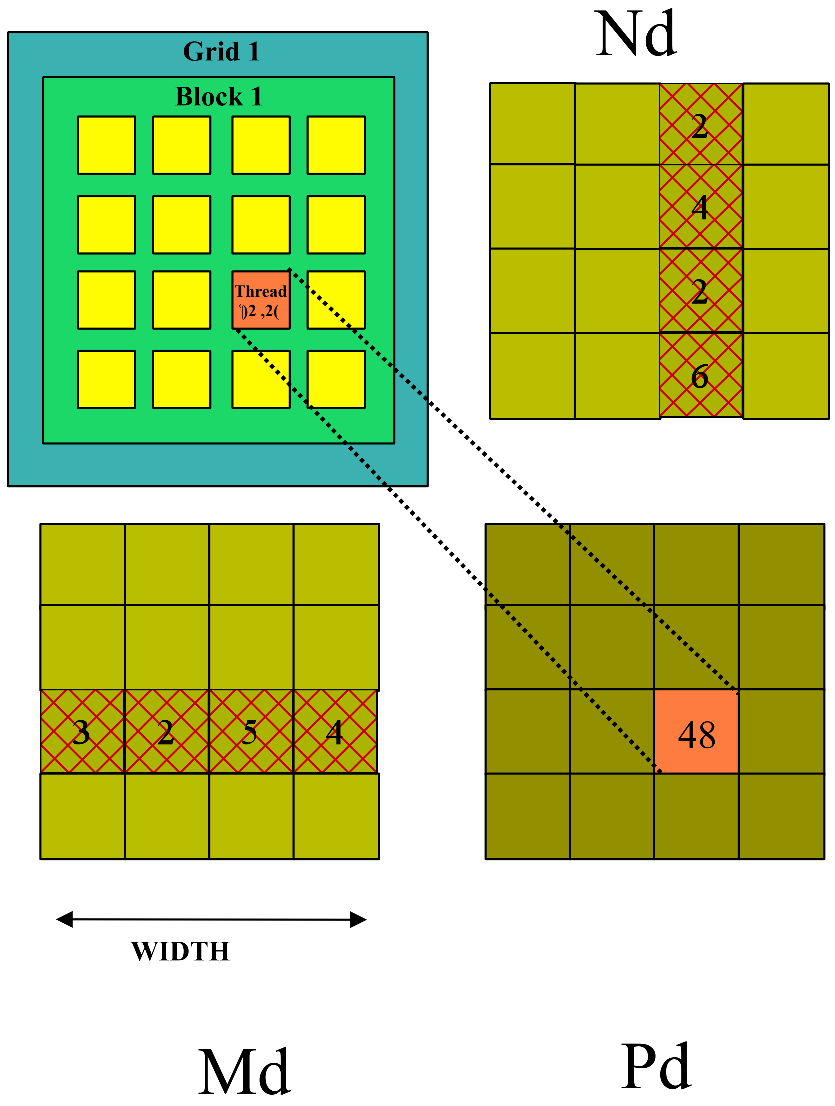


Step 5: Kernel Invocation (Host-side Code)

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

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

Need to Extend to Multiple Block

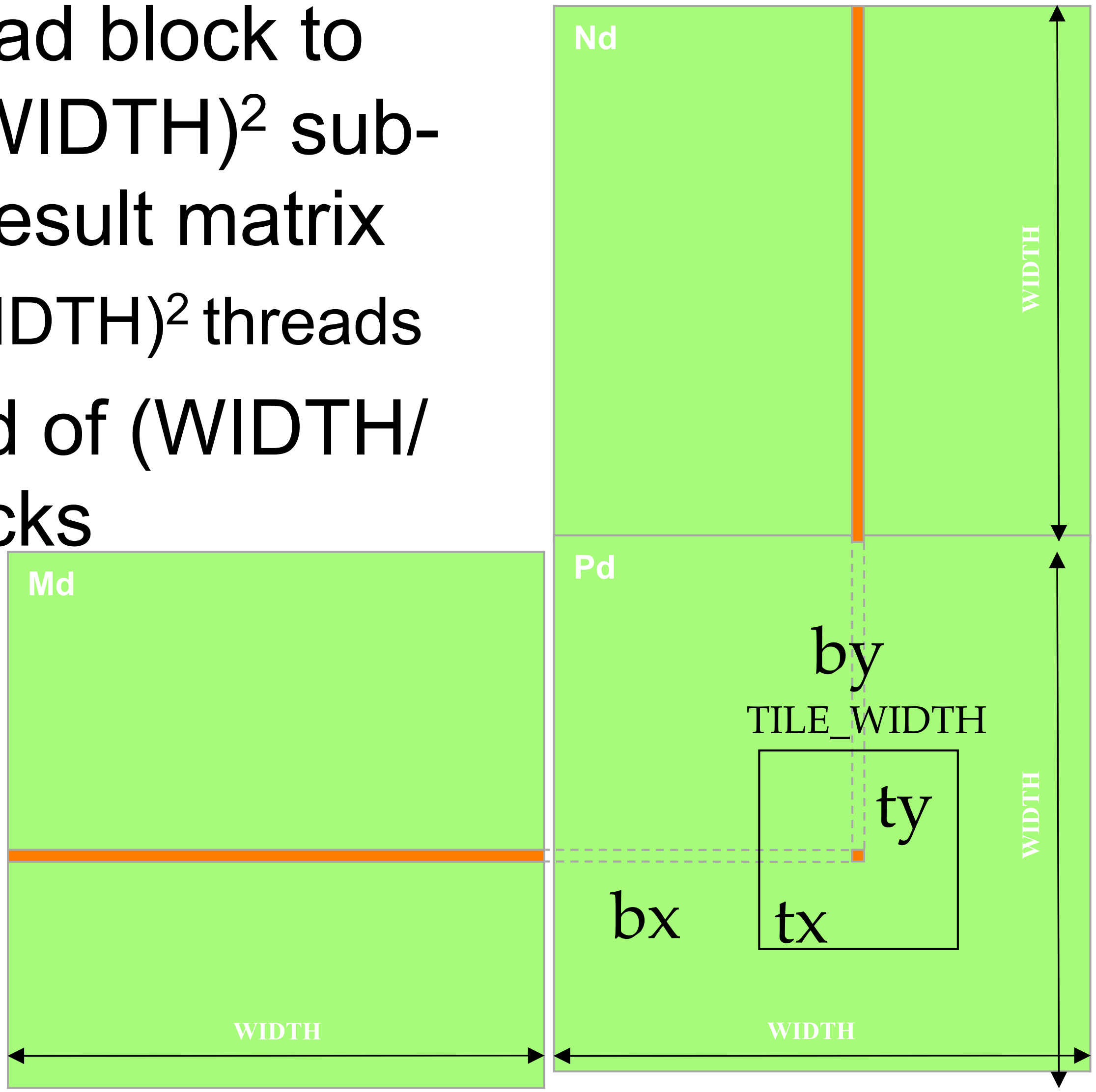
- One Block of threads compute matrix Pd
  - Each thread computes one element of Pd
- Each thread
  - Loads a row of matrix Md
  - Loads a column of matrix Nd
  - Perform one multiply and addition for each pair of Md and Nd elements
  - Compute to off-chip memory access ratio close to 1:1 (not very high)
- Size of matrix limited by the number of threads allowed in a thread block



Step 7: Handling Arbitrary Sized Square Matrices

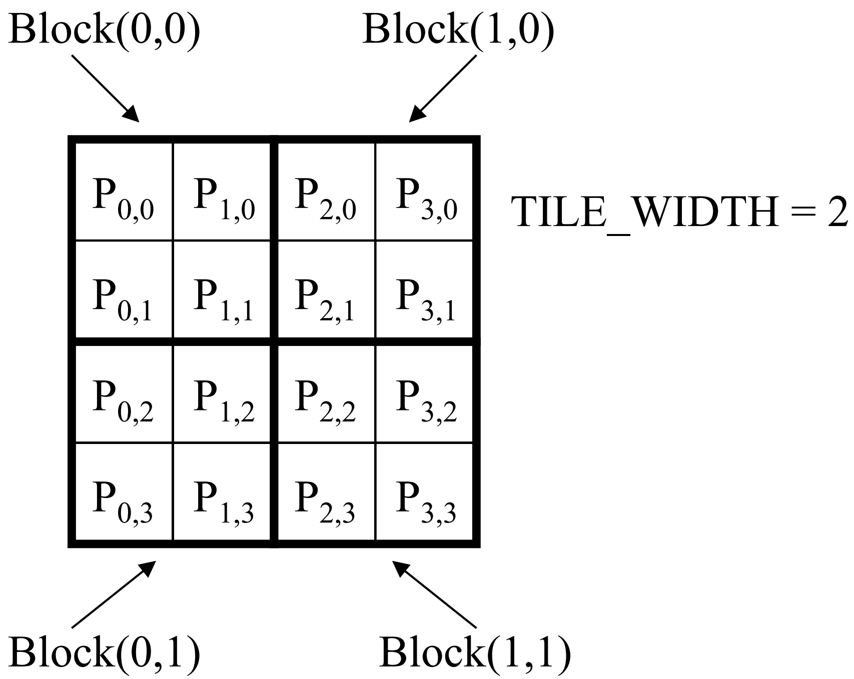
- Have each 2D thread block to compute a (TILE_WIDTH)^2 sub-matrix (tile) of the result matrix
  - Each has (TILE_WIDTH)^2 threads
- Generate a 2D Grid of (WIDTH/ TILE_WIDTH)^2 blocks

You still need to put a loop around the kernel call for cases where WIDTH/ TILE_WIDTH is greater than max grid size (64K)!

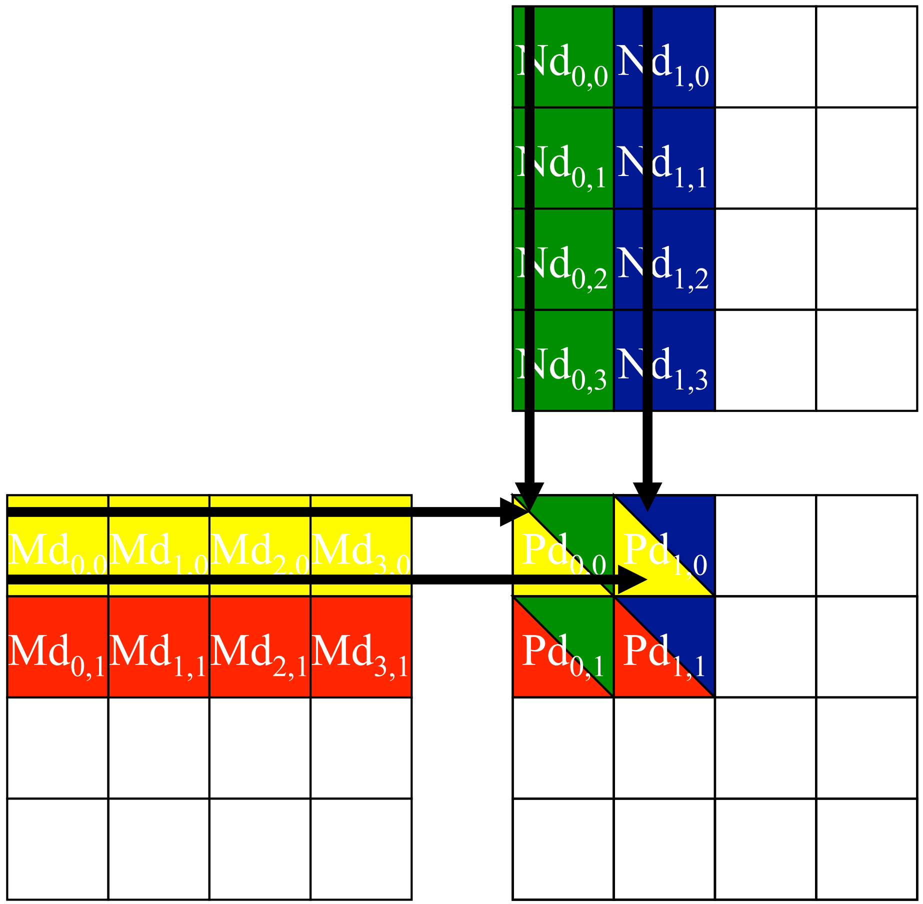


A Small Example

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



A Small Example: Multiplication



Revised Matrix Multiplication Kernel using Multiple Blocks

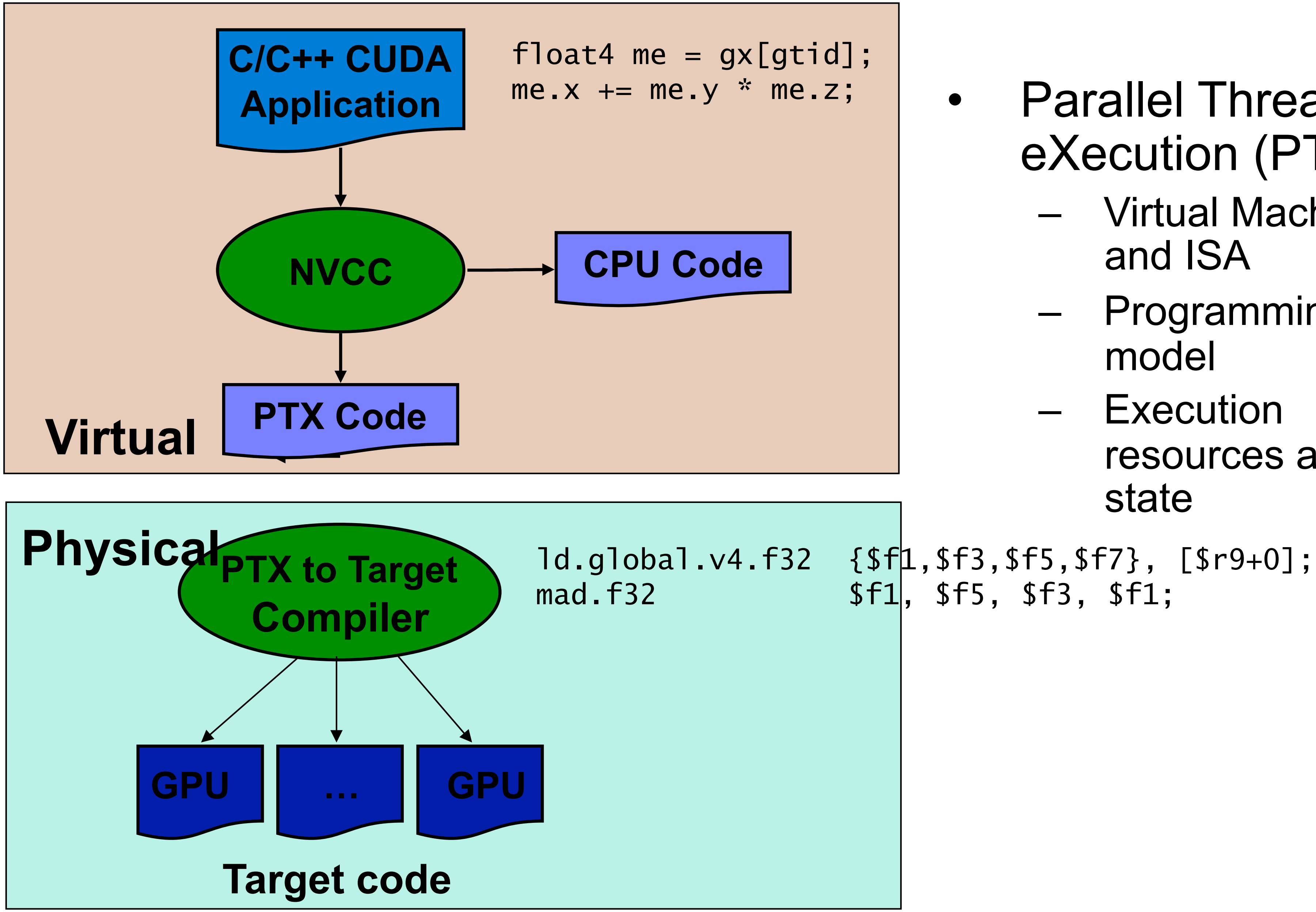
```
__global__ void MatrixMulKernel(float* Md, float* Nd, float* Pd, int Width)
{
// Calculate the row index of the Pd element and M
int Row = blockIdx.y*TILE_WIDTH + threadIdx.y;
// Calculate the column idenx of Pd and N
int Col = blockIdx.x*TILE_WIDTH + threadIdx.x;

float Pvalue = 0;
// each thread computes one element of the block sub-matrix
for (int k = 0; k < Width; ++k)
  Pvalue += Md[Row*Width+k] * Nd[k*Width+Col];

Pd[Row*Width+Col] = Pvalue;
}
```

Revised Step 5: Kernel Invocation (Host-side Code)

```
// Setup the execution configuration
  dim3 dimGrid(Width/TILE_WIDTH, Width/TILE_WIDTH);
  dim3 dimBlock(TILE_WIDTH, TILE_WIDTH);

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

Some Useful Information on Tools

Compiling a CUDA Program



- Parallel Thread eXecution (PTX)
  - Virtual Machine and ISA
  - Programming model
  - Execution resources and state

Compilation

- Any source file containing CUDA language extensions must be compiled with NVCC
- NVCC is a compiler driver
  - Works by invoking all the necessary tools and compilers like cudacc, g++, cl, ...
- NVCC outputs:
  - C code (host CPU Code)
    - Must then be compiled with the rest of the application using another tool
  - PTX
    - Object code directly
    - Or, PTX source, interpreted at runtime

Linking

- Any executable with CUDA code requires two dynamic libraries:
  - The CUDA runtime library (`cudart`)
  - The CUDA core library (`cuda`)