GPU Architecture

National Tsing Hua University

2025, Fall Semester

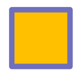
Outline

- Thread execution
  - Execution model
  - Warp
  - Warp Divergence
- Memory hierarchy

Execution Model

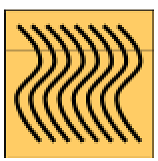
Software | Hardware

Thread

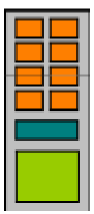


Scalar processor

Threads are executed by scalar processor



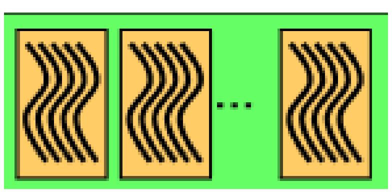
Thread block



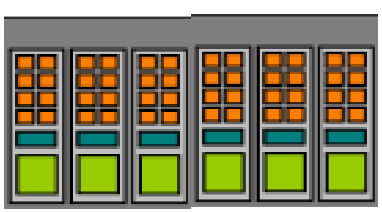
Stream Processor (SM)

Thread blocks are executed on SM

Several concurrent thread block can reside on one SM



Grid



GPU device

A kernel is launched as a grid of thread blocks

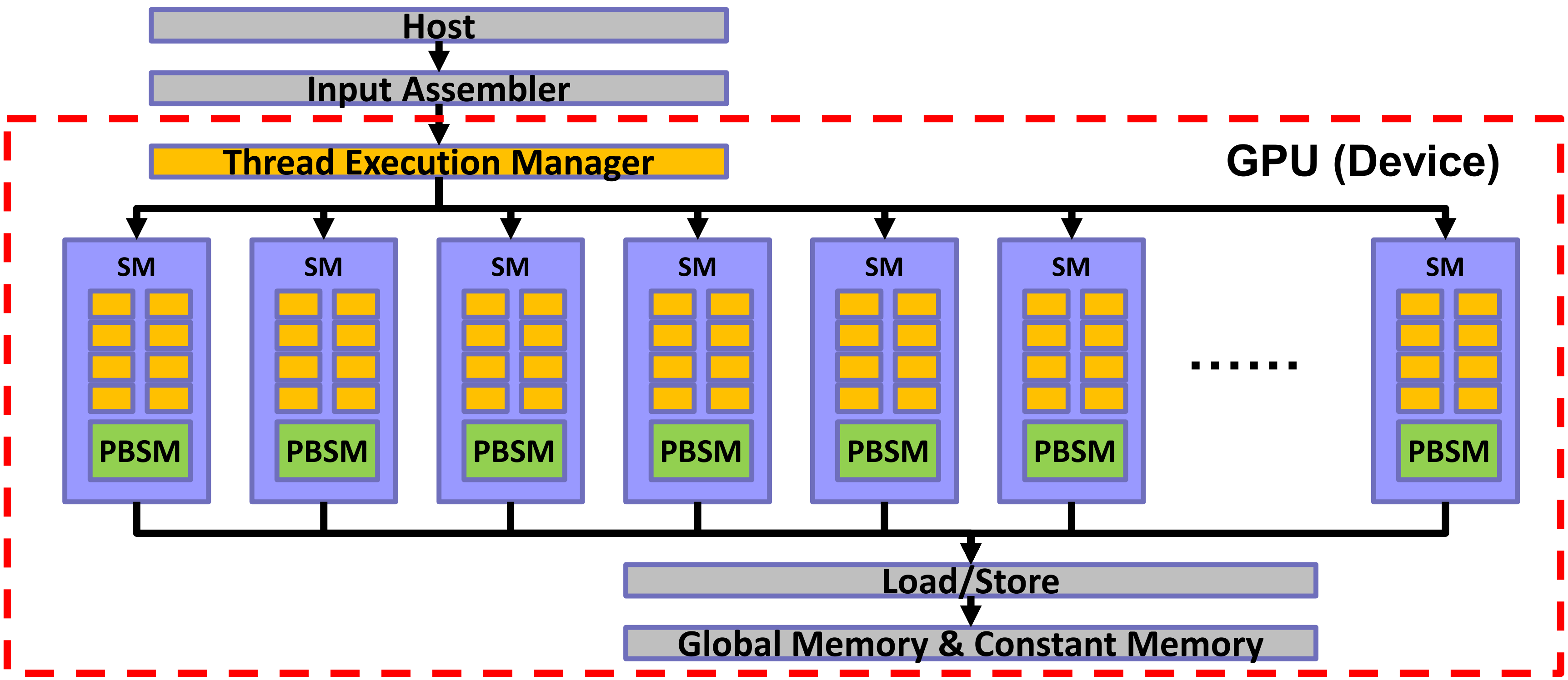
Thread Execution

- CUDA threads are grouped into blocks
  - All threads of the same block are executed in an SM
  - SMs have shared memories, where threads within a block can communicate
  - The entire threads of a block must be executed completely before there is space to schedule another thread block
- Hardware schedules thread blocks onto available SMs
  - No guarantee of order of execution
  - If an SM has more resources, the hardware can schedule more blocks

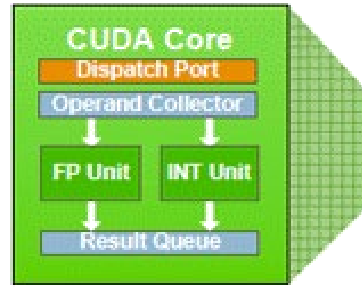
Manycore GPU – Block Diagram

- Consist of multiple stream multi-processors (SM)
- Memory hierarchic:
  - global memory ➔ PBSM/shared memory ➔ local register

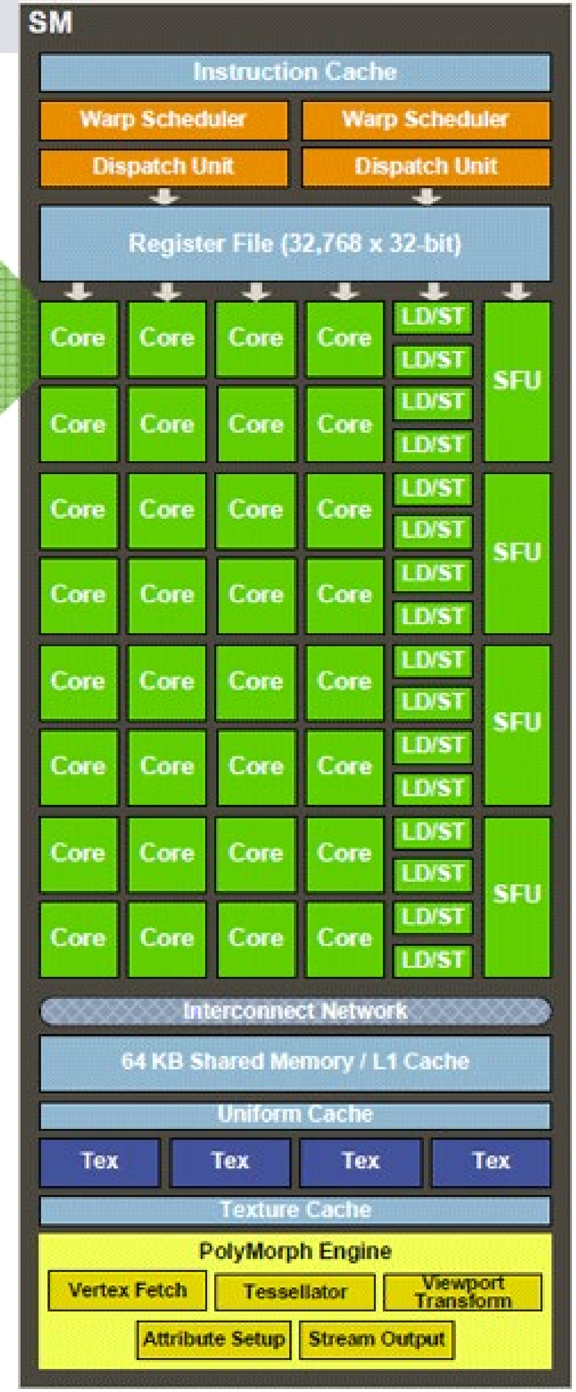
Slow, but large & shared   Fast, but small & local



Stream Multiprocessor

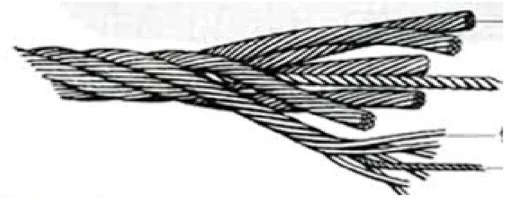


- Each SM is a vector machine
- Shared register files
  - Store local variables
- Programmable cache (shared memory)
  - Shared with a normal L1 cache.
- **Hardware scheduling** for thread execution and **hardware context switch**

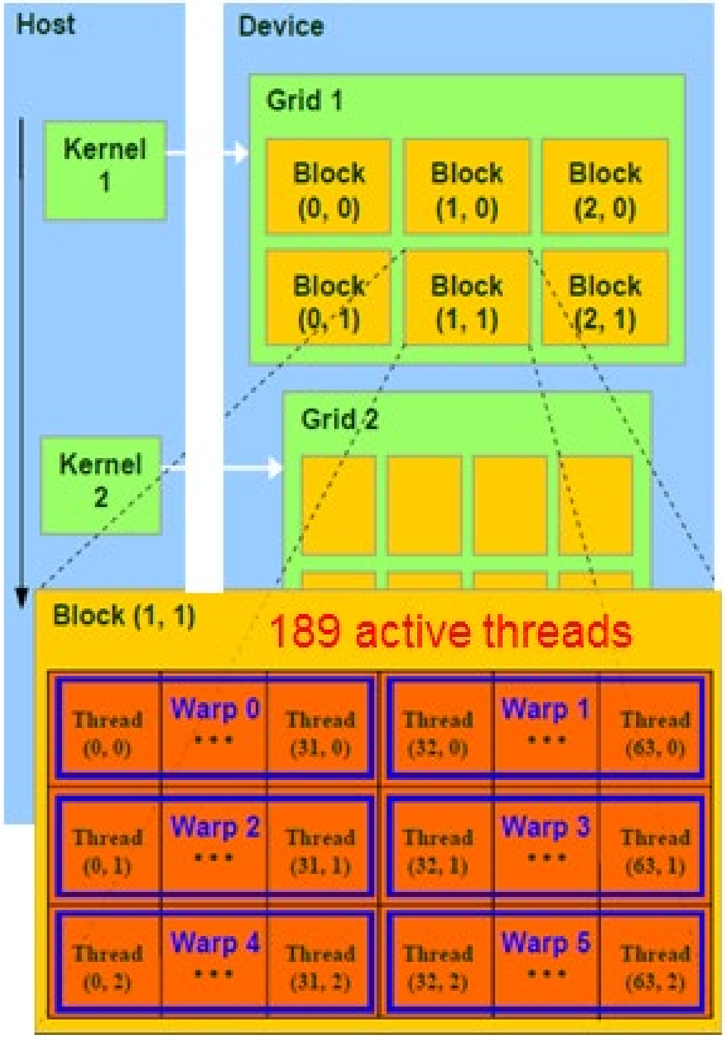


http://hothardware.com/Articles/NVIDIA-GF100-Architecture-and-Feature-Preview/

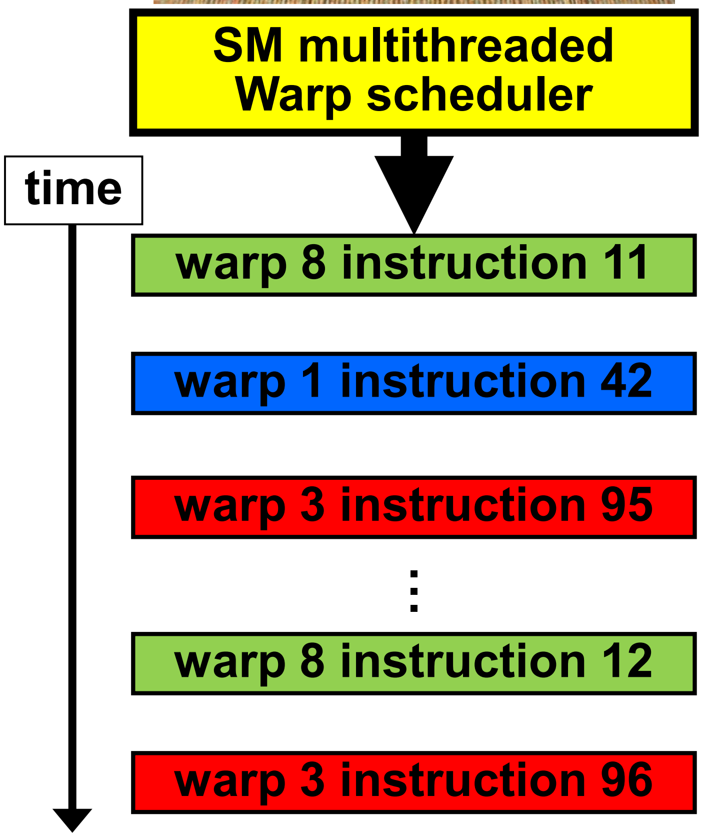
Warp



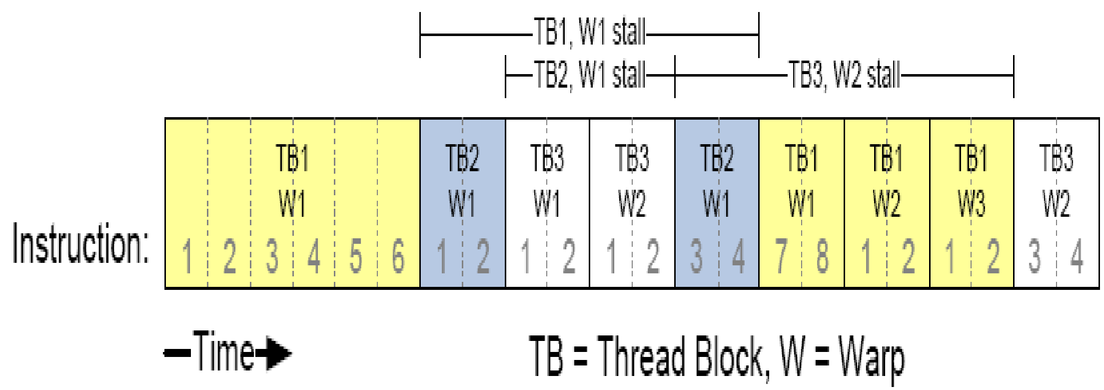
- Inside the SM, threads are launched in groups of 32, called warps
  - Warps share the control part (warp scheduler)
  - At any time, only one warp is executed per SM
  - Threads in a warp will be executing the same instruction (SIMD)
- In other words …
  - Threads in a wrap execute **physically** in parallel
  - Warps and blocks execute **logically** in parallel
  - ➔ Kernel needs to sync threads within a block
- For Fermi:
  - Maximum number of active blocks per SM is 8
  - Maximum number of active warps per SM is 48
  - Maximum number of active threads per SM is 48*32=1,536



Warp Scheduler



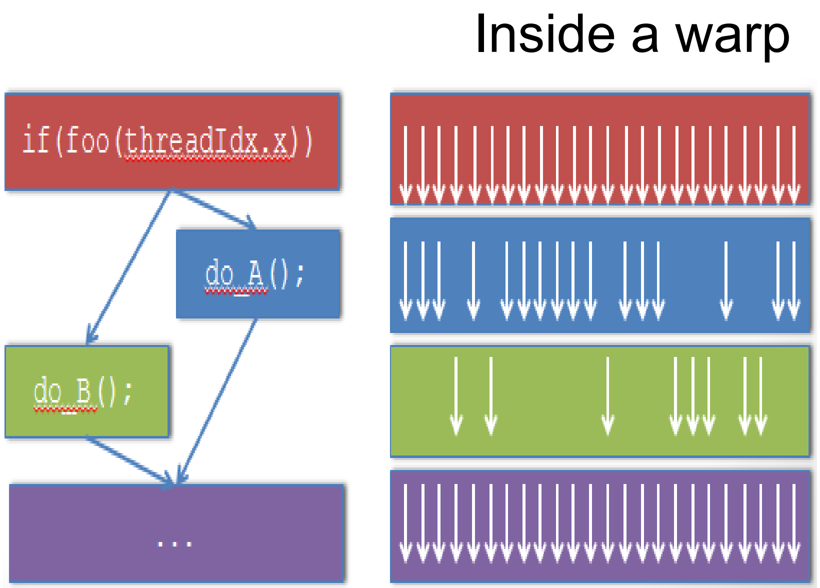
- SM hardware implements zero-overhead Warp scheduling
  - Warps whose next instruction has its operands ready for consumption are eligible for execution
  - Wraps are switched when memory stalls
  - Eligible Warps are selected for execution on prioritized scheduling
  - All threads in a Warp execute the same instruction when selected



Warp Divergence

- What if different threads in a warp need to do different things:
  - Including any flow control instruction (**if, switch, do, for, while**)

```
if(foo(threadIdx.x)){
        do_A();
} else {
        do_B();
}
```



- Different execution paths within a warp are serialized
  - Predicated instructions which are carried out only if logical flag is true
  - All threads compute the logical predicate and two predicated instructions/statements
  - **→ Potential large lost of performance**

Avoid Diverging in a Warp

- Example with divergence:

```
if (threadIdx.x > 2) {...}
else {...}
```

  - Branch granularity < warp size

- Example without divergence:

```
if (threadIdx.x / WARP_SIZE > 2) {...}
else {...}
```

  - Different warps can execute different code with no impact on performance
  - Branch granularity is a whole multiple of warp size

Example: Divergent Iteration

```
__global__ void per_thread_sum
(int *indices, float *data, float *sums){
    ...
    // number of loop iterations is
    // data dependent
    int i = threadIdx.x
    for(int j=indices[i];j<indices[i+1]; j++){
        sum += data[j];
    }
    sums[i] = sum;
}
```

Iteration Divergence

- A single thread can drag a whole warp with it for a long time
- Know your data patterns
- If data is unpredictable, try to flatten peaks by letting threads work on multiple data items

Unroll the for-loop

- Unroll the statements can reduce the branches and increase the pipeline
- Example:

```
for (i=0;i<n;i++) {
    a = a + i;
}
```

  - Unrolled 3 times

```
for (i=0;i<n;i+=3) {
    a = a + i;
    a = a + i+1;
    a = a + i+2;
}
```

#pragma unroll

- The `#pragma unroll` directive can be used to control unrolling of any given loop.
- must be placed immediately before the loop and only applies to that loop
- Example:

```
#pragma unroll 5
for (int i = 0; i < n; ++i)
```

  - the loop will be unrolled 5 times.
  - The compiler will also insert code to ensure correctness
- `#pragma unroll 1` will prevent the compiler from ever unrolling a loop.

Atomic Operations

- Occasionally, an application may need threads to update a counter in **shared** or **global** memory

```
__shared__ int count;
……
if (……) count++;
```

- Synchronization problem: if two (or more) threads execute this statement at the same time
- Solution: use atomic instructions supported by GPU
  - addition / subtraction
  - max / min
  - increment / decrement
  - compare-and-swap

Example: Histogram

```
/* Determine frequency of colors in a picture
colors have already been converted into ints. Each
thread looks at one pixel and increments a counter
atomically*/

__global__ void hist(int* color, int* bin){
    int i = threadIdx.x + blockDim.x *
                          blockIdx.x;
    int c = colors[i];
    atomicAdd(&bin[c], 1);
}
```

Example: Global Min/Max

```
__global__ void global_max(int* values,
int* gl_max){
    int i = threadIdx.x + blockDim.x *
                          blockIdx.x;
    int val = values[i];
    atomicMax(gl_max,val);
}
```

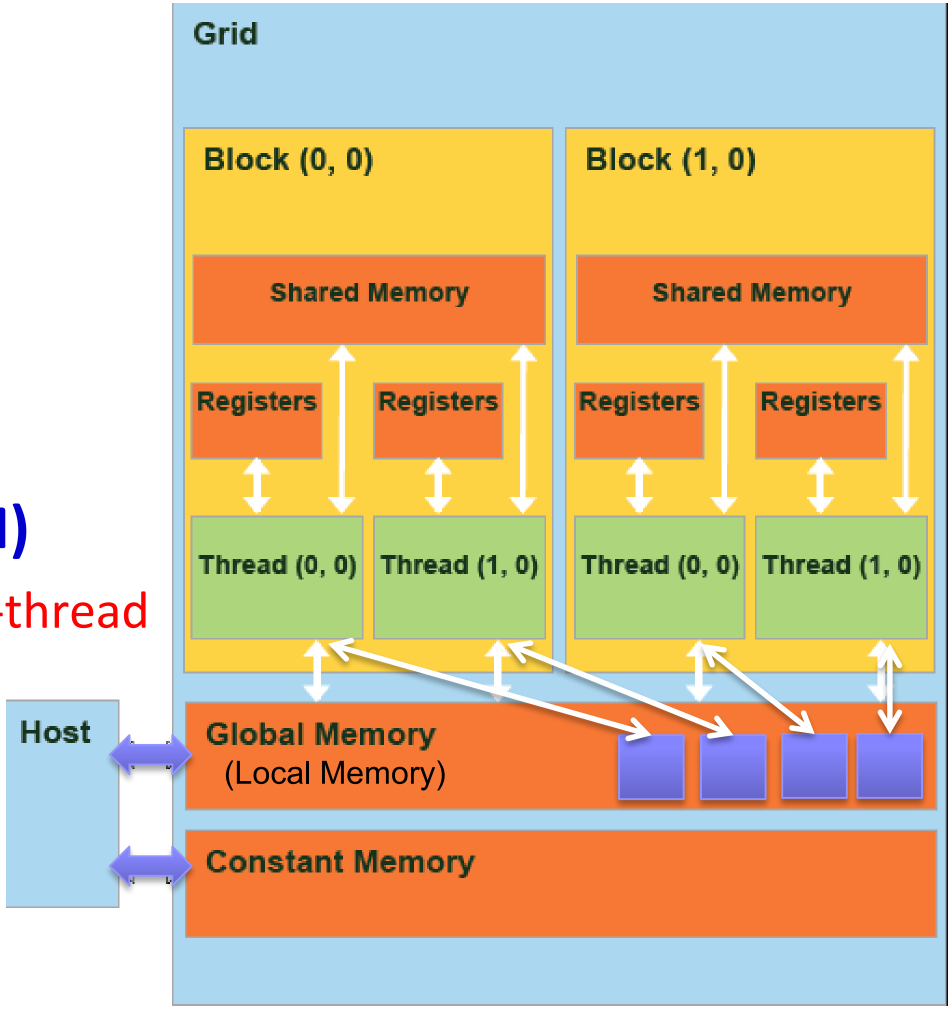
- Not very fast for data in shared memory
- Only slightly slower for data in device memory

Outline

- Thread execution
- Memory hierarchy
  - Register & Local memory
  - Shared memory
  - Global & Constant memory

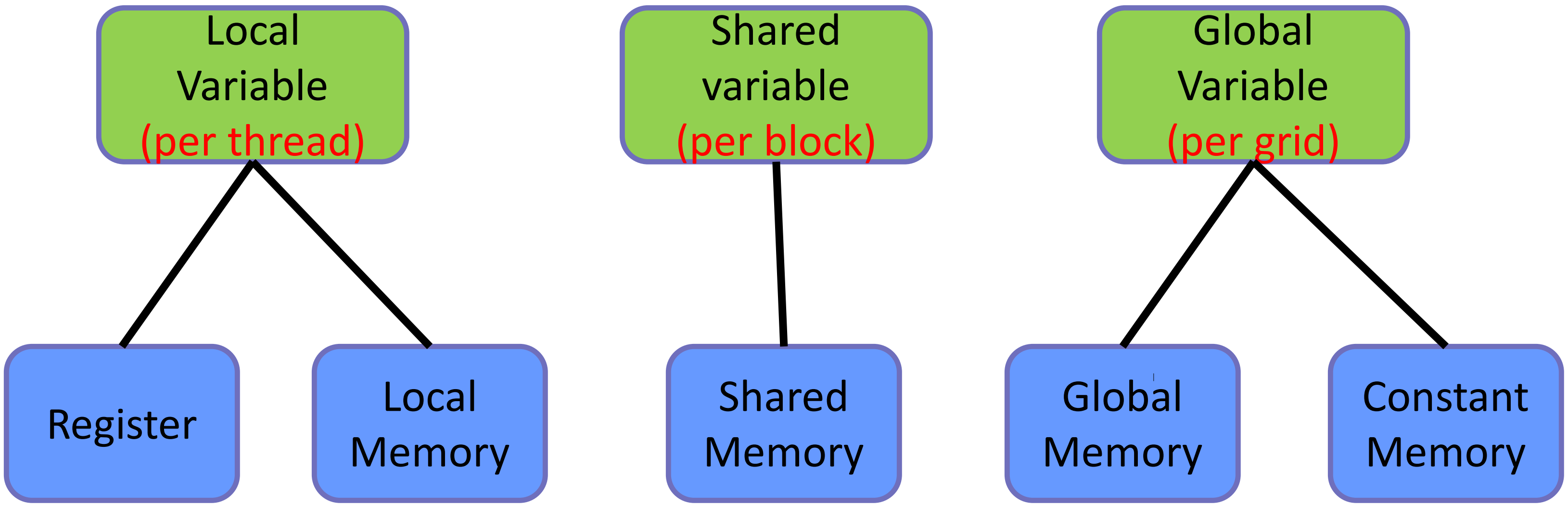
GPU Memory Hierarchy

- **Registers**
  - Read/write per-thread
  - Low latency & High BW
- **Shared memory**
  - Read/write per-block
  - Similar to register performance
- **Global/Local memory (DRAM)**
  - Global is per-grid & Local is per-thread
  - High latency & Low BW
  - Not cached
- **Constant memory**
  - Read only per-grid
  - Cached



Software to Hardware Mapping

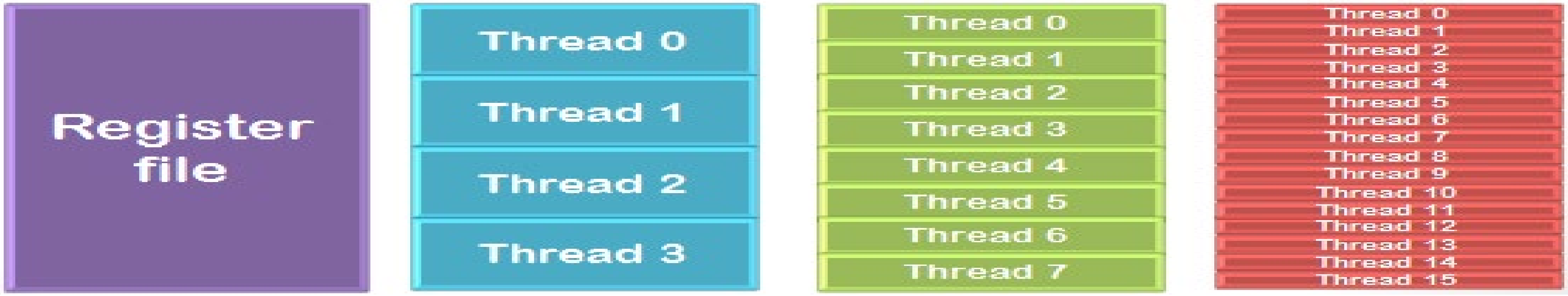
CUDA Variables within a Kernel



GPU Memory Hierarchy

Register

- Register consumes zero extra clock cycles per instruction, except
  - Register **read-after-write dependencies** (24 cycles) and
  - Register memory **bank conflicts**
- Registers aren't indexable
  - **Array variables** always are allocated in **local memory**
- Register spilling
  - Local memory is used if the register limit is met
    - Number of registers available per block (CUDA6.1): 64K
    - Number of registers available per thread (CUDA6.1): 255

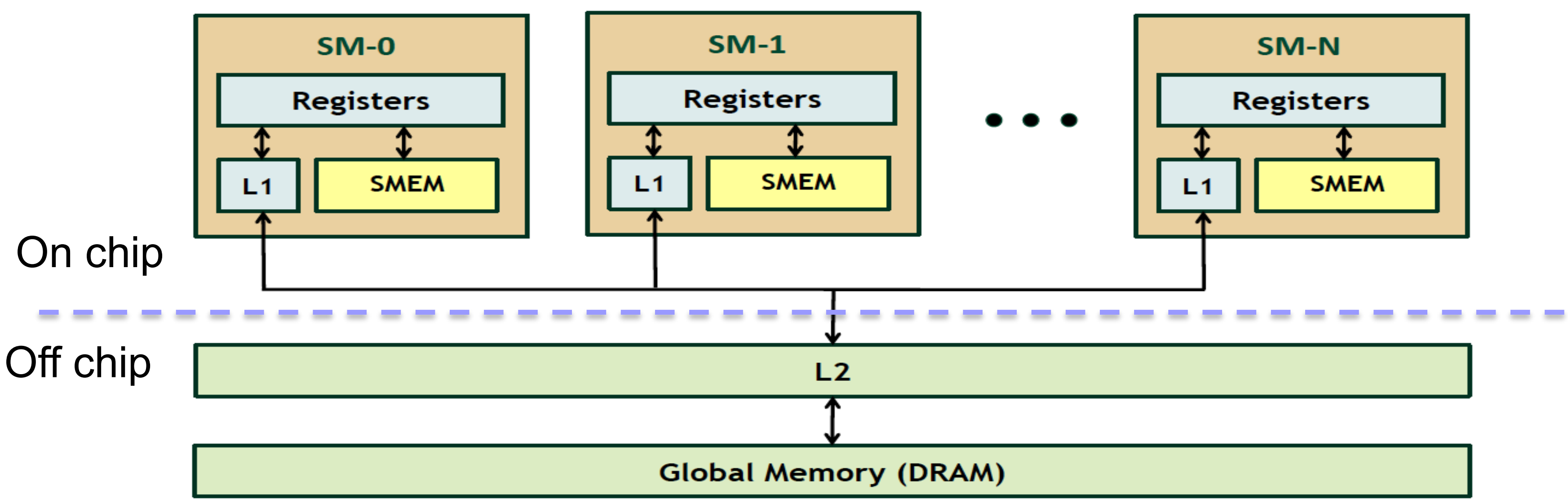


Local Memory

- Name refers to memory where registers and other thread-data is spilled
  - Usually when one runs out of SM resources
  - "Local" because each thread has its own private area
- Details:
  - Not really a "memory" – bytes are stored in **global memory (DRAM)**
- Differences from global memory:
  - Addressing is resolved by the compiler
  - Stores are **cached** in L1

Local Memory Cache

- L1 & L2 are used to cache local memory contents
  - L1: On chip memory (share memory)
  - L2: Off chip memory (global memory)



Example

```
__device__ void distance(int m, int n, int *V){
    int i, j, k;
    int a[10], b[10], c[10];
    ...
}
```

- Variables i, j, k, a, b, c are called “local variables”.
- It is likely that variable i, j, k are stored in registers, and variable a, b, c are stored in “local memory” (off-chip DRAM).
  - Compiler decides which memory space to use.
  - Registers aren’t indexable, so arrays have to be placed in local memory.
  - If not enough registers, local memory will be used.
- Only allowed static array!! ➔ No `int a[m];`

Outline

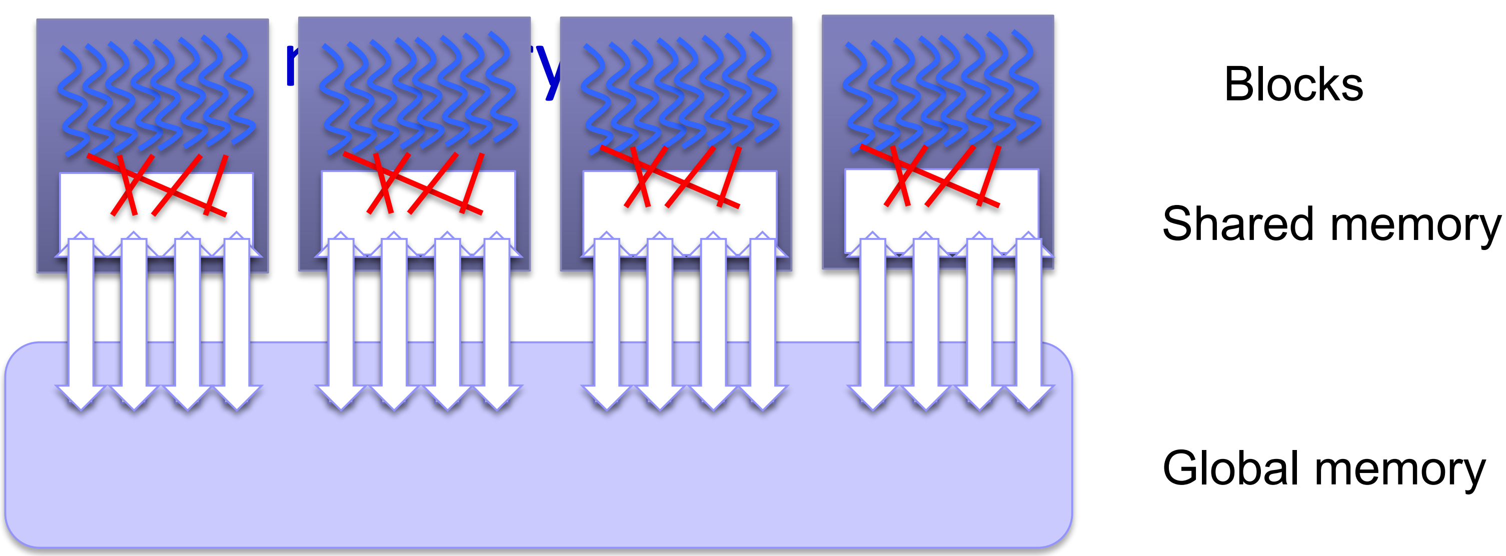
- Thread execution
- Memory hierarchy
  - Register & Local memory
  - Shared memory
  - Global & Constant memory
- Occupancy

Shared Memory

- Programmable cache!!
  - **Almost as fast as registers**
- Scope: shared by all the threads in a block.
  - The threads in the same block can communicate with each other through the shared memory.
  - Threads in different blocks can only communicate with each other through global memory.
- Size: at most 48K per block (CUDA 6.1)
  - On Fermi and Kepler GPU, shared memory and L1 cache use the same memory hardware (64K). The ratio can be adjusted by programmer.
  - But on Pascal and Volta GPU, shared memory is dedicated

General Strategy

1. Load data from global memory to shared memory
2. Process data in the shared memory
3. Write data back from shared memory to



APSP Parallel Implementation Revisit

- Use **n*n threads**.
- Each updates the shortest path of one pair vertices
- Use **global memory** to store the matrix D.

```
__global__ void FW_APSP(int k, int D[n][n]) {
     int i = threadIdx.x;
     int j = threadIdx.y;
     if (D[i][j]>D [i][k]+D[k][j])
        D[i][j]= D[i][k]+D[k][j];
}
int main() { ...
    dim3 threadsPerBlock(n, n);
    for (int k = 0; k<n, k++)
        FW_APSP<<<1, threadsPerBlock >>>(k, D);
}
```

6 global memory access

Using Shared Memory

- This way of using shared memory is called dynamic allocation of shared memory, whose size is specified in the kernel launcher.

```
FW_APSP<<<1,n*n, n*n*sizeof(int)>>>(…);
```

  - The third parameter is the size of shared memory.

```
extern __shared__ int S[][];
__global__ void FW_APSP(int k, int D[n][n]) {
    int i = threadIdx.x;
    int j = threadIdx.y;
    S[i][j]=D[i][j]; // move data to shared memory
    __syncthreads();
    // do computation
    if (S[i][j]>S[i][k]+S[k][j])
        D[i][j]= S[i][k]+S[k][j];
}
```

ONLY 2 global mem access

Limit of Dynamic Allocation

- If you have multiple extern declaration of shared:

```
extern __shared__ float As[];
extern __shared__ float Bs[];
```

  this will lead to As pointing to the same address as Bs.

- Solution: keep `As` and `Bs` inside the 1D-array.

```
extern __shared__ float smem[];
```

- Need to do the memory management yourself
  - When calling kernel, launch it with size of `sAs+sBs`, where `sAs` and `sBs` are the size of `As` and `Bs` respectively.
  - When indexing elements in `As`, use `smem[0:sAs-1]`; when indexing elements in `Bs`, use `smem[sAs:sAs+sBs]`.

Using Shared Memory

- `FW_APSP<<<1,n*n, n*n*sizeof(int)>>>(…);`
  - The third parameter is the size of shared memory.

```
extern __shared__ int S[];
__global__ void FW_APSP(int* k, int* D,int* n) {
    int i = threadIdx.x;
    int j = threadIdx.y;
    S[i*(*n)+j]=D[i*(*n)+j]; //move data to shared memory
    __syncthreads();
    // do computation
    if (S[i*(*n)+j]>S[i*(*n)+k]+S[k*(*n)+j])
        D[i*(*n)+j]= S[i*(*n)+k]+S[k*(*n)+j];
}
```

Static Shared Memory Allocation

- If the size of shared memory is known in compilation time, shared memory can be allocated statically.

```
__global__ void FW_APSP(int k, int D[][]){
    __shared__ int DS[10*10];
    ...
}
```

Must know n=10 at compile time

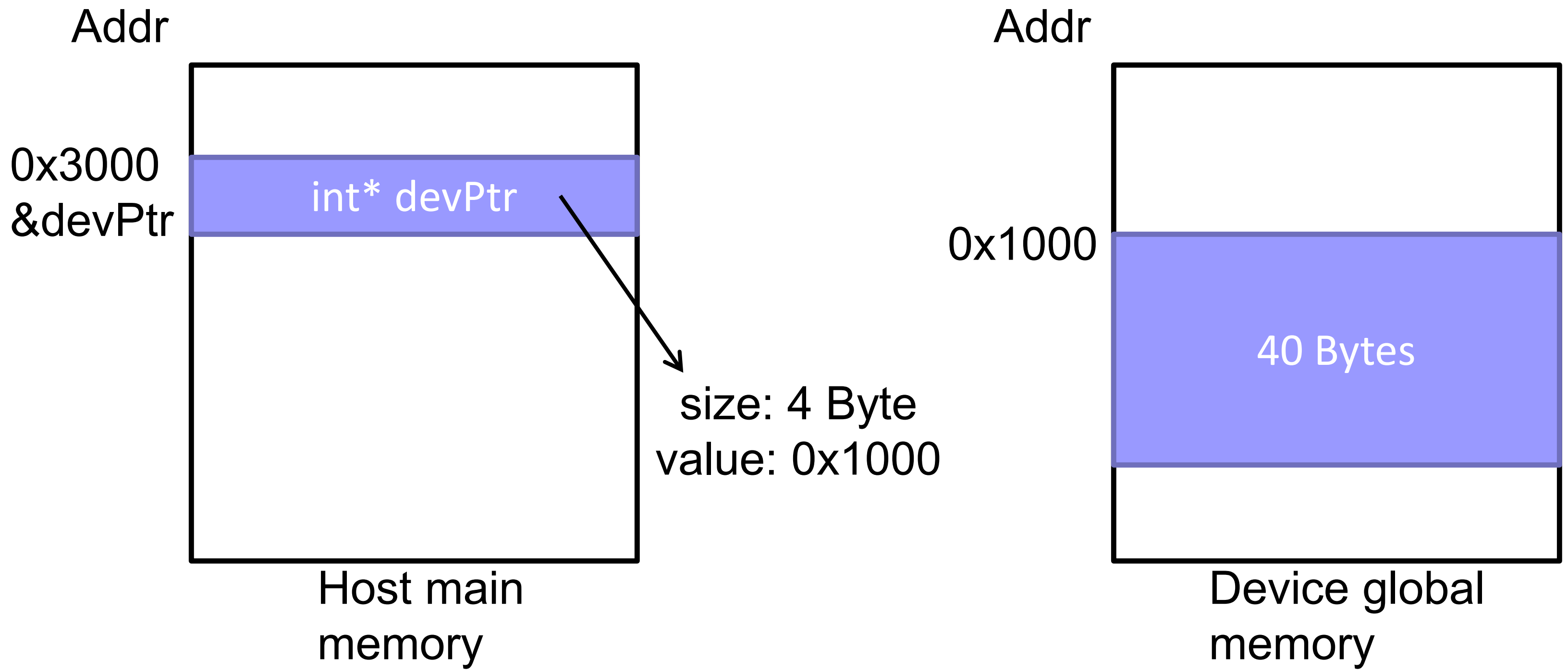
Outline

- Thread execution
- Memory hierarchy
  - Register & Local memory
  - Shared memory
  - Global & Constant memory

How to Allocate Device (Global) Memory

1. `cudaMalloc(void **devPtr, size_t size)`
   - `devPtr`: return the address of the allocated memory on **device**
   - `size`: the allocated memory size (**bytes**)

2. `cudaFree (void *devPtr)`



Synchronous Global Memory Copy

- `cudaMemcpy( void *dst, const void *src, size_t count, enum` **`cudaMemcpyKind`** `kind)`
  - `count`: size in **bytes** to copy

`cudaMemcpyKind`	**Meaning**	`dst`	`src`
`cudaMemcpyHostToHost`	Host → Host	host	host
`cudaMemcpyHostToDevice`	Host → Device	device	host
`cudaMemcpyDeviceToHost`	Device → Host	host	device
`cudaMemcpyDeviceToDevice`	Device → Device	device	device

host to host has the same effect as memcpy()

Complier does not distinguish between the device pointer & host pointer.
You have to check by yourself very carefully.

Copy 3 Int between Device & Host

```
int main(void) {
   int a=1, b=2, c; // host copies of a, b, c
   int *d_a, *d_b, *d_c; // device copies of a, b, c
   // Allocate space for device copies of a, b, c
   cudaMalloc((void **)&d_a, sizeof(int));
   cudaMalloc((void **)&d_b, sizeof(int));
   cudaMalloc((void **)&d_c, sizeof(int));
   // Copy inputs to device
   cudaMemcpy(d_a,&a,sizeof(int),cudaMemcpyHostToDevice);
   cudaMemcpy(d_b,&b,sizeof(int),cudaMemcpyHostToDevice);
   // Launch add() kernel on GPU
   add<<<1,1>>>(d_a, d_b, d_c);
   // Copy result back to host
   cudaMemcpy(&c, d_c, sizeof(int), cudaMemcpyDeviceToHost);
   // Cleanup
   cudaFree(d_a); cudaFree(d_b); cudaFree(d_c);
   return 0;
}
```

Constant Memory

- Same usage and scope as the global memory except
  - **Read only**
  - Declare by variable qualifier `__constant__`
  - Move by `cudaMemcpyToSymbol()` & `cudaMemcpyFromSymbol()`
- Each SM has its own constant memory
  - The constant memory on each SM is of size 64K, and has a separated cache, of size 8K.

```
__constant__ int constData[100];
int main(void) {
    int A[100];
    cudaMemcpyToSymbol(constData, A, sizeof(A));
    add<<<grid_size,blk_size>>>();
    cudaMemcpyFromSymbol(A, constData, sizeof(A));
}
__global__ kernel() {
    int v = constData[threadIdx];
}
```

CUDA Variables within a Kernel

Variable declaration	Memory	Scope	Lifetime
`int var`	Register	Thread	Thread
`int array_var[10]`	Local	Thread	Thread
`__shared__ int shared_var`	Shared	Block	Block
`__device__ int global_var`	Global	Grid	App
`__constant__ int constant_var`	Constant	Grid	App

- Scalar variables without qualifier reside in a register
  - Compiler will spill to thread local memory
- Array variables without qualifier reside in thread-local memory

Memory Speed

Variable declaration	Memory	Speed
`int var`	Register	1x
`int array_var[10]`	Local	100x
`__shared__ int shared_var`	Shared	1x
`__device__ int global_var`	Global	100x
`__constant__ int constant_var`	Constant	1x

- Scalar variables reside in fast, on-chip registers
- Shared variables reside in fast, on-chip memories
- Thread-local arrays & global variables reside in uncached off-chip memory
- Constant variables reside in cached off-chip memory

Memory Scale

Variable declaration	Total no. of variables	Visible by no. of threads
`int var`	100,000	1
`int array_var[10]`	100,000	1
`__shared__ int shared_var`	100	100
`__device__ int global_var`	1	100,000
`__constant__ int constant_var`	1	100,000

- 100Ks per-thread variables, R/W by 1 thread
- 100s shared variables, each R/W by 100s of threads
- Global variable is R/W by 100Ks threads
- 1 constant variable is readable by 100Ks threads

Reference

- **NVIDIA CUDA Library Documentation**
  - http://developer.download.nvidia.com/compute/cuda/4_1/rel/toolkit/docs/online/index.html
- **NVIDIA CUDA Warps and Occupancy**
  - http://on-demand.gputechconf.com/gtc-express/2011/presentations/cuda_webinars_WarpsAndOccupancy.pdf