GPU Parallel Programming: CUDA

National Tsing-Hua University 2019, Summer Semester

Outline

- **CUDA Basic**
- Example Code Study
 - > Hello world
 - > All pairs shortest path
- Time Measurement & Debug API
- Multi-GPUs
- Dynamic Parallelism



What is CUDA?

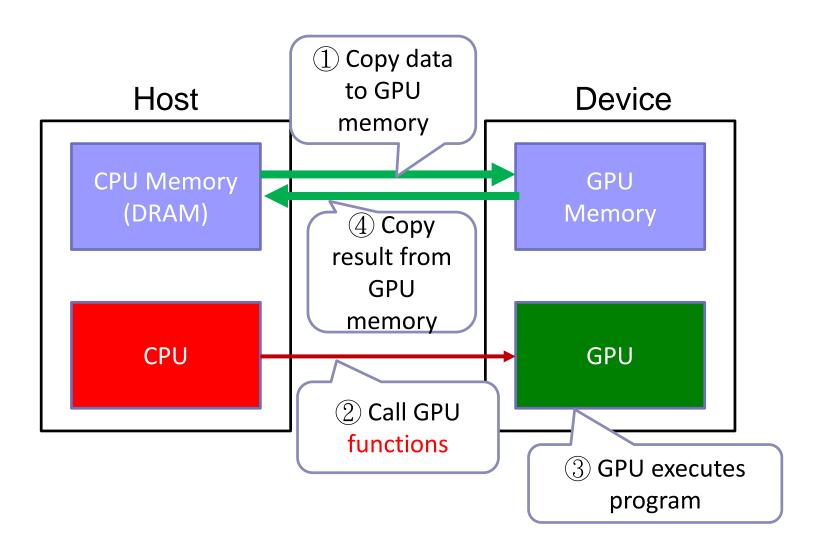
- CUDA: Compute Unified Device Architecture
 - > CUDA is a compiler and toolkit for programming NVIDIA GPUs
 - > Enable heterogeneous computing and horsepower of GPUs
 - CUDA API extends the C/C++ programming language
 - Express SIMD parallelism
 - Give a high level abstraction from hardware

CUDA version

- > The latest version is 7.5
- ➤ We will learn the syntax of 4.2 first, because we will use it in the optimization lectures



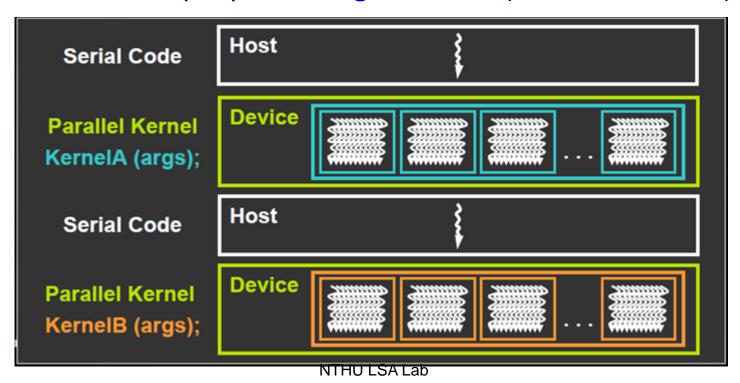
CUDA program flow



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- CUDA = serial program with parallel kernels, all in C
 - Serial C code executes in a host thread (i.e. CPU thread)
 - ➤ Parallel kernel C code executes in many devices threads across multiple processing elements (i.e. GPU threads)





GPU code (parallel)

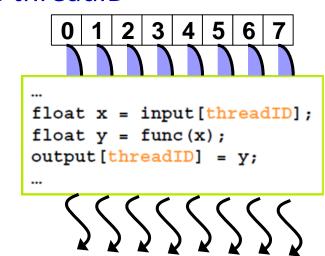
CPU code (serial or parallel if p-thread/ OpenMP/T BB/MPI is used.)

```
#include <cuda_runtime.h>
  global void my_kernel(...) {
int main() {
   cudaMalloc(...)
   cudaMemcpy(...)
      my_kernel<<<nblock,blocksize>>>(...)
   cudaMemcpy(...)
```



Kernel = Many Concurrent Threads

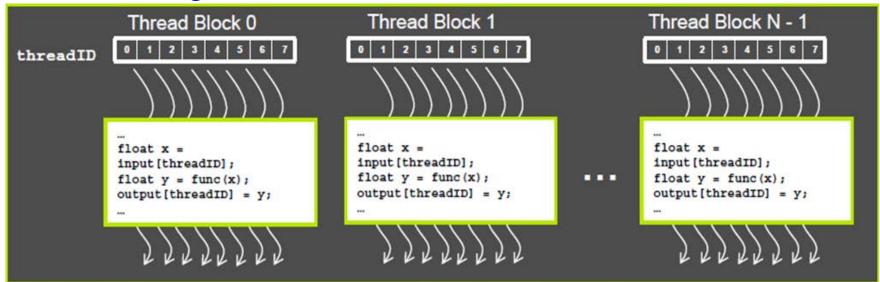
- One kernel is executed at a time on the device
- Many thread execute each kernel
 - > Each thread executes the same code
 - ... on the different data based on its threadID
- CUDA thread might be
 - Physical threads
 - As on NVIDIA GPUs
 - GPU thread creation and context switching are essentially free
 - Or virtual threads
 - E.g. 1 CPU core might execute multiple CUDA threads





Hierarchy of Concurrent Threads

- Threads are grouped into thread blocks
 - Kernel = gird of thread blocks



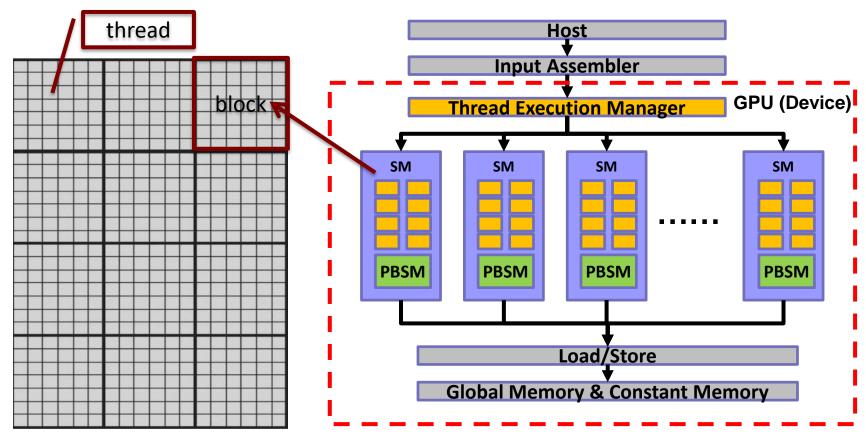
 By definition, threads in the same block may synchronized with barriers, but not between blocks

```
scratch[threadID] = begin[threadID];
__syncthreads();
int left = scratch[threadID - 1];
```



Software Mapping

- Software: grid → blocks→ threads
- Hardware: GPU(device) → SM(multicore processor) → core

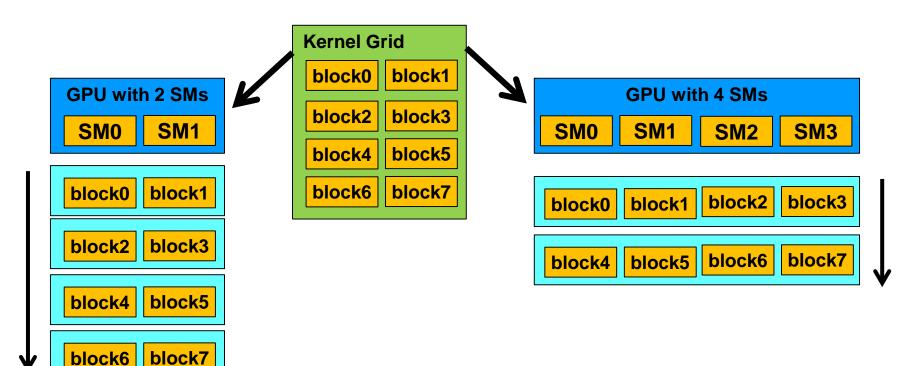


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Transparent Scalability

- Thread blocks cannot synchronize
 - So they can run in any order, concurrently or sequentially
- This independence gives scalability:
 - A kernel scales across any number of parallel cores



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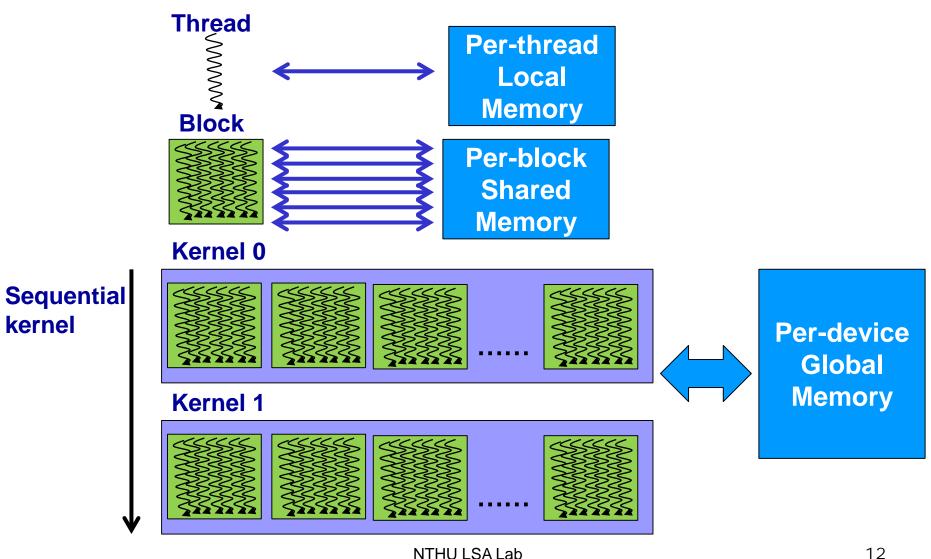
Thread group limits

- The maximum number of threads per block is limited
 - 512 before CUDA 2.0
 - > 1024 after CUDA 2.0
- The maximum number of blocks is limited
 - 65535 before CUDA 3
 - \geq 2³¹-1 after CUDA 3
- Total number of threads = threads per block * number of blocks

Use deviceQuery.cpp to find out your limits



Memory Hierarchy



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CUDA Programming Terminology

■ Host : CPU

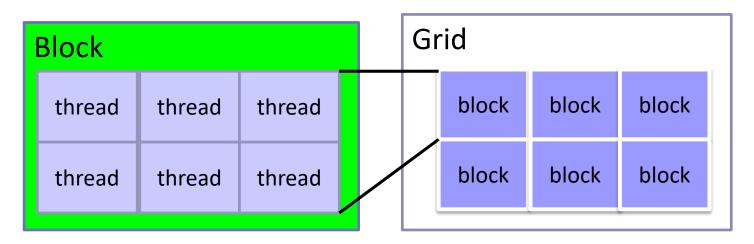
Device : GPU

Kernel: functions executed on GPU

Thread: the basic execution unit

■ Block : a group of threads

Grid: a group of blocks





Quiz

- What is a CUDA kernel?
- What are the 4 steps of CUDA program flow?
- Can a kernel run on two different devices at the same time?
- Can a kernel run across multiple SM processors?
- Can the threads from a same block run across multiple SM processors?
- Why shared block memory can only be accessed by the threads in the same blocks?
- Why __syncthreads() is not supported across blocks?



CUDA Language

Philosophy: provide minimal set of extensions necessary

Kernel launch

- Build-in device variables
 - threadIdx; blockIdx; blockDim; gridDim
- Intrinsic functions that expose operations in kernel code __syncthreads();
- Declaration specifier to indicate where things live

```
__global__ void KernelFunc(...); // kernel function, run on device
__device__ void GlobalVar; // variable in device memory
__shared__ void SharedVar; // variable in per-block shared memory
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```

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Thread and Block IDs

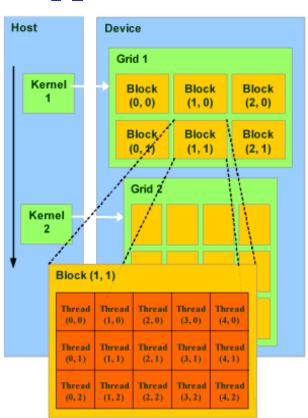
- The index of threads and blocks is a 3-tuple: dim3
- dim3 is a struct defined in vector_types.h

```
struct dim3 { x; y; z; };
```

Example:

```
> dim3 grid(3, 2);
> dim3 blk(5, 3);
> my_kernel<<< grid, blk >>>();
```

■ Each thread can be uniquely identified by a pair of index (x,y).



Function Qualifiers

Function qualifiers	limitations
device function	Executed on the device Callable from the device only
globalfunction	Executed on the device Callable from the host only (must have void return type!)
host function	Executed on the host Callable from the host only
Functions without qualifiers	Compiled for the host only
host devicefunction	Compiled for both the host and the device



Variable Type Qualifiers

Variable qualifiers	limitations
devicevar	 Resides in device's global memory space
constantvar	 Has the lifetime of an application Is accessible from all the threads within the grid and from the host through the runtime library
	• Resides in device's constant memory space
sharedvar	 Resides in the shared memory space of a thread block Has the lifetime of the block Is only accessible from all the threads within the block



Device memory operations

- Three functions:
 - > cudaMalloc(), cudaFree(), cudaMemcpy()
 - Similar to the C's malloc(), free(), memcpy()
 - 1. cudaMalloc(void **devPtr, size_t size)
 - devPtr: return the address of the allocated device memory
 - size: the allocated memory size (bytes)
 - 2. cudaFree (void *devPtr)
 - 3. cudaMemcpy(void *dst, const void *src, size_t count, enum cudaMemcpyKind kind)
 - count: size in bytes to copy



one of the following four values

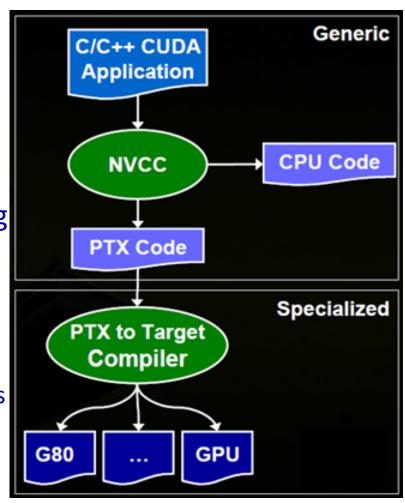
cudaMemcpyKind	Meaning	dst	src
cudaMemcpyHostToHost	Host → Host	host	host
cudaMemcpyHostToDevice	Host → Device	device	host
cudaMemcpyDeviceToHost	Device → Host	host	device
cudaMemcpyDeviceToDevice	Device → Device	device	device

host to host has the same effect as memcpy()



Program Compilation

- Any source file containing CUDA language must be compiled with NVCC
 - NVCC separates code running on the host from code running on the device
- Two-stage complication:
 - Virtual ISA
 - PTX: Parallel Threads executions
 - Device-specific binary object





Quiz

How to index a 100 elements of an array under the following kernel launch setting?

```
int i = A[i] = A[i] + 1;
}

1. my_kernel <<< 1, 100 >>>(A);
2. my_kernel <<< 100, 1 >>>(A);
3. my_kernel <<< 10, 10 >>>(A);
4. size=10; dim3 blk(size, size);
my_kernel <<< 1, blk >>>(A, size);
```

__global__ void VecAdd(float* A)

// Kernel definition

Quiz

Function qualifiers	limitations
devicefunction	
globalfunction	
Functions without qualifiers	

Variable qualifiers	Limitations (Lifetime, Data Scope)
devicevar	
constantvar	
sharedvar	

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Example 1: Hello World!

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

- Two new syntactic elements...
 - 1. __global__ indicates a function that runs on the device and is called from host code
 - mykernel<<<1,1>>>();
 Triple angle brackets mark a call from host code to device code, which is called a "kernel launch".



Example 2: add 2 numbers

```
__global___ void add(int *a, int *b, int *c) {
    *c = *a + *b;
}
int main(void) {
    int ha=1,hb=2,hc;
    add<<<1,1>>>(&ha, &hb, &hc);
    printf("c=%d\n",hc);
    return 0;
}
```

- This does not work!!
- int ha, hb, hc are in the host memory (DRAM), which cannot be used by device (GPU).
- We need to allocate variables in "device memory".



The correct main()

```
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, size, cudaMemcpyDeviceToHost);
  // Cleanup
   cudaFree(d_a); cudaFree(d_b); cudaFree(d_c);
  return 0;
```



Example 3: add 2 vectors

■ Let's first look at the sequential code!

```
// function definition
void VecAdd(int N, float* A, float* B, float* C)
{
     for(int i = 0; i<N; i++)
           C[i] = A[i] + B[i];
int main()
{ ...
   VecAdd (N, Ah, Bh, Ch);
```



Parallel CUDA code

- Use blockIdx.x as the index of the arrays
 - ➤ Each thread processes 1 addition, for the elements indexed at blockIdx.x.

```
// Kernel definition
__global__ void VecAdd(float* A, float* B, float* C)
{
     int i = threadIdx.x;
     C[i] = A[i] + B[i];
int main()
{ ...
     // Kernel invocation with N threads
     VecAdd<<<1, N>>>(Ah, Bh, Ch); ...
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```

Alternative implementation

Using parallel thread instead

```
__global___ void add(int *a, int *b, int *c) {
    c[blockIdx.x] = a[blockIdx.x] + b[blockIdx.x];
}
int main(void) {
    int a[N], b[N], c[N];
    int *d_a, *d_b, *d_c;
    ...
    add<<< N, 1 >>>(d_a, d_b, d_c);
    ...
}
```

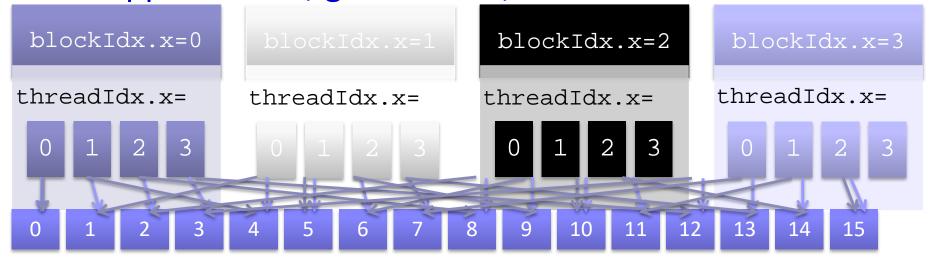
- N blocks and each block has 1 thread.
- Which one is better?
 - Threads in the same block can communicate, synchronize with others, but the number of threads per block is limited.

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3rd implementation

- Using multiple threads and multiple blocks
- Suppose N=16, grid size = 4, and block size = 4



- How to index 16 elements of an array?
 - Method 1: index = blockIdx.x*4+threadIdx.x
 - ➤ Method 2: index = threadIdx.x*4+blockIdx.x
- Which one is better?



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

```
__global___ void add(int *a, int *b, int *c) {
   int index = threadIdx.x + blockIdx.x * blockDim.x;
   c[index] = a[index] + b[index];
}
int main(void) {
   int a[N], b[N], c[N];
   int *d_a, *d_b, *d_c;
   ...
   add<<< N/BS,BS>>>(d_a, d_b, d_c);
   ...
}
What if N is not a
   multiple of BS?
...
add<<< N/BS,BS>>>(d_a, d_b, d_c);
...
}
```

■ BS is block size (number of threads per block)



A even more general case

```
__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];
}
int main(void) {
   int a[N], b[N], c[N];
   int *d_a, *d_b, *d_c;
   ...
   add<<< (N+BS-1)/BS, BS>>>(d_a, d_b, d_c, N);
   ...
}
```

■ The kernel function can have branches, but with a price to pay...



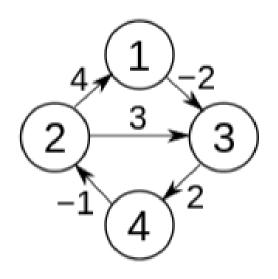
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APSP

- Given a weighted directed graph G(V, E, W), where |V| = n, |W|=m, and W>0, find the shortest path of all pairs of vertices (vi,vj).
- **■** Example:



0	INF	-2	INF
4	0	3	INF
INF	INF	0	2
INF	-1	INF	0

Initial weight

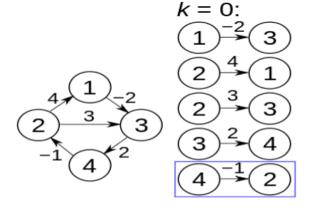
0	-1	-2	0
4	0	2	4
5	1	0	2
3	-1	1	0

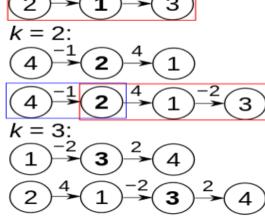
Final result

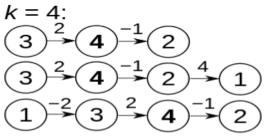


Floyd-Warshall (Sequential code)

k = 1:









Implementation I

- 1 block and *n* threads.
- Thread i updates the SP for vertex i.

```
_global__ void FW_APSP(int k, int D[n][n]) {
     int i = threadIdx.x;
       for (int j = 0; j < n; j++)
            if (D[i][j]>D [i][k]+D[k][j])
                  D[i][j] = D[i][k] + D[k][j];
int main() { ...
     for (int k = 0; k < n, k++)
         FW APSP<<<1, n>>>(k, D);
```

Simple! But can it be faster?



Implementation 2

- Each thread updates one pair of vertices
 - ➤ Increase parallelism from n to n²

```
__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);
}
```

■ How about the for-loop of k?



Implementation 3

```
global void FW_APSP(int D[n][n]) {
    int i = threadIdx.x;
   int j = threadIdx.y;
    for (int k = 0; k < n, k++)
        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);
    FW APSP<<<1, threadsPerBlock >>>(D);
```

- It is a synchronous computation
 - There are data dependency on k...



Add __syncthreads()

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



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Execution time: in host

CUDA provides functions to measure the execution time between events.

- ms: time between start and end in ms
- start: starting event
- end: ending event
- The time unit is milliseconds, whose resolution is 0.5 microseconds



CUDA event

- Data type : cudaEvent_t
- cudaError_t cudaEventCreate(cudaEvent_t* event)
 - Create CUDA event
- cudaError_t cudaEventRecord(cudaEvent_t event, cudaStream_t stream = 0)
 - Record CUDA event
 - If stream is non-zero, the event is recorded after all preceding operations in the stream have been completed
 - Since operation is asynchronous, cudaEventQuery() and/or cudaEventSynchronize() must be used to determine when the event has actually been recorded
- cudaError_t cudaEventSynchronize(cudaEvent_t event)
 - Wait until the completion of all device work preceding the most recent call to cudaEventRecord()



Example

```
cudaEvent_t start, stop;
                                         Create event
   cudaEventCreate(&start);
2.
   cudaEventCreate(&stop);
3.
                                       Record event
   cudaEventRecord(start);
4.
   kernel<<<blook, thread>>>();
                                           Record event and
   cudaEventRecord(stop);
                                             synchronize
6.
   cudaEventSynchronize(stop);
7.
   float time;
8.
   cudaEventElapsedTime(&time, start, stop);
9.
                                  Compute the event duration
```

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Reporting errors

- All CUDA 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)



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Using CUDA with pthread

Launch the kernel function for a GPU in a thread

```
void* GPUthread(void* arg){
   struct HYBctx* ctx = (struct HYBctx*)arg;
   int *dA, A[32]=...;
   cudaMalloc((void**)&dA, sizeof(int)*32);
   cudaMemcpy(dA, A, sizeof(int)*32,
              cudaMemcpyHostToDevice);
   kernel <<<1, 32>>> (dA);
   cudaMemcpy(A, dA, sizeof(int)*32,
              cudaMemcpyDeviceToHost);
   cudaFree(dA);
   cudaDown(ctx);
   return NULL;
```



Using CUDA with OpenMP

- Put CUDA functions inside the parallel region
- General setting:
 - ➤ The number of CPU threads is the same as the number of CUDA devices. Each CPU thread controls a different device, processing its portion of the data.
- It's possible to use more CPU threads than there are CUDA devices.
 - Several CPU threads will be allocating resources and launching kernel on the same device, which will slow down the performance.



Example: cudaOMP.cu

```
cudaGetDeviceCount(&num qpus);
. . .
omp_set_num_threads(num_gpus);
// create as many CPU threads as there are CUDA devices
#pragma omp parallel
   unsigned int cpu_thread_id = omp_get_thread_num();
   unsigned int num_cpu_threads = omp_get_num_threads();
   CUDA_SAFE_CALL(cudaSetDevice(cpu_thread_id));
   int qpu id = -1;
   CUDA_SAFE_CALL(cudaGetDevice(&gpu_id));
   printf("CPU thread %d (of %d) uses CUDA device %d\n",
           cpu_thread_id, num_cpu_threads, gpu_id);
```

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Using CUDA with MPI

```
int main(int argc, char* argv[]){
   int rank, size;
   int A[32];
   int i;
   MPI_Init(&argc, &argv);
   MPI Comm rank(MPI COMM WORLD, &rank);
   MPI_Comm_size(MPI_COMM_WORLD, &size);
   printf("I am %d of %d\n", rank, size);
   for(i = 0; i < 32; i++) A[i] = rank+1;
   launch(A); // a call to launch CUDA kernel
   MPI_Barrier(MPI_COMM_WORLD);
   MPI Finalize();
   return 0;
```



Example: launch(A)

```
extern "C"
void launch(int *A){
    int *dA;
    cudaMalloc((void**)&dA, sizeof(int)*32);
    cudaMemcpy(dA, A, sizeof(int)*32,
                cudaMemcpyHostToDevice);
    kernel <<<1, 32>>> (dA);
    cudaMemcpy(A, dA, sizeof(int)*32,
                cudaMemcpyDeviceToHost);
    cudaFree(dA);
```



Compilation and execution

Compilation

```
> nvcc -c kernel.cu
> mpicc -o mpicuda mpi.c kernel.o
-L /usr/local/cuda/lib -lcudart
-I /usr/local/cuda/include
```

■ Execution

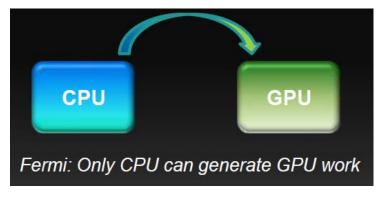
➤ mpirun -l -np 4 ./mpicuda

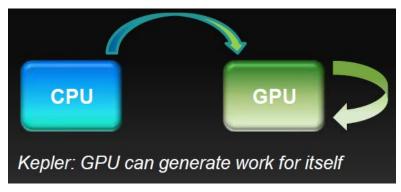
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Dynamic parallelism

- The ability to launch new grids from the GPU
 - Dynamically
 - Simultaneously
 - Independently
- Supported from CUDA5.0 on devices of Compute Capability 3.5 or higher



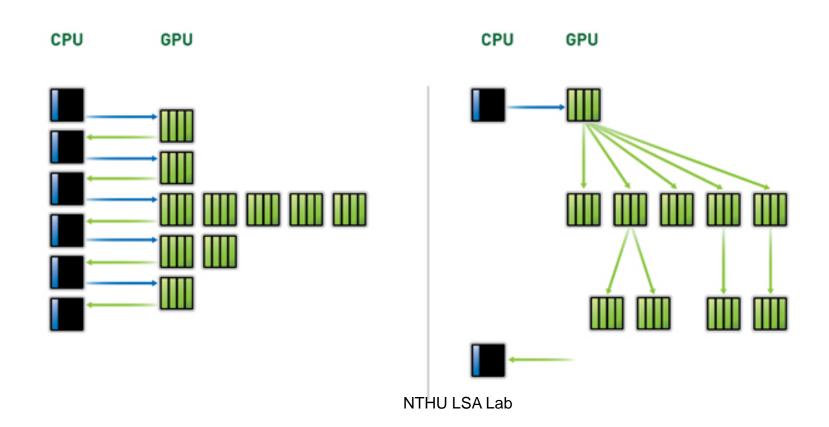




What does it mean?

■ Reduce the number of kernel launches

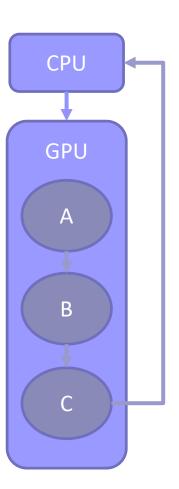
DYNAMIC PARALLELISM





Dependency in CUDA

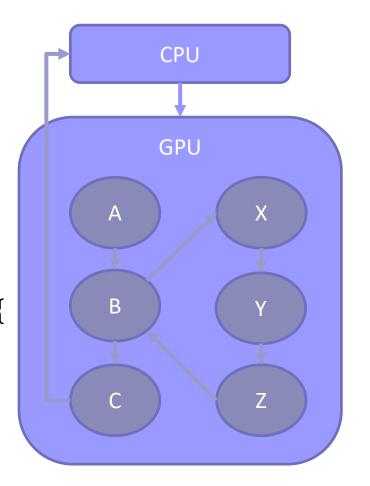
```
void main() {
   float *data;
   do_stuff(data);
   A <<< ... >>> (data);
   B <<< ... >>> (data);
   C <<< ... >>> (data);
   cudaDeviceSynchronize();
   do_more_stuff(data);
}
```





Nested dependency

```
void main() {
   float *data;
   do_stuff(data);
   A <<< ... >>> (data);
   B <<< ... >>> (data);
   C <<< ... >>> (data);
   cudaDeviceSynchronize();
   do more stuff(data);
 global___ void B(float *data){
  do stuff(data);
  X <<< ... >>> (data);
  Y <<< ... >>> (data);
  Z <<< ... >>> (data);
  cudaDeviceSynchronize();
  do_more_stuff(data);
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```



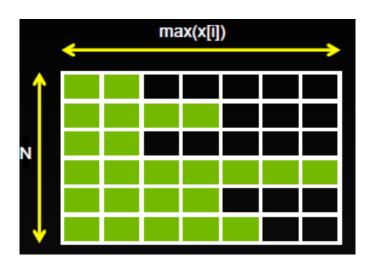


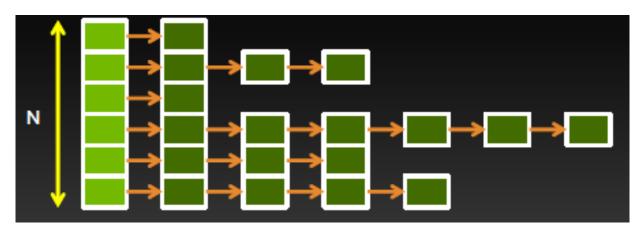
What is DP good for?

- Dynamic block size and grid size
- Dynamic work generation
- Nested parallelism
- Library calls
- Parallel recursion



```
for i = 1 to N
  for j = 1 to x[i]
     convolution(i, j)
  next j
next i
```

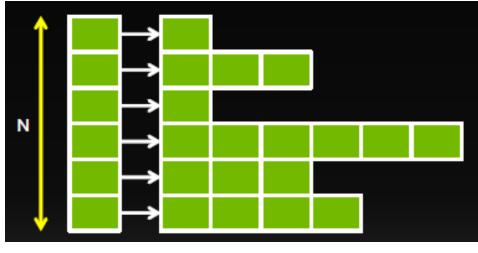






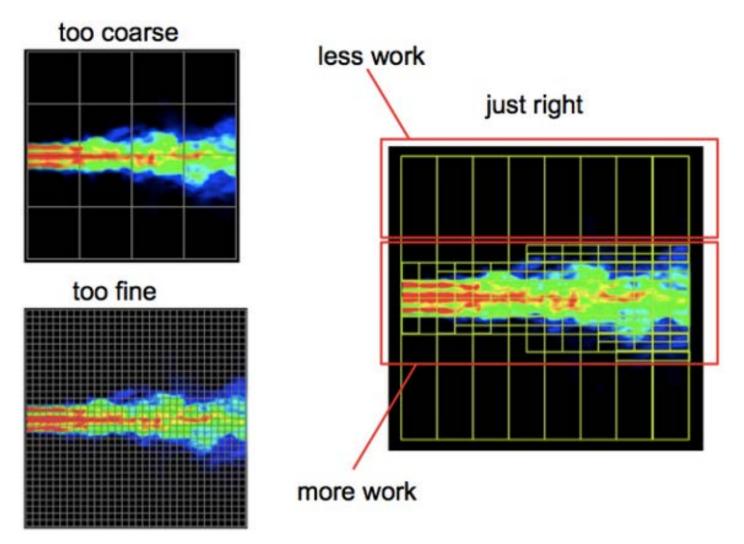
1. Dynamic block size with DP

```
__global___ void convolution(int x[]){
   for j = 1 to x[blockIdx]
        kernel<<< ... >>>(blockIdx, j)
}
...
convolution<<< N, 1 >>>(x);
```

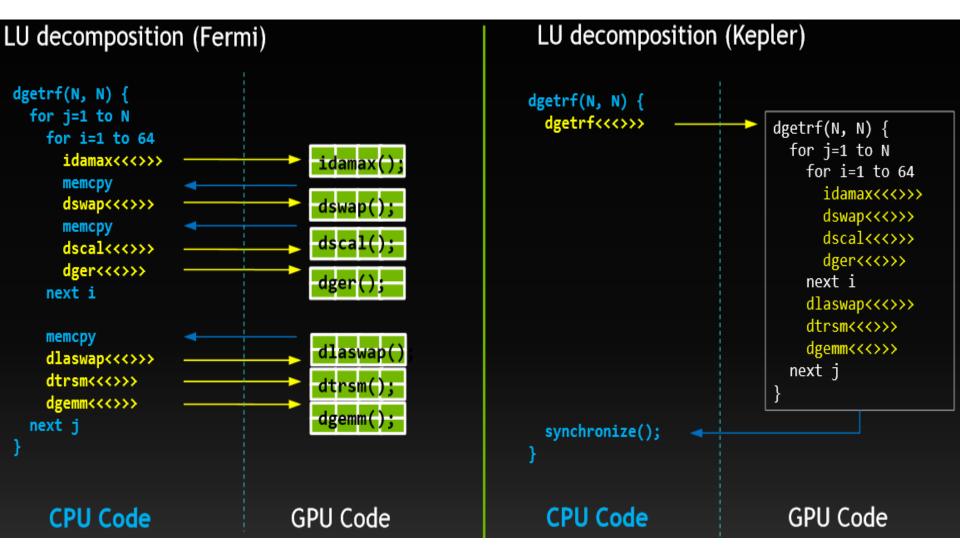


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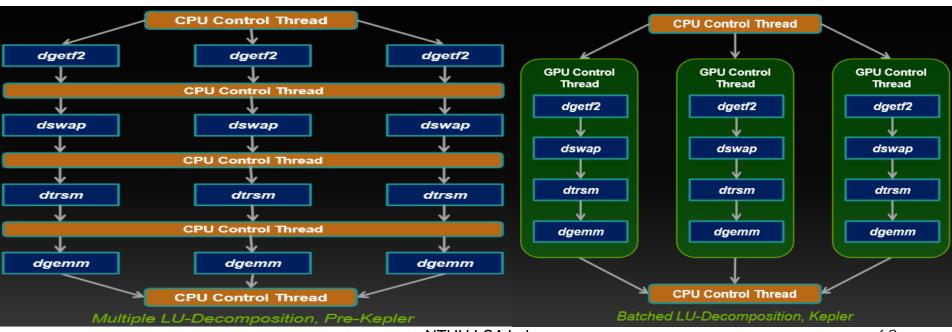


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LU Decomposition

- CPU controlled batching
 - Limited by single point control
 - Can run at most 10s of threads
 - CPU is fully consumed with controlling launches

- Batching via DP
 - Move top loop to GPU
 - Run thousands of independent tasks
 - Release CPU for other work



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4. Library call

```
global___ void libraryCall(float *a,float *b,float *c){
 // All threads generate data
 createData(a, b);
 __syncthreads();
 // Only one thread calls library
 if(threadIdx.x == 0) {
     cublasDgemm(a, b, c);
     cudaDeviceSynchronize();
 // All threads wait for dtrsm
 __syncthreads();
 // Now continue
 consumeData(c);
```



5. Parallel Recursion

Quick sort

```
<u>__global___</u> void qsort(int *data, int l, int r) {
  int pivot = data[0];
  int *lptr = data+l, *rptr = data+r;
  // Partition data around pivot value
  partition(data, 1, r, lptr, rptr, pivot);
  // Launch next stage recursively
  if(1 < (rptr-data))
      qsort <<< ... >>> (data, l, rptr-data);
  if(r > (lptr-data))
      qsort <<< ... >>> (data, lptr-data, r);
```



Reference

■ NVIDIA CUDA Library Documentation

http://developer.download.nvidia.com/compute/cuda/4_1/rel/toolkit/docs/online/index.html

Heterogeneous computing course slides from Prof.
 Che-Rung Lee