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?

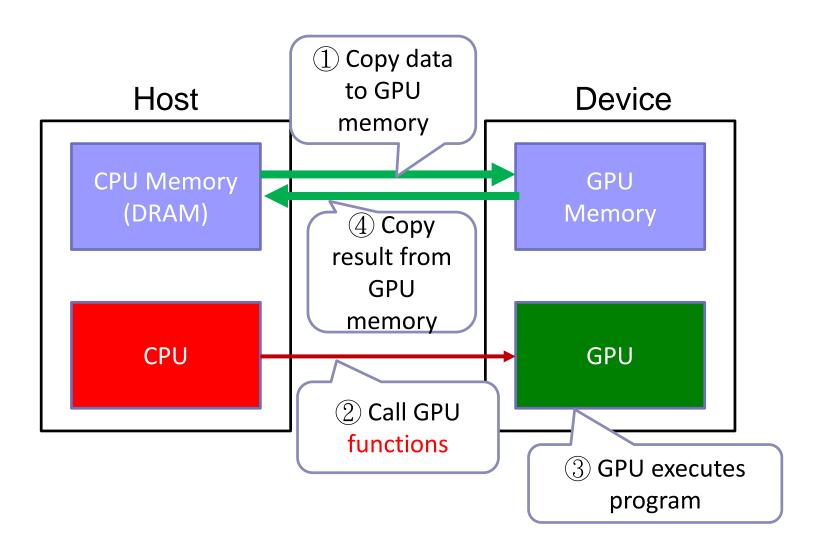
- CUDA: Compute Unified Device Architecture
 - > CUDA is a compiler and toolkit for programming NVIDIA GPUs
 - > Enable heterogeneous computing and horsepower of GPUs
 - CUDA API extends the C/C++ programming language
 - Express SIMD parallelism
 - Give a high level abstraction from hardware

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



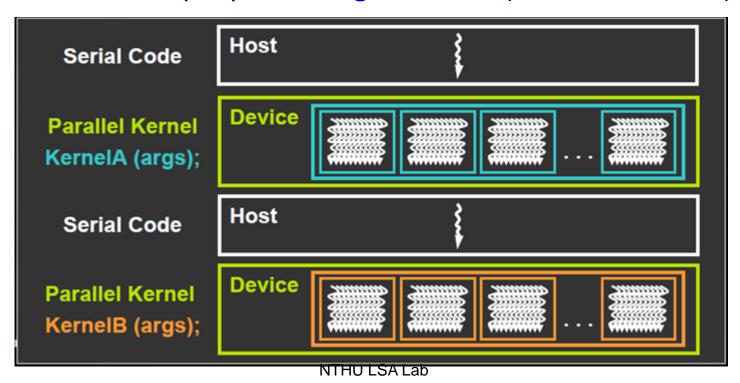
CUDA program flow



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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)

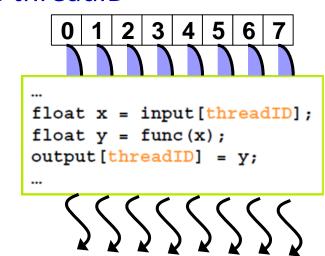
CPU code (serial or parallel if p-thread/ OpenMP/T BB/MPI is used.)

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



Kernel = Many Concurrent Threads

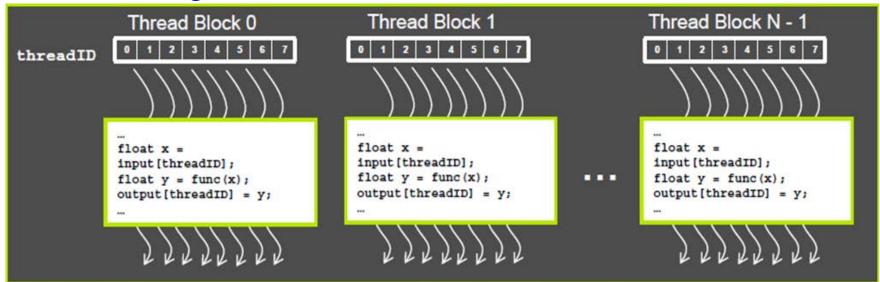
- One kernel is executed at a time on the device
- Many thread execute each kernel
 - > Each thread executes the same code
 - ... on the different data based on its threadID
- CUDA thread might be
 - Physical threads
 - As on NVIDIA GPUs
 - GPU thread creation and context switching are essentially free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



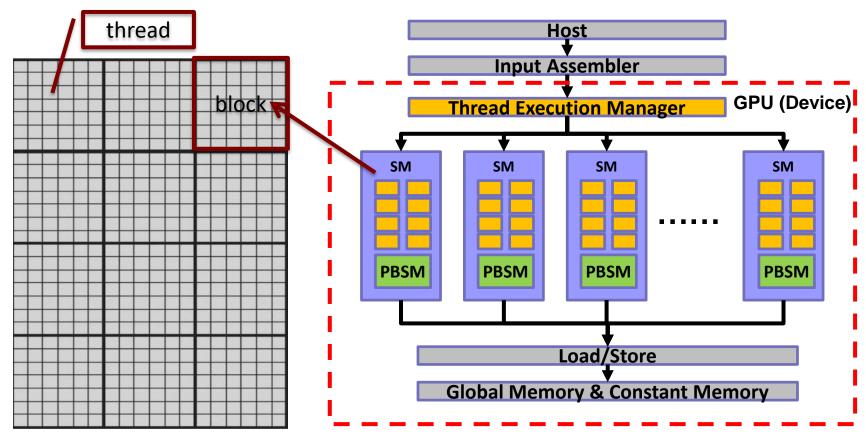
 By definition, threads in the same block may synchronized with barriers, but not between blocks

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



Software Mapping

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

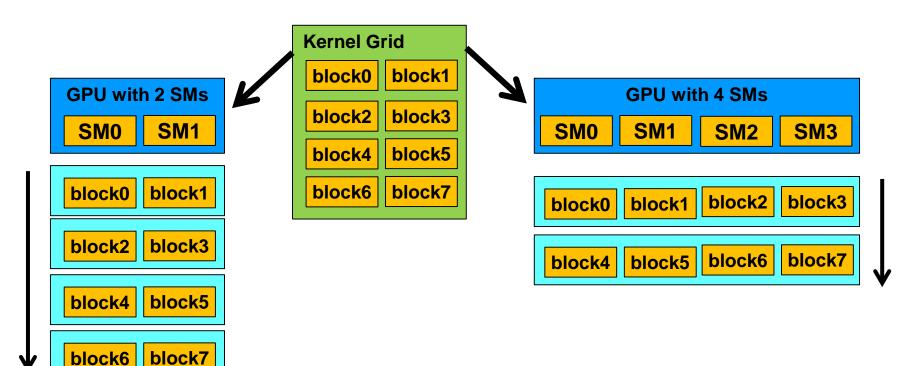


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Transparent Scalability

- 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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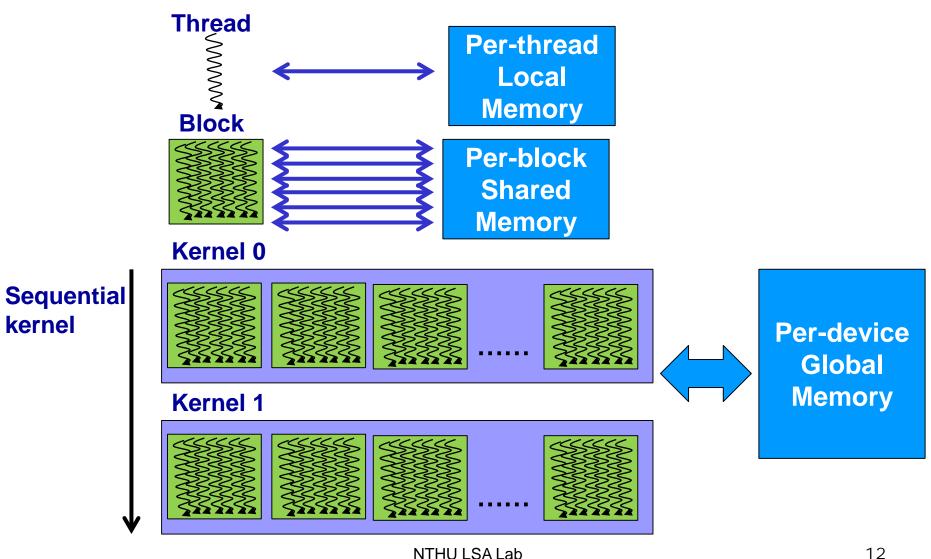
Thread group limits

- 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

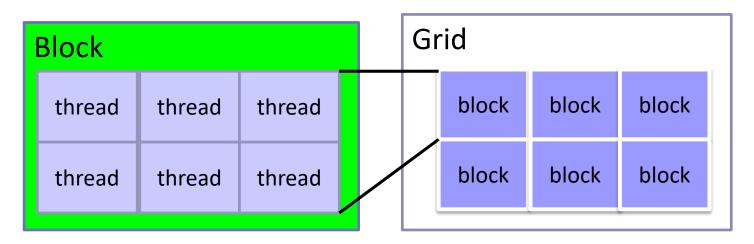
Device : GPU

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

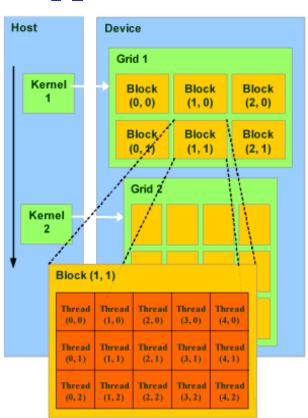
- The index of threads and blocks is a 3-tuple: dim3
- dim3 is a struct defined in vector_types.h

```
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

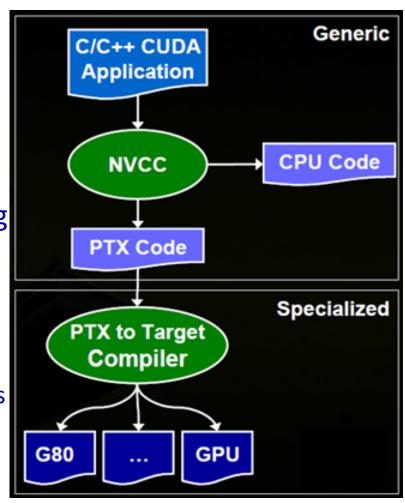
| cudaMemcpyKind | Meaning | dst | src |
|--------------------------|-----------------|--------|--------|
| cudaMemcpyHostToHost | Host → Host | host | host |
| cudaMemcpyHostToDevice | Host → Device | device | host |
| cudaMemcpyDeviceToHost | Device → Host | host | device |
| cudaMemcpyDeviceToDevice | 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);
    ...
}
```

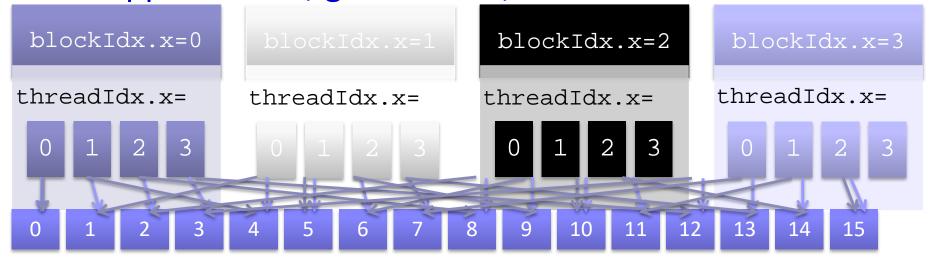
- N blocks and each block has 1 thread.
- Which one is better?
 - Threads in the same block can communicate, synchronize with others, but the number of threads per block is limited.

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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...



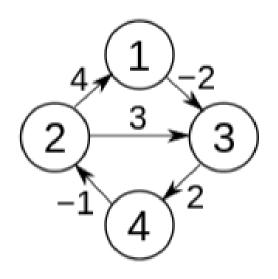
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APSP

- 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

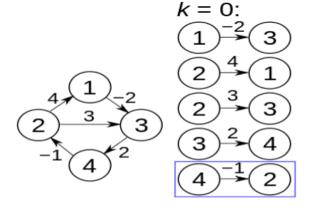
| 0 | -1 | -2 | 0 |
|---|----|----|---|
| 4 | 0 | 2 | 4 |
| 5 | 1 | 0 | 2 |
| 3 | -1 | 1 | 0 |

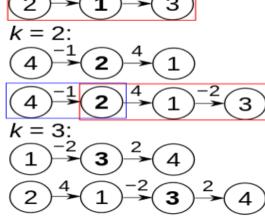
Final result

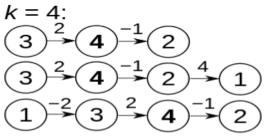


Floyd-Warshall (Sequential code)

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

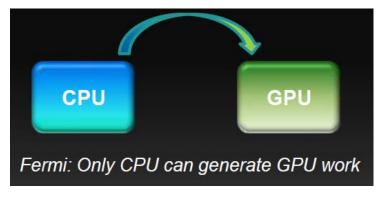
➤ mpirun -l -np 4 ./mpicuda

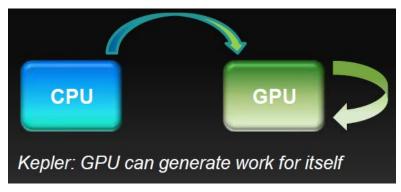
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Dynamic parallelism

- 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



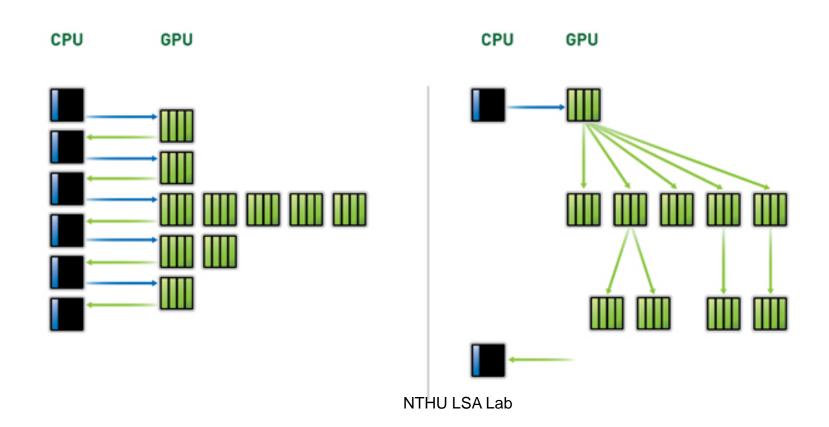




What does it mean?

■ Reduce the number of kernel launches

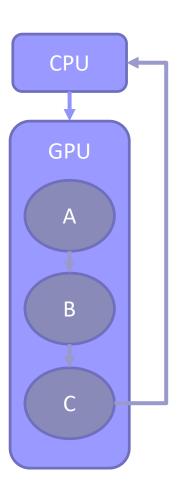
DYNAMIC PARALLELISM





Dependency in CUDA

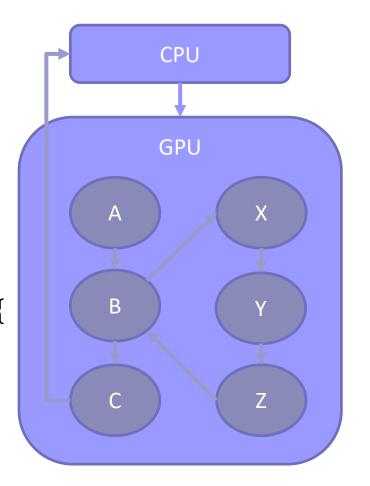
```
void main() {
   float *data;
   do_stuff(data);
   A <<< ... >>> (data);
   B <<< ... >>> (data);
   C <<< ... >>> (data);
   cudaDeviceSynchronize();
   do_more_stuff(data);
}
```





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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```



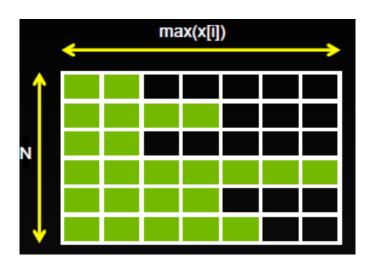


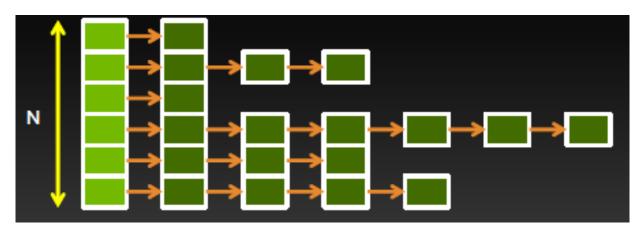
What is DP good for?

- 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
```

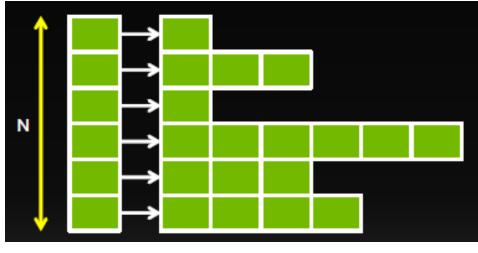






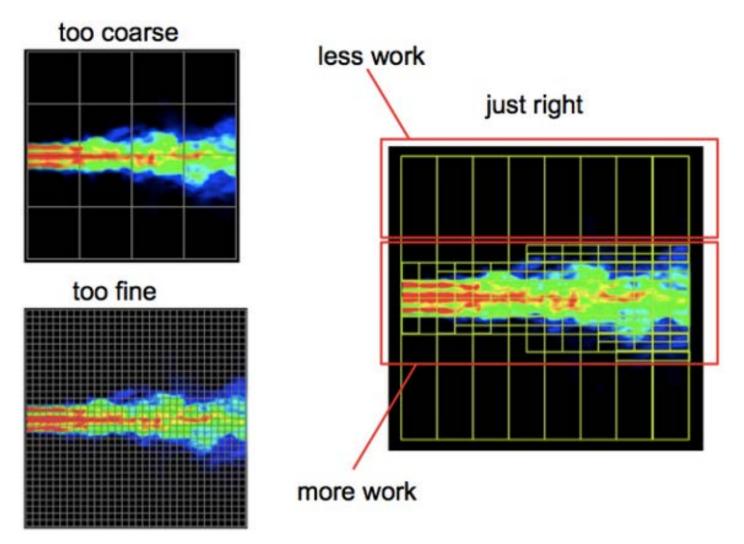
1. Dynamic block size with DP

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

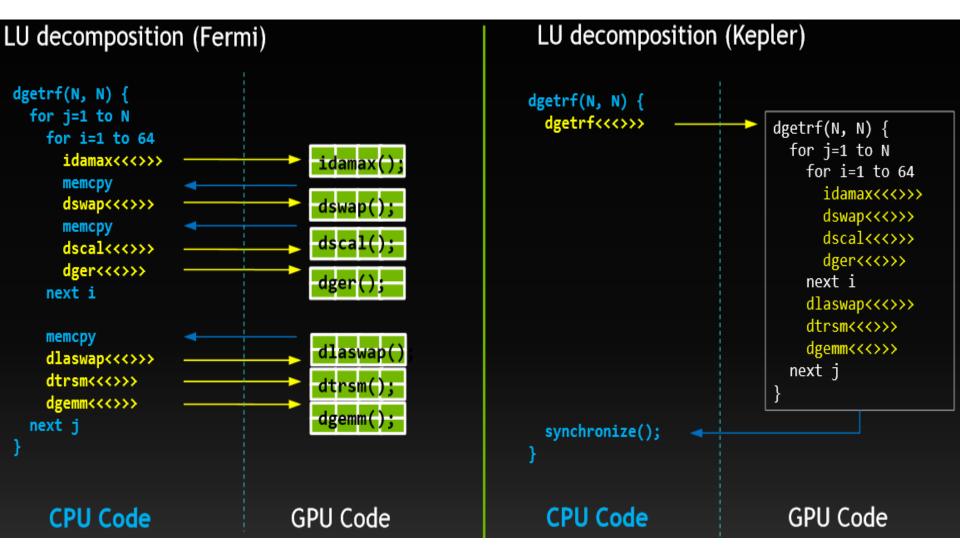


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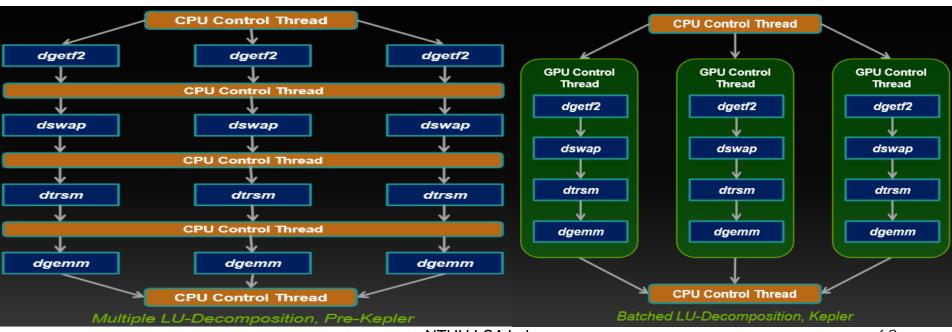


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LU Decomposition

- 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