COMP 4901Q: High Performance Computing (HPC)

Tutorial 2:
Programming with CUDA on GPUs

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Part 1:
Programming environment setup

CUDA Environment on CS Lab2

- CUDA version: 8.0
  - path:/usr/local/cuda-8.0/
- Check your CUDA environment first in the terminal:
  - Use nvcc --version
- If you cannot found nvcc command (or it is not CUDA 8.0), please add the CUDA toolkit installation path to the end of your

  ~/.cshrc_user file

```
csl2wk01:ywanghz:156> nvcc --version
nvcc: NVIDIA (R) Cuda compiler driver
Copyright (c) 2005-2016 NVIDIA Corporation
Built on Tue_Jan_10_13:22:03_CST_2017
Cuda compilation tools, release 8.0, V8.0.61
csl2wk01:ywanghz:157>
```

```
#####################################################
#       File : .cshrc_user
#       Generic Version 1.1. CS. HKUST
#####################################################

setenv MANPATH /usr/local/share/man:${MANPATH}
setenv PATH "${PATH}:/usr/local/software/openmpi/bin"
setenv PATH "${PATH}:/usr/local/cuda-8.0/bin/"
#export CUDA_DEBUGGER_SOFTWARE_PREEMPTION=1
set cuda software_preemption on
~
```

CUDA Environment on CS Lab2

- Check available GPUs:

```
$ nvidia-smi
```

- Detailed description of the installed GPUs

```
$ mkdir ~/cuda-samples
$ cp -r /usr/local/cuda-8.0/samples/1_Utilities ~/cuda-samples/
$ cp -r /usr/local/cuda-8.0/samples/common ~/cuda-samples/
$ cd ~/cuda-samples/1_Utilities/deviceQuery
$ make
$ ./deviceQuery
```

CUDA Environment on CS Lab2

```
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 460.27.04    Driver Version: 460.27.04    CUDA Version: 11.2     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|                               |                      |               MIG M. |
|===============================+======================+======================|
|   0  GeForce GTX 960     Off  | 00000000:01:00.0 Off |                  N/A |
| 39%   27C    P0    26W / 130W |      0MiB /  2001MiB |      0%      Default |
|                               |                      |                  N/A |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                                  |
|  GPU   GI   CI        PID   Type   Process name                  GPU Memory |
|        ID   ID                                                   Usage      |
|=============================================================================|
|  No running processes found                                                 |
+-----------------------------------------------------------------------------+
```

```
./deviceQuery Starting...

 CUDA Device Query (Runtime API) version (CUDART static linking)

Detected 1 CUDA Capable device(s)

Device 0: "GeForce GTX 960"
  CUDA Driver Version / Runtime Version          11.2 / 8.0
  CUDA Capability Major/Minor version number:    5.2
  Total amount of global memory:                 2002 MBytes (2099052544 bytes)
  ( 8) Multiprocessors, (128) CUDA Cores/MP:     1024 CUDA Cores
  GPU Max Clock rate:                            1240 MHz (1.24 GHz)
  Memory Clock rate:                             3505 Mhz
  Memory Bus Width:                              128-bit
  L2 Cache Size:                                 1048576 bytes
  Maximum Texture Dimension Size (x,y,z)         1D=(65536), 2D=(65536, 65536), 3D=(4096, 4096, 4096)
  Maximum Layered 1D Texture Size, (num) layers  1D=(16384), 2048 layers
  Maximum Layered 2D Texture Size, (num) layers  2D=(16384, 16384), 2048 layers
  Total amount of constant memory:               65536 bytes
  Total amount of shared memory per block:       49152 bytes
  Total number of registers available per block: 65536
  Warp size:                                     32
  Maximum number of threads per multiprocessor:  2048
  Maximum number of threads per block:           1024
  Max dimension size of a thread block (x,y,z): (1024, 1024, 64)
  Max dimension size of a grid size    (x,y,z): (2147483647, 65535, 65535)
  Maximum memory pitch:                          2147483647 bytes
  Texture alignment:                             512 bytes
  Concurrent copy and kernel execution:          Yes with 2 copy engine(s)
  Run time limit on kernels:                     No
  Integrated GPU sharing Host Memory:            No
  Support host page-locked memory mapping:       Yes
  Alignment requirement for Surfaces:            Yes
  Device has ECC support:                        Disabled
  Device supports Unified Addressing (UVA):      Yes
  Device PCI Domain ID / Bus ID / location ID:   0 / 1 / 0
  Compute Mode:
     < Default (multiple host threads can use ::cudaSetDevice() with device simultaneously) >

deviceQuery, CUDA Driver = CUDART, CUDA Driver Version = 11.2, CUDA Runtime Version = 8.0, NumDevs = 1, Device0 = GeForce GTX 960
Result = PASS
```

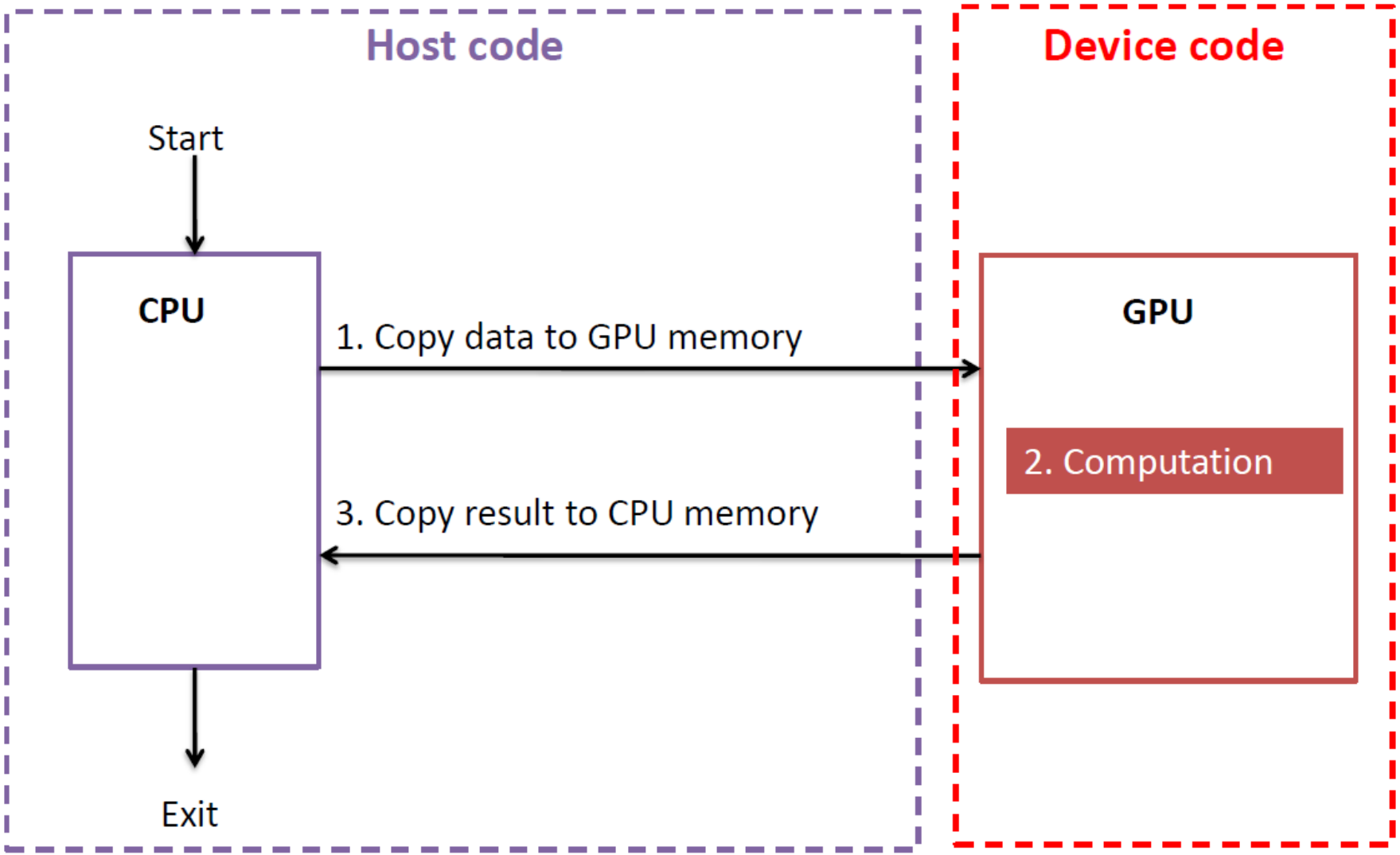
Part 2:
Programming with CUDA

Demo / Compile /Run / Debug

Host and Device code

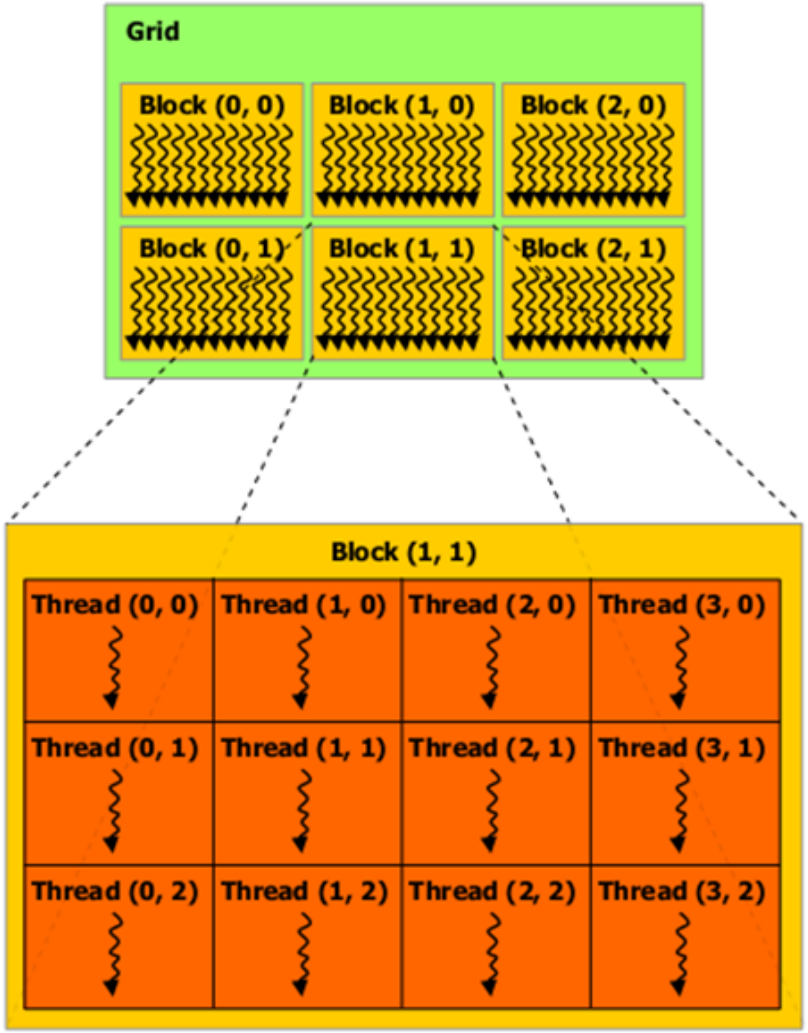
- A CUDA program consists of two parts: *host* and *device* (or *kernel*) code.
- Host code: executed on the CPU
  - Memory copy between the GPU and the CPU
  - Computation on the CPU and call GPU kernel
- Device code: executed on the GPU
  - GPU-based computation
- A CUDA program always starts from the host code, and then invokes the GPU kernels.

Processing Flow of a CUDA Program



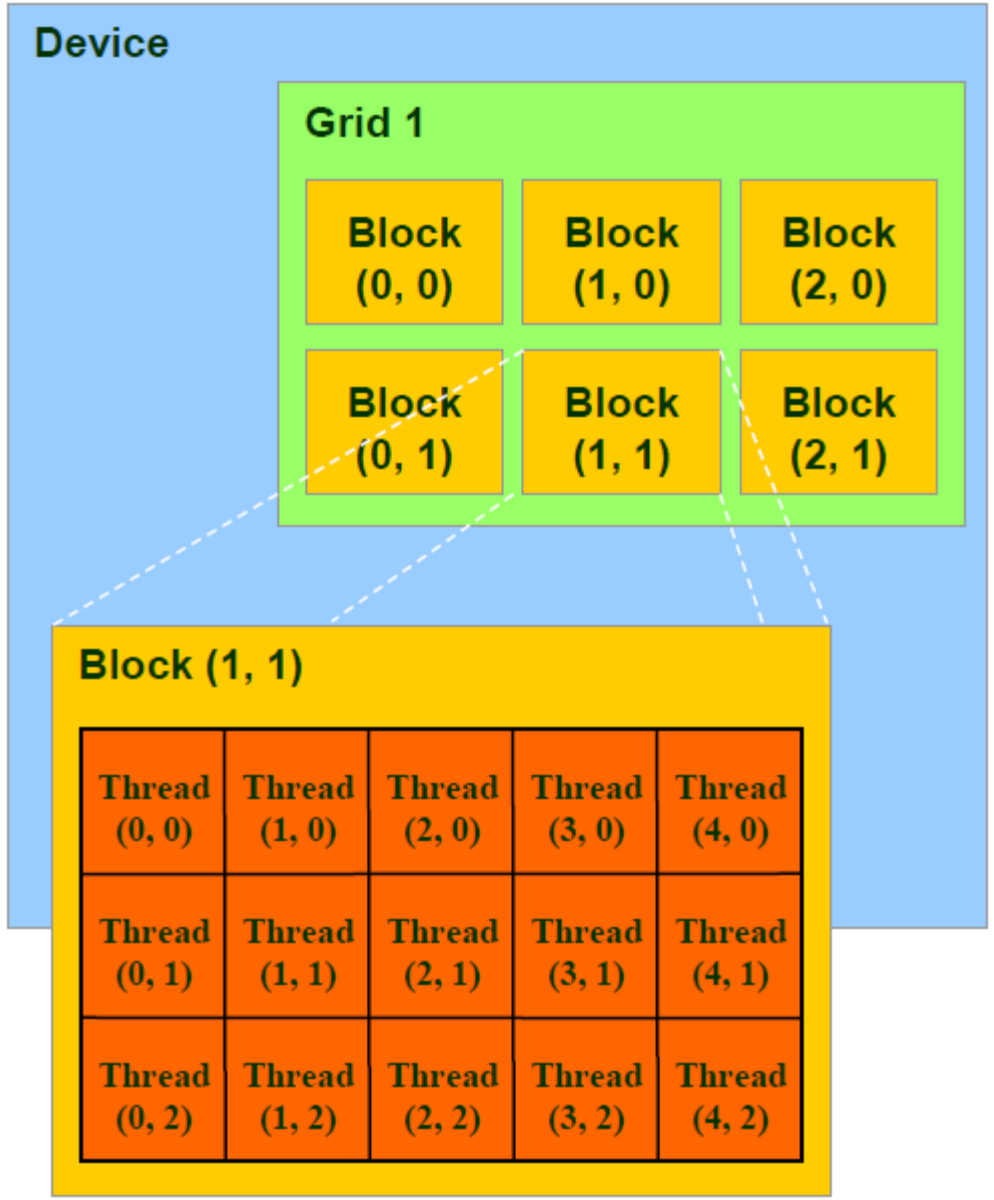
Grid, blocks and threads

- Each kernel corresponds to a ***grid*** of threads.
- Each grid consists of multiple thread ***blocks***.
- Each thread block contains multiple ***threads***.
- A grid consists of i-dimension (i=1,2,3) **blocks**
  - gridDim.x, gridDim.y, gridDim.z
- A thread block contains **threads** organized in 1-3 dimensions
  - blockDim.x, blockDim.y, blockDim.z
- Any unspecified dimension is set to size 1.



Block and Thread IDs

- Threads and blocks have built-in IDs
  - Block ID: (blockIdx.x, blockIdx.y, blockIdx.z)
  - Thread ID: 1D, 2D, or 3D **within a block** (threadIdx.x, threadIdx.y, threadIdx.z)



Device Code (Kernel)

- The device code is the same for each thread.
- A kernel function has the prefix *__global__*, and has a *void* return type.

  __global__ void kernel1*(param1, …)*

- Note: device code has no direct access to main memory.

Kernel Invocation in Host Code

***kernelName*<<<*#block*, *#thread*, *shared_size*, *s*>>>** **(*param1*, …)**

#block: number of thread blocks in the grid

#thread: number of threads per block

shared_size: optional; size of shared memory per block, default 0.

s: optional; the associated stream, default 0.

Memory Management

- In CUDA, host (i.e., CPU) and device (i.e., GPU) have separate memory spaces
- To execute a kernel on GPU, we need to
  1. allocate memory on the device
  2. transfer data from host memory to allocated device memory
- After device execution, we need to transfer the result data from device memory back to host

GPU memory management functions

– GPU memory allocation:
cudaMalloc(*devPtr, size*)
cudaFree(*devPtr*)

– Memory copy:
cudaMemcpy(*dst, src, size, direction*)
direction*: *cudaMemcpyHostToDevice,
cudaMemcpyDeviceToHost

Demo 1

- Allocate CPU memory for *n* integers
- Allocate GPU memory for *n* integers
- Initialize GPU memory to 0s
- Copy from GPU to CPU
- Print the values

Demo 1

```
#include <cuda.h>
#include <stdio.h>
int main() {
        int dimx= 16;
        int num_bytes= dimx* sizeof(int);
        int*d_a= 0, *h_a= 0;   // device and host pointers
        h_a= (int*)malloc(num_bytes);
        cudaMalloc((void**)&d_a, num_bytes);
        if (0 == h_a|| 0 == d_a) {
                printf("couldn't allocate memory\n");
                return 1;
        }
        cudaMemset(d_a, 0, num_bytes);
        cudaMemcpy(h_a, d_a, num_bytes, cudaMemcpyDeviceToHost);
        for (int i= 0; i< dimx; i++)
                printf("%d\n", h_a[i]);
        free(h_a);
        cudaFree(d_a);
        return 0;
}
```

Demo 1

- Compile
  - nvcc source_file -o output_file
- Run
  - ./output_file

Demo 2

- Use GPU to initialize an array by thread IDs
- Copy the array to CPU
- Print the values

A kernel function:

```
__global__  void  mykernel(int*  a)
{
        int idx= blockIdx.x* blockDim.x+ threadIdx.x;
        a[idx] = 7;
}
```

```
#include <cuda.h>
#include <stdio.h>

__global__ void mykernel(int* a) {
        int idx= blockIdx.x* blockDim.x+ threadIdx.x;  // locate the data item handled by this thread
        a[idx] = threadIdx.x;
}

int main() {
        int dimx= 16, num_bytes= dimx*sizeof(int);
        int*d_a= 0, *h_a= 0; // device and host pointers
        h_a= (int*)malloc(num_bytes);
        cudaMalloc((void**)&d_a, num_bytes);
        cudaMemset(d_a, 0, num_bytes);
        dim3  grid, block;
        block.x= 4;                             // each block has 4 threads
        grid.x= dimx / block.x;                 // # of blocks is calculated
        mykernel<<<grid,  block>>>(d_a);
        cudaMemcpy(h_a, d_a, num_bytes, cudaMemcpyDeviceToHost);
        for(inti= 0; i< dimx; i++)
                printf("%d\n", h_a[i]);
        free(h_a);
        cudaFree(d_a);
        return 0;
}
```

The output will be:
0 1 2 3 0 1 2 3 0 1 2 3 0 1 2 3

Debugging using CUDA-GDB

- What does CUDA-GDB do?
  - Control the execution of the application
    - Breakpoints
    - Single-step
    - CTRL-C
  - Inspect the current state of the application
    - Kernels, blocks, threads
    - Devices, SMs, warps
  - Inspect and Modify
    - Code memory (disassemble)
    - Global, shared, and local memory
    - Hardware registers
    - Textures (read-only)

Debugging using CUDA-GDB

- Compile:
  - nvcc -g -G XXX.cu -o XXX
- Enter debug mode:
  - cuda-gdb debug_file
  - **set cuda software_preemption on**

Debugging using CUDA-GDB

- Execution control
  - launch the application
    - (cuda-gdb) run [arguments]
  - resume the application (all host and dev threads)
    - (cuda-gdb) continue
  - kill the application
    - (cuda-gdb) kill
  - interrupt the application
    - CTRL-C

Debugging using CUDA-GDB

- Breakpoints
  - Symbolic breakpoints
    - (cuda-gdb) break my_kernel
  - Line number breakpoints
    - (cuda-gdb) break my_app.cu:380
  - Address breakpoints
    - (cuda-gdb) break *0x3e840a8
  - Kernel entry breakpoints
    - (cuda-gdb) set cuda break_on_launch application
  - List of breakpoints
    - (cuda-gdb) info breakpoints

Debugging using CUDA-GDB

- Focus Query
  - Query commands
    - cuda <list of coordinates>
    - thread
  - If focus set to device thread
    - **(cuda-gdb) cuda kernel block thread**
      - kernel 1, block (0, 0, 0), thread (0, 0, 0)
    - **(cuda-gdb) cuda device kernel block warp thread**
      - kernel 1, block (0, 0, 0), thread (0, 0 ,0), device 0,warp 0
  - If focus set to host thread
    - **(cuda-gdb) thread**
      - [Current thread is 1 …]
    - **(cuda-gdb) cuda thread**
      - Focus not set on any active CUDA kernel

Debugging using CUDA-GDB

- Focus Switch
  - Switch command
    - cuda <list of coordinate-value pairs>
    - thread <host thread id>
  - Only switch the specified coordinates
    - current coordinates are assumed in case of non-specified coordinates
    - if no current coordinates, best effort to match request
    - error if cannot match request

Debugging using CUDA-GDB

- Focus Switch
  - **(cuda-gdb) cuda kernel 1 block 1 thread 2,0**
    - [Switching focus to CUDA kernel 1, grid 2, block (1, 0, 0), thread (2, 0, 0), device 0, sm 5, warp 0, lane 2]
  - **(cuda-gdb) cuda kernel 1**
    - [Switching focus to CUDA kernel 1, grid 2, block (0, 0, 0), thread (0, 0, 0), device 0, sm 1, warp 0, lane 0]
  - **(cuda-gdb) cuda thread 256**
    - Request cannot be satisfied. CUDA focus unchanged.

Debugging using CUDA-GDB

Step 1: compile using –g –G augments

nvcc -g -G demo2.cu -o demo2

Step 2: enter cuda-gdb

cuda-gdb -q demo2

Step 3: display some codes

list

Step 4: Set break point

break mykernel

```
(cuda-gdb) list
3
4       // Device code
5       __global__ void mykernel(int* a) {
6           int idx= blockIdx.x* blockDim.x+
threadIdx.x;  // locate the data item handled by
this thread
7           a[idx] = threadIdx.x;
8       }
9
10      // Host code
11      int main() {
12          int dimx= 16, num_bytes=
dimx*sizeof(int);

(cuda-gdb) break mykernel
Breakpoint 1 at 0x402c00: file demo2.cu, line 5.

(cuda-gdb) break mykernel
Breakpoint 1 at 0x402c00: file demo2.cu, line 5.
```

Debugging using CUDA-G

Step 5: Run the program

run

Step 6: run next line

next

Step 7: check cuda threads

info cuda threads

```
(cuda-gdb) run
Starting program: /homes/yxingag/hpc/lab02/demo2
[Thread debugging using libthread_db enabled]
Using host libthread_db library "/lib64/libthread_db.so.1".
[New Thread 0x7ffff54ef700 (LWP 27647)]
[New Thread 0x7ffff4cee700 (LWP 27648)]
[New Thread 0x7ffff44ed700 (LWP 27649)]
[Switching focus to CUDA kernel 0, grid 1, block (0,0,0),
thread (0,0,0), device 0, sm 0, warp 0, lane 0]

Breakpoint 1, mykernel<<<(4,1,1),(4,1,1)>>> (a=0x4026e0000)
at demo2.cu:6
6           int idx= blockIdx.x* blockDim.x+ threadIdx.x;
// locate the data item handled by this thread

(cuda-gdb) next
7  a[idx] = threadIdx.x;

(cuda-gdb) info cuda threads
 BlockIdx ThreadIdx To BlockIdx ThreadIdx Count
Virtual PC Filename  Line
Kernel 0
*  (0,0,0)    (0,0,0)      (0,0,0)    (3,0,0)      4
0x0000000000a85a38 demo2.cu     7
   (1,0,0)    (0,0,0)      (3,0,0)    (3,0,0)     12
0x0000000000a859e8 demo2.cu     6
```

Debugging using CUDA-GDB

Step 8: print local variables

info locals

Step 9: print variables

print idx

Step 10: continue execution

continue

```
(cuda-gdb) info locals
idx = 0

(cuda-gdb) print idx
$1 = 0

(cuda-gdb) continue
Continuing.
0
1
2
3
…
1
2
3
[Thread 0x7ffff4cee700 (LWP 27648) exited]
[Thread 0x7ffff54ef700 (LWP 27647) exited]
[Thread 0x7ffff7fc9740 (LWP 27599) exited]
[Inferior 1 (process 27599) exited normally]
```

Demo 3: Vector addition

A kernel function which will be executed on GPU

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

Demo 3: Vector addition

Host code which will be executed on CPU

```
int main ()
{
        int n = 10000;
        // allocate and initialize host (CPU) memory
        float *H_A = …, *H_B = …, *H_C = …;
        // allocate device (GPU) memory
        float *A_d, *B_d, *C_d;
        cudaMalloc(…); …
        // copy host memory to device
        cudaMemcpy(…);…
        // run 16 blocks of 256 threads each
        vecAdd<<< ceil(n/256.0), 256 >>>(d_A, d_B, d_C, n);
        // copy result to host
        cudaMemcpy(…);
        cudaFree(A_d);…
}
```

Try to debug by yourself!

Error Handling

- It is very common to use an error-handling macro to wrap all CUDA API calls
  - To simplify the error checking process

```
#define CHECK(call)
{
   const cudaError_t error = call;
   if (error != cudaSuccess)
   {
      printf("Error: %s:%d, ", __FILE__, __LINE__);
      printf("code:%d, reason: %s\n", error, cudaGetErrorString(error);
      exit(1);
   }
}
```

E.g.:

```
CHECK(cudaMemcpy(…));
```

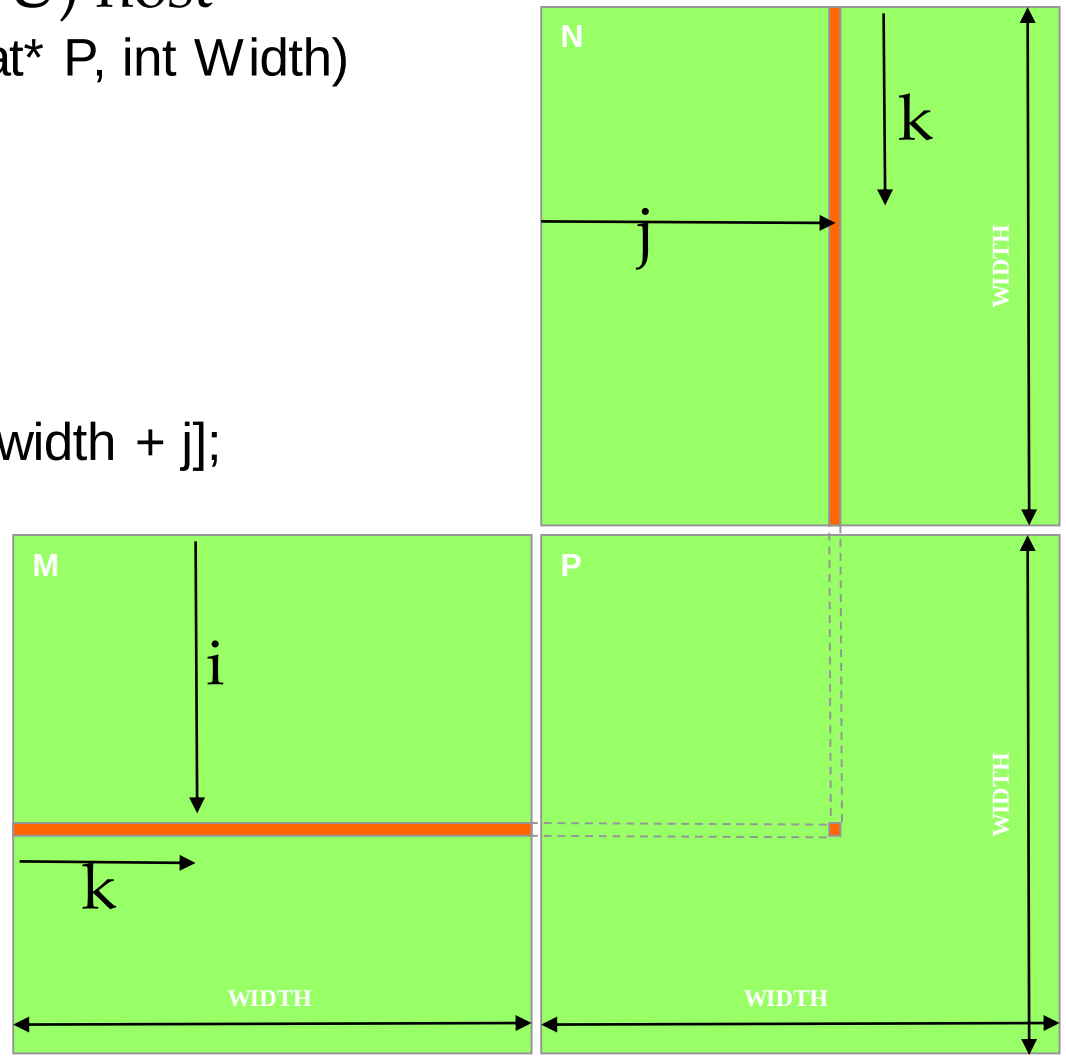
__FILE__ and __LINE__ are standard predefined macros that represent the current input file and input line number, respectively.

Appendix: Matrix multiplication

- Problem: P = M x N
- M, N, P are square matrix: WIDTH x WIDTH
- Parallelization on GPU
  - The calculation of each item in *P* is done by a GPU thread
    - To perform a dot product of two vectors
  - Question: How to organize the threads into blocks?

Appendix: Serial Solution

```
// Matrix multiplication on the (CPU) host
void MatMulOnHost(float* M, float* N, float* P, int Width)
{
    for (int i = 0; i < Width; i++)
        for (int j = 0; j < Width; j++) {
            float sum = 0.0;
            for (int k = 0; k < Width; k++) {
                sum += M[i * width + k] * N[k * width + j];
            }
            P[i * Width + j] = sum;
        }
}
```



Appendix: Matrix multiplication

Please refer to the attached codes of this tutorial!

```
#include <iostream>
#include <cstdio>
#include <cuda_runtime.h>
#include <device_launch_parameters.h>
#include <cmath>
using namespace std;

const int TILE_WIDTH = 16;
__global__ void MatrixMulKernel(int *d_M,int *d_N,int *d_P,int m,int n,int k)
{
  __shared__ int ds_M[TILE_WIDTH][TILE_WIDTH];
  __shared__ int ds_N[TILE_WIDTH][TILE_WIDTH];

  int bx = blockIdx.x;
  int by = blockIdx.y;

  int tx = threadIdx.x;
  int ty = threadIdx.y;

  //Identify the row and column of the Pd element to work on
  int row = by * TILE_WIDTH + ty;
  int col = bx * TILE_WIDTH + tx;
  int pValue = 0;
                ....
```