Programming Basics

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IT4INNOVATIONS
NATIONAL SUPERCOMPUTING
CENTER

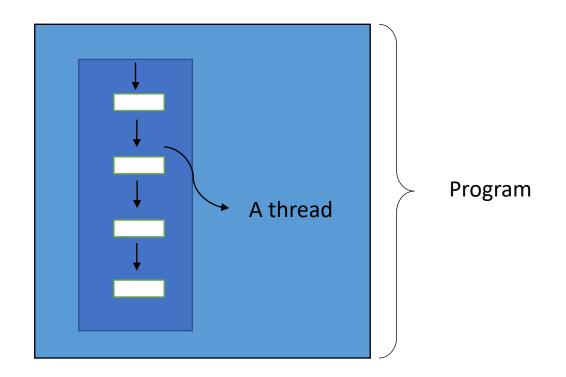


Thread



Thread

- A thread is a single sequential flow of instructions within a program.
- A sequential code in one processor has one thread.



C - pointers



Pointer

A variable that points to the storage/memory address of another variable.

A variable of type certain type will store a value

 This variable has its address (where it is located the memory). This address can be obtained by using '&'

A pointer stores the address of the variable

The value of the variable can be accessed using the variable or the pointer



Malloc()



malloc()

- Dynamically allocates a single large block of memory
 - Syntax

```
pointer = (type*) malloc(byte - size)
```

Example

Vector Addition - C



EXERCISE 1: Vector Addition using C program

Source code

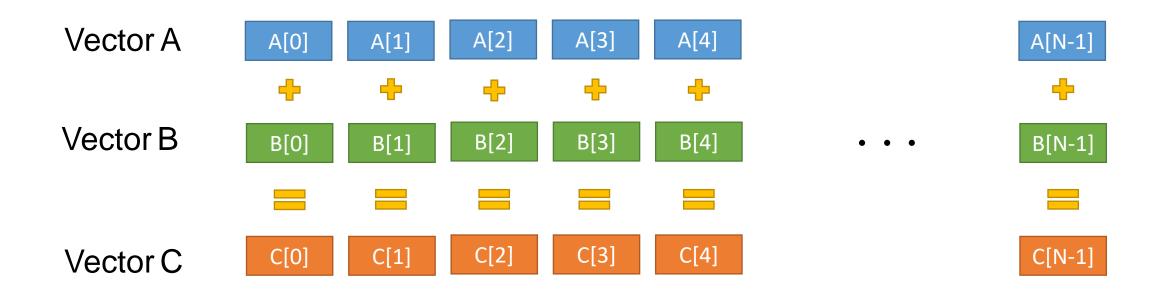
FOLDER: EX1_VECTOR_ADDITION

vector_add.c

Vector Addition



$$A + B = C$$



C program for Vector Addition



C programming – Vector addition

```
#include <stdio.h>
#include <time.h>
#include <stdlib.h>
```

The "include" tells the pre-processor to include the content of the named header file.



```
#define array_size 10000000
```

Define size of the array as global variable

C program for Vector Addition



```
int main(){
}
```

The main body of the code.



```
float *a, *b, *c;

a = (float*)malloc(sizeof(float) * array_size);
b = (float*)malloc(sizeof(float) * array_size);
c = (float*)malloc(sizeof(float) * array_size);
```

Memory Allocation for the variables

```
// Initialize array
for(int i = 0; i < array_size; i++){</pre>
    a[i] = 1.0f;
    b[i] = 2.0f;
```

Initializing the variables



```
for(int i=0; i < array_size; i++){</pre>
    c[i] = a[i] + b[i];
```

Addition of vectors

C program for Vector Addition SCtrain KNOWLEDGE PARTNERSHIP



```
free(a); free(b); free(c);
    Deallocation of
       Memory
```

```
clock_t t;
t = clock()
t = clock() - t;
double time_taken =
((double)t)/CLOCKS_PER_SEC;
```

Measuring time

Slurm - Running programs



#!/bin/bash
#SBATCH --job-name=test
#SBATCH --output=res1.txt
#SBATCH --ntasks=1

#SBATCH --time=03:00 #SBATCH --partition=gpu #SBATCH --nodelist=gpu01

module purge module load icc module load CUDA

Operations
echo "Job start"
./matvec_onethread
Operations
echo "Job end"

To run the compiled code "matvec_onethread"

Create the file by the name: submit.sh

Command to launch: sbatch submit.sh

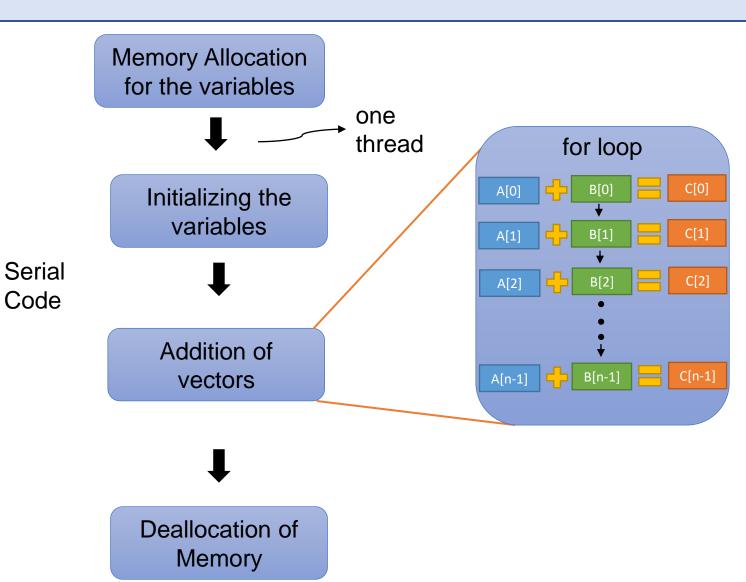
The output from the file is stored in "res1.txt"

This file launches a slot for 3 minutes in the core with gpu.

C program for Vector Addition

SCtrain SUPERCOMPUTING KNOWLEDGE PARTNERSHIP

```
#include <stdio.h>
#include <time.h>
#include <stdlib.h>
#define array_size 100000000
int main(){
    float *a, *b, *c;
    a = (float*)malloc(sizeof(float) * array_size);
       = (float*)malloc(sizeof(float) * array_size);
       = (float*)malloc(sizeof(float) * array size);
    // Initialize array
    for(int i = 0; i < array_size; i++){</pre>
        a[i] = 1.0f; b[i] = 2.0f;
    clock t t;
    t = clock();
    // vector addition
    for(int i = 0;i < array_size; i++){</pre>
        c[i] = a[i] + b[i];
    t = clock() - t;
    double time taken = ((double)t)/CLOCKS PER SEC; // in
seconds
    printf("fun() took %f seconds to execute \n",
time_taken);
    free(a); free(b); free(c);
```



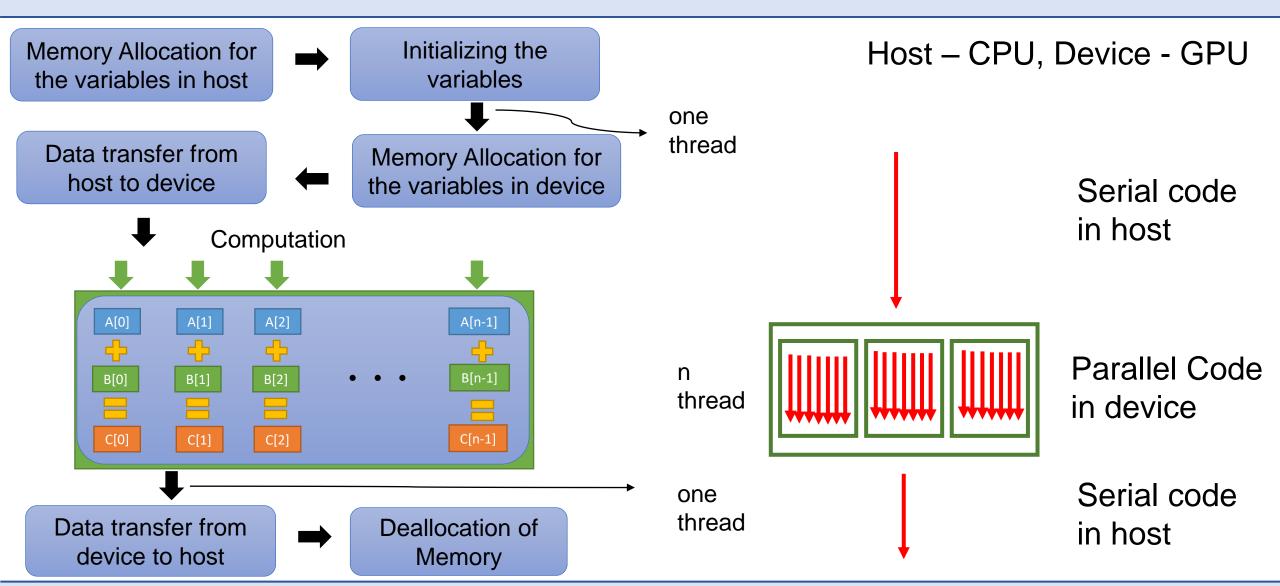
Heterogenous Program



```
Memory Allocation
int main(){
   float *a, *b, *out, *d a, *d b, *d out;
                                                                                                                           for the variables
   // Allocate host memory
      = (float*)malloc(sizeof(float) * array_size);
      = (float*)malloc(sizeof(float) * array size);
   out = (float*)malloc(sizeof(float) * array size);
                                                                                                                                                                          one
                                                                                                                              Initializing the
   // Initialize array
                                                                                                                                                                          thread
   for(int i = 0; i < array size; i++){</pre>
                                                                                                                                  variables
       a[i] = 1.0f;
                       b[i] = 2.0f;
                                                                                  Serial
   // Allocate device memory
                                                                                  Code
   cudaMalloc((void**)&d a, sizeof(float)*array size);
   cudaMalloc((void**)&d b, sizeof(float)*array size);
   cudaMalloc((void**)&d out, sizeof(float)*array size);
   // Transfer data from host to device memory
   cudaMemcpy(d_a, a, sizeof(float)*array_size, cudaMemcpyHostToDevice);
   cudaMemcpy(d b, b, sizeof(float)*array size, cudaMemcpyHostToDevice);
                                                                                                        A[0]
                                                                                                                    A[1]
                                                                                                                                                              A[n-1]
   int block size = 256;
                                                                                  Parallel
   int grid size = (array size + block size) / block size;
   // Vector addition
                                                                                                                                                                                n
                                                                                                        B[0]
                                                                                                                    B[1]
                                                                                                                                                              B[n-1]
   vector_add<<<grid size, block size>>>(d out, d a, d b, array size);
                                                                                   Code
                                                                                                                                                                                thread
   // Transfer data from device to host memory
   cudaMemcpy(out, d out, sizeof(float)*array size, cudaMemcpyDeviceToHost);
                                                                                                                                                              C[n-1]
                                                                                                        C[0]
   // Deallocate device memory
   cudaFree(d a);
                                                                                  Serial
   cudaFree(d b);
   cudaFree(d_out);
                                                                                  Code
   // Deallocate host memory
   free(a);
                                                                                                                             Deallocation of
                                                                                                                                                                          one
   free(b);
                                                                                                                                                                          thread
   free(out);
                                                                                                                                  Memory
```

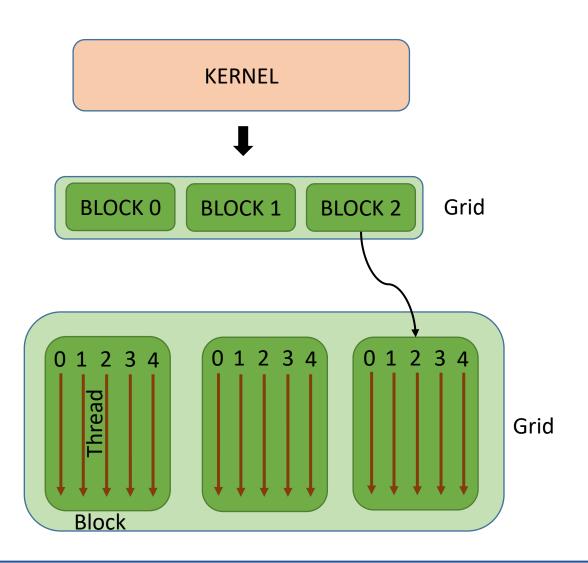
Heterogenous Program





GPU Architecture

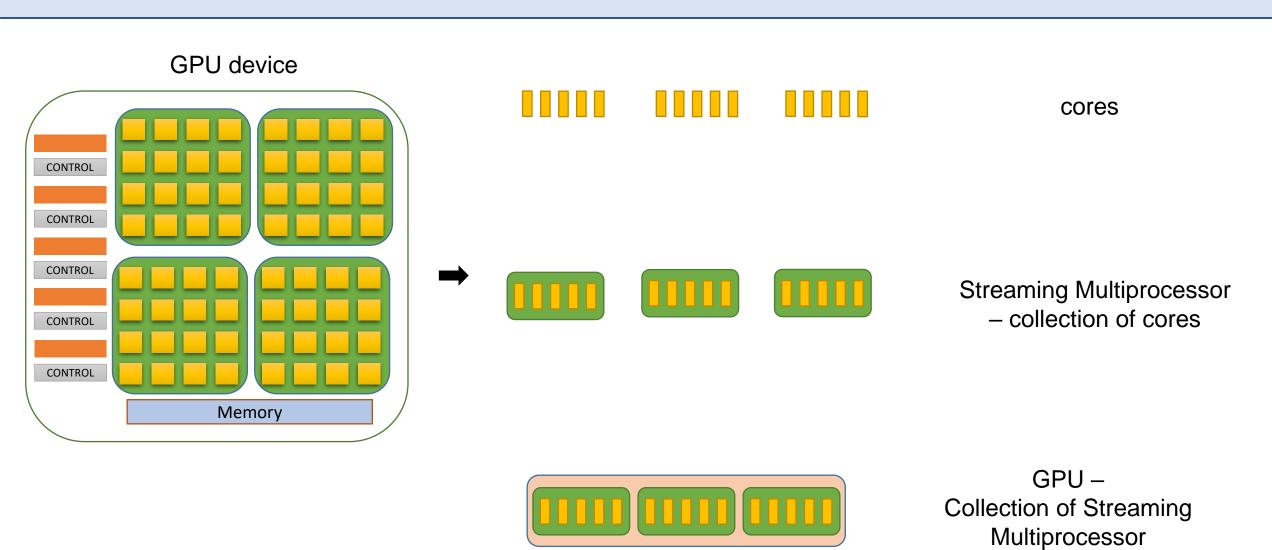




- > A kernel is executed as a grid
- > A grid is broken into blocks
- > Each block is broken into threads

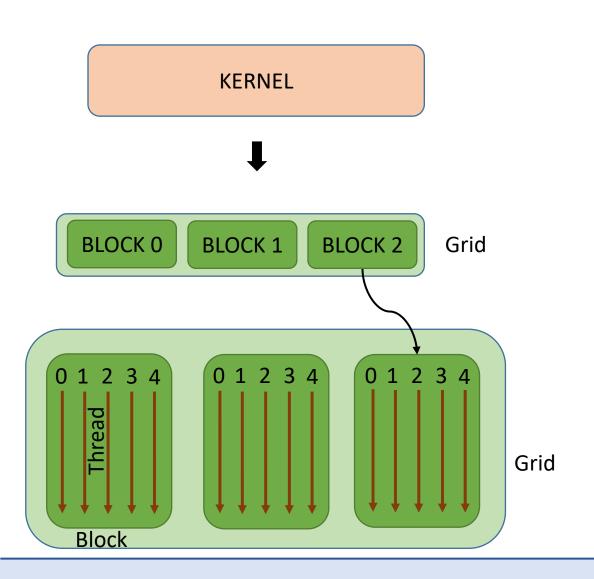
GPU Architecture



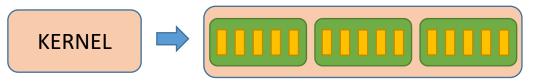


GPU Architecture

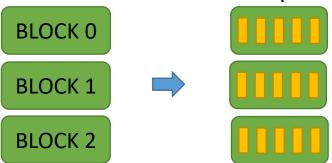




A kernel is executed in a CUDA-enabled GPU



One block is executed in one Streaming Multiprocessor. The three blocks are executed in parallel



- Depending on the number of SM, blocks are distributed and executed in parallel
- ➤ More SM a device has, faster is the execution

A thread is executed in a core

Vector Addition - GPU

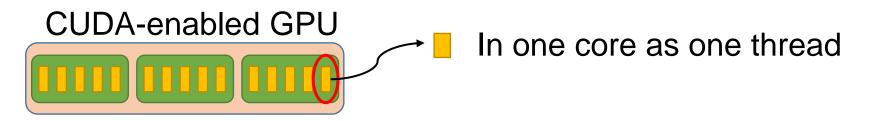


Vector Addition using GPU

- In one core as one thread
- In one streaming multiprocessor as one block
- In the entire GPU device as multiple blocks

Vector Addition – One core





```
for loop
                 C[0]
                 C[1]
B[1]
B[2]
                 C[2]
                C[n-1]
```

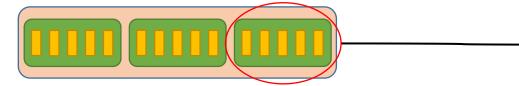
```
__global__ void vector_add(float *out, float *a, float *b, int
n){
for(int i = 0; i < n; i++){
   out[i] = a[i] + b[i];}
}</pre>
```

Vector Addition – One SM



CUDA-enabled GPU

A streaming multiprocessor has a number of cores

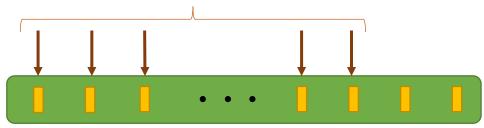




When the kernel is called, the number of blocks and the number of threads in each block is specified

```
vector_add <<<1,256>>> (d_out, d_a, d_b, N)
```

256 threads



```
__global__ void vector_add(float *out, float *a, float *b, int n){
int index = threadIdx.x;
int stride = blockDim.x;

for(int i=index; i<n; i+=stride){
   out[i] = a[i] + b[i];}
}</pre>
```

Vector Addition - One SM



- Each thread performs the vector addition on a certain chunk of the array.
- Strategy for distributing the array between the threads
 - Requisite
 - 1. The threads should not communicate with each other.
 - 2. The array should be equally split between the threads.
 - Constraint
 - 1. Each thread will run the same function.

- The array is in the device memory.
- It is available for all the threads.

What's available?

Each thread can have its local variables.

We define two local variables:

1. It has an unique id : threadIdx.x

2. The number of threads : blockDim.x

Vector Addition – One SM



```
thread 0
```

```
__global__ void vector_add(float *out, float *a, float *b, int n){
int index = threadIdx.x;
int stride = blockDim.x;

for(int i=index; i<n; i+=stride){
   out[i] = a[i] + b[i];}
}</pre>
```

```
thread 1
```

```
Local variables for this thread:
```

```
index = threadIdx.x = 0
stride = blockDim.x = 256
```

For loop

```
first loop:
    i = index = 0
    out[i=0] = a[i=0] + b[i=0]
second loop:
    i = i + stride = 256
    out[i=256] = a[i=256] + b[i=256]
third loop:
    i = i + stride = 512
    out[i=512] = a[i=512] + b[i = 512]
until: i < n</pre>
```

```
Local variables for this thread:
```

```
index = threadIdx.x = 1
stride = blockDim.x = 256
```

For loop

```
first loop:
    i = index = 1
    out[i=1] = a[i=1] + b[i=1]
second loop:
    i = i + stride = 257
    out[i=257] = a[i=257] + b[i=257]
third loop:
    i = i + stride = 513
    out[i=513] = a[i=513] + b[i = 513]
until: i < n</pre>
```

Vector Addition – One SM



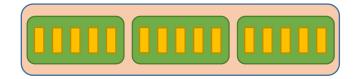
```
1<sup>st</sup> loop
                                                                                                                    2<sup>nd</sup> loop
                                                  255
                                                                                                                                                255
                                                                    threadIdx.x
                                                                                              0
                                                  255
                                                                                                        257
                                                                              i
                                                                                                                   258
                                                                                                                                                511
                                                                                             256
                       A[2]
A[0]
           A[1]
                                                 A[255]
                                                                                             A[256]
                                                                                                                                                A[511]
                                                                                                        A[257]
                                                                                                                   A[258]
                                                 B[255]
                                                                                                                                                B[511]
                                                                                             B[256]
                                                                                                        B[257]
                                                                                                                   B[258]
                       C[2]
                                                 C[255]
                                                                                                                                                C[511]
                                                                                                                   C[258]
```

```
__global___ void vector_add(float *out, float *a, float *b, int n){
int index = threadIdx.x;
int stride = blockDim.x;

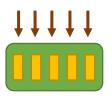
for(int i = index; i < n; i+ = stride){
    out[i] = a[i] + b[i];}
}</pre>
```

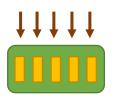


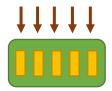
CUDA-enabled GPU



Many streaming multiprocessors can be used







- Each thread accesses one element in the array. We predefine the number of threads in a block.
- The number of blocks is calculated based on the array size and the number of threads in a block.

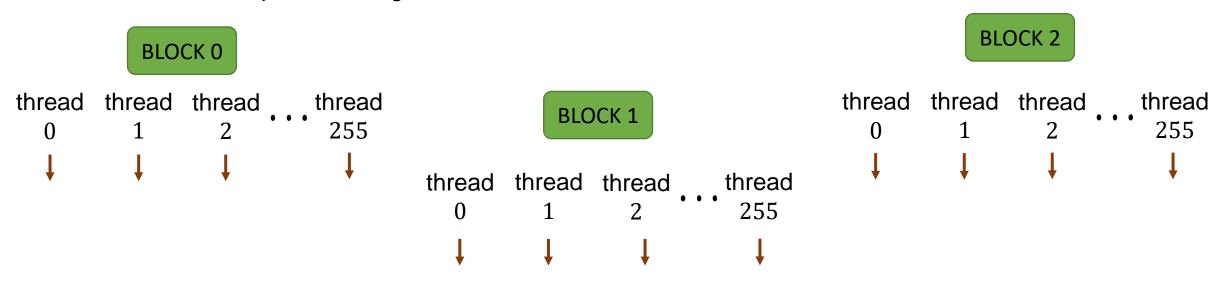
number of blocks
$$\frac{n}{n} = \frac{\text{array size}}{\text{number of threads in each block}}$$



When the kernel is called, the number of blocks and the number of threads in each block is specified:

The above command instantiates n blocks with 256 threads in each block.

Each thread in a block has an unique id starting from 0. Each block has an unique id starting from 0.

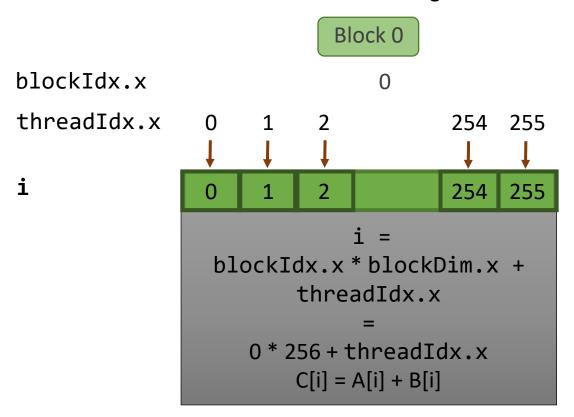


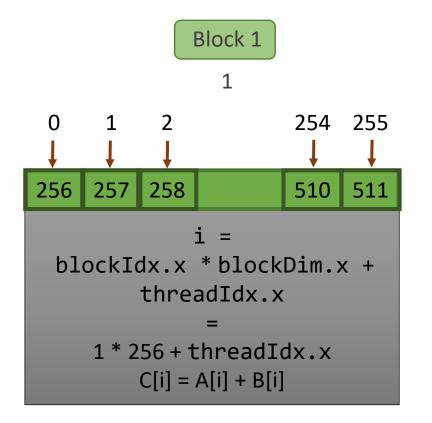


SUPERCOMPUTING

Each thread can have its local variables. We define three local variables:

- The id of the thread :threadIdx.x
- The number of threads in the block : blockDim.x = 256
- :blockIdx.x The block to which the thread belongs to





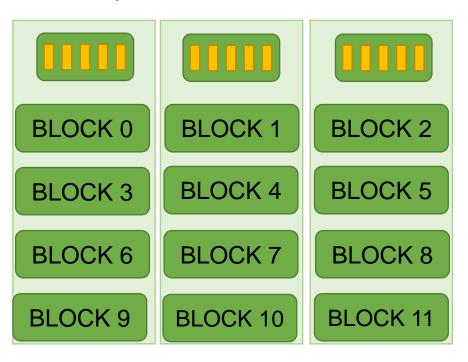


255

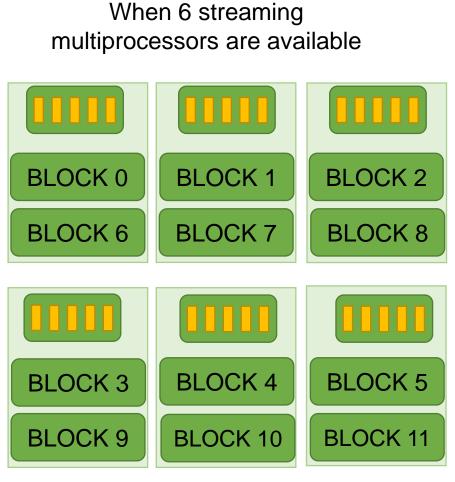


The blocks are distributed among the streaming multiprocessors

When 3 streaming multiprocessors are available



BLOCK 0	BLOCK 1
BLOCK 2	BLOCK 3
BLOCK 4	BLOCK 5
BLOCK 6	BLOCK 7
BLOCK 8	BLOCK 9
BLOCK 10	BLOCK 11



GPU Programming Syntax

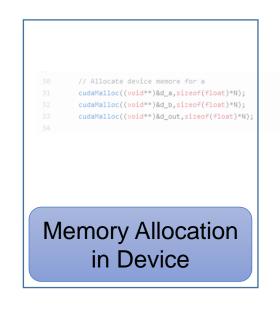


- Functions that run on GPU are usually enclosed in "<<< >>>".
- The file has extension ".cu".
- It is complied using nvcc compiler driver.

Heterogenous Program













```
// Main function
int block_size = 256;
int grid_size = (N+block_size)/block_size;
vector_add<<<grid_size,block_size>>>>(d_out, d_a, d_b, N);

Computation in Device
```

```
// Deallocate device memory
cudaFree(d_a);
48 cudaFree(d_b);
49 cudaFree(d_out);
50
51 // Deallocate host memory
52 free(a);
53 free(b);
54 free(out);
```

Deallocation of Memory



Data transfer from Device to Host

cudaMemcpy(out, d_out, sizeof(float)*N, cudaMemcpyDeviceToHost)



GPU Programming Functions



The CPU manages both device and host memory

- Allocate the memory in the CPU (type*) malloc(byte – size)
- Allocate the memory in the GPU cudaMalloc((void**) pointer,malloc(byte - size)
- Data is transferred from host memory to device memory cudaMemcpy(device_variable, host_variable, size of variable, CudaMemcpyHosttoDevice)
- After the kernel execution and data is transferred from device to host memory cudaMemcpy(host_variable, device_variable, size of variable, CudaMemcpyDevicetoHost)
- The memory in GPU is deallocated cudaFree(pointer)
- Finally, the memory in CPU is deallocated free(pointer)

GPU Programming Functions



EXERCISE 1: Vector Addition using GPU program

Source code

FOLDER: EX1_VECTOR_ADDITION

```
#include <stdio.h>
#include <time.h>
#include <stdlib.h>
#include <cuda.h>
#include <sys/time.h>
```

Host – CPU, Device - GPU

The "include" statement to tell the pre-processor to include the content of the named header file.



#define array_size 268435456

Define size of the array as global variable

Host – CPU, Device - GPU

```
float *a, *b, *out;
float *d a, *d b, *d out;
  = (float *)malloc(sizeof(float) * array_size);
   = (float *)malloc(sizeof(float) * array_size);
out = (float *)malloc(sizeof(float) * array_size);
// Initialize array
for(int i = 0; i < array_size ; i++){</pre>
    a[i] = 1.0f;
   b[i] = 2.0f;
```

Memory Allocation in Host and initialization of data

Host – CPU, Device - GPU

```
// Allocate device memory for variables
cudaMalloc((void**)&d_a, sizeof(float) * array_size);
cudaMalloc((void**)&d_b, sizeof(float) * array_size);
cudaMalloc((void**)&d_out, sizeof(float) * array_size);
```

Memory Allocation in Device

Host – CPU, Device - GPU

```
// Transfer data from host to device memory
cudaMemcpy(d_a, a, sizeof(float) * array_size, cudaMemcpyHostToDevice);
cudaMemcpy(d_b, b, sizeof(float) * array_size, cudaMemcpyHostToDevice);
```

Data transfer from Host to Device

```
cudaMemcpy(out, d_out, sizeof(float) * array_size, cudaMemcpyDeviceToHost);
```

Data transfer from Device to Host



```
// Deallocate device memory
cudaFree(d_a);
cudaFree(d_b);
cudaFree(d_out);

// Deallocate host memory
free(a);
free(b);
free(out);
```

Deallocation of Memory

Host – CPU, Device - GPU

One thread

Host - CPU, Device - GPU

Computation in Device

Kernel

```
__global__ void vector_add(float *out, float *a, float *b, int n){
for(int i = 0; i < n; i++){
   out[i] = a[i] + b[i];}
}</pre>
```

```
// Main function
int block_size = 1;
int grid_size = 1;
vector_add<<<grid_size,block_size>>>(d_out, d_a, d_b, N);
cudaDeviceSynchronize();
```

One block

Host – CPU, Device - GPU

Computation in Device

Kernel

```
__global__ void vector_add(float *out, float *a, float *b, int n){
int index = threadIdx.x;
int stride = blockDim.x;

for(int i = index; i < n; i += stride){
   out[i] = a[i] + b[i];}
}</pre>
```

```
// Main function
int block_size = 256;
int grid_size = 1;
vector_add<<<grid_size,block_size>>>(d_out, d_a, d_b, N);
cudaDeviceSynchronize();
```

Multiple block

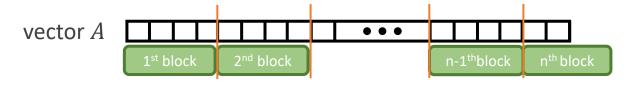
Computation in Device

Host – CPU, Device - GPU

```
__global__ void vector_add(float *out, float *a, float *b, int n){
int index = blockIdx.x * blockDim.x + threadIdx.x;
if (index < n){
   out[index] = a[index] + b[index];}
}</pre>
```

```
// Main function
int block_size = 256;
int grid_size = (N + block_size) / block_size;
vector_add<<<grid_size,block_size>>>(d_out, d_a, d_b, N);
cudaDeviceSynchronize();
```

Remark: We ensure the tail of the array is processed by launching one extra block.



Slurm - Running programs



```
#!/bin/bash
#SBATCH --job-name=test
#SBATCH --output=res1.txt
#SBATCH --ntasks=1
```

#SBATCH --time=03:00 #SBATCH --partition=gpu #SBATCH --nodelist=gpu01

module purge module load icc module load CUDA

Operations echo "Job start" ./matvec_onethread # Operations echo "Job end" To run the compiled code "matvec_onethread"

Create the file by the name: submit.sh

Command to launch: sbatch submit.sh

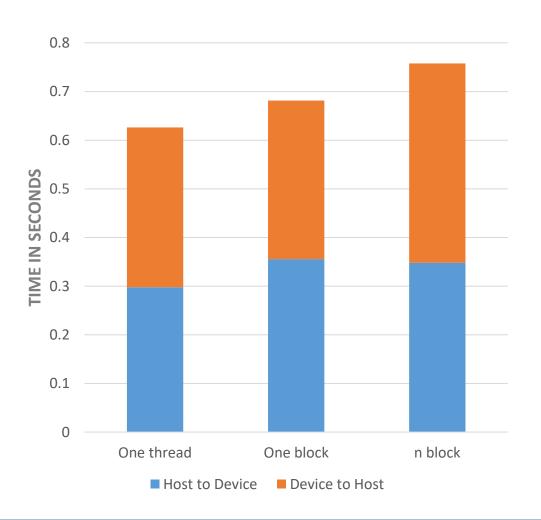
The output from the file is stored in "res1.txt"

This file launches a slot for 3 minutes in the core with gpu.

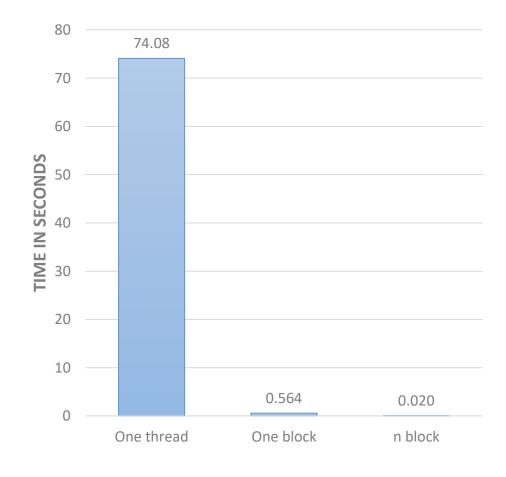
Time comparison



Time for data transfer



Kernel execution time



Code Profiling



Code profiling – nvprof ./####

1 thread

```
==8304== Profiling application: ./vector_add_onethread
==8304== Profiling result:
Type Time(%) Time Calls Avg Min Max Name
GPU activities: 99.45% 111.230s 111.230s 111.230s 111.230s vector_add(float*, float*, float*, int)
0.30% 335.78ms 1 335.78ms 335.78ms [CUDA memcpy DtoH]
0.25% 283.87ms 2 141.93ms 141.51ms 142.35ms [CUDA memcpy HtoD]
```

1 block with 256 threads

```
==8354== Profiling application: ./vector add oneblock
==8354== Profiling result:
           Type Time(%)
                            Time
                                     Calls
                                                         Min
                                                Avq
                                                                   Max Name
GPU activities:
                                                    695.40ms 695.40ms vector add(float*, float*, float*, int)
                 46.94% 695.40ms
                                        1 695.40ms
                                        2 226.74ms 226.60ms 226.87ms [CUDA memcpy HtoD]
                 30.61% 453.48ms
                 22.45% 332.56ms
                                        1 332.56ms 332.56ms [CUDA memcpy DtoH]
```

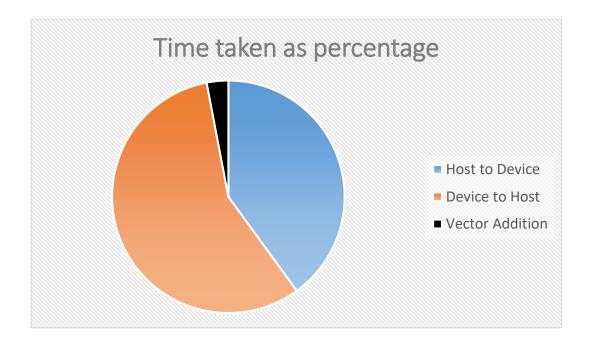
N blocks with all threads

```
==11178== Profiling application: ./vector add nblock
==11178== Profiling result:
           Type Time(%)
                             Time
                                      Calls
                                                 Avg
                                                           Min
                                                                         Name
                                                                     Max
GPU activities:
                 57.10% 410.44ms
                                          1 410.44ms 410.44ms 410.44ms [CUDA memcpy DtoH]
                  39.65% 284.97ms
                                          2 142.49ms 142.12ms 142.85ms [CUDA memcpy HtoD]
                                            23.336ms 23.336ms 23.336ms vector add(float*, float*, float*, int)
                   3.25% 23.336ms
```

Code Profiling

```
==11178== Profiling application: ./vector_add_nblock
==11178== Profiling result:
Type Time(%) Time Calls Avg Min Max Name
GPU activities: 57.10% 410.44ms 1 410.44ms 410.44ms [CUDA memcpy DtoH]
39.65% 284.97ms 2 142.49ms 142.12ms 142.85ms [CUDA memcpy HtoD]
3.25% 23.336ms 1 23.336ms 23.336ms vector_add(float*, float*, float*, int)
```

Expensive step is the memory transfer



GPU computation



- For a task involving single computation on a data,
 - When a GPU is used most of the time will be spent on copying data between CPU and GPU memory.
- One way to circumvent this problem, if the task allows it, then:
 - □Perform simultaneous data transfer and computation
 - ➤ Overlap computation and data transfer
- GPU is ideal when many computations needs to be done for a given data.

Thank you for your attention!

http://sctrain.eu/

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