Practical Parallel Computing (実践的並列コンピューティング)

2025 Class No.8
[CUDA Part] (1)
Introduction to CUDA

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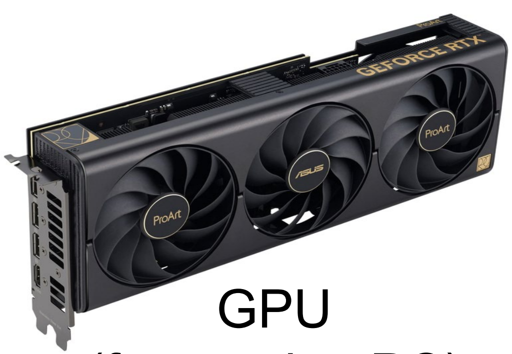
Overview of This Course

- Introduction Part
  - 2 classes
- OpenMP (OMP) Part
  - 4 classes
  - Report (required)
- OpenACC (ACC) Part
  - 2 classes
  - Report (required)
- CUDA Part
  - 3 classes ← We are here (1/3)
  - Report (elective)
- MPI Part
  - 3 classes
  - Report (elective)

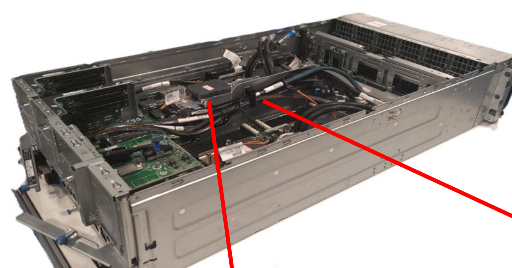
OpenACC and CUDA for GPUs

- OpenACC
  - C/Fortran + directives (#pragma acc …), Easier programming
  - Basically for data parallel programs with for-loops
- CUDA
  - Most popular and suitable for higher performance

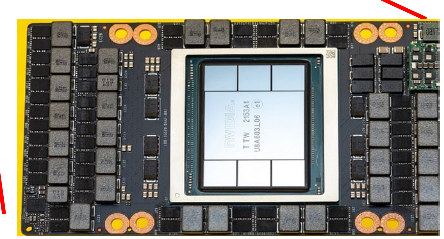
Programming is harder, but more general



GPU
(for gaming PC)



TSUBAME4
node



GPU

Why is CUDA Harder?

- Like OpenACC,
  - We program code for GPUs and CPUs
  - We program data copying
- Unlike OpenACC,
  - We must specify number of threads (& thread blocks)
  - No “#pragma acc kernel” ➔ we write kernel functions
  - No “#pragma acc loop” ➔ we write code for “what each thread does”
  - No “#pragma acc data” ➔ we must use different arrays/pointers on CPUs and GPUs

  :

An OpenACC Program Look Like

```
   int A[100], B[100];
   int i;
#pragma acc data copy(A,B)
#pragma acc kernels
#pragma acc loop independent
   for (i = 0; i < 100; i++) {
       A[i] += B[i];
   }
```

Executed on GPU in parallel

A CUDA Program Look Like

Sample:
ppcomp-ex/cuda/add/

```
int A[100], B[100];
int *DA, *DB;
int i;
cudaMalloc(&DA, sizeof(int)*100);
cudaMalloc(&DB, sizeof(int)*100);
cudaMemcpy(DA,A,sizeof(int)*100,
    cudaMemcpyHostToDevice);
cudaMemcpy(DB,B,sizeof(int)*100,
    cudaMemcpyHostToDevice);

add<<<20, 5>>>(DA, DB);

cudaMemcpy(A,DA,sizeof(int)*100,
    cudaMemcpyDeviceToHost);
```

```
__global__ void add
   (int *DA, int *DB)
{
   int i = blockIdx.x*blockDim.x
        + threadIdx.x;
   DA[i] += DB[i];
}
```

Executed on GPU
(called a *kernel function*)

We have to separate code regions executed on CPU and GPU

Using cuda/add Sample

```
[make sure that you are at a interactive node (rXn11) ]
module load nvhpc    [Do once after login]
[please go to your ppcomp-ex directory]
cd cuda/add
make
[An executable file “add” is created]
./add
```

Meaning of the program is very simple:

for (i = 0; i < 100; i++) { A[i] += B[i]; }

Notes on “module load”

- Either is ok for CUDA programming
  - module load nvhpc ➔ Both OpenACC and CUDA are ok
  - module load cuda ➔ CUDA is ok
- If “module load cuda” fails:

```
Loading cuda/12.8.0
  ERROR: Module cannot be loaded due to a conflict.
    HINT: Might try "module unload nvhpc/25.1 cuda12.6" first.
```

➔ On TSUBAME4, “nvhpc” and “cuda” cannot be used together

  - Try “module unload nvhpc” and then “module load cuda”
  - Another method: “module purge” unload all modules (in the same shell)

Preparing Data on Device Memory

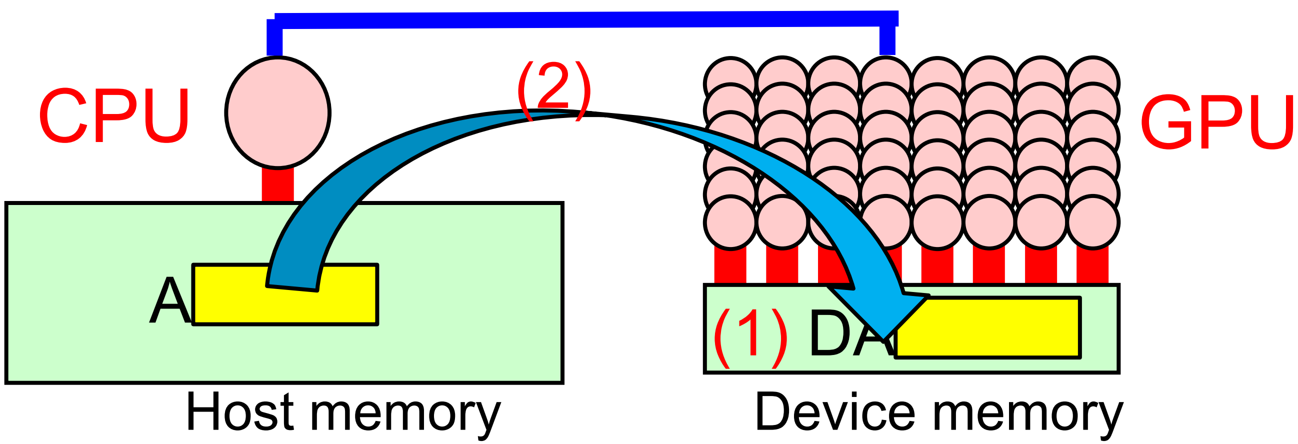
Before computation on GPU, we need to prepare data on device memory

- Allocate a region on device memory (1)

  cf) cudaMalloc((void**)&DA, *size*); ➔ DA is a pointer on device memory

- Copy data from host to device (2)

  cf) cudaMemcpy(DA, A, *size*, cudaMemcpyDefault);



Note: cudaMalloc and cudaMemcpy must be called on CPU, NOT on GPU

In CUDA, No “acc data”

OpenACC

Both allocation and copy are done by acc data copyin

One variable name A may represent both

- A on host memory
- A on device memory

```
  int A[100];  ← on CPU
#pragma acc data copy(A)
#pragma acc kernels
 {
   … A[i] …
 }      ↖ on GPU
```

CUDA

cudaMalloc and cudaMemcpy are separated

Programmer have to prepare two pointers, such as A and DA

```
int A[100];  ← on CPU
int *DA;     ← on GPU
cudaMalloc(&DA, …);
cudaMemcpy(DA, A, …, …);
// Here CPU cannot access DA[i]

func<<<…, …>>>(DA, …);
```

Calling A GPU Kernel Function from CPU

- We need to write functions on GPU and functions on CPU separately
  - A functions on GPU is called a GPU kernel function

[CPU side]

```
func<<<20, 5>>>(…);
```

In this case, 20x5=100 threads run on GPU

call

return

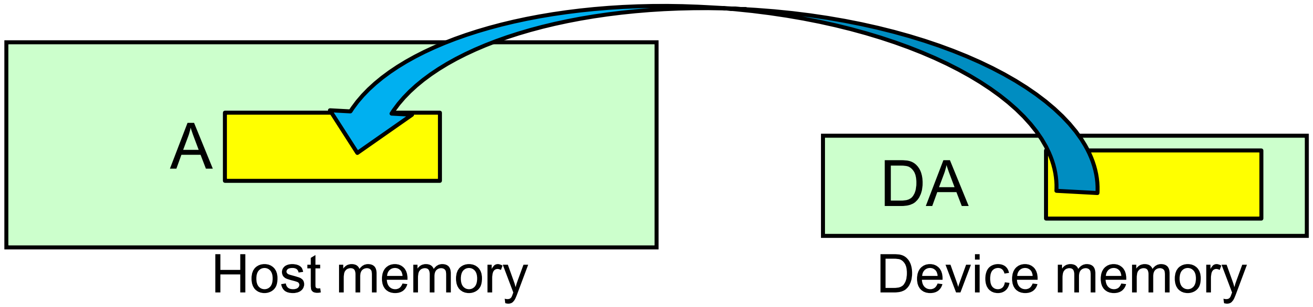
[GPU side]

```
__global__ void func(…)
{
      :
  return;
}
```

A GPU kernel function (called from CPU)

- needs __global__ keyword
- can take parameters
- can NOT return value; return type must be void

Copying Back Data from GPU

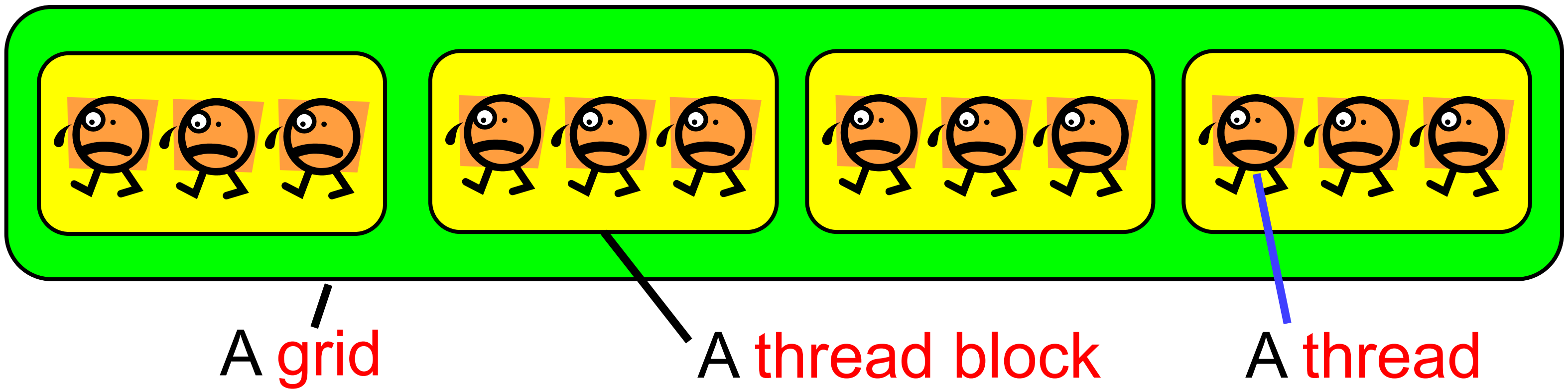


- Copy data using cudaMemcpy
  - cf) cudaMemcpy(A, DA, *size*, cudaMemcpyDefault);
  - 4th argument is one of
    - cudaMemcpyHostToDevice
    - cudaMemcpyDeviceToHost
    - cudaMemcpyDefault ← Detect memory type automatically ☺

- When a memory area is unnecessary, free it
  - cf) cudaFree(DA);

Threads in CUDA

When calling a GPU kernel function, specify <u>2 numbers </u>(at least) for number of threads



cf) func <<< 4, 3 >>> (); → 12 threads

Number of thread blocks = gridDim

Number of threads per block = blockDim

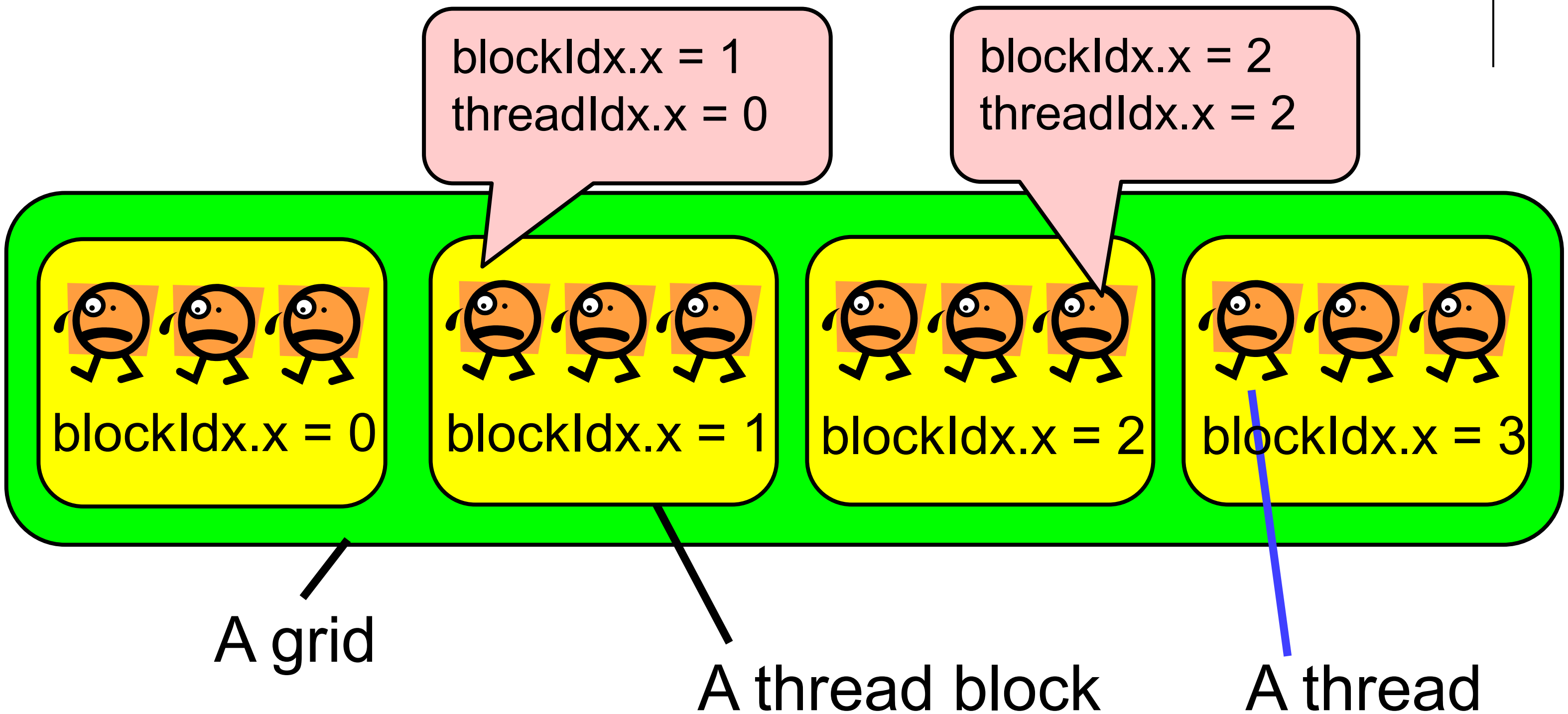
The reason is related to GPU hardware

Thread block ⇔ SMX, Thread ⇔ CUDA core

To See Who am I

- By reading the following special variables, each thread can see its thread ID in GPU kernel function
- My ID
  - blockIdx.x: Index of the block the thread belong to (≧0)
  - threadIdx.x: Index of the thread (inside the block) (≧0)
- Number of thread/blocks
  - gridDim.x: How many blocks are running
  - blockDim.x: How many threads (per block) are running

Thread Block ID, Thread ID



For every thread, gridDim.x = 4, blockDim.x = 3

Note: In order to see the entire sequential ID, we should compute
blockIdx.x * blockDim.x + threadIdx.x

The Case of cuda/add Sample

- ppcomp-ex/cuda/add
- We want to do

```
for (i = 0; i < 100; i++) { DA[i] += DB[i]; }
```

[CPU side]

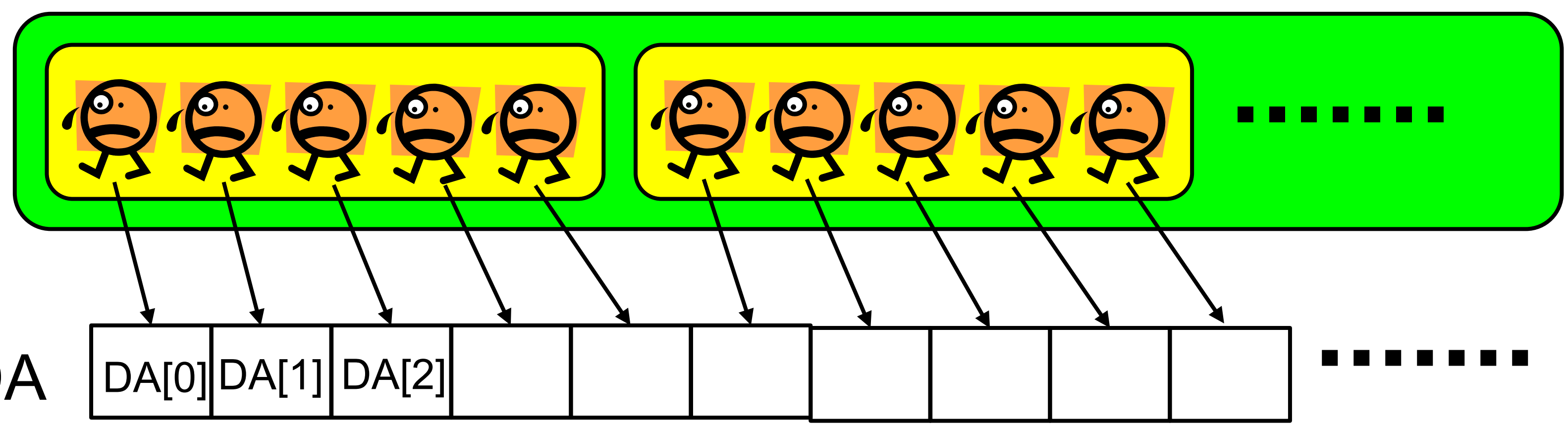
```
add<<<20, 5>>>(…);
```

20x5=100 threads
will execute add function

[GPU side]

```
__global__ void add(int *DA, int *DB)
{
    int i = blockIdx.x * blockDim.x + threadIdx.x;
    DA[i] += DB[i];
    return;
}
```

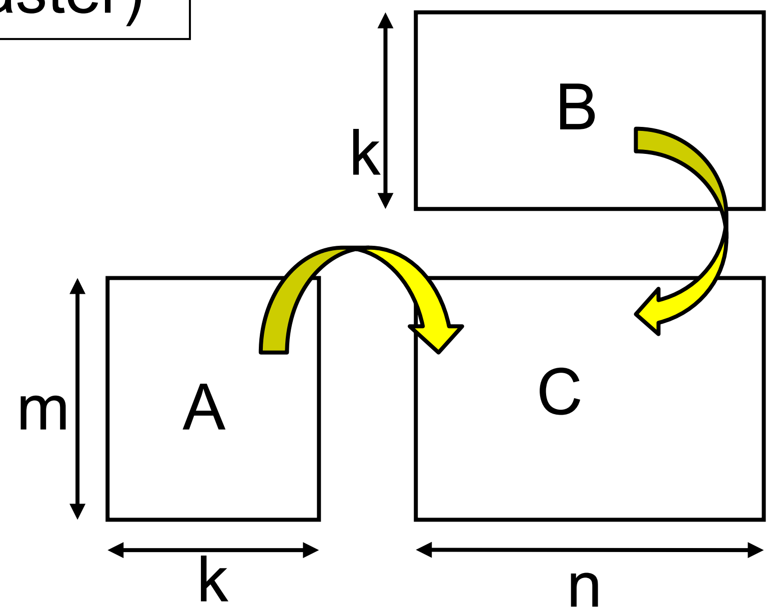
DA



“mm” sample: Matrix Multiply (related to [C3])

CUDA versions are at
- ppcomp-ex/cuda/mm-1dpar/ (slow)
- ppcomp-ex/cuda/mm/ (faster)

A: a (m × k) matrix, B: a (k × n) matrix
C: a (m × n) matrix
$C \leftarrow A \times B$



- Supports variable matrix size
- Execution:./mm [m] [n] [k]

Using cuda/mm-1dpar Sample

[make sure that you are at a interactive node (rXn11)]
module load nvhpc *[Do once after login]*
[please go to your ppcomp-ex directory]
cd cuda/mm-1dpar
make
[An executable file "mm" is created]
./mm 2000 2000 2000

When you try cuda/mm,
replace cuda/mm-1dpar to cuda/mm

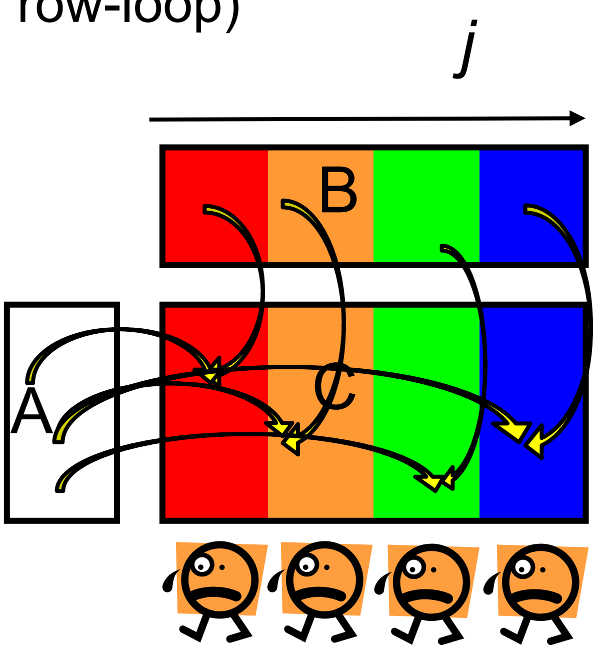
How We Parallelize Computation

In mm, we can compute different C elements in parallel

•On the other hand, it is harder to parallelize dot-product loop

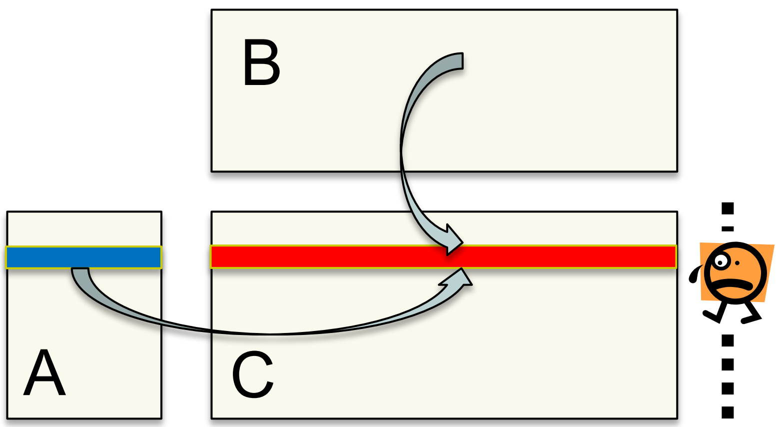
OpenMP

- Parallelize column-loop (or row-loop)



CUDA (mm-1dpar)

- We can create many threads
- 1 thread computes 1 row
    - We use m threads



※ This is not the unique way

Parallelism in cuda/mm-1dpar

- It is ok to make >1000, >10000 threads on CUDA
- We use *m* threads for *m* rows computation

```
matmul_kernel<<<m/BS, BS>>>(.....);
```

gridDim

blockDim (BS=64 in this sample)

1 element for 1 row → No need of "i" loop in this sample

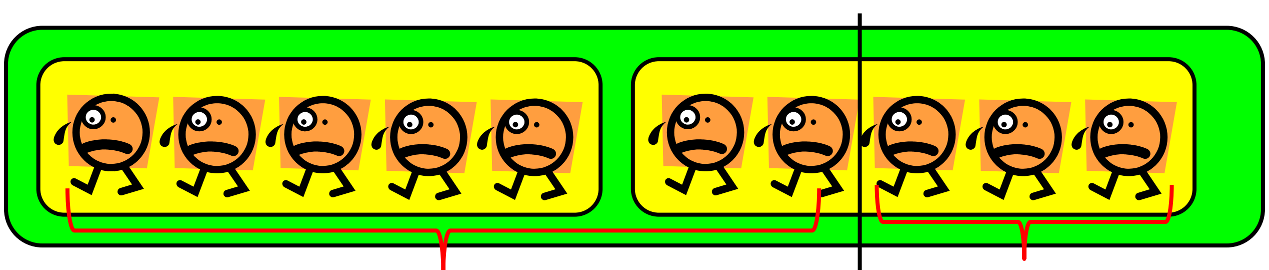
Note:
<<<m, 1>>> also works, but speed is even slower ☹
<<<1, m>>> causes an error if m>1024 (CUDA's rule)

If Number of Threads is Indivisible by BlockDim

- m: the number of threads
- BS: BlockDim
- If m may be indivisible by BS, we should use
  <<<(m+BS-1)/BS, BS>>>

→ But # of threads may be larger m. “Extra” threads (id≧m) <u>should not work</u>. See cuda/mm-1dpar/mm.cu

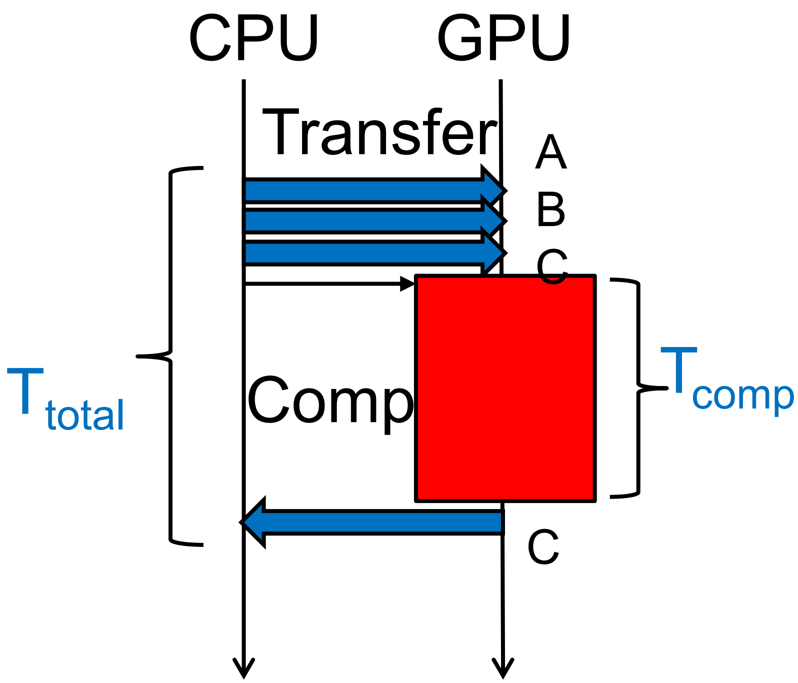
Example: m=7, BS=5 → <<<2,5>>>
10 threads start working, but 3 threads should do nothing



7 threads work

3 threads should return immediately

Data Transfer in cuda/mm-1dpar



(1) A, B, C are copied from CPU to GPU

- cudaMemcpy(DA, A, …)
- cudaMemcpy(DB, B, …)
- cudaMemcpy(DC, C, …)

(2) Computation is done on GPU

(3) C is copied from GPU to CPU

- cudaMemcpy(C, DC, …)

Notes in Time Measurement

- clock(), gettimeofday() must be called from CPU
- For accurate measurement, we should call cudaDeviceSynchronize() before measurement
  - Actually GPU kernel function call and cudaMemcpy(HostToDevice) are non-blocking

Discussion on Speed

Bad news: cuda/mm-1dpar is much slower than OpenACC! ☹
(even slower than OpenMP?)

- In acc/mm, i-loop and j-loop has "loop independent"
  → m × n elements are computed in parallel

- In mm-1dpar, we use m threads
  - → We should use more threads on a GPU!
  - We see m=1000~8000 threads are still insufficient, and slow

➔ cuda/mm uses mxn threads. Explained in next class

How is Number of Threads Determined? (1)

Difference between OpenMP and CUDA

- On OpenMP, number of threads (OMP_NUM_THREADS) should be ≦ CPU cores (or hyper threads)
  - The number is basically determined by hardware
  - ≦48 on an interactive (node_o) node, ≦384 on node_f

- On CUDA, it is better to use number of thread >> GPU cores
  - >> 7,680 on an interactive (node_o) node with ½ GPU
  - >> 16,896 on gpu_1, node_q ...
  - You can use >1,000,000 threads!

How is Number of Threads Determined? (2)

We have to deicide 2 numbers in kernel call

<<<number of blocks, block size>>>

A better way would be

(1)We decide total number of threads P

(2)We tune each block size BS

- Good candidates are 32, <u>64</u>, 128, … 1024

(3)Then block number is P/BS

- For indivisible cases, (P+BS-1)/P

Comparing OpenMP/OpenACC/CUDA

	OpenMP	OpenACC	CUDA
Processors	CPU	CPU+GPU	
File extension	.c, .cc		.cu
To start parallel (GPU) region	#pragma omp parallel	#pragma acc kernels	func<<<…, …>>>()
To specify # of threads	export OMP_NUM_THREADS=…	(num_gangs, vector_length etc)	
Desirable # of threads	# of CPU cores or less	# of GPU cores or “more”	
To get thread ID	omp_thread_num()	-	blockIdx, threadIdx
Parallel for loop	#pragma omp for	#pragma acc loop	-
Task parallel	#pragma omp task	-	-
To allocate device memory	-	#pragma acc data	cudaMalloc()
To copy to/from device memory	-	#pragma acc data #pragma acc update	cudaMemcpy()
Functions on GPU	-	#pragma acc routine	__global__,__device__

※ “# of XXX” = “The number of XXX”

Assignments in this Course

- There is homework for each part.

Part	Problems	
OMP Part	[O1] diffusion [O2] bsort [O3] qsort [O4] free	*Select 1 problem*
ACC Part	[A1] diffusion [A2] bsort [A3] mm speed [A4] free	*Select 1 problem*
CUDA Part	[C1] diffusion [C2] bsort [C3] mm speed [C4] free	*Select 1 problem from 2 parts*
MPI Part	[M1] [M2] [M3] [M4]	

Assignments in CUDA Part (1)

If you choose this part,

choose one of [C1]—[C4], and submit a report

Due date: May 26 (Monday)

[C1] Parallelize “diffusion” sample program by CUDA

- You can start from /ppcomp-ex/cuda/diffusion

Optional：

- To make array sizes variable parameters
- To compare CUDA vs OpenMP (vs OpenACC?)
- To improve performance further

Assignments in CUDA Part (2)

[C2] Parallelize "bsort" sample program by CUDA

- You can start from /ppcomp-ex/cuda/bsort

Optional:

- Comparison with other sort algorithms
  - Quick sort (qsort), Heap sort, Merge sort, …
- Comparison with OpenMP or OpenACC...

Assignments in CUDA Part (3)

[C3] Evaluate speed of “cuda/mm” sample in detail

ppcomp-ex/cuda/mm/

- Compare speed of cuda/mm and cuda/mm-1dpar
- Use various matrices sizes
- Evaluate effects of data transfer cost

Optional：

- Compare with OpenMP or OpenACC
- To use different loop orders
- To change/improve the program
  - Cache blocking?

Assignments in CUDA Part (4)

[C4] (Freestyle) Parallelize *any* program by CUDA

- cf) A problem related to your research
- Challenging one for parallelization is better
  - cf) Partial computations have dependency with each other

Notes in Report Submission (1)

- Submit the followings via LMS

  (1) A report document

  - PDF, MS-Word or text file
  - 2 pages or more
  - in English or Japanese (日本語もok)

  (2) Source code files of your program

- Try “zip” to submit multiple files

Notes in Report Submission (2)

The report document should include:

- Which problem you have chosen
- How you parallelized
  - It is even better if you mention efforts for high performance or new functions
  - [CUDA] How many threads? What computations do threads do?
- Performance evaluation on TSUBAME
  - With varying number of threads
  - With varying problem sizes
  - Discussion with your findings
  - Other machines than TSUBAME are ok, if available

Plan of CUDA Part

- Class #9 (Today)
  - Introduction to CUDA, kernel functions
- Class #10
  - Characteristics of grid, thread blocks, threads
- Class #11
  - Performance improvement on GPU