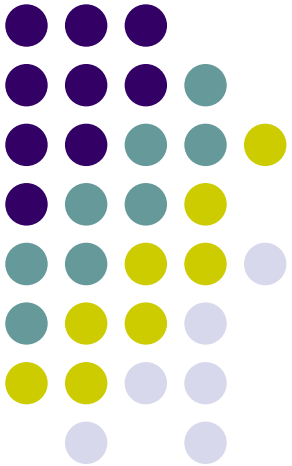
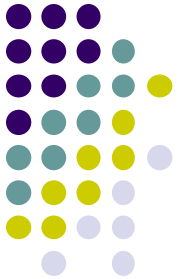
Practical Parallel Computing (実践的並列コンピューティング) 2021 No. 10

Part2: GPU (4)
May 17, 2021



Toshio Endo
School of Computing & GSIC
endo@is.titech.ac.jp

Overview of This Course



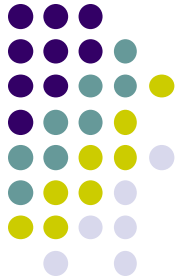
- Part 0: Introduction
  - 2 classes
- Part 1: OpenMP for shared memory programming
  - 4 classes
- Part 2: GPU programming
  - 4 classes ← We are here (4/4)
  - OpenACC (1.5 classes) and CUDA (2.5 classes)
- Part 3: MPI for distributed memory programming
  - 3 classes

Comparing OpenMP/OpenACC/CUDA

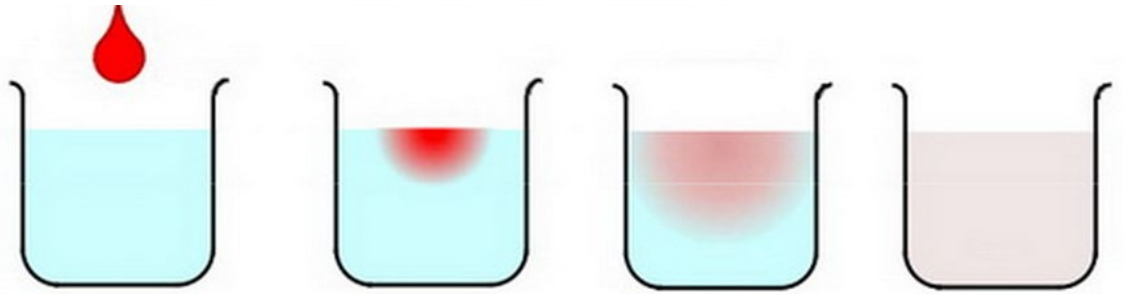
	OpenMP	OpenACC	CUDA
Processors	CPU	CPU+GPU	
File extension	.c, .cc		.cu
To start parallel (GPU) region	#pragma omp parallel	#pragma acc kernels	func<<<…, …>>>()
To specify # of threads	export OMP_NUM _THREADS=…	(num_gangs, vector_length etc)	
Desirable # of threads	# of CPU cores or less	# of GPU cores 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()
Function on GPU	-	#pragma acc routine	__global__,__device__

※ “# of XXX” = “The number of XXX”

“diffusion” Sample Program
related to [G1]



An example of diffusion phenomena:

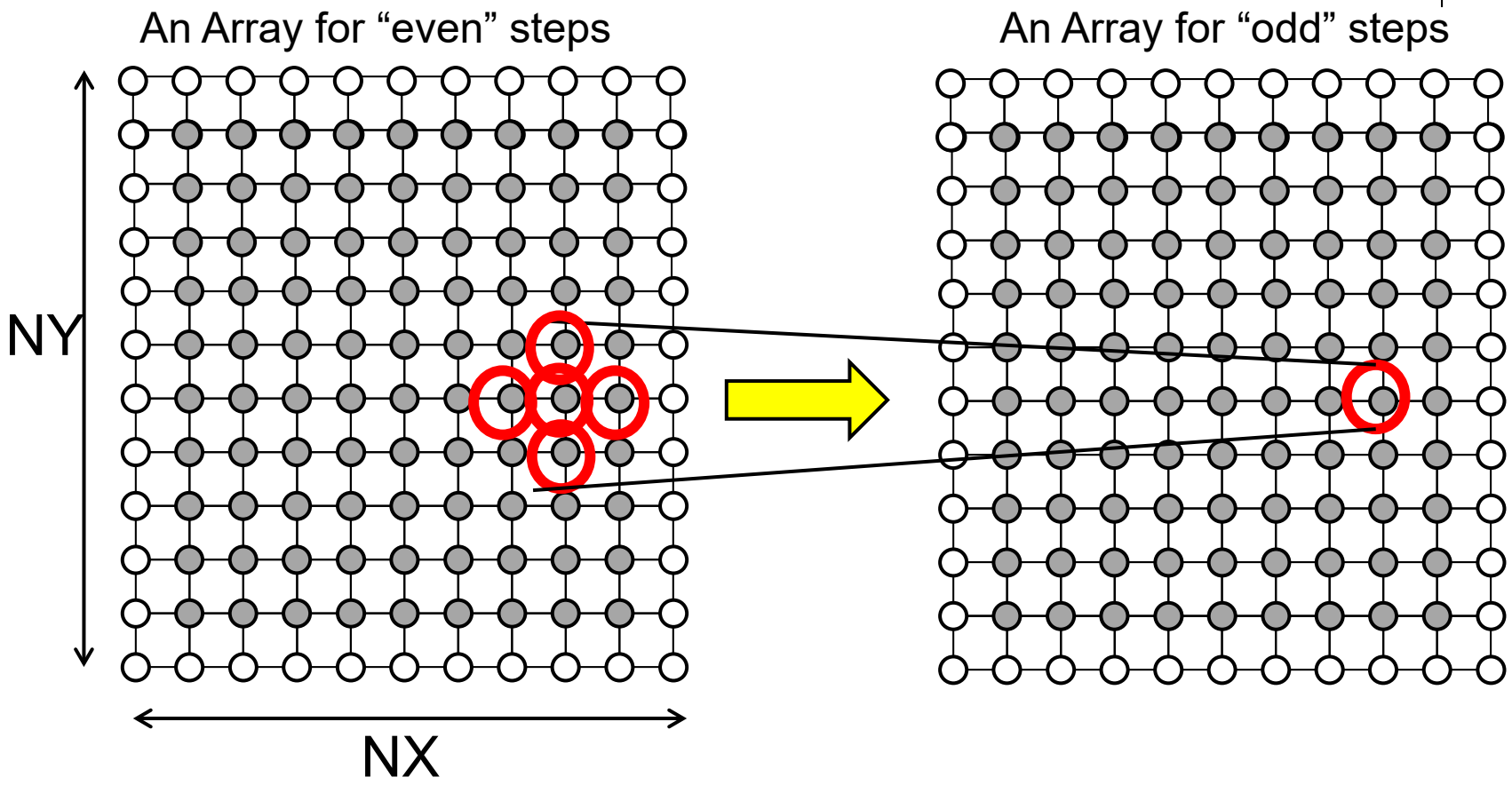


The ink spreads gradually, and finally the density becomes uniform (Figure by Prof. T. Aoki)

Available at /gs/hs1/tga-ppcomp/21/diffusion/
You can use /gs/hs1/tga-ppcomp/21/diffusion-cuda/

- Execution：./diffusion [nt]
  - nt: Number of time steps

Discussion on diffusion sample



Both arrays have to be on GPU device memory when computations are done

Consideration of Parallelizing Diffusion with CUDA
related to [G1]

- x, y loops can be parallelized
- t loop cannot be parallelized

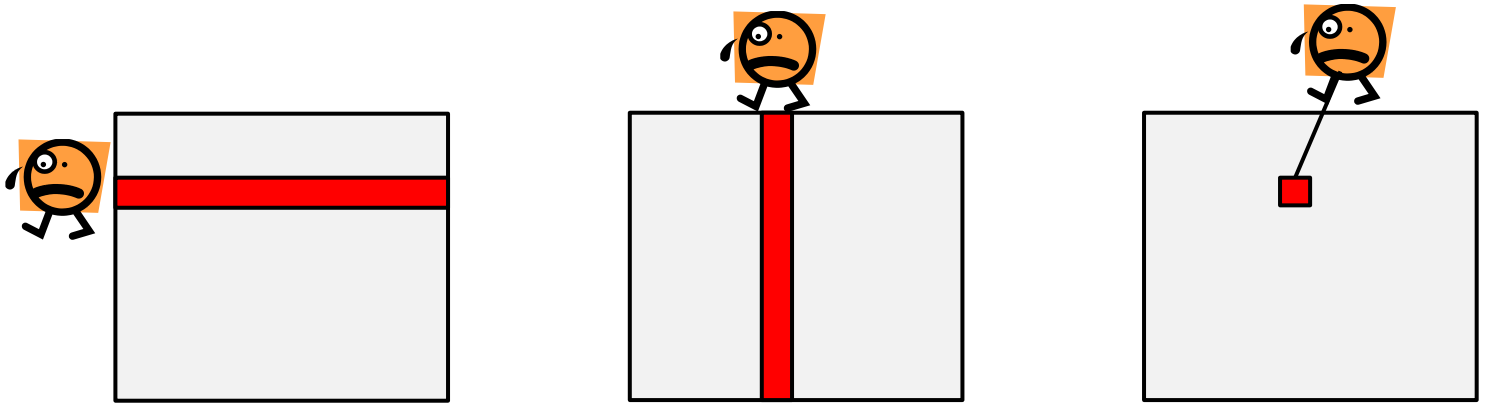
```
[Data transfer from CPU to GPU]
for (t = 0; t < nt; t++) {

  for (y = 1; y < NY-1; y++) {
    for (x = 1; x < NX-1; x++) {
            :
    }
  }
}
[Data transfer from GPU to CPU]
```

GPU computation must be a distinct function (GPU kernel function)

It's better to transfer data *out of* t-loop

Considering CUDA Threads

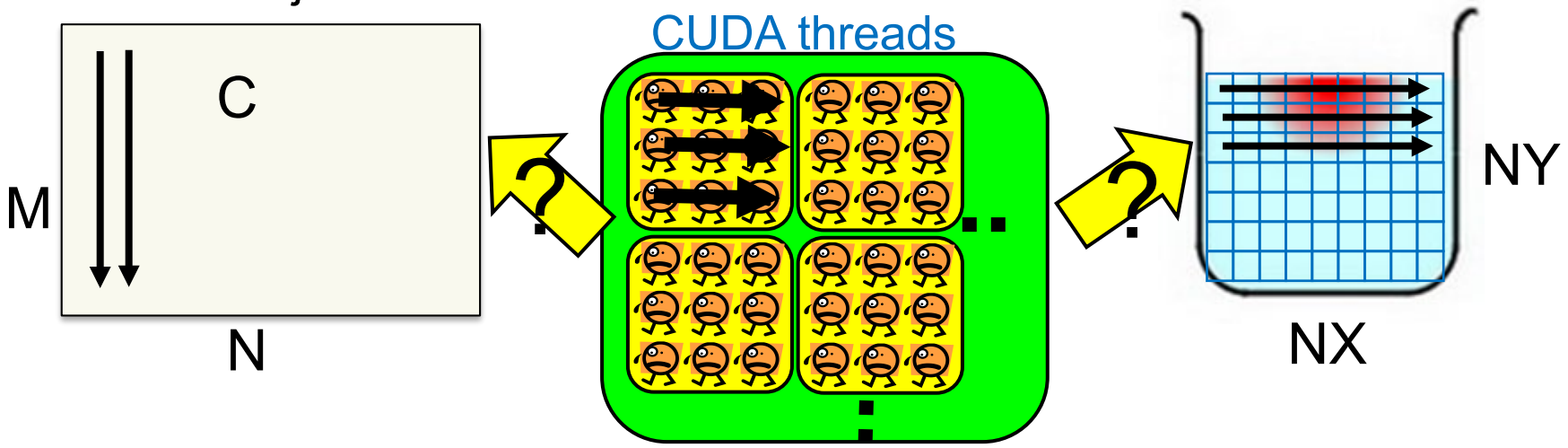
- How do we design threads on CUDA?
- There are several choices in [G1]
  - 1thread = 1row
    - We use NY threads in total → only x-loop in kernel function
  - 1thread = 1column
    - We use NX threads in total → only y-loop in kernel function
  - 1thread = 1element
    - We use NX x NY threads in total → No loop in kernel function!
    - This looks fast since the number of threads is very large



Mapping between Threads and Data

mm-cuda:
Matrices has
column-major format

diffusion:
2D array has
row-major format




```
j = blockIdx.y * blockDim.y +
threadIdx.y;
i = blockIdx.x * blockDim.x +
threadIdx.x;
 : This thread computes Cij
```

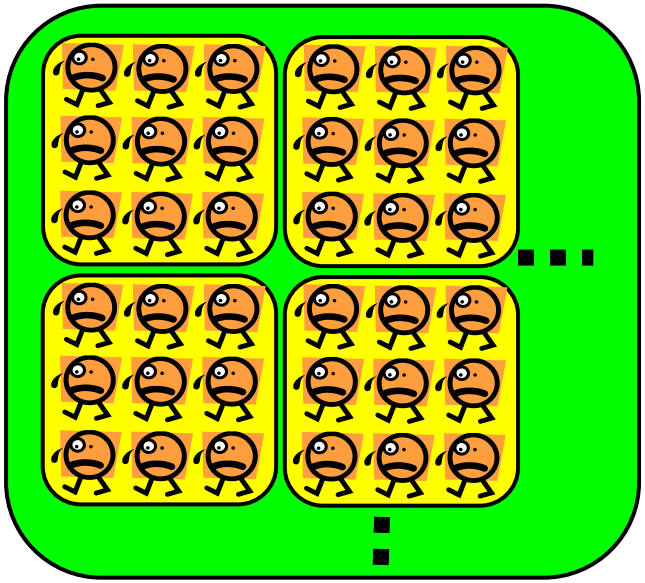
```
y = blockIdx.y * blockDim.y +
threadIdx.y;
x = blockIdx.x * blockDim.x +
threadIdx.x;
 : This thread computes[y][x]
```

[Q] What if the dimensions are exchanged?

Considering gridDim/blockDim (1)

```
func <<< dim3 (?, ?, ?), dim3 (?, ?, ?) >>>(…);
```

gridDim　　blockDim



(1) We decide total number of threads

➔ (NX, NY, 1) threads

- See notes on the next page

(2) We tune each block size (blockDim)

➔ Good candidates are (4, 4, 1), (8, 8, 1), (16, 16, 1), (32, 32, 1)

- The number must be ≦ 1024
- How about non-square blocks?

(3) Then block number (gridDim) is determined

We should consider indivisible cases

Considering gridDim/blockDim (2)

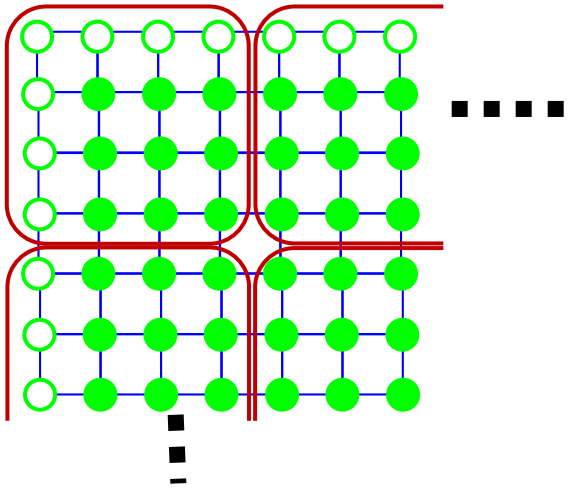
- In diffusion, Points [1, NX-1) × [1, NY-1), excluded boundary, should be computed

  There are choices:

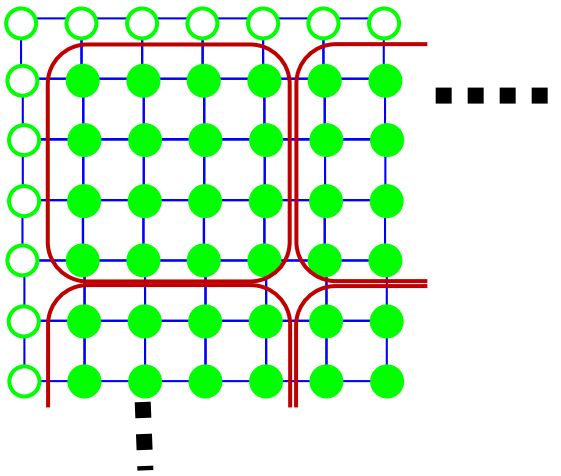
  (A) Create NX x NY threads
  - Thread (x,y) computes (x,y)
  - Threads with below IDs do nothing
    - x == 0 or y == 0 or x ≧ NX-1 or y ≧ NY-1

  (B) Create (NX-2) x (NY-2) threads
  - Thread (x,y) computes (x+1,y+1)
  - Threads with below IDs do nothing
    - x ≧ NX-2 or y ≧ NY-2

(A)



(B)



Either is ok ☺

Discussion on Data Transfer of Diffusion

Both codes will work, but how about speeds?

```
[Data transfer from CPU to GPU]
for (t = 0; t < nt; t++) {
                :

  for (y = 1; y < NY-1; y++) {
    for (x = 1; x < NX-1; x++) {
                :
     }
   }

}
[Data transfer from GPU to CPU]
```

Computation: O(NX NY nt)
Transfer: O(NX NY)

```
for (t = 0; t < nt; t++) {
                :
  [Data transfer from CPU to GPU]
  for (y = 1; y < NY-1; y++) {
    for (x = 1; x < NX-1; x++) {
                :
     }
   }
   [Data transfer from GPU to CPU]
}
```

Computation: O(NX NY nt)
Transfer: O(NX NY nt)

Speed of GPU Programs and GPU Architecture

Advanced topic

Case 1: How should block-size be determined?

When creating 1,000,000 threads,

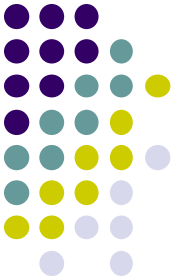
- <<<1, 1000000>>> causes an error
  - blockDim must be <= 1024
- <<<1000000, 1>>> can work, but slow
- <<<1000, 1000>>> is faster → Why?

Case 2: How should each thread access memory?

- In mm-cuda, (x = row,y = col) and (x = col, y = row) shows different speed

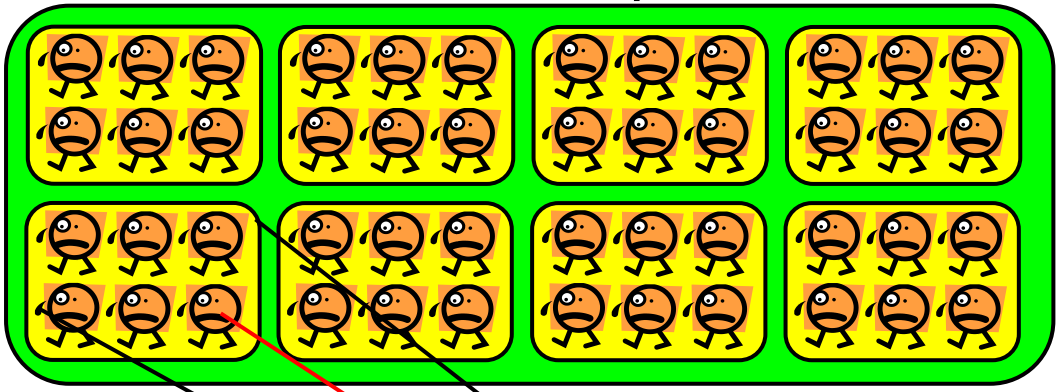
Knowledge of GPU architecture helps understanding of speeds

Why Do We Have to Specify both gridDim and blockDim?



- and why did NVIDIA decide so?

→ Hierarchical structure of GPU processor is considered

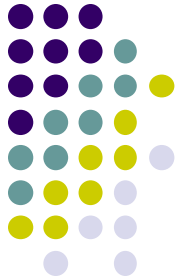


Structure of P100 GPU
(16nm, 15Billion transistors)

1 GPU = 56 SMXs
1 SMX = 64 CUDA cores
(16 cores x 4 groups)

→ 1GPU=3,584 CUDA cores

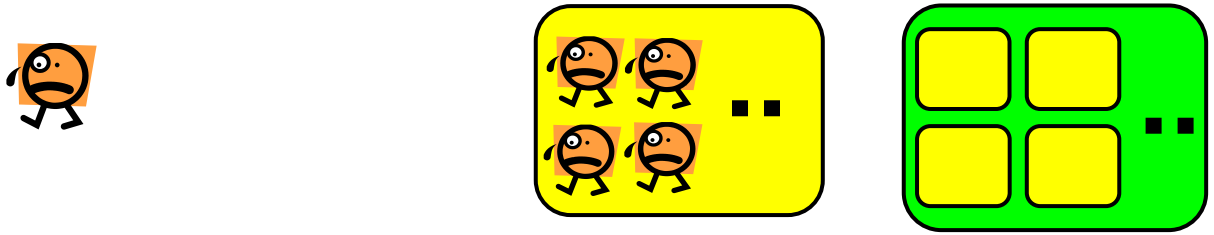
Mapping between Threads and Cores



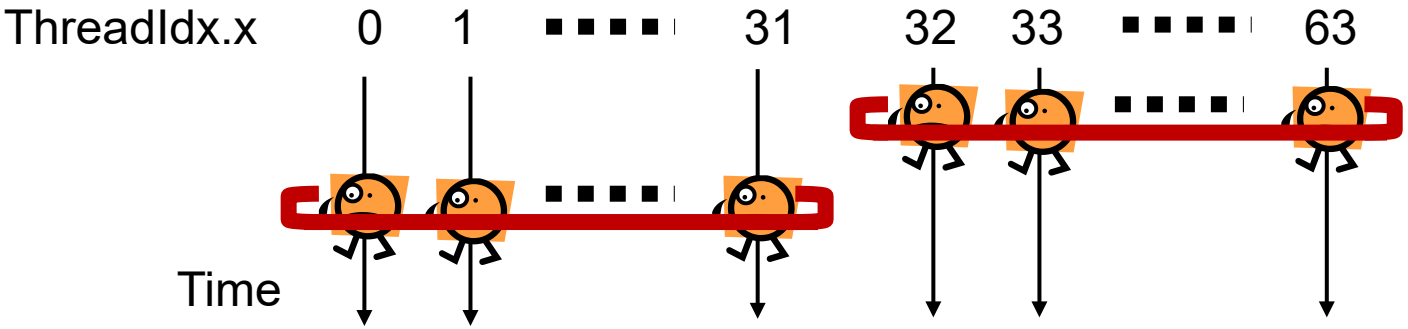
- 1 thread blocks (or more) run on 1 SMX
  - → At least 56 blocks are needed to use all SMXs on P100
  - → gridDim (gx*gy*gz) should be ≧56
- 1 thread (or more) run on a CUDA core
  - → At least 56*64=3584 threads in total are needed to use all CUDA cores on P100
  - → Total threads (gx*gy*gz * bx*by*bz) should be ≧3584
- 32 consective threads (in a block) are batched (called a *warp*) and scheduled
  - → At least 32 threads per block are needed for performance
  - → blockDim (bx*by*bz) should be ≧32

Warp: Internal Execution Unit

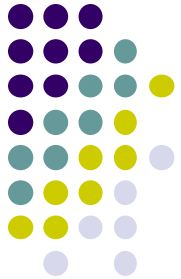
thread < warp < thread block < grid



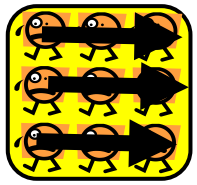
- Threads in a thread block are internally divided into "warp", a group of contiguous 32 threads
- 32 threads in a warp always are executed synchronously
  - They execute the same instruction simultaneously
  - Only 1 program counter for 32 threads → GPU hardware is simplified
  - Actually 32 threads are executed on 16 CUDA cores



Observations due to Warps



- If number of threads per block (blockDim) is not *32 x n*, it is inefficient
  - Even if blockDim=1, the system creates a warp for it
- Characteristics in memory addresses accessed by threads in a warp affect the performance
  - Coalesced accesses are fast

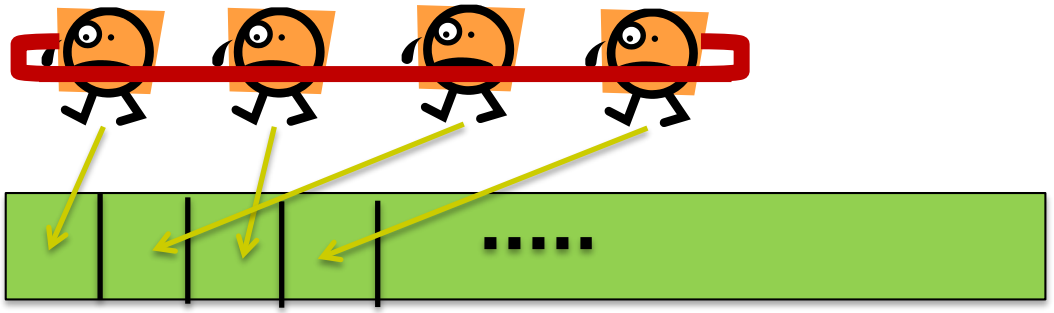


※ In multi-dimensional cases (blockDim.y>1 or blockDim.z>1), “neighborhood” is defined by x-dimension

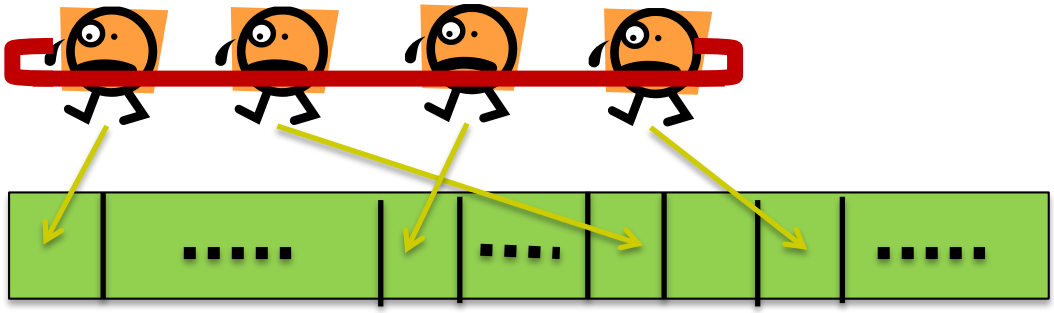
Coalesced Memory Access

- When threads in a warp access “neighbor” address on memory (coalesced access), it is more efficient

Coalesced access
→ **Faster**



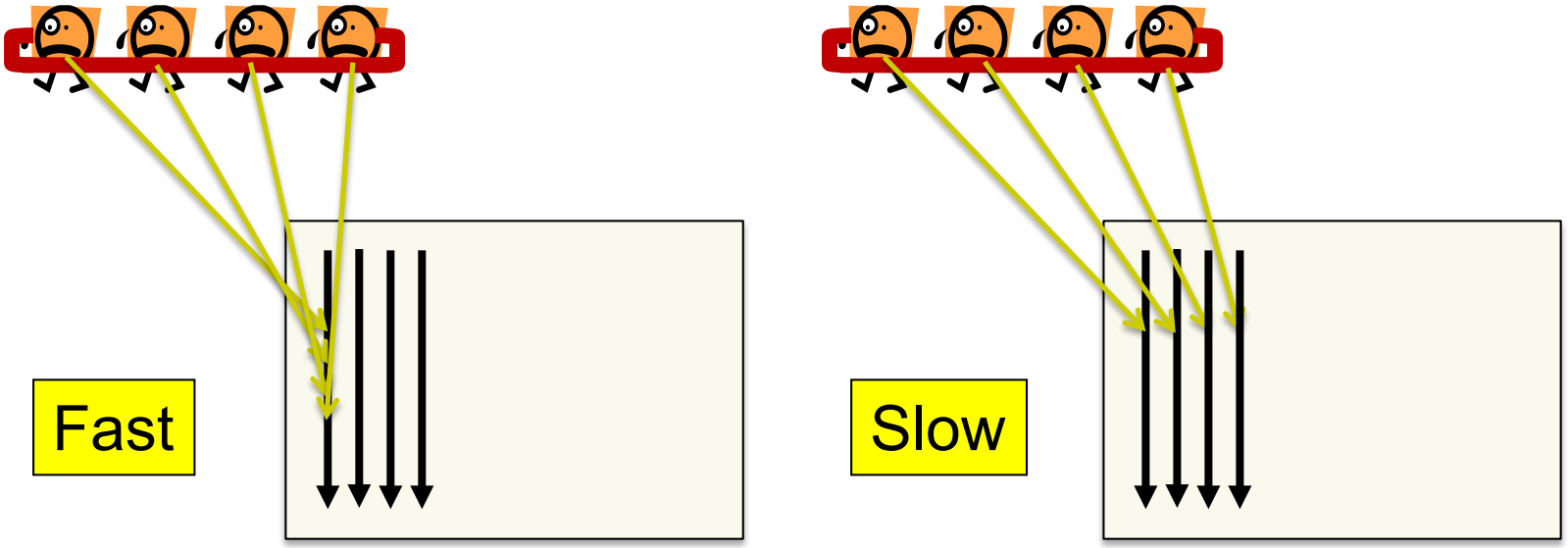
Non-coalesced access
→ **Slower**



Accesses in mm-cuda Sample

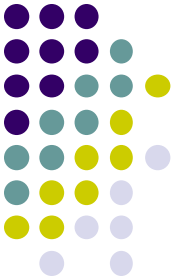
- mm-cuda: (x = row,y = col) → coalesced and fast
- mm-nc-cuda: (x = col, y = row) → non-coalesced and slow

We should see "what data are accessed by threads in a warp simultaneously"



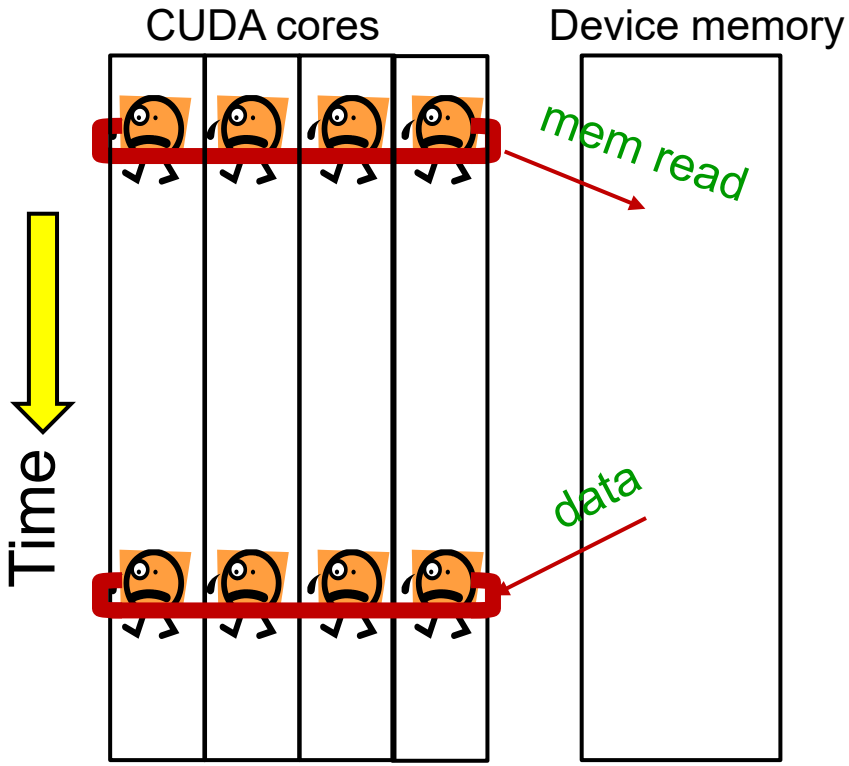
matrices in column-major format

Why #threads >> #cores Works Well on GPUs?

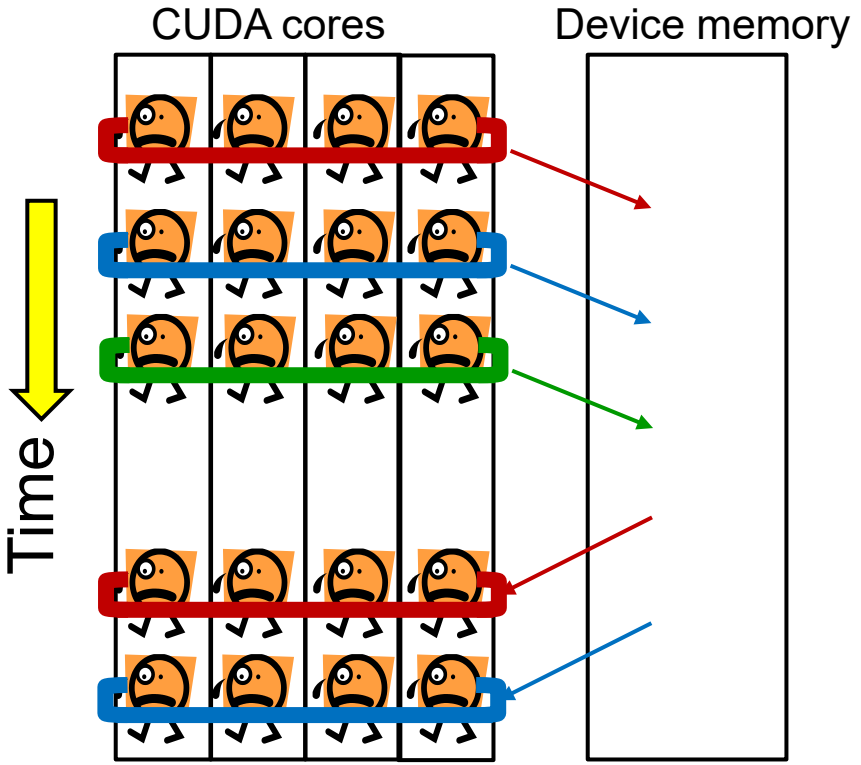


- GPU supports very fast (~1 clock) context switches
  - ➔ With many threads, memory access latency can be hidden

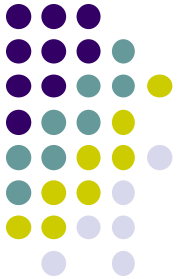
#threads == #cores



#threads > #cores



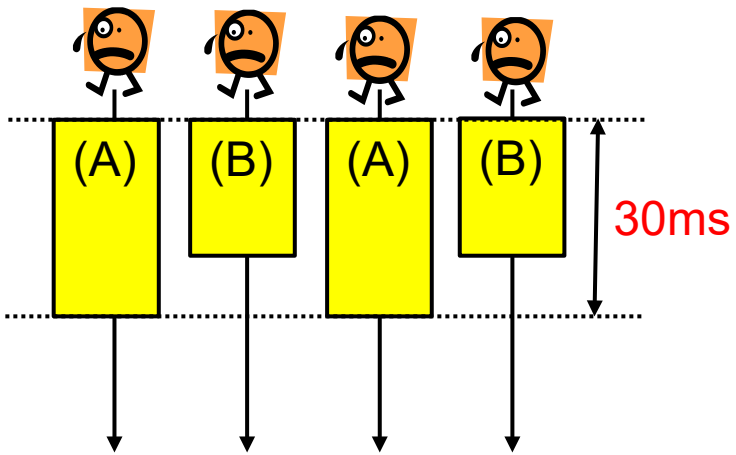
Considering Branches in Parallel Programs



Consider this code. How long is execution time?

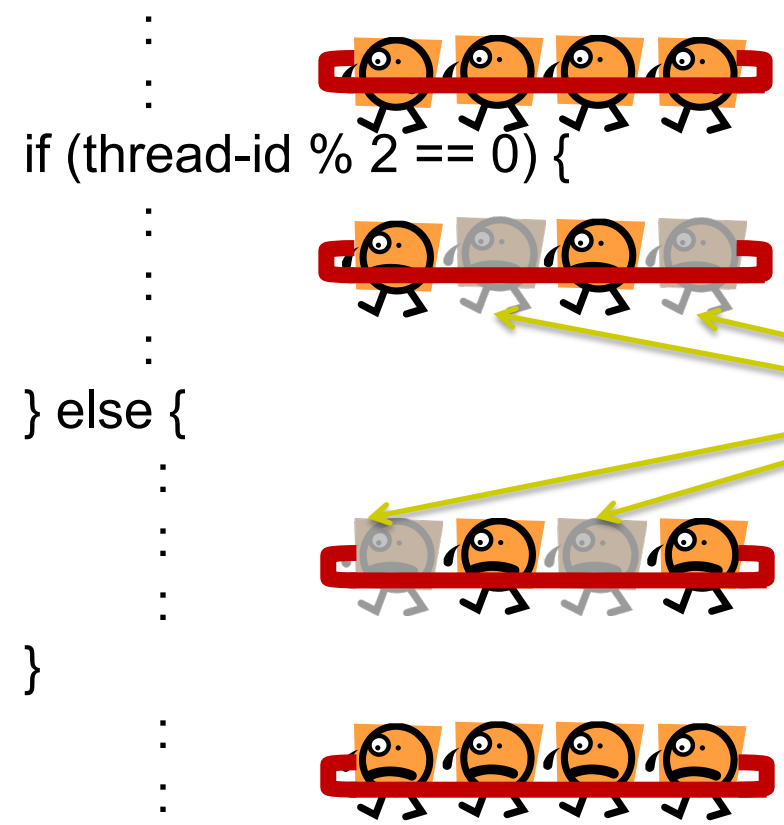
```
if (thread-id % 2 == 0) {
        :  // (A) 30msec
} else {
        :  // (B) 20msec
}
```

On CPU (OpenMP)



On GPU, threads in a warp must execute the same instruction. What happens?

Branches on GPU (1)

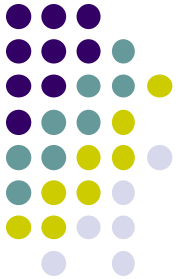


Some threads are made sleep
Both “then” and “else” are executed!

→ Answer to previous question is 50ms !

※ Similar cases happen in for, while…

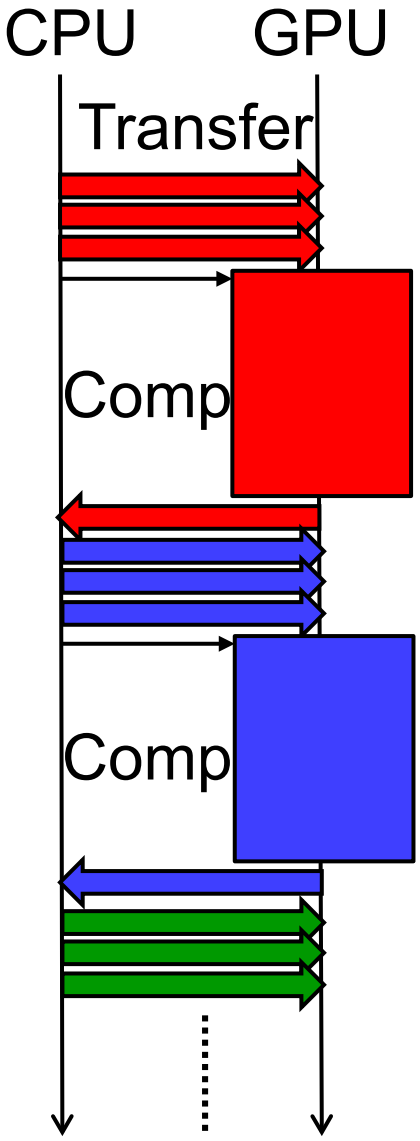
Branches on GPU (2)



- As exceptional cases, if threads in a warp “agree” in branch condition, either “then” part or “else” part is executed → Efficient!
- If there is difference of opinion (previous page), it is called a divergent branch

→ Agreement among buddies (threads in a warp) is important for speed

Considering Data Transfer Costs



Example case: We are going to compute multiply for different matrices

- Input data are on host memory
  - C1 = A1 × B1
  - C2 = A2 × B2

    ….
  - Cn = An × Bn

- In default, GPU cannot compute during transfer

→ cudaStream is useful for hiding transfer costs

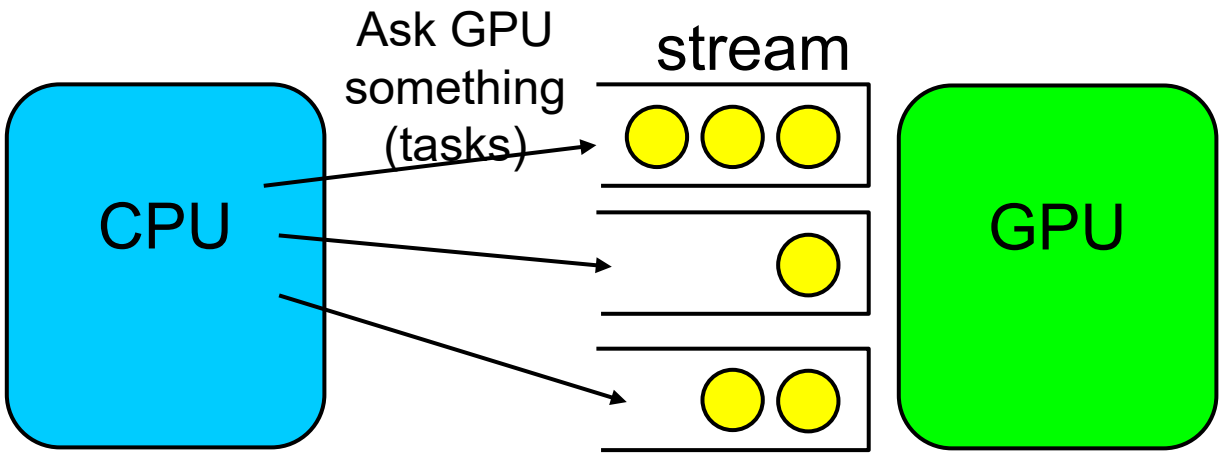
This is also useful for speed-up of mm-cuda, by dividing matrices into pieces

Asynchronous Executions with cudaStream (1)

What are streams?

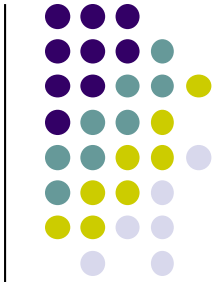
- GPU's "service counters" that accept tasks from CPU
  - Each stream looks like a queue
- "Tasks" from CPU to GPU include
  - Data transfer (Host → Device)
  - GPU kernel function call
  - Data transfer (Device → Host)

"Tasks" here are a bit different from "omp task"



All of sample programs are using the "default stream"

Asynchronous Executions with cudaStream (2)



Create a stream

```
cudaStream_t str;
cudaStreamCreate(&str); // Create a stream
```

Data transfer using a specific stream

```
cudaMemcpyAsync(dst, src, size, type, str);
```

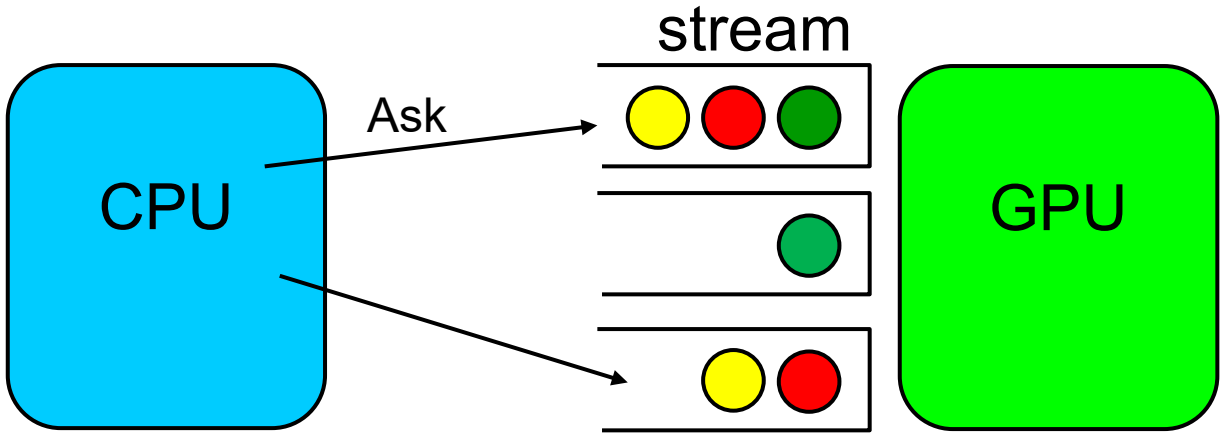
Call GPU kernel function using a stream

```
func<<<gs, bs, 0, str>>>( … );
// 3rd parameter is related to for “shared memory”
```

Wait until all tasks on a stream are finished

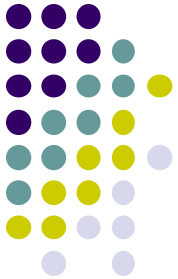
```
cudaStreamSynchronize(str);
```

How GPU Executes Tasks



- Tasks on the same stream is done in FIFO
- If tasks are in different streams, and have different kinds, they may be done simultaneously
  - Kinds: H→D, kernel, D→H
  - Note: If tasks are in the same kind, no speed up

Speed Up with Overlap of Computation and Transfer



n streams can be used for n independent tasks

- C1 = A1 × B1 (includes H->D, Calc, D->H)
- C2 = A2 × B2

….

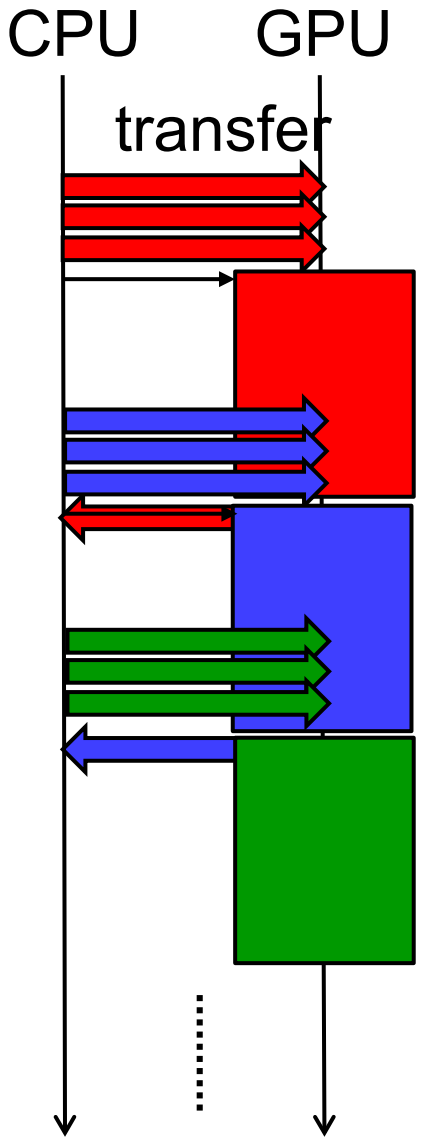
- Cn = An × Bn

→ We will see speed up since

(Total comp time + Total trans time)

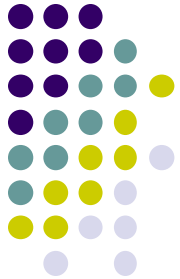
is improved to

max(Total comp time, Total trans time)



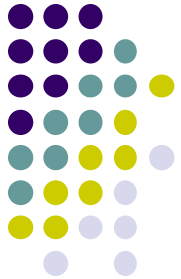
This is not a unique solution;
Use 2 or 3 streams repeatedly → we can save memory and stream resources

More Things to Study



- Using CUDA shared memory
  - fast and small memory than device memory
- Unified memory in recent CUDA
  - cudaMemcpy can be omitted for automatic data transfer
- Using Tensor-core to accelerate deep learning
  - Only on V100 GPUs or later
  - Unfortunately, TSUBAME3 has older P100 ☹
- Using multiple GPUs towards petascale computation
  - MPI+CUDA, MPI+OpenACC
- More and more…

Assignments in GPU Part (Abstract)



Choose one of [G1]—[G3], and submit a report

Due date: May 27 (Thursday)

[G1] Parallelize “diffusion” sample program by OpenACC or CUDA

[G2] Evaluate speed of “mm-acc” or “mm-cuda” in detail

[G3] (Freestyle) Parallelize *any* program by OpenACC or CUDA.

Next Class:

- Part 3: MPI Programming (1)
  - Introduction to distributed memory parallel programming