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

Part 2: GPU

No 1: Overview and OpenACC

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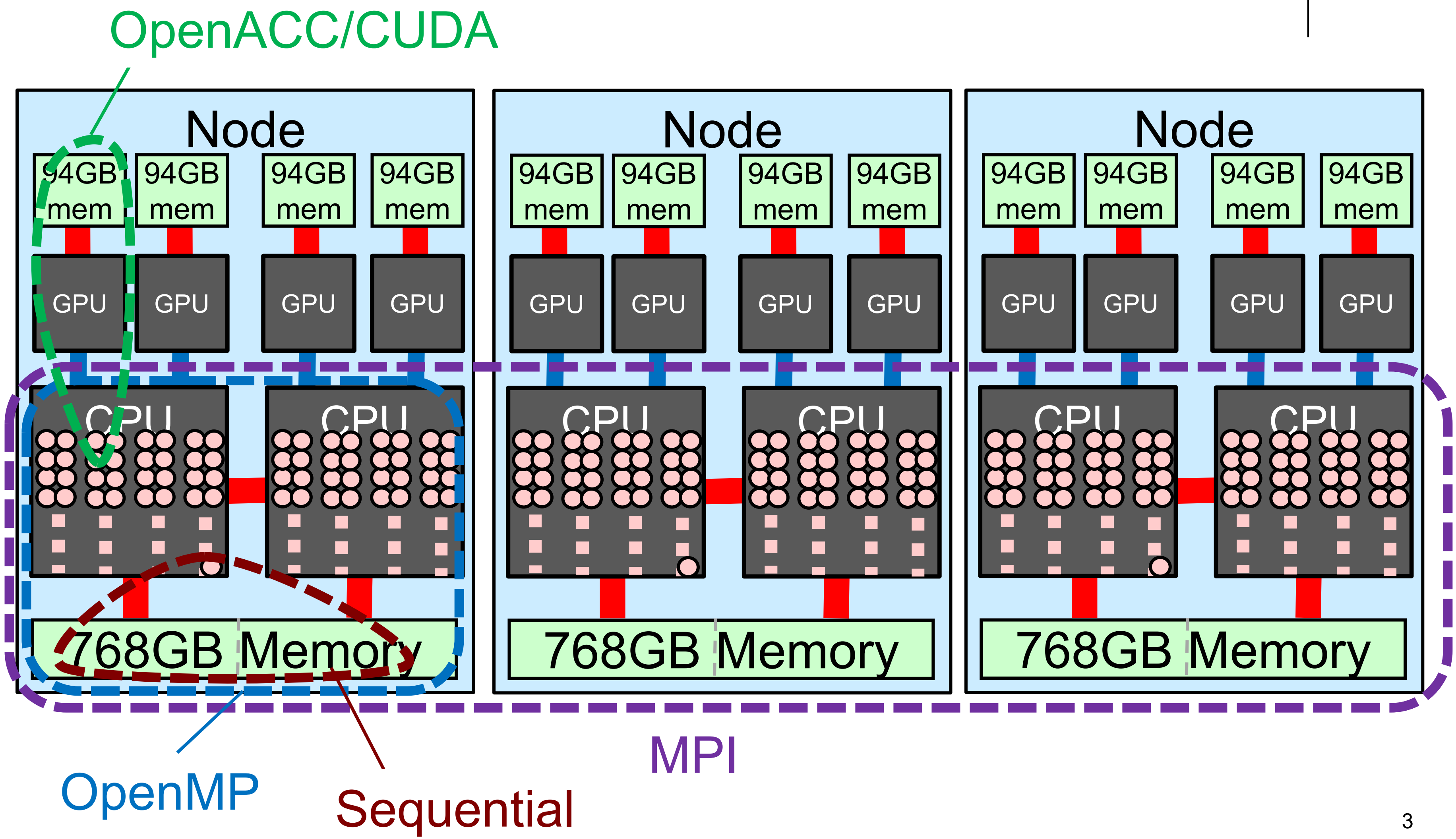
Overview of This Course

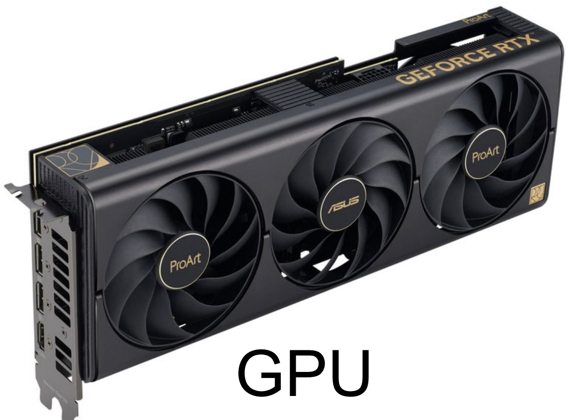
- Part 0: Introduction
    - 2 classes
- Part 1: OpenMP for shared memory programming
    - 4 classes
- Part 2: GPU programming
    - 4 classes ← We are here (1/4)
    - OpenACC (1.5 classes) and CUDA (2.5 classes)
- Part 3: MPI for distributed memory programming
    - 3 classes

Parallel Programming Methods on TSUBAME

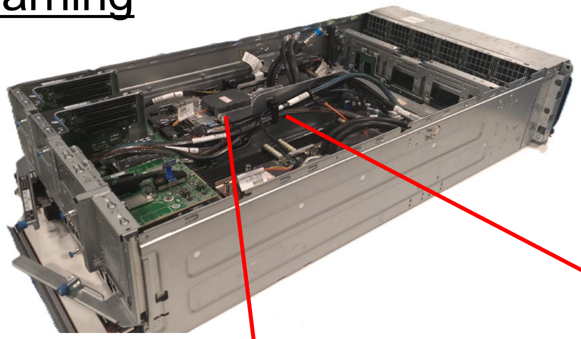


GPU Computing

- Graphic processing units (GPU) have been originally used for computing graphics (including video games)
- A high performance GPU has many cores
  - CPU: 2 to 32 cores. GPU: >1000 cores
  - The concept is called GPGPU (General-Purpose computing on GPU)
- GPGPU became popular since NVIDIA invented CUDA language in 2007
  - Recently it is popular for deep learning

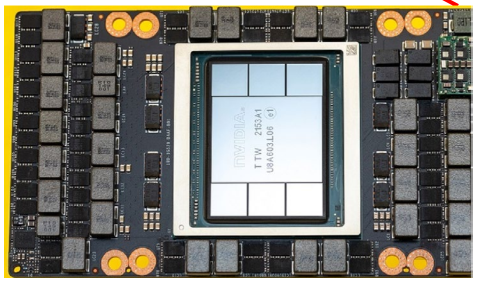


GPU
(for gaming PC)

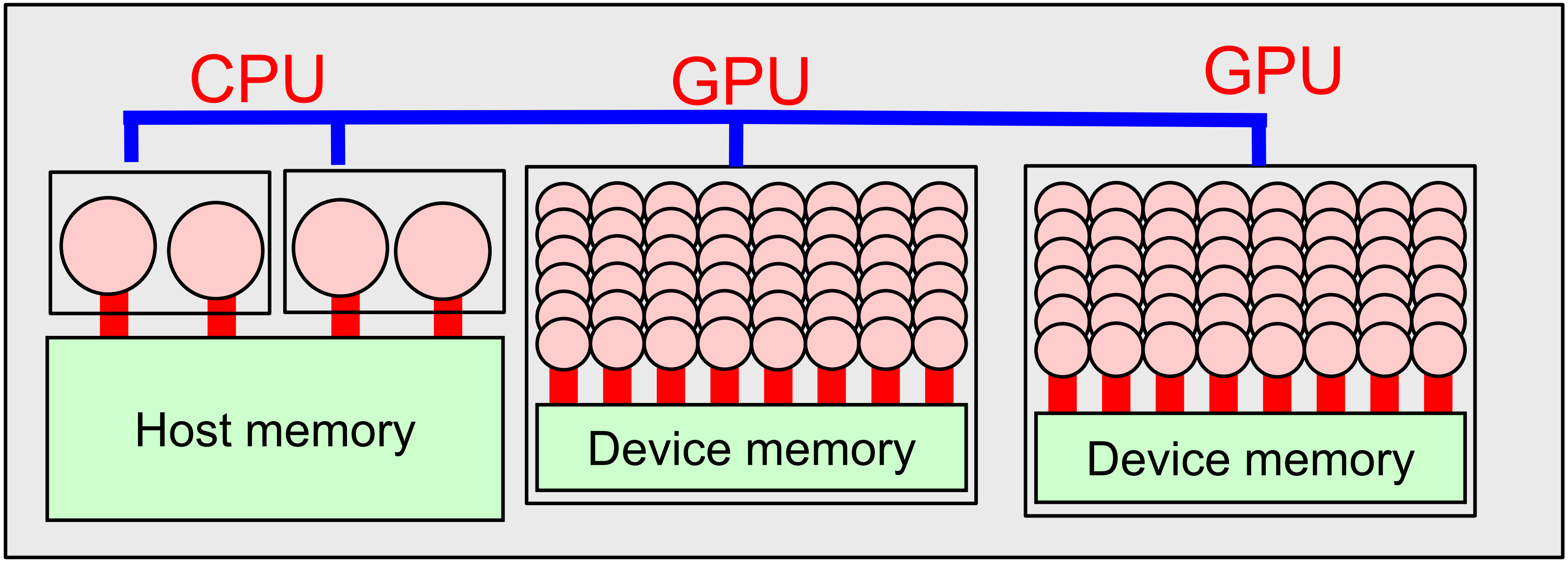


TSUBAME4
node

GPU



A Compute Node with GPU



- A GPU has its distinct memory (device memory)
  - CPU memory is called host memory
- Many cores in a GPU share its device memory
- If there are multiple GPUs, each has its device memory

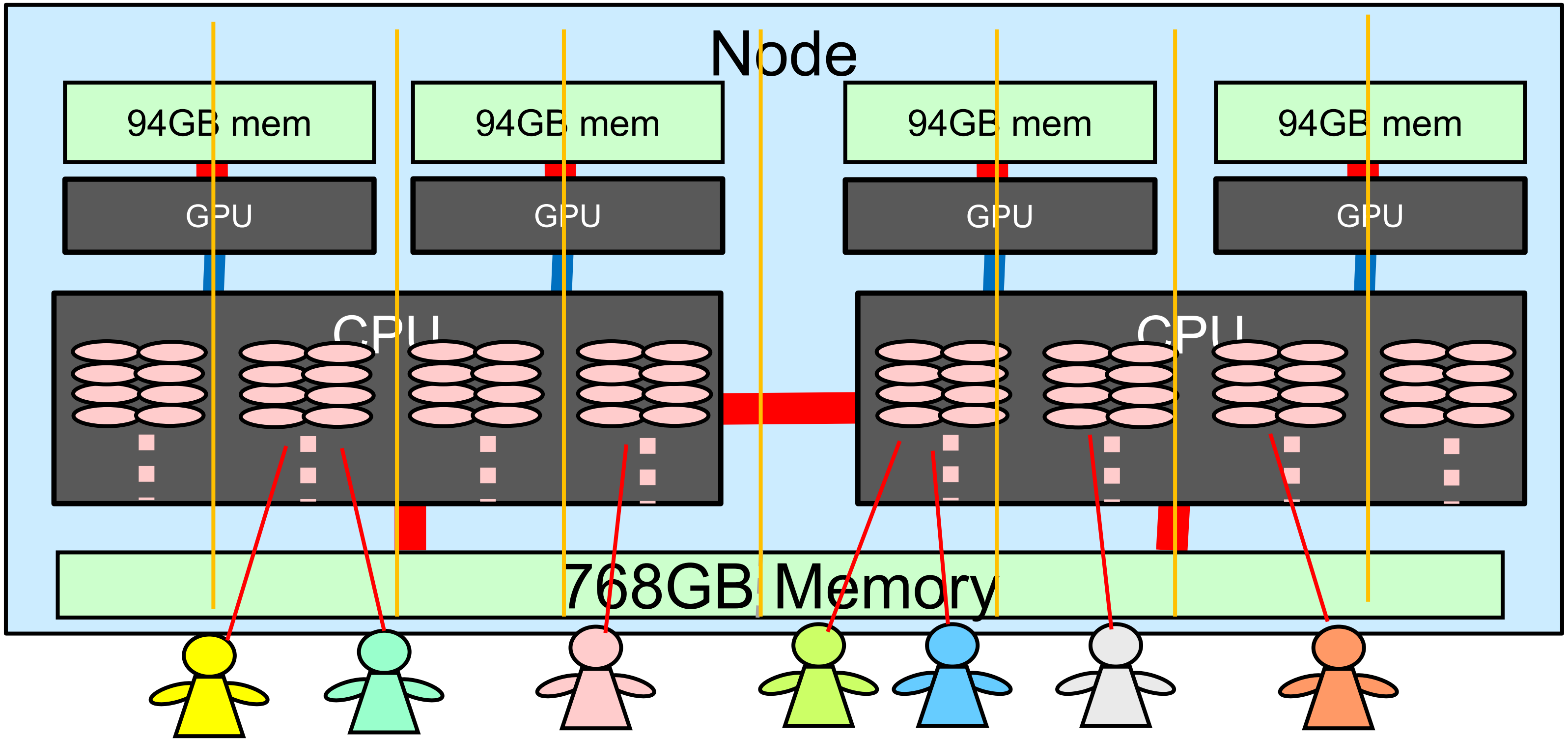
Characteristics of GPUs

A GPU is a board or a card attached to computers
→ It cannot work alone. Driven by CPUs
→ Different programming methods

Comparing EPYC 9654 (TSUBAME4's CPU) and
Tesla H100-94GB (TSUBAME4's GPU)

	1 CPU		1 GPU
Number of cores	96 cores (192 cores with 2CPUs)	<<<	16,896 CUDA cores (=128 x 132SMXs)
Clock Frequency	3.55GHz (with boost)	>	1.98GHz
Peak Computation Speed (double precision)	5.45TFlops	<<	66.9TFlops
Memory Capacity	384GB (768GB shared by 2CPUs)	>	94GB

Notes on TSUBAME Interactive Node



In an interactive node, each user uses 0.5 GPU

- 7,680 CUDA cores (128x60SMs), ~46GB memory

If you want use “a full GPU”, you may try “qsub” (described later)

Programming Environments for NVIDIA GPUs

- CUDA 🡐 We will use after OpenACC
  - The most famous environment, designed by NVIDIA
  - C/Fortran + new syntaxes
  - Use “nvcc” command for compile
    - module load cuda
    - nvcc … XXX.cu
  - For more general programs than OpenACC ☺
- OpenACC 🡐 Today’s topic
  - C/Fortran + directives (#pragma acc …), Easier programming ☺
  - Supported by NVIDIA HPC SDK
    - module load nvhpc
    - nvc -acc … XXX.c
  - For parallel programs with for-loops
- OpenMP 5, OpenCL…

An OpenACC Program Looks Like

C/C++/Fortran + directives

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

Examples of OpenACC *directives*

In this case, each directive has an effect on the following block/sentence

OpenACC is not so popular as OpenMP, unfortunately☹
- gcc’s support is not so good
- On TSUBAME4, we use NVIDIA HPC SDK

OpenACC Version of “mm” sample

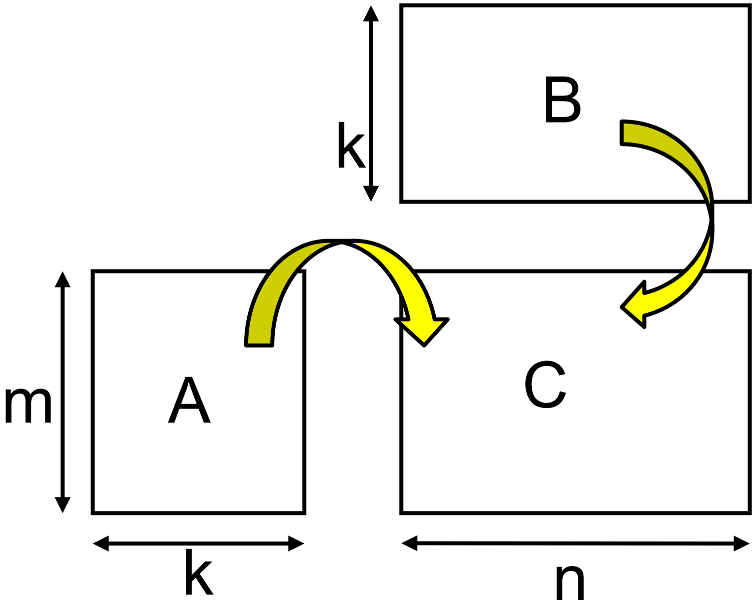
Available at /gs/bs/tga-ppcomp/24/mm-acc/

A: a (m × k) matrix, B: a (k × n) matrix

C: a (m × n) matrix

C ← A × B

- Algorithm with a triply-nested for-loop
- Supports variable matrix size.
  - Each matrix is expressed as a 1D array by *column-major* format



- Execution: ./mm [m] [n] [k]

Using mm-acc Sample

```
[make sure that you are at a interactive node (rXn11) ]
module load nvhpc    [Do once after login]
cd ~/ppc24
cp -r /gs/bs/tga-ppcomp/24/mm-acc  .
cd mm-acc
make
[You will see some messages, and an executable file
"mm" is created]
./mm 2000 2000 2000
```

Notes on Compiling OpenACC Programs

- NVIDIA HPC SDK on TSUBAME4.0
  - module load nvhpc, and then use nvc command
  - Use -acc option in compiling and linking
  - -Minfo=accel option outputs many information on parallelization

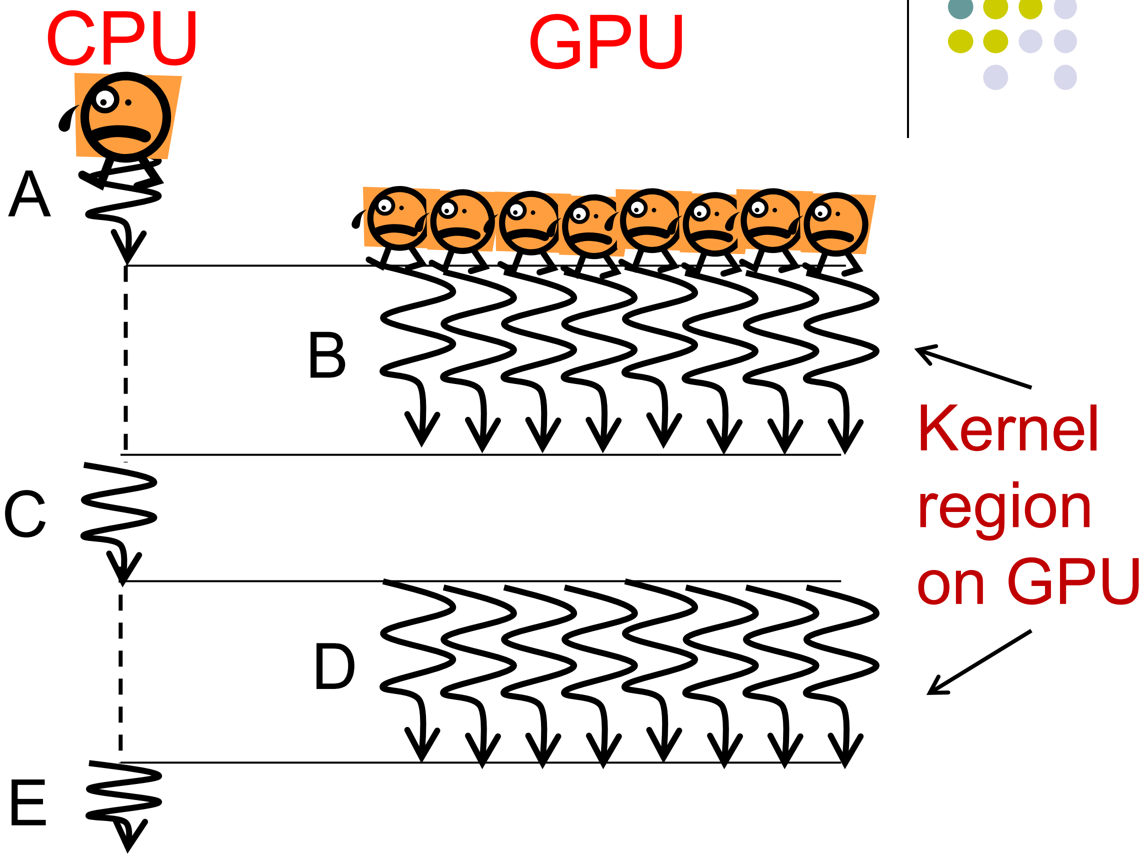
Example of output

```
          :
   26, Generating copyin(A[:m*k])
       Generating copy(C[:m*n])
       Generating copyin(B[:k*n])
       Loop is parallelizable
          :
```

They are not errors ☺

Kernel Region in OpenACC

```
int main()
{
    A;
#pragma acc kernels
    {
          B;
    }
    C;
#pragma acc kernels
    D;
    E;
}
```



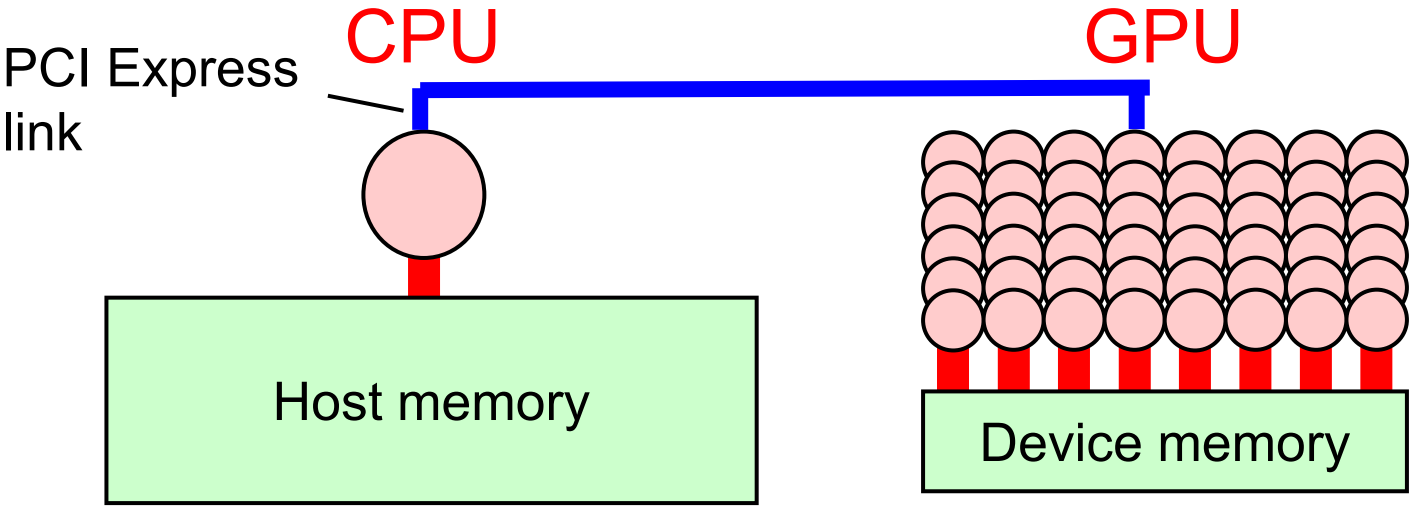
Kernel region on GPU

A sentence/block immediately after #pragma acc kernels is called a kernel region, executed on GPU

- We don't need to specify number of threads (it is hard to specify explicitly)

Data Movement between CPU and GPU

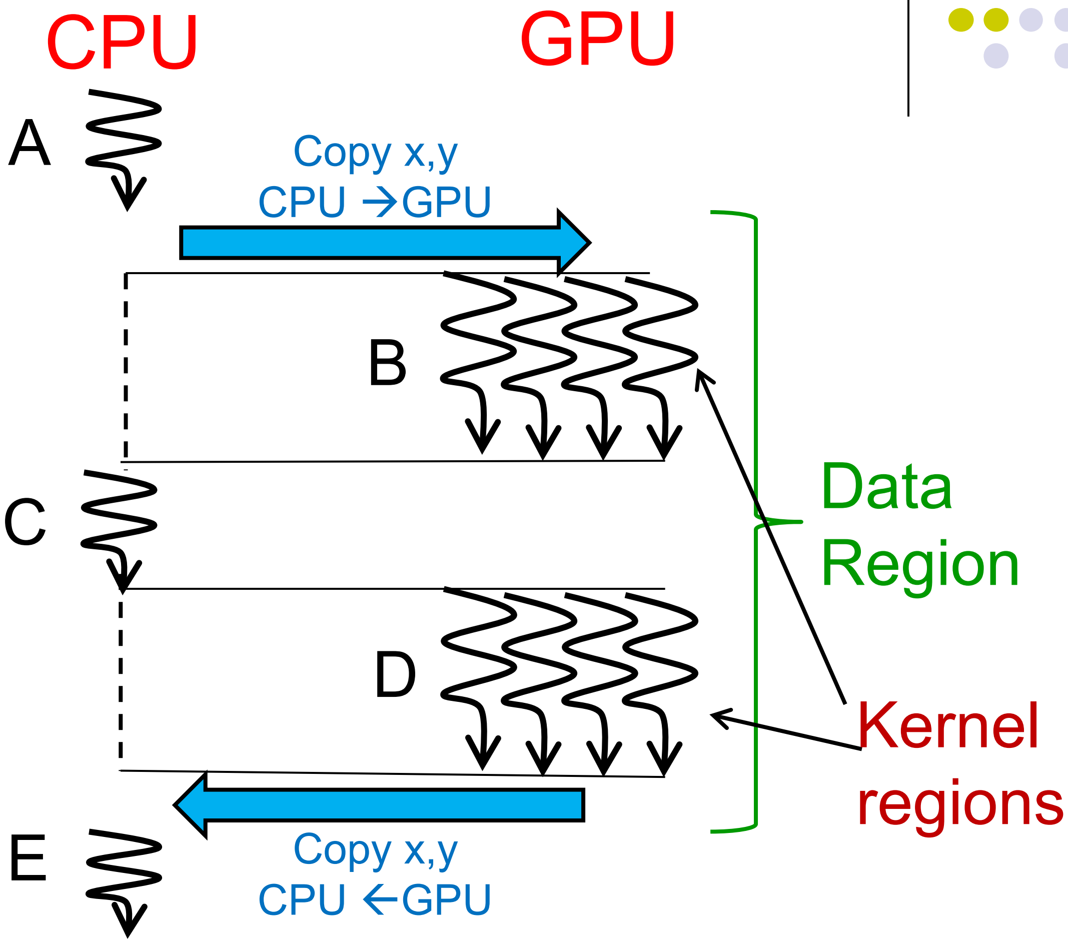
- We need to move data between CPU and GPU
  - Host (CPU) memory and Device (GPU) memory are distinct, like distributed memory
  - Threads on a GPU share the device memory



For this purpose, we use #pragma acc data directive
→ This defines a data region

Data Directives to use GPU memory

```
int main()
{
    A;
#pragma acc data copy(x,y)
    {
#pragma acc kernels
       {
          B;
       }
       C;
#pragma acc kernels
       D;
    }
    E;
}
```



- Data region may contain 1 or more kernel regions
- Data movement occurs at beginning and end of data region

Data Directive (1)

- Arrays (like a):
  - we can write array names if the sizes are statically declared → entire array is copied
- Pointers as arrays (like b):

  cf) b [0 : 20]

  start index number of elements

  - Partial copying like b[10:5] or a[4:4] work
- Scalar variables (like x):
  - You can omit copy(x) ➔ The compiler detects automatically ☺

```
    int x;
    float a[10];
    double *b = (double*)
         malloc(20*sizeof(double));
          :
#pragma acc data copy(x, a, b[0:20])
          :
```

Same meaning

```
#pragma acc data copy(a[0:10], b[0:20])
```

Data Directive (2)

- Directions of copying
  - … data copyin(…): Copy CPU→GPU at the begininng
  - … data copyout(…): Copy GPU→CPU at the end
  - … data copy(…): Do both

  Optimization of data movement will help speedup

Loop Directive

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

- #pragma acc loop must be included in "acc kernels" or "acc parallel"
- Directly followed by "for" loop
  - The loop must have a loop counter, as in OpenMP
  - List/tree traversal is NG

- … loop independent: Iterations are done in parallel by multiple GPU threads
- … loop seq: Done sequentially. Not be parallelized
- … loop: Compiler decides

OpenACC Version of mm (mm-acc/mm.c)

```
#pragma acc data copyin(A[0:m*k],B[0:k*n]),copy(C[0:m*n])
#pragma acc kernels
#pragma acc loop independent
  for (j = 0; j < n; j++) {
#pragma acc loop seq
    for (l = 0; l < k; l++) {
#pragma acc loop independent
      for (i = 0; i < m; i++) {
        Ci,j += Ai,l * Bl,j;
      } } }
```

We can omit GPU➔CPU copy of A,B

←For each column in C

←For dot product

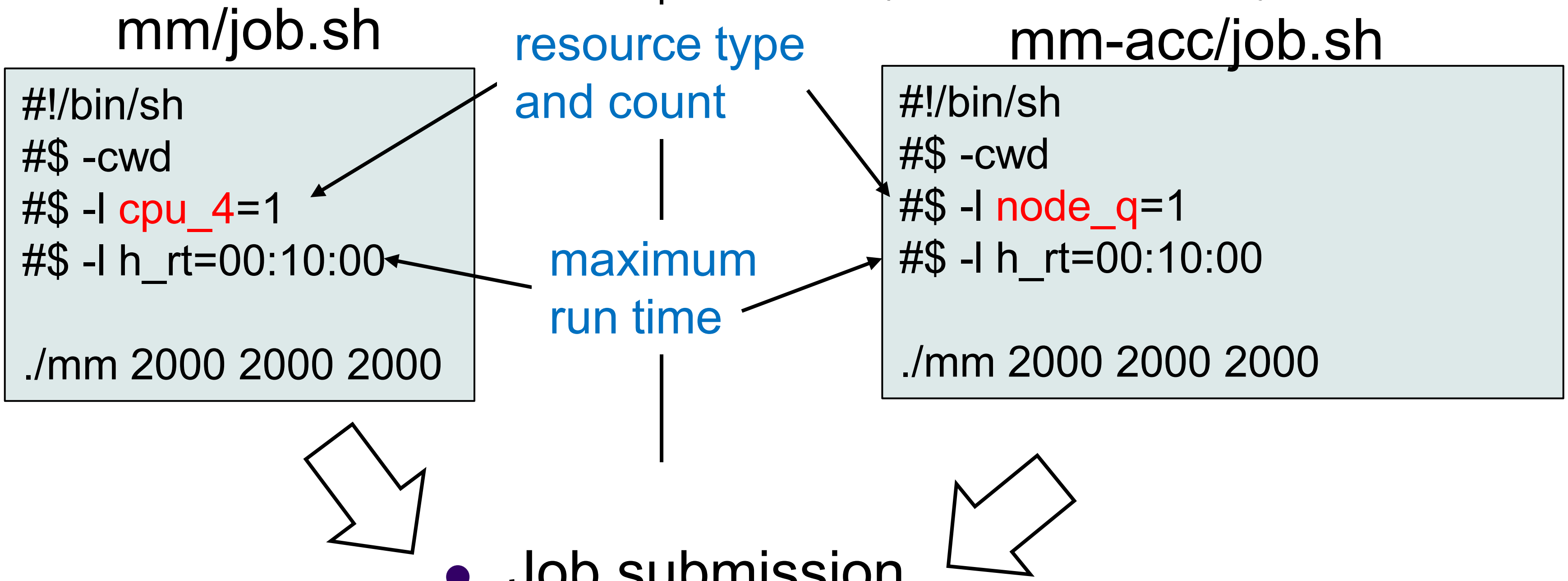
←For each row in C

- Each element in C can be computed in parallel (i-loop, j-loop)
- Computation of a single C element is sequential (l-loop)

Submitting a GPU Job to the Job Scheduler

- Sequential version
  - see mm directory

- OpenACC version
  - see mm-acc directory
  - To use a GPU, use node_q type
  - (node_h or node_f types for multi-GPU)



mm/job.sh

```
#!/bin/sh
#$ -cwd
#$ -l cpu_4=1
#$ -l h_rt=00:10:00

./mm 2000 2000 2000
```

resource type and count

maximum run time

mm-acc/job.sh

```
#!/bin/sh
#$ -cwd
#$ -l node_q=1
#$ -l h_rt=00:10:00

./mm 2000 2000 2000
```

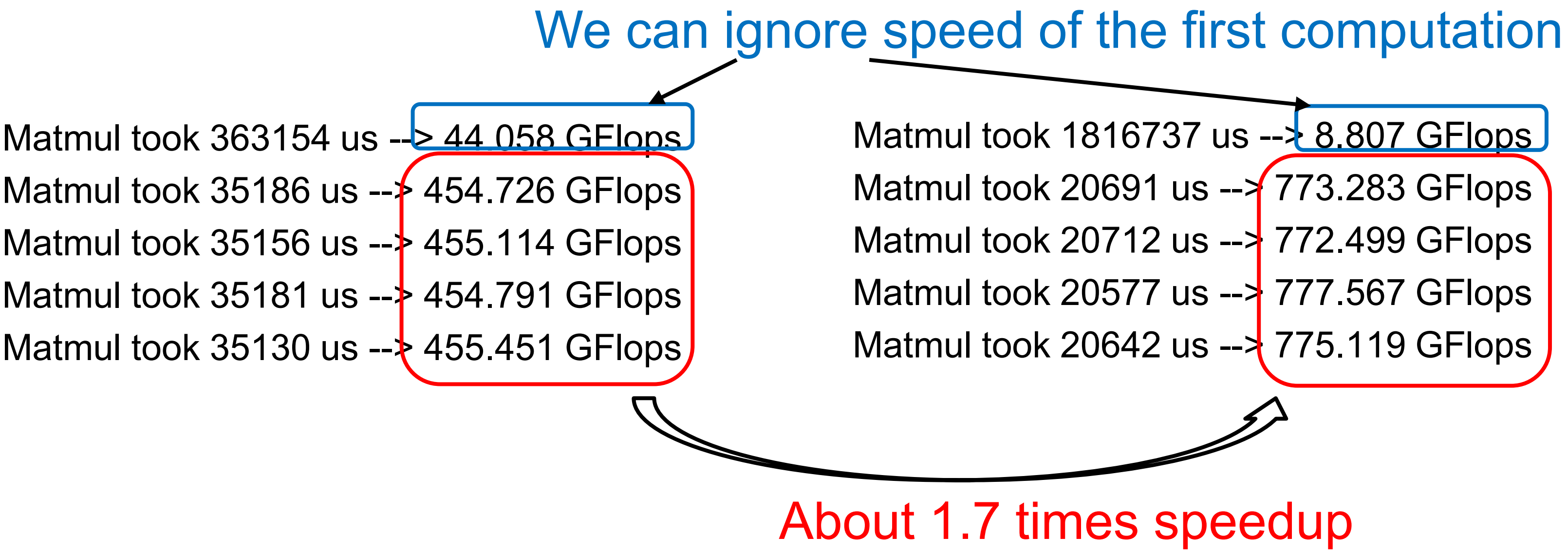
- Job submission
  - qsub job.sh

0.5 GPU vs 1 GPU

m=n=k=2000

Interactive node (0.5GPU)

node_q (1GPU)



We can ignore speed of the first computation

```
Matmul took 363154 us --> 44.058 GFlops
Matmul took 35186 us --> 454.726 GFlops
Matmul took 35156 us --> 455.114 GFlops
Matmul took 35181 us --> 454.791 GFlops
Matmul took 35130 us --> 455.451 GFlops
```

```
Matmul took 1816737 us --> 8.807 GFlops
Matmul took 20691 us --> 773.283 GFlops
Matmul took 20712 us --> 772.499 GFlops
Matmul took 20577 us --> 777.567 GFlops
Matmul took 20642 us --> 775.119 GFlops
```

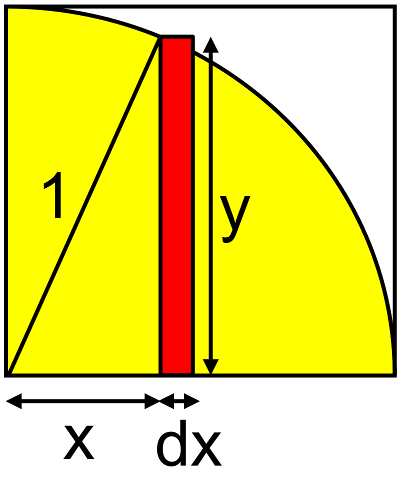
About 1.7 times speedup

The first computation suffers slowdown by initialization of GPU etc.
The similar slowdown also occurs in CPU programs

OpenACC version of “pi” sample

Estimate approximation of π (circumference/diameter) by approximation of integration

- Available at /gs/bs/tga-ppcomp/24/pi-acc/
- Method
  - Let SUM be approximation of the yellow area
  - 4 x SUM → π
- Execution：./pi [n]
  - n: Number of division
  - Cf) ./pi 100000000
- Compute complexity：O(n)



dx = 1/n
y = sqrt(1-x*x)

Algorithm of “pi”

OpenMP

```
double pi(int n) {
    int i;
    double sum = 0.0;
    double dx = 1.0 / (double)n;

#pragma omp parallel
#pragma omp for reduction(+:sum)
    for (i = 0; i < n; i++) {
        double x = (double)i * dx;
        double y = sqrt(1.0 - x*x);
        sum += dx*y;
    }

    return 4.0*sum; }
```

OpenACC

```
double pi(int n) {
    int i;
    double sum = 0.0;
    double dx = 1.0 / (double)n;

#pragma acc kernels
#pragma acc loop independent reduction(+:sum)
    for (i = 0; i < n; i++) {
        double x = (double)i * dx;
        double y = sqrt(1.0 - x*x);
        sum += dx*y;
    }

    return 4.0*sum; }
```

※ For scalar variables, “data copy” is omitted

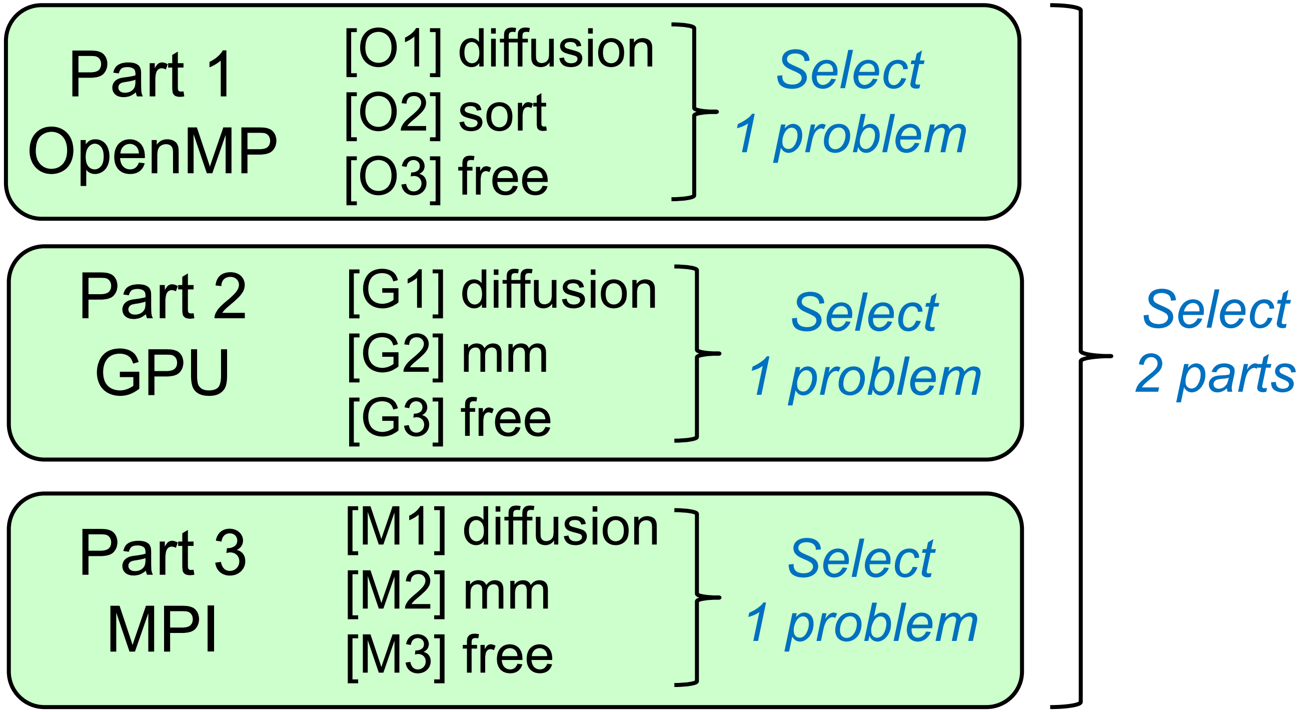
Notes on Number of Threads

- In OpenMP, the number of threads is set by OMP_NUM_THREADS
- In OpenACC, the number is automatically determined per loop

- In OpenMP, thread ID is obtained by omp_get_thread_num()
- In OpenACC, we cannot see thread ID

Assignments in this Course

- There is homework for each part. Submissions of reports for 2 parts are required



Part 1
OpenMP

[O1] diffusion
[O2] sort
[O3] free

Select 1 problem

Part 2
GPU

[G1] diffusion
[G2] mm
[G3] free

Select 1 problem

Part 3
MPI

[M1] diffusion
[M2] mm
[M3] free

Select 1 problem

Select 2 parts

Assignments in GPU Part (1)

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

Due date: May 30 (Thursday)

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

- You can use Makefile in /gs/bs/tga-ppcomp/24/diffusion-acc/ or /gs/bs/tga-ppcomp/24/diffusion-cuda/

Optional:

- To make array sizes variable parameters
- To compare OpenACC vs CUDA
- To improve performance further
  - Different assignment of threads and elements (CUDA), etc

Assignments in GPU Part(2)

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

mm-acc: /gs/bs/tga-ppcomp/24/mm-acc/

mm-cuda: /gs/bs/tga-ppcomp/24/mm-cuda/

- Use various matrices sizes
- Evaluate effects of data transfer cost
- Compare with CPU (OpenMP) version

Optional :

- To use different loop orders
- To evaluate both mm-acc and mm-cuda
- To change/improve the program
  - Different assignment of threads and elements (CUDA) etc

Assignments in GPU Part (3)

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

- cf) A problem related to your research
- “sort” sample on GPU?
  - The quick sort may be hard on GPU (There is no “task” syntax)
  - → Bitonic sort?
- More challenging one for parallelization is better
  - cf) Partial computations have dependency with each other

Notes in Report Submission (1)

- Submit the followings via T2SCHOLA

  (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
  - In Part 2, describe which you used, OpenACC or CUDA?
- How you parallelized
  - It is even better if you mention efforts for high performance or new functions
- 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

Next Class:

- GPU Programming (2)
  - OpenACC
    - Improving data copy
    - Improving loop parallelization
  - Introduction of CUDA

- Schedule
  - Mon, May 6: No classes (national holiday)
  - Thu, May 9: GPU (2)
  - Mon, May 13: GPU (3)
  - Thu, May 16: No classes (cancelled/休講)