2020
Practical Parallel Computing
(実践的並列コンピューティング)
No. 2

Introduction (2)
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Overview of This Course

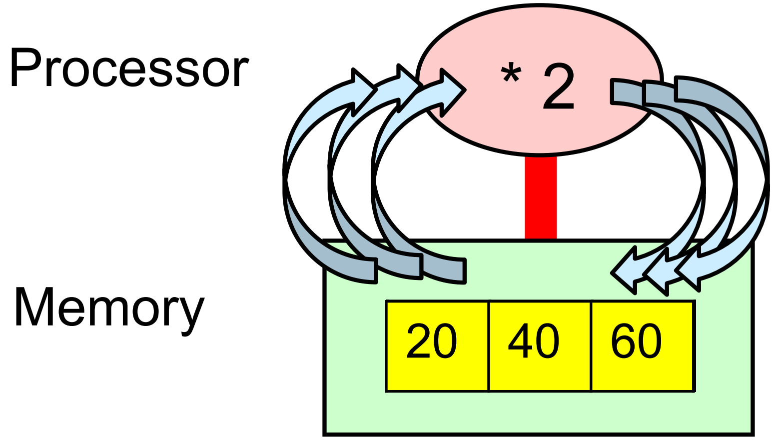
- Part 0: Introduction
  - 2 classes ← We are here (2/2)
- Part 1: OpenMP for shared memory programming
  - 4 classes
- Part 2: GPU programming
  - OpenACC and CUDA
  - 4 classes
- Part 3: MPI for distributed memory programming
  - 3 classes

Computation on Computer Architecture

- Computation (Software) = Algorithm + Data
- Architecture (Hardware) = Processor + Memory

Note: This is so simplified discussion

Computer Architecture



Computation Example

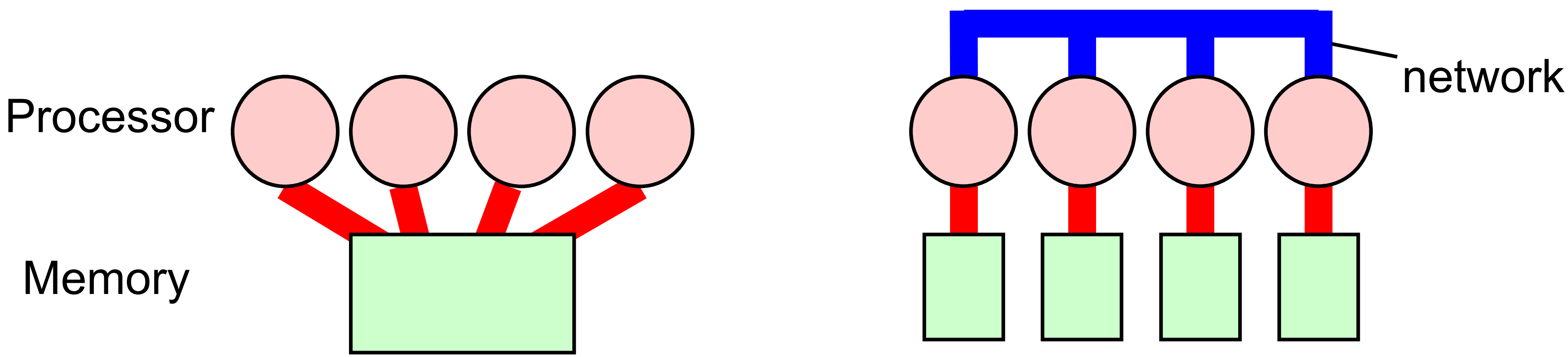
```
int a[3] = {10, 20, 30};
int i;

for (i = 0; i < 3; i++) {
   a[i] = a[i] *2;
}
```

What is Parallel Architecture?

- Parallel architecture has MULTIPLE components
- Two basic types:

Shared memory parallel architecture

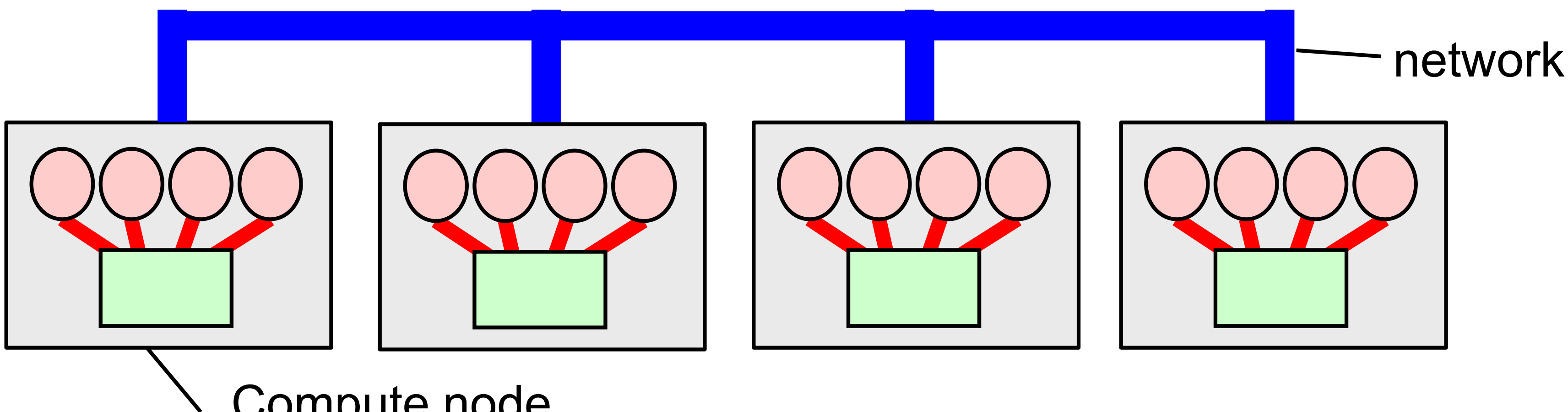
Distributed memory parallel architecture



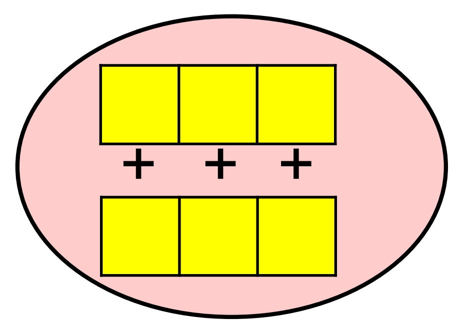
- Different programming methods are used for different architecture

Modern SCs use Both!

Modern SCs are combination of "shared" and "distributed"
"shared memory" in a node
"distributed memory" among nodes, connected by network

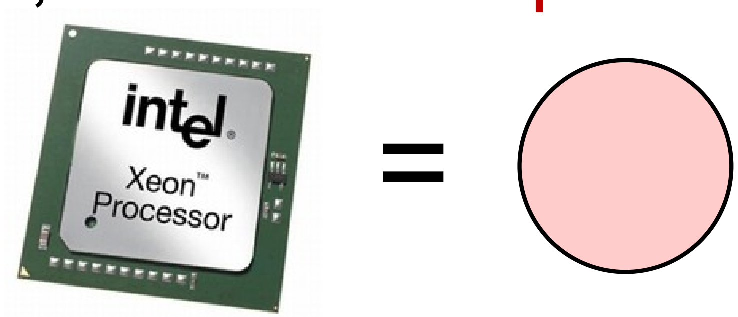


※ Moreover, each processor (core) may have *SIMD parallelism* , such as SSE, AVX…
A processor (core) can do several computations at once
SIMD is out of scope of this class

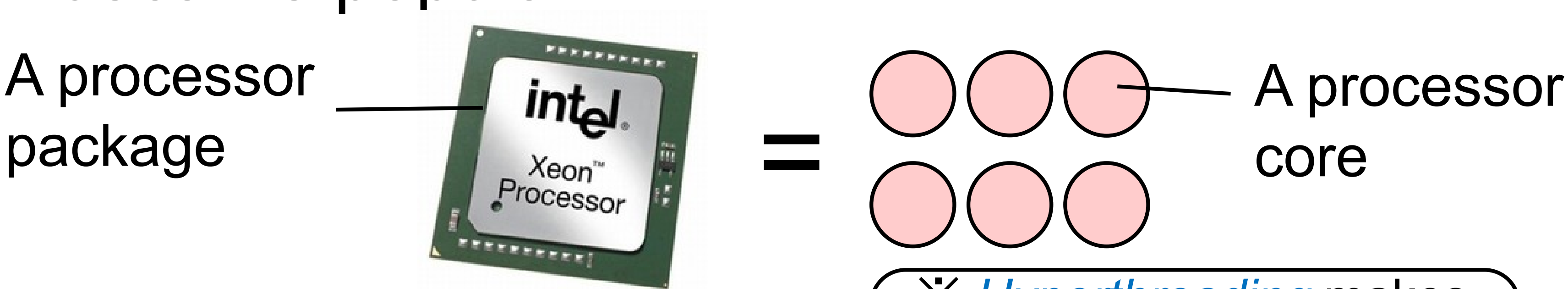


(Confusing) Terminology

- In old days, definition of "processor" was simple



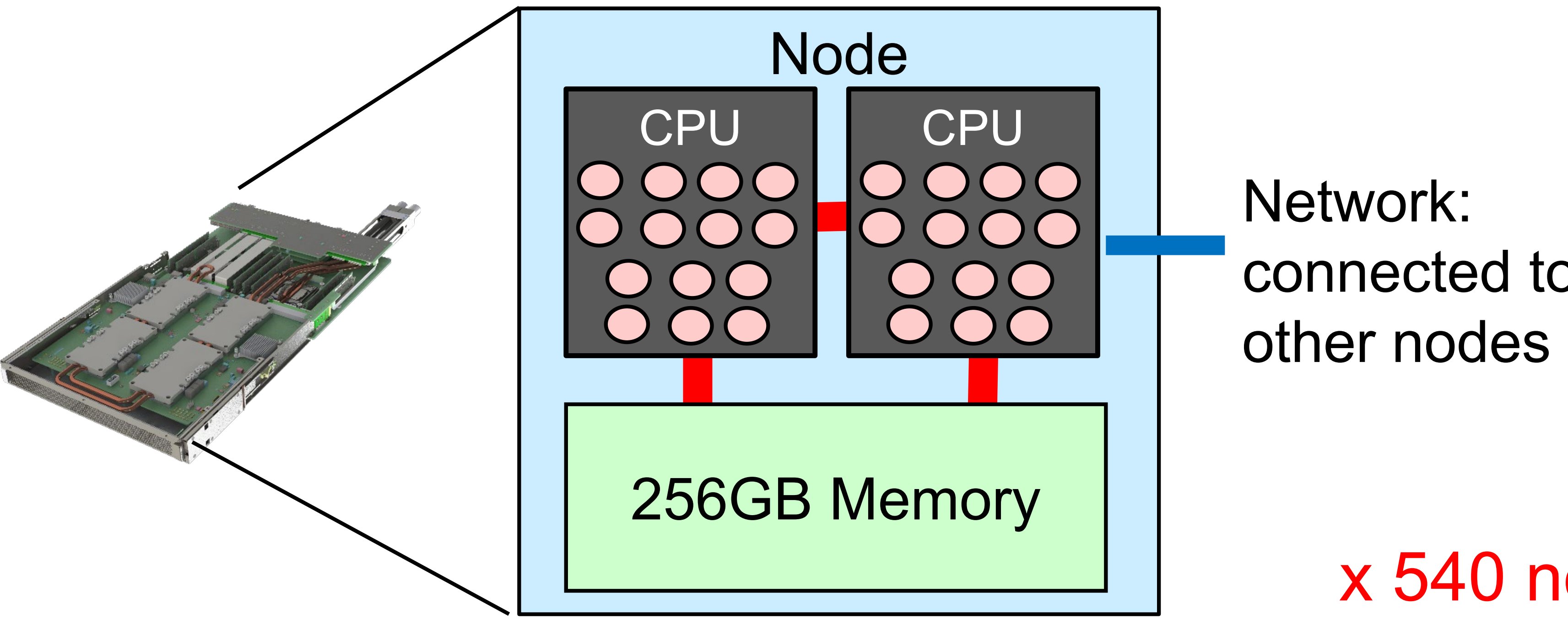
- Since around 2005, "multicore processor" became popular



※ *Hyperthreading* makes discussion more complex, but skipped

A TSUBAME3 Node

- 2 processor packages (CPU) × 14 cores
  - 28 cores share memory

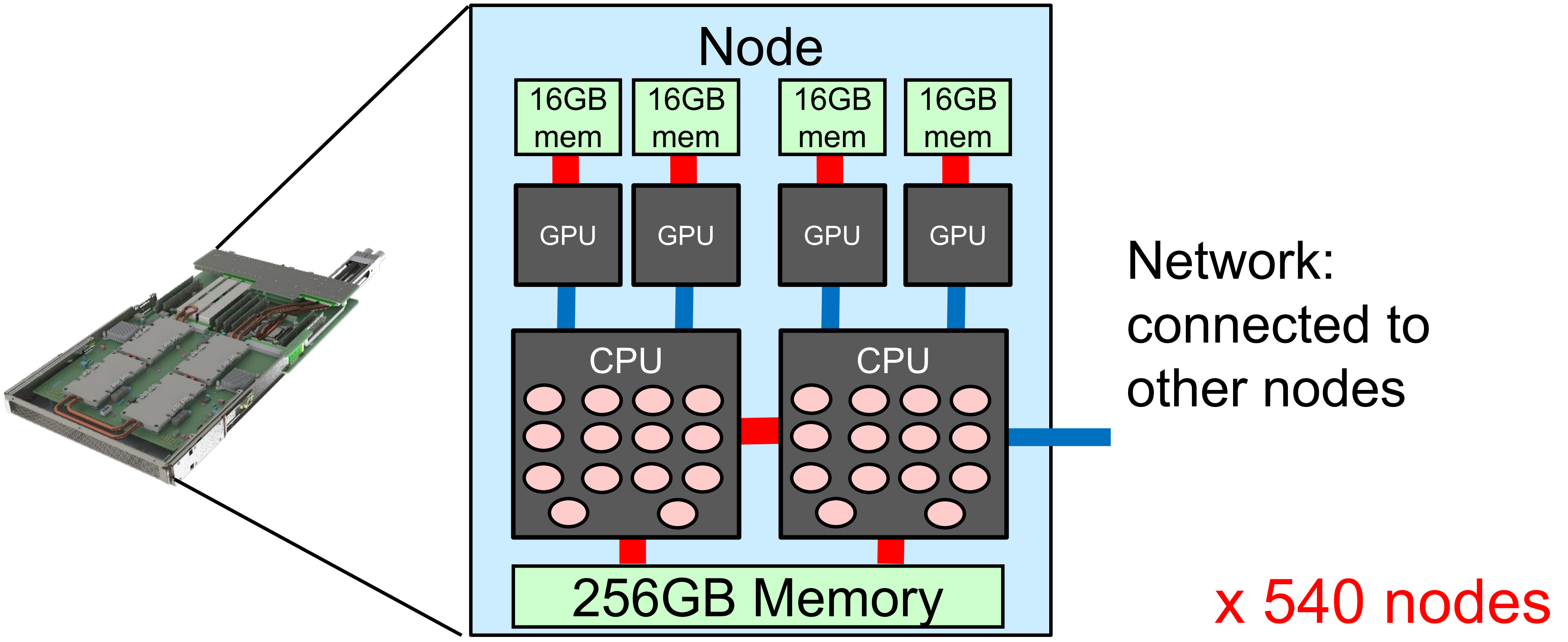


x 540 nodes

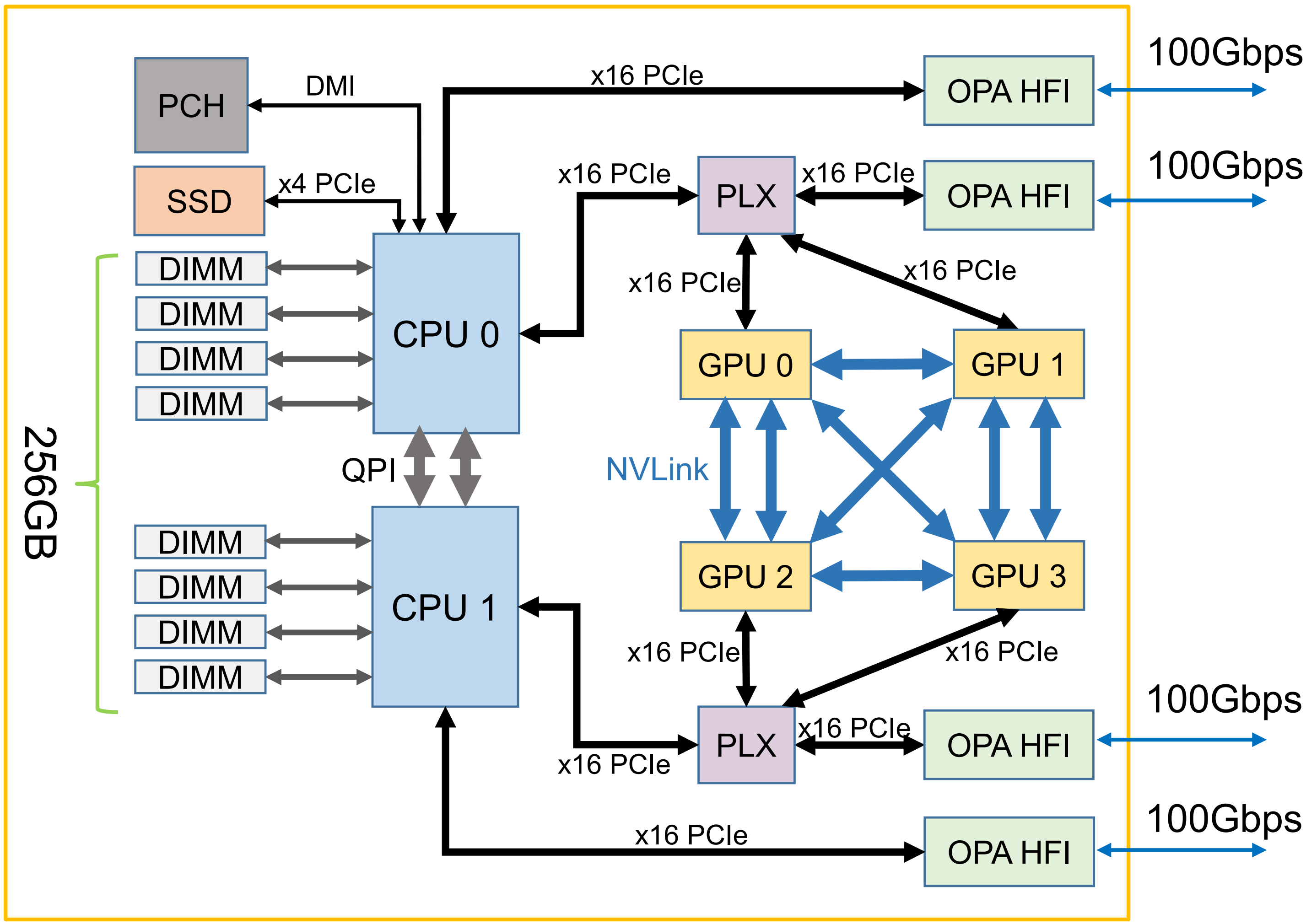
- GPUs are (still) omitted in this figure

A TSUBAME3 Node with GPUs

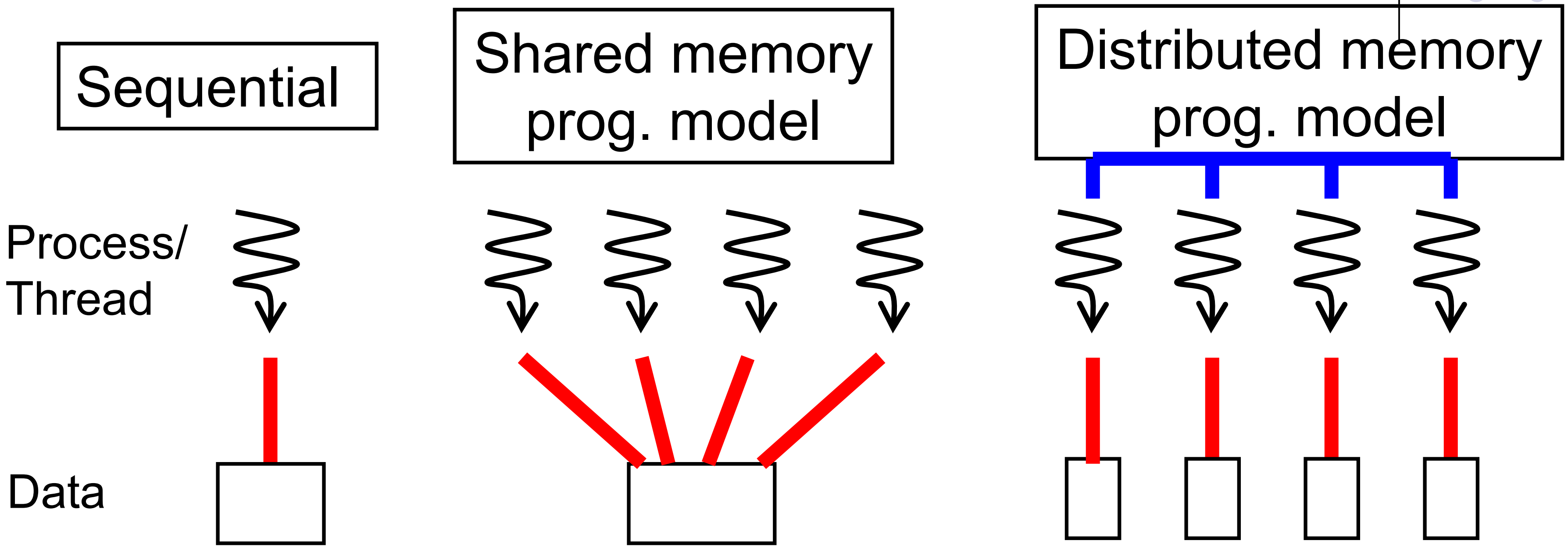
- A node has 2 CPUs + 4 GPUs
  - Each GPU (Tesla P100) has 3,584 cores



A TSUBAME3 Node in More Detail

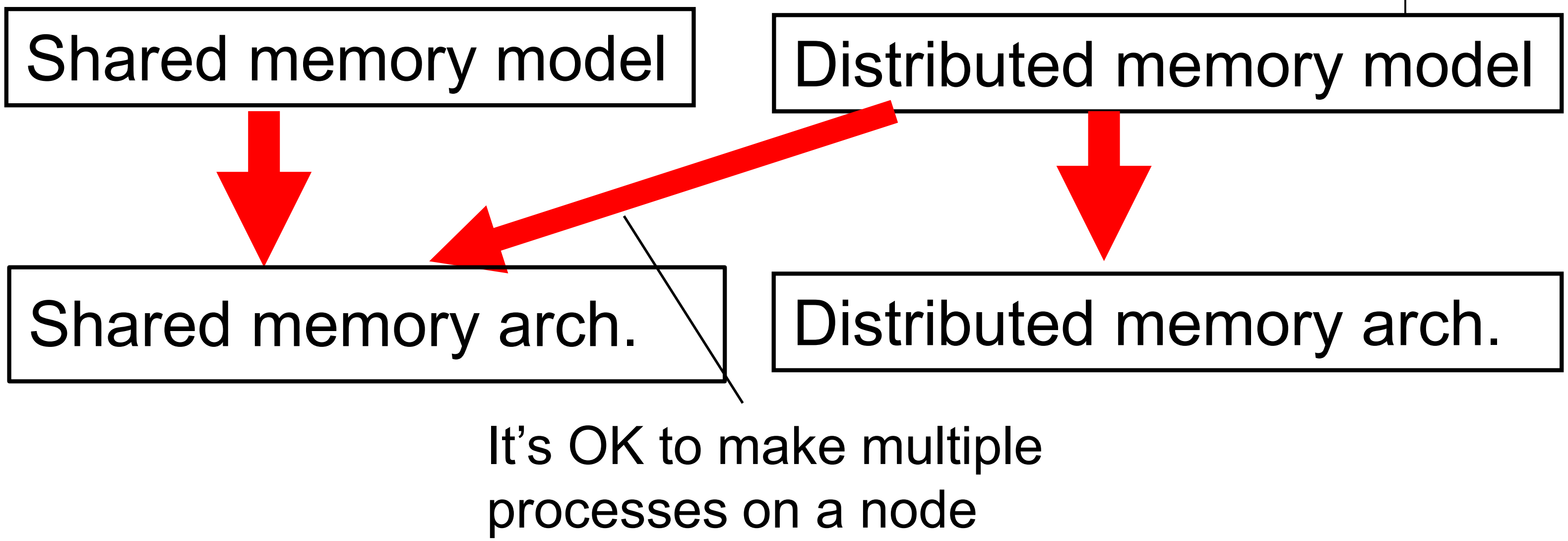


Classification of Parallel Programming Models



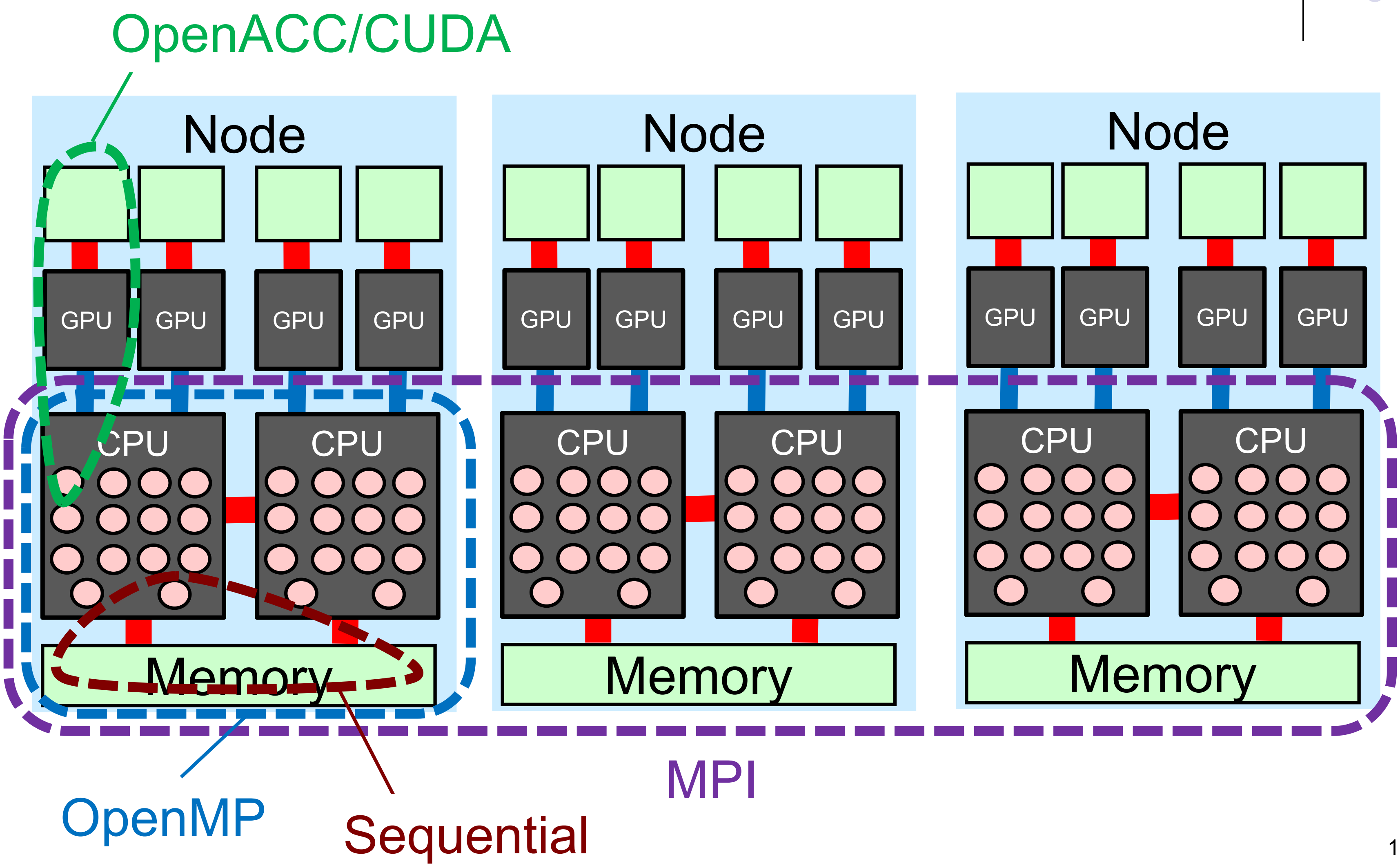
Sequential	Shared memory	Distributed memory
Programming without parallelsim	Threads have access to shared data • OpenMP • pthread • Java thread…	Need communication among processes • MPI • socket • Hadoop, Spark…

Programming Models on Architecture



- Shared memory model (Part 1) can use only cores in a single node (up to 28 cores on TSUBAME3)
- Distributed memory model (Part 3) supports large scale parallelism (~15,000 cores on TSUBAME3)

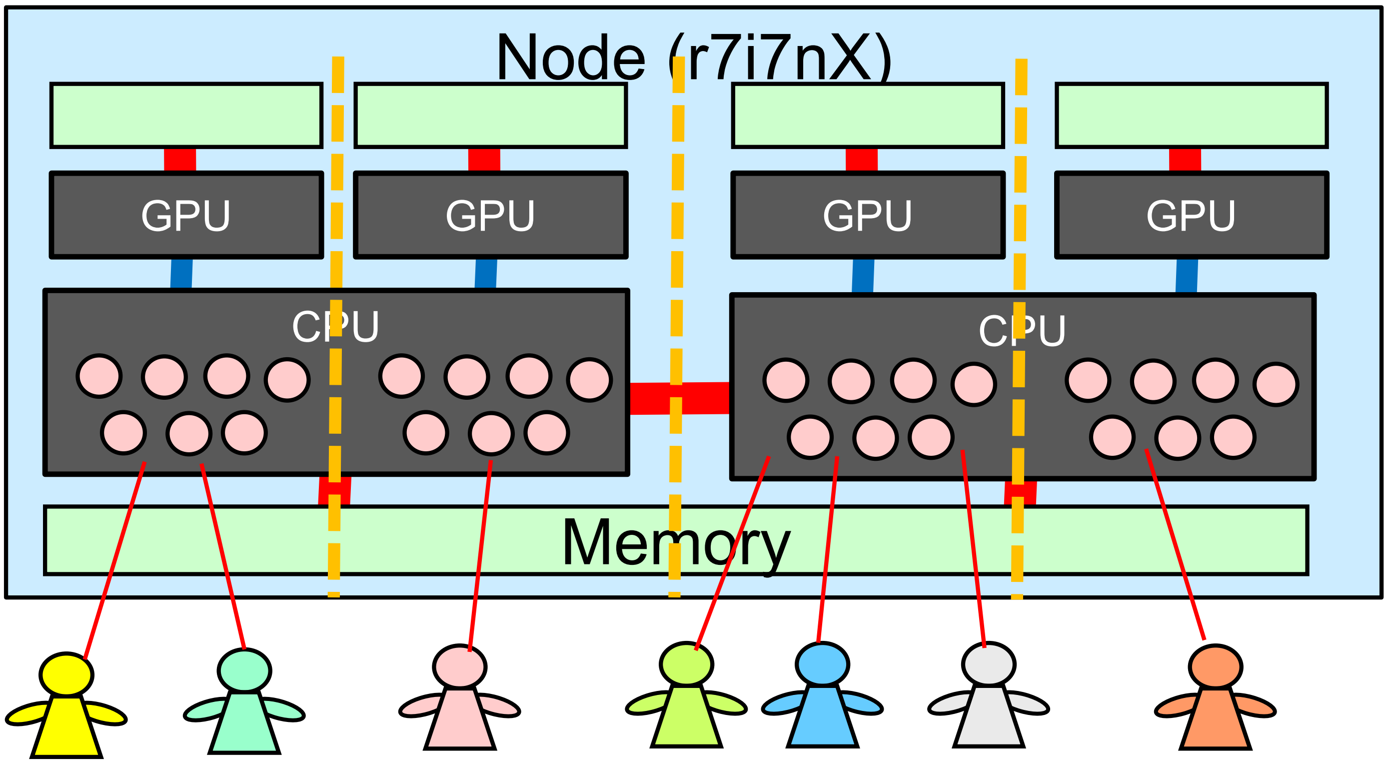
Parallel Programming Methods on TSUBAME



Standard route

Web-only route

TSUBAME Interactive Node



A node is partitioned into 4. Each user can use

- ¼ node = 7 CPU cores + 60GB memory + 1 GPU (3584cores+16GB mem)
- Only one partition simultaneously

A partition may be shared by several users → you may suffer from slow down

Sample Programs in this Lecture

- /gs/hs1/tga-ppcomp/20/ directory
  - You have to a member of tga-ppcomp group
  - There are sub-directories per sample
- Sequential sample programs
  - pi: approximation of pi (π)
  - mm: matrix multiplication
  - diffusion: simple simulation of diffusion phenomena
  - fib: Fibonacci number
  - sort: quick-sort sample

Using Sample Programs (1) Make Copies

- Samples in /gs/… are "*read-only*", so make copies of samples into somewhere in your home directory
  - Where is somewhere? If you are using web-only route, ~/t3workspace looks good
  - In the case of "mm" sample

```
[make sure that you are at a interactive node (r7i7nX) ]
cd ~/t3workspace    [In web-only route]
cp –r /gs/hs1/tga-ppcomp/20/mm .
cd mm
```

don't forget space & dot

Using Sample Programs (2) Executing mm

- In the case of “mm” sample

```
[make sure that you are at mm directory]
ls
[you will see 3 files of mm.c, Makefile, job.sh]
make
[this creates an executable file “mm”]
./mm 1000 1000 1000
[this is the execution of mm sample]
```

Using Sample Programs (3) Executing Samples

Before execution, please do “copy” and “make” for each sample

- mm

```
./mm 1000 1000 1000
```

Options are matrix sizes *m,n,k*

- pi

```
./pi 10000000
```

Option is number of samples *n*

- diffusion

```
./diffusion 20
```

Option is number of time steps *nt*

- fib

```
./fib 40
```

Option is sequence index *n*

- sort

```
./sort 10000000
```

Option is array length *n* to be sorted

“mm” sample: Matrix Multiply

Available at /gs/hs1/tga-ppcomp/20/mm/

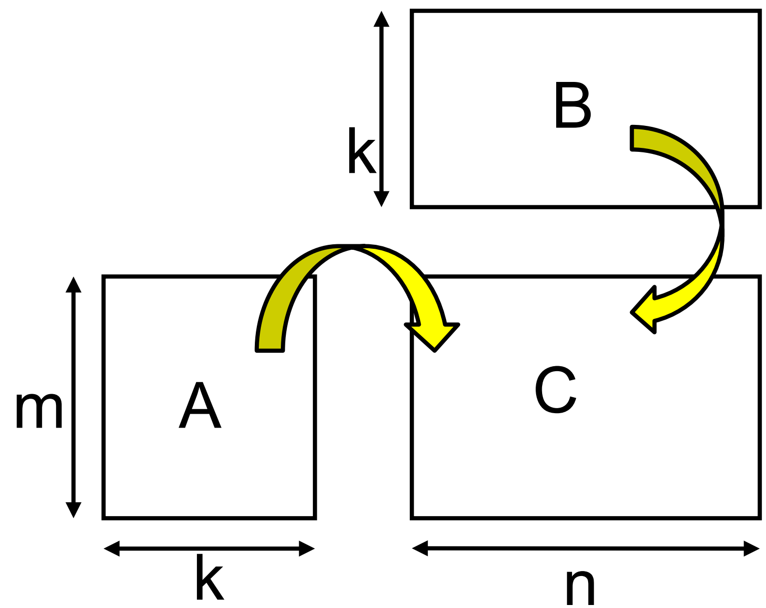
A: a ($m \times k$) matrix

B: a ($k \times n$) matrix

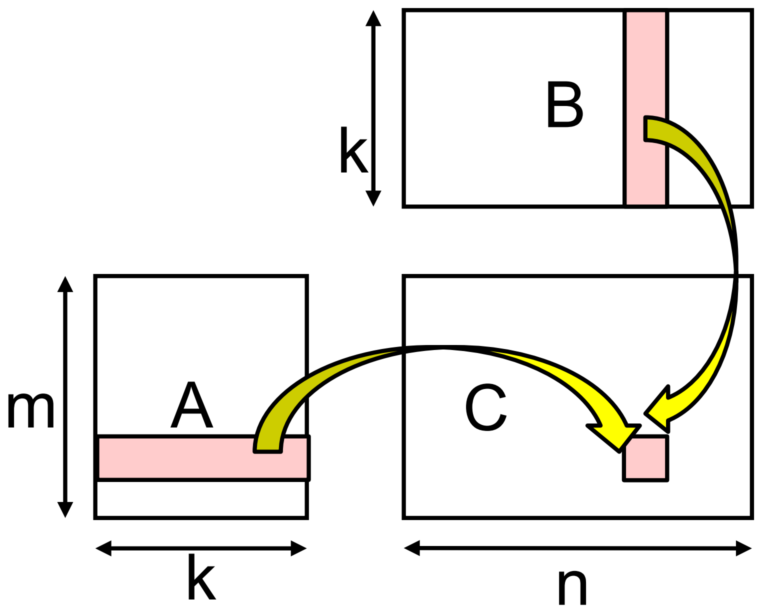
C: a ($m \times n$) matrix

$C \leftarrow A \ B$

- This sample supports variable matrix sizes
- Execution: ./mm [m] [n] [k]



Matrix Multiply Algorithm (1)



$C_{i,j}$ is defined as the dot product of

- A's i-th row
- B's j-th column

The algorithm uses triply-nested loop

```
for (i = 0; i < m; i++) {           ←For each row in C
  for (j = 0; j < n; j++) {         ←For each column in C
    for (l = 0; l < k; l++) {       ←For dot product
      Ci,j += Ai,l * Bl,j;
    } } }
```

Matrix Multiply Algorithm (2)

```
for (i = 0; i < m; i++) {           ←For each row in C
  for (j = 0; j < n; j++) {         ←For each column in C
    for (l = 0; l < k; l++) {       ←For dot product
      Ci,j += Ai,l * Bl,j;
    } } }
```

- The innermost statement is executed for *mnk* times
- Compute Complexity：O(mnk)
  - Computation speed (Flops) is obtained as 2mnk/t, where *t* is execution time

The innermost statement includes 2 (floating point) calculations: *, +

- [Q] What if loop order is changed?
  - Number of operations does not change. But how is the speed?

Variable Length Arrays in (Classical) C Language

- double C[n]; raises an error. How do we do?
- void *malloc(size_t size);

  ⇒ Allocates a memory region of *size* bytes from “heap region”, and returns its head pointer
- When it becomes unnecessary, it should be discarded with free() function

A fixed length array

```
double C[5];

… C[i] can be used …
```

A variable length array

```
double *C;
C = (double *)malloc(sizeof(double)*n);

… C[i] can be used …

free(C);
```

array length

※ Exceptionally, C99 specification includes variable length arrays

How We Do for Multiple Dimensional Arrays

double C[m][n]; raises an error. How do we do?

Not in a straightforward way. Instead, we do either of:

(1) Use a pointer of pointers

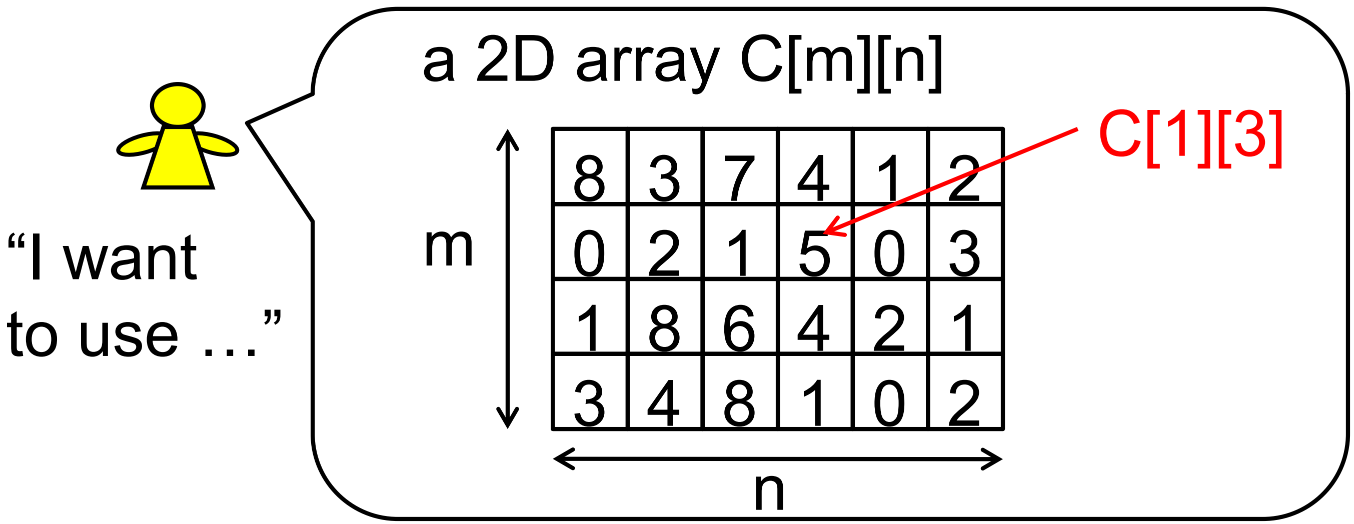
- We *malloc* m 1D arrays for every row (each has n length)
- We malloc 1D array of m length to store the above pointers

(2) Use a 1D array with length of $m \times n$

(mm sample uses this method)

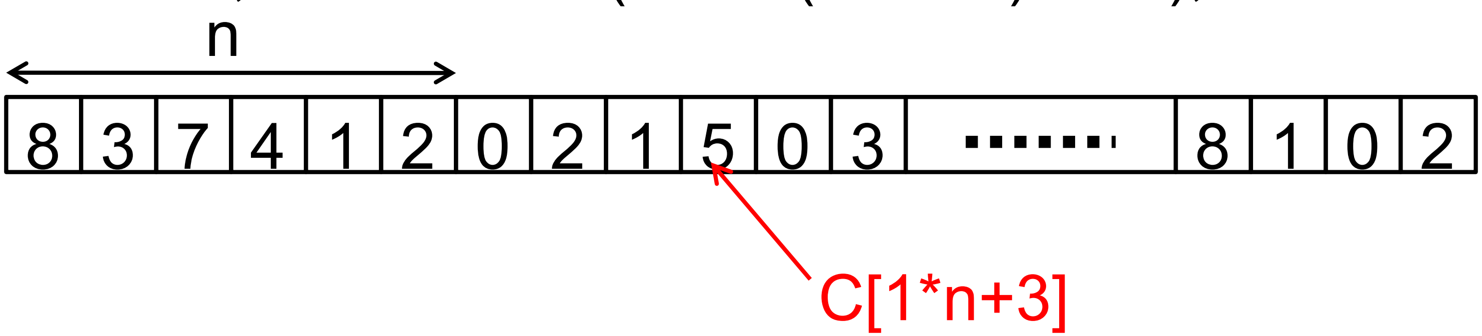
- To access an array element, we should use C[i*n+j] or C[i+j*m], instead of C[i][j]

Express a 2D array using a 1D array



Expressions in C language (Example)

double *C;   C = malloc(sizeof(double)*m*n);



In this case, an element $C_{i,j}$ is C[i*n+j]

Two Data Formats

Row major format

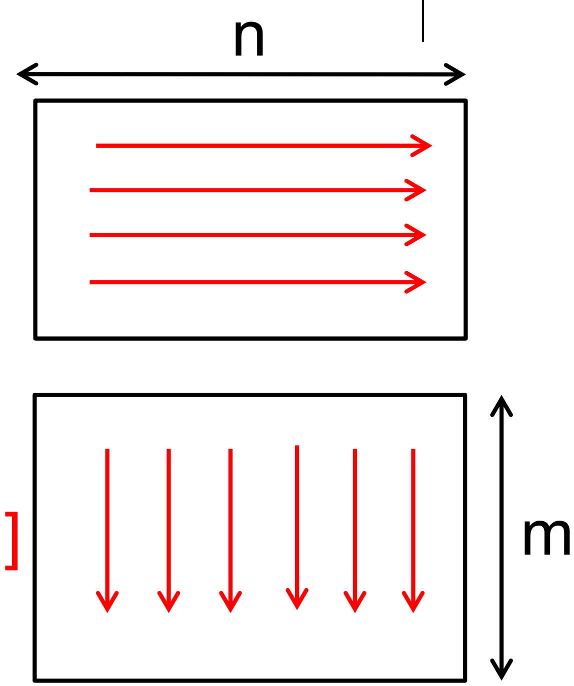
- More natural for C programmers

$C_{i,j} \Rightarrow C[i*n+j]$

Column major format

- BLAS library
- mm sample uses this

$C_{i,j} \Rightarrow C[i+j*m]$



- We have more choices for 3D, 4D… arrays

[Q] Does the format affect the execution speed?

Actual Codes in mm Sample

```
for (i = 0; i < m; i++) {
  for (j = 0; j < n; j++) {
    for (l = 0; l < k; l++) {
      Ci,j += Ai,l * Bl,j;
    } } }
```

IJL order

```
for (j = 0; j < n; j++) {
  for (l = 0; l < k; l++) {
    double blj = B[l+j*ldb];
    for (i = 0; i < m; i++) {
      double ail = A[i+l*lda];
      C[i+j*ldc] += ail*blj;
    }}}
```

Changed to JLI order
(a bit faster)

=k

=m

Time Measurement in Samples

- gettimeofday() function is used
  - It provides wall-clock time, not CPU time
  - Time resolution is better than clock()

```
#include <stdio.h>
#include <sys/time.h>
      :
{
   struct timeval st, et;
   long us;
   gettimeofday(&st, NULL); /* Starting time */
   ・・・Part for measurement ・・・
   gettimeofday(&et, NULL); /* Finishing time */
   us = (et.tv_sec-st.tv_sec)*1000000+
        (et.tv_usec-st.tv_usec);
   /* us is difference between st & et in microseconds */
}
```

If You Have Not Done This Yet

Please do the followings as soon as possible

- Please make your account on TSUBAME
- Please send an e-mail to ppcomp@el.gsic.titech.ac.jp

Subject: TSUBAME3 ppcomp account
To: ppcomp@el.gsic.titech.ac.jp

Department name:
School year:
Name:
Your TSUBAME account name:

Then we will invite you to the TSUBAME group, please click URL and accept the invitation

その後、TSUBAMEグループへの招待を送ります。メール中のURLをクリックして参加承諾してください

Next Class : Introduction to OpenMP

- Shared memory parallel programming API
- Extensions to C/C++, Fortran
- Includes directives& library functions
  - Directives : #pragma omp ~~

```
  int i;
#pragma omp parallel for
  for (i = 0; i < 100; i++) {
        a[i] = b[i]+c[i];
  }
```