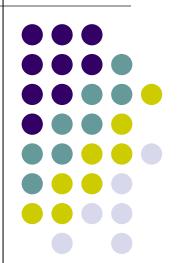
## Practical Parallel Computing (実践的並列コンピューティング)

2025 Class No.3
[OpenMP Part] (1)
Introduction to OpenMP



Toshio Endo endo@scrc.iir.isct.ac.jp



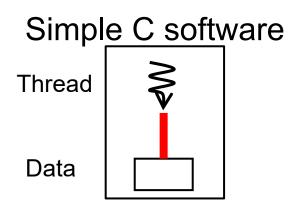
- Introduction Part
  - 2 classes
- OpenMP (OMP) Part
  - 4 classes
- ← We are here (1/4)
- Report (required)
- OpenACC (ACC) Part
  - 2 classes
  - Report (required)
- CUDA Part
  - 3 classes
  - Report (elective)
- MPI Part
  - 3 classes
  - Report (elective)

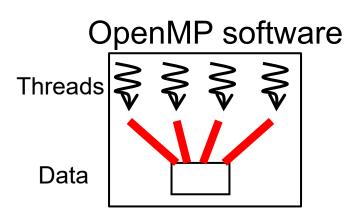
Slack channel in Science Tokyo Workspace

#dp-ppcomp-mcs-t418-2025

### What is OpenMP?

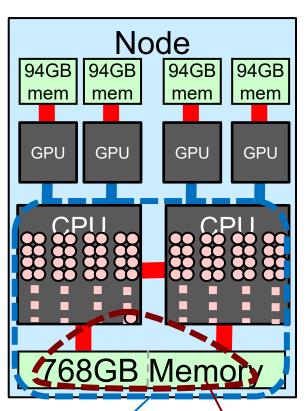
- One of programming APIs based on shared-memory parallel model
  - Multiple threads work cooperatively using multiple cores
  - Threads can share data
  - Threads (in a program) are on a single node
- → If we can divide computations into threads efficiently, the program speed is improved!

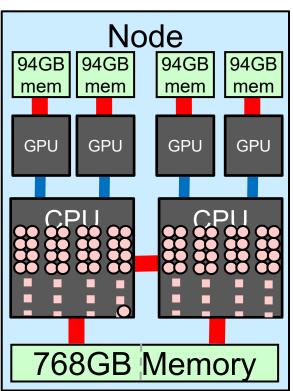


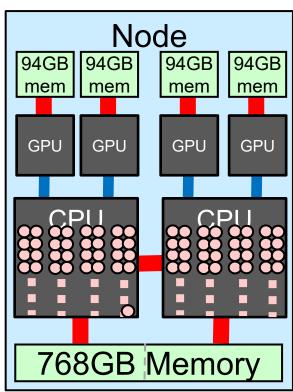


## With OpenMP, We Can Use Multiple Cores





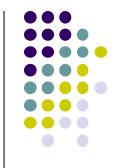






Sequential





- OpenMP defines extensions to C/C++/Fortran
- Directive syntaxes & library functions
  - Directives look like: #pragma omp ~~

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

## An example of OpenMP directive

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

### Sample Programs

- At github
  - If not yet, you can download by git clone <a href="https://github.com/toshioendo/ppcomp-ex.git">https://github.com/toshioendo/ppcomp-ex.git</a>
  - For details, please see #2 slides
- Samples related to today's class
  - A simple sample
    - omp/hello
  - matrix multiplication
    - base/mm sequential version
    - omp/mm OpenMP version
    - omp/mm-mkl Using Intel MKL library







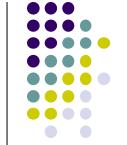
[make sure that you are at an interactive node (rXn11)] [make sure that you have downloaded samples] cd ppcomp-ex [please go to your ppcomp-ex directory] cd omp/hello

make

[this creates an executable file "hello"]

./hello

### **Compiling OpenMP Programs**



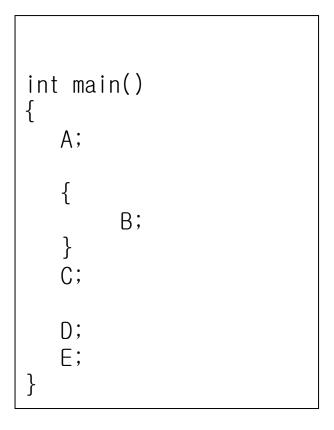
All famous compilers support OpenMP (fortunately<sup>⊚</sup>), but require different options (unfortunately<sup>⊗</sup>)

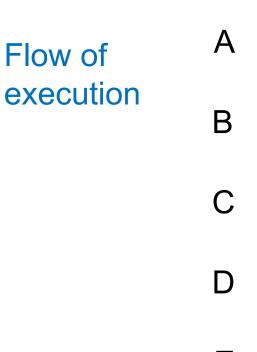
- gcc
  - -fopenmp option in compiling and linking

Our samples use gcc

- NVIDIA HPC SDK (called PGI compiler in past)
  - module load nvhpc, and then use pgcc
  - -mp option in compiling and linking
- Intel compiler
  - module load intel, and then use icx
    - "icc" was deprecated
  - -qopenmp option in compiling and linking



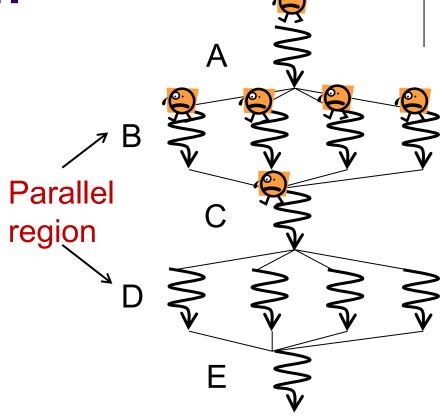






## Basic Parallelism in OpenMP: Parallel Region

```
#include <omp.h>
int main()
#pragma omp parallel
        Β;
#pragma omp parallel
```



Sentence/block immediately after #pragma omp parallel is called parallel region, executed by multiple threads

- Here a "block" is a region surrounded by braces {}
- Functions called from parallel region are also in parallel region

#### Number of Threads 9 9











How is the number of threads in parallel region determined?

- Default: number of cores (including HyperThreads) are used
  - On a TSUBAME4 interactive node, it is 24x2 = 48
- We can specify number of threads by **OMP NUM THREADS** environment variable
  - this is done out of program execution

```
export OMP_NUM_THREADS=4
      [executed with 4 threads]
./hello
```

- For "environment variables" (環境変数), please check
- 3. We can overwrite it inside the program
  - cf) omp\_set\_num\_threads(6);

### Outputs of hello-omp



Before the parallel region

Hello OpenMP World

I'm 8-th thread out of 48 threads

I'm 6-th thread out of 48 threads

I'm 9-th thread out of 48 threads

I'm 1-th thread out of 48 threads

I'm 0-th thread out of 48 threads

I'm 7 th thread out of 48 threads

Good Bye OpenMP World

Inside the parallel region, each thread prints a message for several (5) times

omp\_get\_num\_threads()

omp get thread num()

After the parallel region

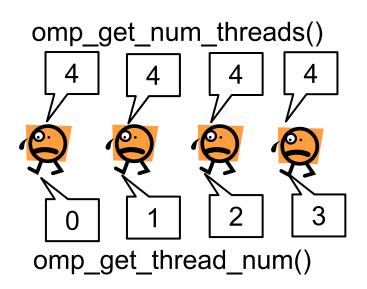
# Who am I?

## To Know ID of Threads

In some programs, threads can distinguish each other Each thread has an "ID number" (0, 1, 2 ...)

- To obtain number of threads
  - cf) n = omp\_get\_num\_threads();

- To obtain my ID of calling thread
  - cf) id = omp\_get\_thread\_num();
    - 0 ≤ id < n (total number)</li>



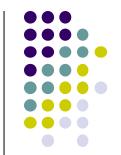
## **Executing a Sample with Various Number of Threads**



```
export OMP NUM THREADS=1
./hello
export OMP NUM THREADS=8
./hello
export OMP NUM THREADS=48
./hello
export -n OMP NUM THREADS
[This deletes the environment variable]
./hello
```

[make sure that there is an executable file "hello"]

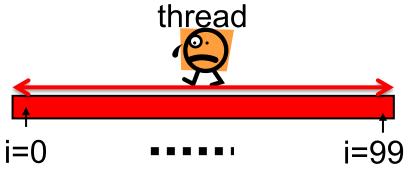
### How Can We Make a Program Faster?



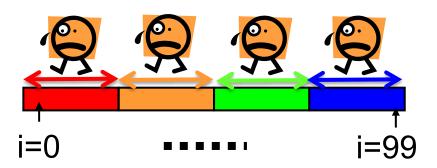
```
for (i = 0; i < 100; i++) { some computation; }
```

assumption: 100 tasks are independent with each other

Only with one thread



With 4 threads



```
thread 0: for (i = 0 ; i < 25; ...
thread 1: for (i = 25; i < 50; ...
thread 2: for (i = 50; i < 75; ...
thread 3: for (i = 75; i < 100; ...
```



## #pragma omp for for Easy Parallel Programming



"for" loop with simple forms can parallelized easily

#pragma omp for must be

- inside a parallel region
- right before a "for" loop
- → Computations in the loop are distributed among threads (work distribution)
- With 4 threads, each thread take 100/4=25 iterations → speed up!!
  - Indivisible cases are ok, such as 7 threads

Abbreviation: omp parallel + omp for = omp parallel for

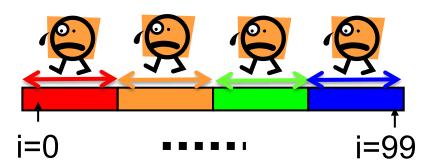
### Why "omp for" Reduces Execution Time



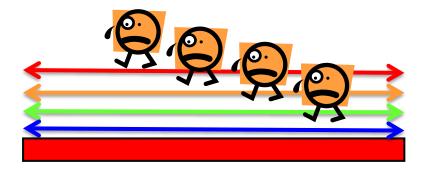
Only with one thread thread



With several threads



What if we use "omp parallel", but forget to write "omp for"?



Every thread would work for all iterations

- → No speed up ⊗
- → Answer will be wrong ⊗

### "mm" sample: Matrix Multiply



In class #2, we tested base/mm/, which is sequential

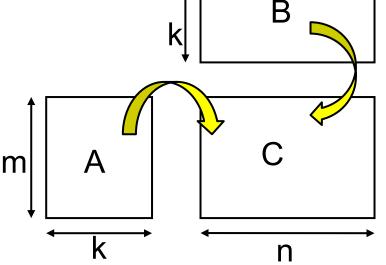
```
A: a (m \times k) matrix
```

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

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

$$C \leftarrow A B$$

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



You can try the parallel version at omp/mm/

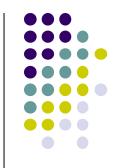
[please go to your ppcomp-ex directory]
cd omp/mm
make
[this creates an executable file "mm"]
./mm 2000 2000 2000

## OpenMP Version of mm (mm-omp)

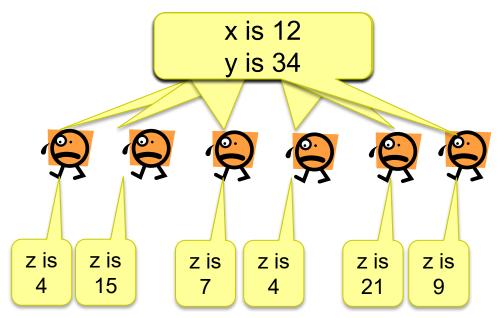
- matmul() function uses 3 loops
- Out of them, j loop is parallelized

"private" option is explained later

## **Shared Variables & Private Variables (1)**



While OpenMP uses "shared memory model", not all are shared Two types of variables: shared variables and private variables cf) Here variables *x*, *y* are shared, and *z* is private



#### Shared ->

Single instance for each x, y are shared by threads

#### Private >

Each thread has its own instance for z

- When a thread updates a shared variable, other threads are affected
  - We should be careful

## **Shared Variables & Private Variables (2)**



In the default rule, variables are classified as follows

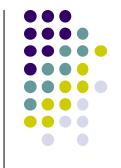
- Variables declared out of parallel region ⇒ Shared variables
- Global variables

- ⇒ Shared variables
- Variables declared inside parallel region ⇒ Private variables

```
f
  int s = 1000;
#pragma omp paralle

{
    int i;
    i = func(s, omp_get_thread_num());
    printf( "%d\f", i);
}
}
```





- The following code looks ok, but it has a bug
  - We do not see compile errors, but answers would be wrong ⊗

```
#pragma omp parallel
#pragma omp for
  for (i = 0; i < m; i++) {
    for (j = 0; j < n; j++) {
```

Both i, j are declared outside parallel region → Considered "shared" It is a problem to share

cf) Thread A is executing i=5 loop Thread B is executing i=8 loop

The executions should be independent Each execution must include j=0, j=1...j=n-1 correctly 22 j must be private

## Pitfall in Nested Loops (2)

#### Two possible modifications (Either is ok)

```
int i, j;
#pragma omp parallel for private(j)
    // j is forcibly private
    for (i = 0; i < m; i++) {
        for (j = 0; j < n; j++) {
            ...
        } }</pre>
```



## OpenMP Version of mm (Again)



#pragma omp parallel private(i,l) → i, I made private forcibly #pragma omp for

```
for (j = 0; j < n; j++) {

for (l = 0; l < k; l++) {

for (i = 0; i < m; i++) {

    C[i+j*ldc] += A[i+l*lda] * B[l+j*ldb];

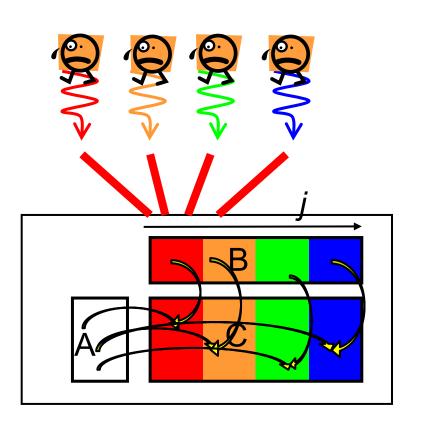
} }
```

In this sample, *j* loop is parallelized

→ Each thread executes computations only for subset of [0, n)

## How Arrays are Accessed in mm-omp





 It is programmers responsibility to make each thread does independent computation

j loop is parallelized

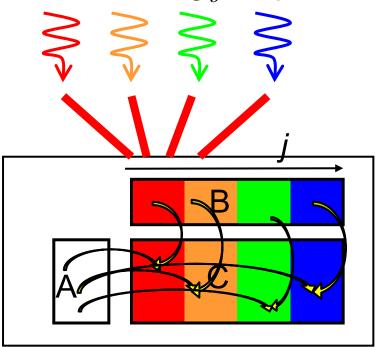
→ Each thread executes computations only for subset of [0, n)

- [Q] What if we parallelize other loops?
- $\rightarrow$  i loop is ok for correct answers, but may be slow
- → *l* loop causes wrong answers!

## **Correct Parallelization and Bad Parallelization**



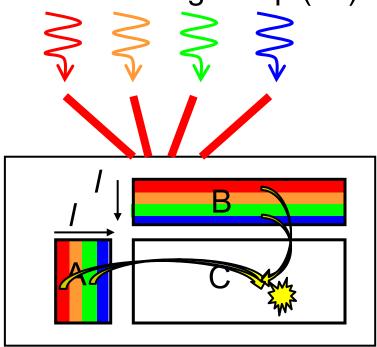
Parallelizing *j* loop



Simultaneous read from same data (in this case, A) is OK

Similarly, parallelizing *i* loop is ok

Parallelizing *l* loop (??)



Possible simultaneous write to same data

→ "Race condition" problem may occur.

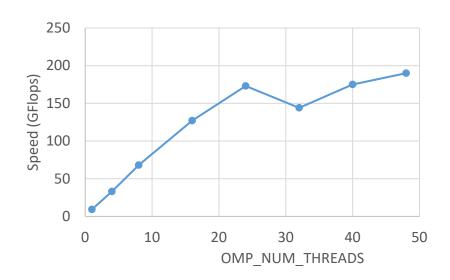
Answers may be wrong !!

### Performance of mm-omp sample



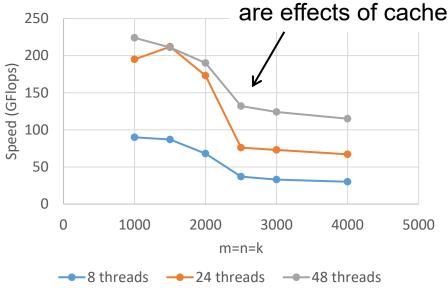
- On a TSUBAME4 interactive node (24 cores)
- Speed is (2mnk/t)

m=n=k=2000, Varying # of threads



#### Varying m=n=k

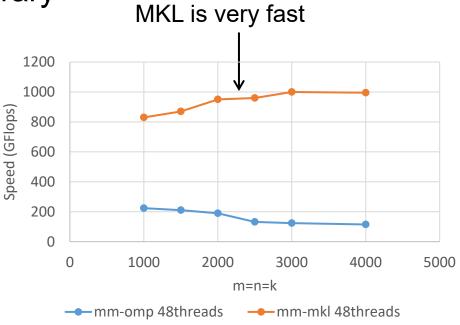
Should be constant "theoretically". There are effects of cache





- Each processor vendor has optimized (fast) libraries including matrix operations or deep learning kernels
  - Such as Intel MKL, NVIDIA cuBLAS/cuDNN...
- mm-mkl sample uses MKL library

[please go to your ppcomp-ex directory] cd omp/mm-mkl module load intel make export OMP\_NUM\_THREADS=48 ./mm 2000 2000 2000







#### Such libraries use many optimizing techniques

- Using multiple threads to use multiple cores
  - ↑ This lecture focuses on this
- Using SIMD instructions
- Using cache blocking techniques to harness cache memory
  - Unfortunately, MKL is not open-source
  - Some libraries such as OpenBLAS are open-source

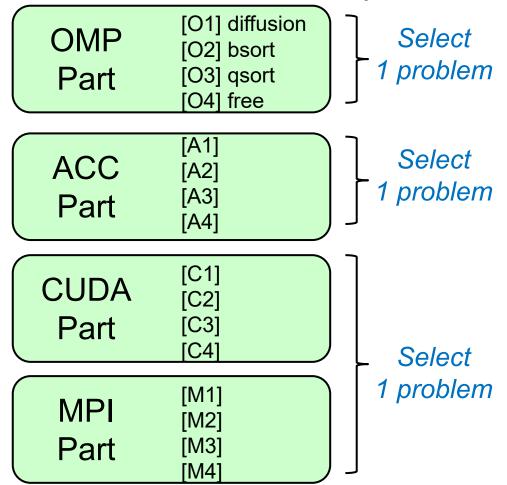
#### "Python is slow" may not be true

- "numpy" linear algebra package may call a fast library automatically
  - C = numpy.matmul(A, B)
- Writing 3 loops in Python is very slow

### **Assignments in this Course**



There is homework for each part.



### **Assignments in OpenMP Part**

Choose one of [O1]—[O4], and submit a report via LM\$

Due date: May 1 (Thu)

[O1] Parallelize "diffusion" sample program by OpenMP.

(seq/diffusion, omp/diffusion)

#### Optional:

- To make array sizes variable parameters, which are specified by execution options. "malloc" will be needed.
- To parallelize it without "omp for"
  - omp\_get\_thread\_num(), omp\_get\_num\_threads() are needed

## Assignments in OpenMP Part (cont)



[O2] Parallelize "bsort" sample program by OpenMP.

(seq/bsort, omp/bsort)

#### Optional:

- Comparison with other sort algorithms
  - Quick sort (qsort), Heap sort, Merge sort, ...

[O3] Parallelize "qsort" sample program by OpenMP.

(seq/qsort, omp/qsort)

#### Optional:

- Comparison with other sort algorithms
  - Bitonic sort (bsort), Heap sort, Merge sort, ...

## Assignments in OpenMP Part (cont)



#### [O4] (Freestyle) Parallelize any program by OpenMP.

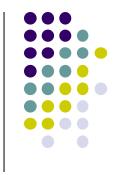
- cf) A problem related to your research
- More challenging one for parallelization is better
  - cf) Partial computations have dependency with each other
  - cf) Uniform task division is not good for load balancing

### **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

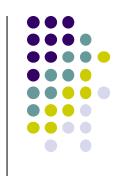
### **Notes in Report Submission (2)**



#### 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
- Performance evaluation on TSUBAME
  - With varying number of threads
    - On an interactive nodes, 1 ≤ OMP\_NUM\_THREADS ≤ 48
    - To use more CPU cores, you need to do "job submission"
  - With varying problem sizes
  - Discussion with your findings
  - Other machines than TSUBAME are ok, if available





Introduction to OpenMP parallel programming

- Multiple threads work simultaneously with #pragma omp parallel
- With #pragma omp for, loop-based programs can be parallelized easily
- But it is programmer's responsibility to avoid bugs caused by race conditions

#### Plan of OMP Part

- Class #3 (Today)
  - Introduction to OpenMP
- Class #4
  - Data parallelism with for loops
  - diffusion sample [O1], bsort sample [O2]
- Class #5
  - Task parallelism
  - qsort sample [O3]
- Class #6
  - What are bottlenecks, race conditions?