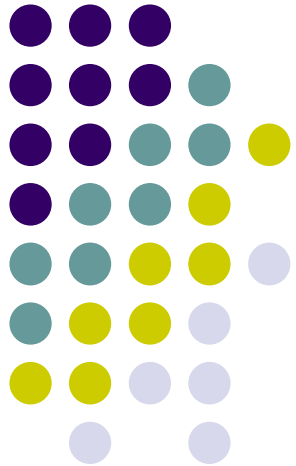
Practical Parallel Computing (実践的並列コンピューティング)



Part 1: OpenMP

No 1: Introduction to OpenMP

uploaded to github as ppcomp-1-1.pdf

Apr 17, 2023

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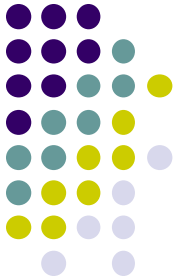
Overview of This Course

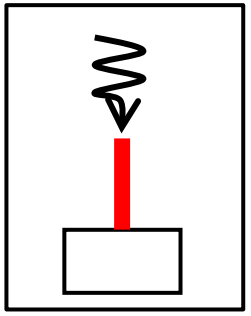


- Part 0: Introduction
  - 2 classes
- Part 1: OpenMP for shared memory programming
  - 4 classes ← We are here (1/4)
- Part 2: GPU programming
  - OpenACC and CUDA
  - 4 classes
- Part 3: MPI for distributed memory programming
  - 3 or 4 classes

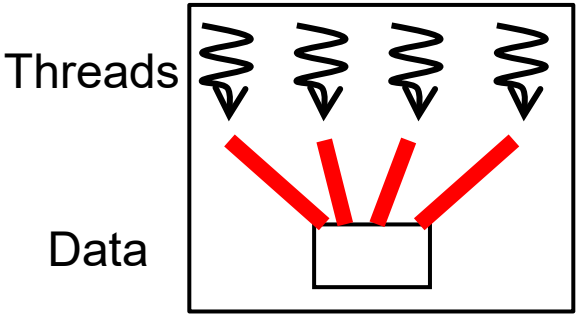
What is OpenMP?

- 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

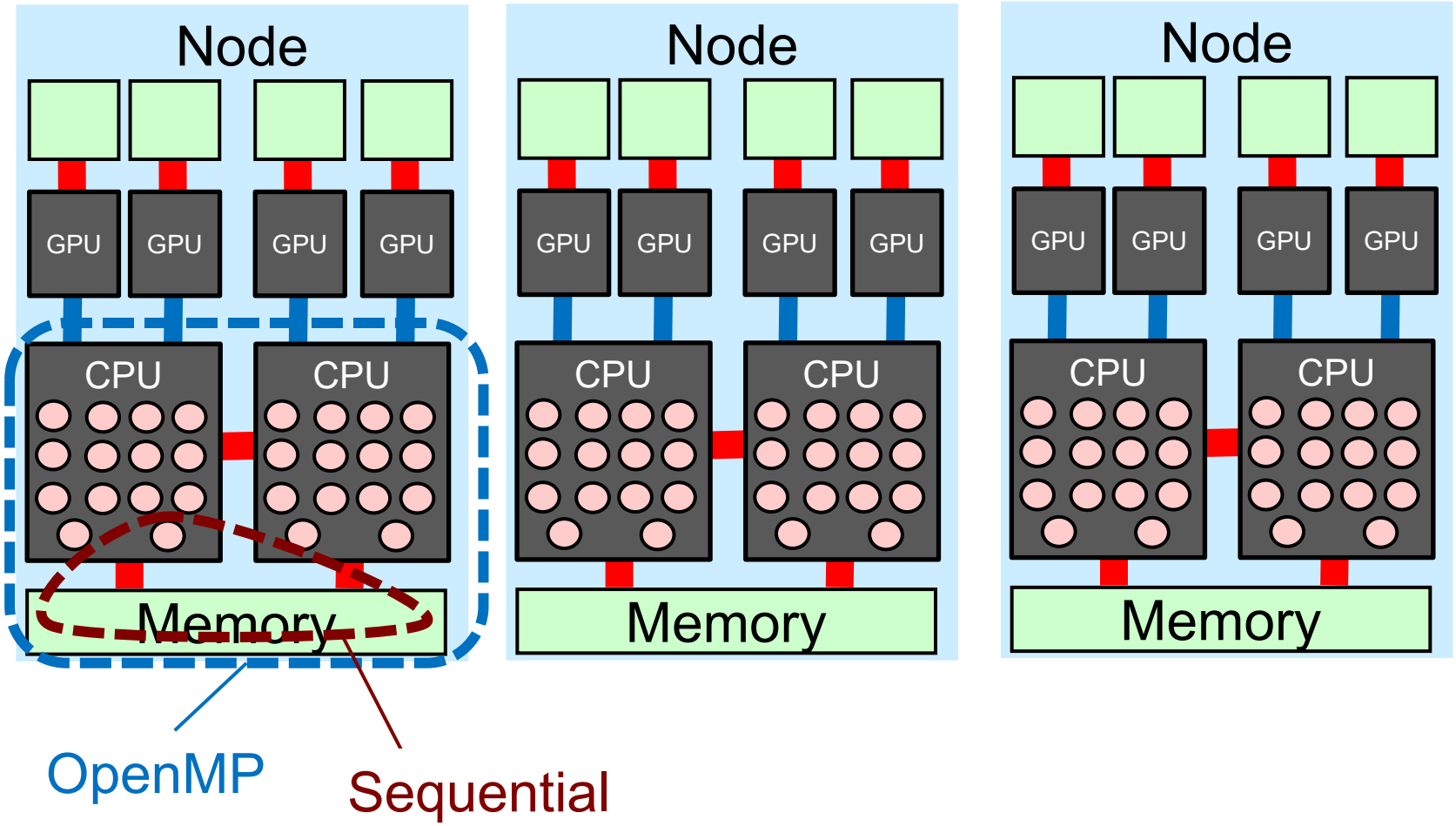
Simple C software



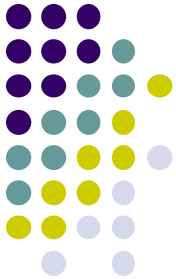
OpenMP software



With OpenMP, We Can Use Multiple Cores



OpenMP Programs Look Like



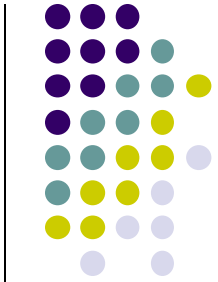
- OpenMP defines extensions to C/C++/Fortran
- Directive syntaxes & library functions
  - Directives look like: #pragma omp ~~

```
   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];
   }
```

An example of OpenMP *directive*

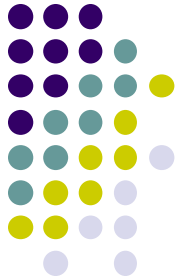
In this case, a directive has an effect on the following block/sentence

Sample Programs



- /gs/hs1/tga-ppcomp/23/ directory
  - You have to be a member of tga-ppcomp group
  - There are sub-directories per sample
- Samples related to today's class
  - hello-omp
  - matrix multiplication
    - mm: sequential version
    - mm-omp: OpenMP version
    - mm-mkl: Using Intel MKL library

Using hello-omp Sample



[make sure that you are at a interactive node (r7i7nX)]
cd ~/t3workspace *[Example in web-only route]*
cp -r /gs/hs1/tga-ppcomp/23/hello-omp .
cd hello-omp
make
[this creates an executable file “hello”]
./hello

Compiling OpenMP Programs

All famous compilers support OpenMP (fortunately☺), but require different options (unfortunately☹)

- gcc
  - -fopenmp option in compiling and linking

Our samples use gcc

- NVIDIA HPC SDK (called PGI compiler)
  - module load nvhpc, and then use pgcc
  - -mp option in compiling and linking
- Intel compiler
  - module load intel, and then use icc
  - -openmp option in compiling and linking

Check outputs of “make” in OpenMP sample directory

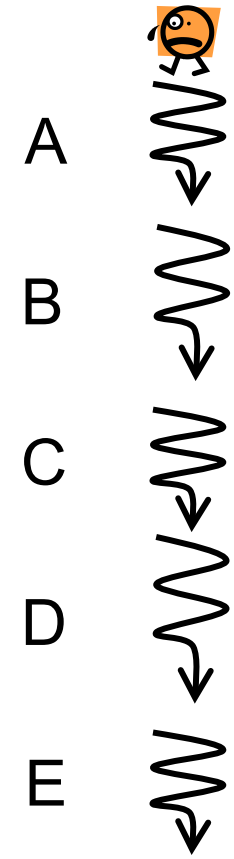
A Sequential Example

```
int main()
{
   A;

   {
        B;
   }
   C;

   D;
   E;
}
```

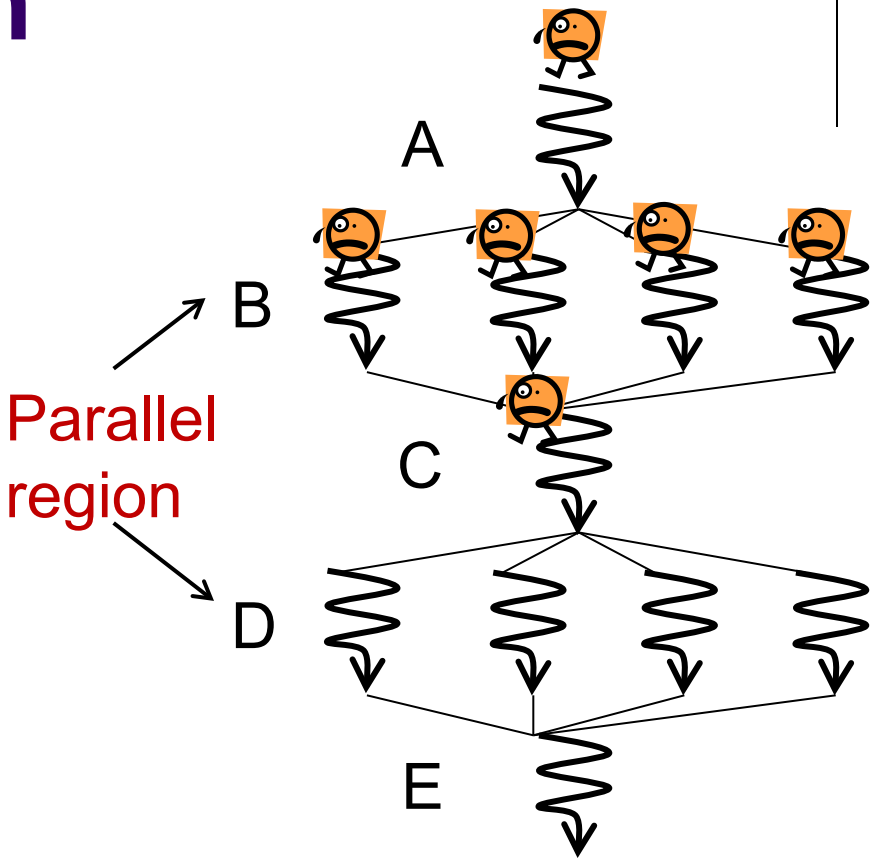
Flow of execution



Basic Parallelism in OpenMP: Parallel Region

```
#include <omp.h>

int main()
{
    A;
#pragma omp parallel
    {
        B;
    }
    C;
#pragma omp parallel
    D;
    E;
}
```



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

How is the number of threads in parallel region determined?

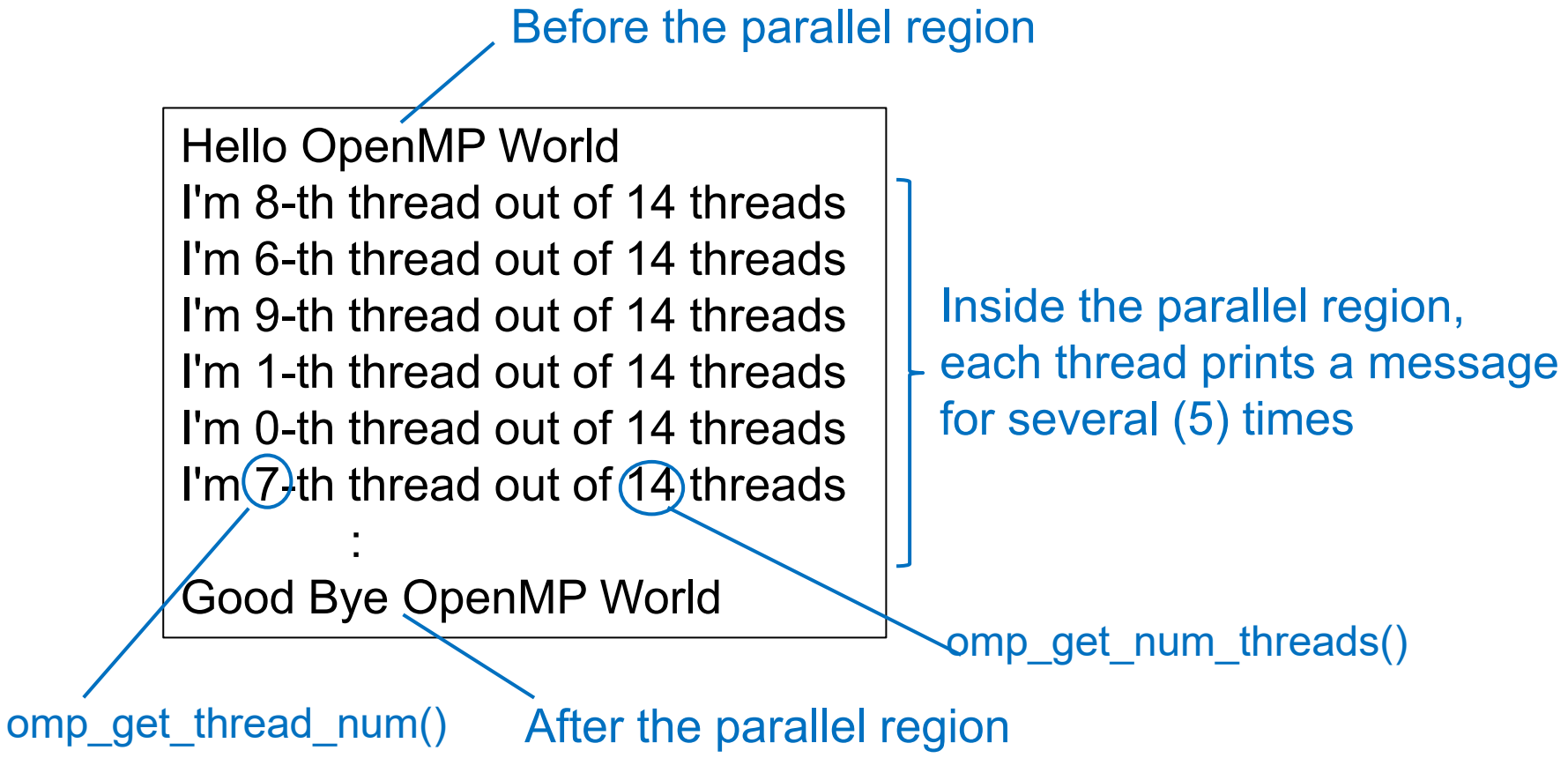
1. Default: number of cores (including HyperThreads) are used
   - On a TSUBAME3 interactive node, it is 7x2 = 14

2. We can specify number of threads by OMP_NUM_THREADS environment variable
   - this is done out of program execution

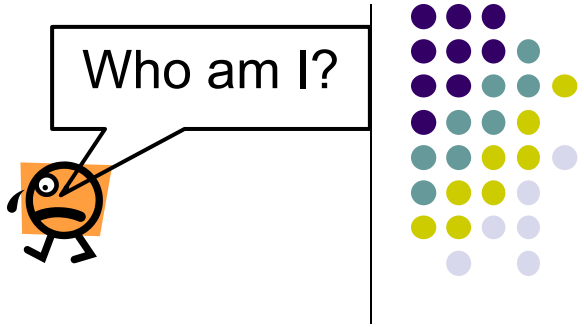
```
export OMP_NUM_THREADS=4
./hello     [executed with 4 threads]
```

3. We can overwrite it inside the program
   - cf) omp_set_num_threads(6);

Outputs of hello-omp

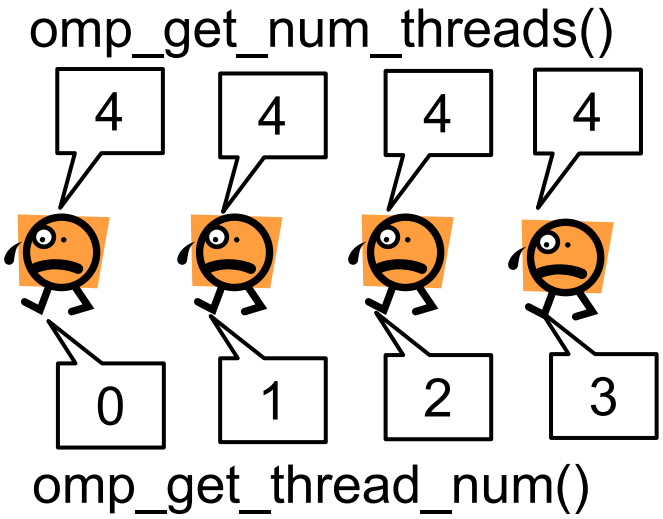


To Know ID of Threads

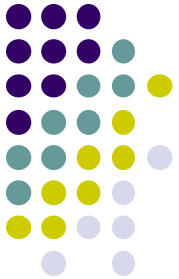


In some programs, threads can distinguish each other
Each thread has an “ID number” (0, 1, 2 …)

- 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)



Executing a Sample with Various Number of Threads



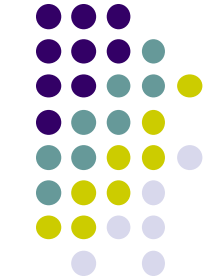
```
[make sure that there is an executable file “hello”]
export OMP_NUM_THREADS=1
./hello

export OMP_NUM_THREADS=4
./hello

export OMP_NUM_THREADS=7
./hello

export OMP_NUM_THREADS=14
./hello
```

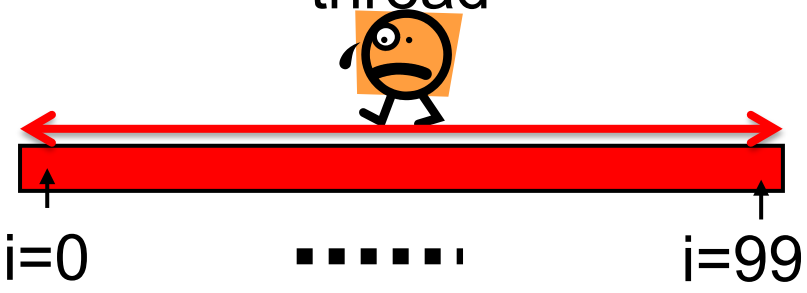
How Can We Make a Program Faster?



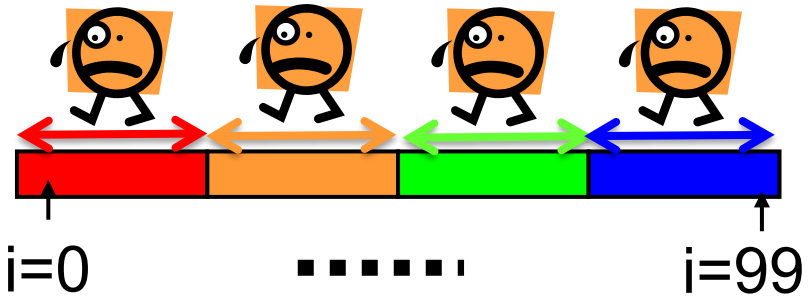
```
for (i = 0; i < 100; i++) { some computation; }
```

assumption: 100 tasks are independent with each other

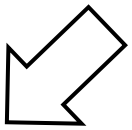
Only with one thread



With 4 threads

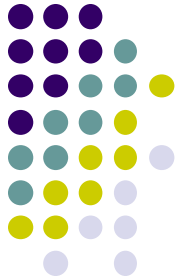


thread 0: for (i = 0 ; i < 25; …
thread 1: for (i = 25; i < 50; …
thread 2: for (i = 50; i < 75; …
thread 3: for (i = 75; i < 100; …



Fortunately, OpenMP makes this program very easy!

#pragma omp for for Easy Parallel Programming



"for" loop with simple forms can parallelized easily

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

#pragma omp for must be

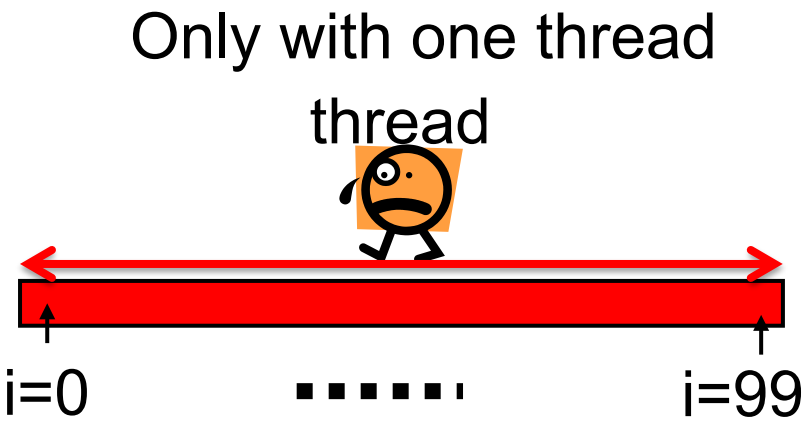
- inside a parallel region
- right before a "for" loop

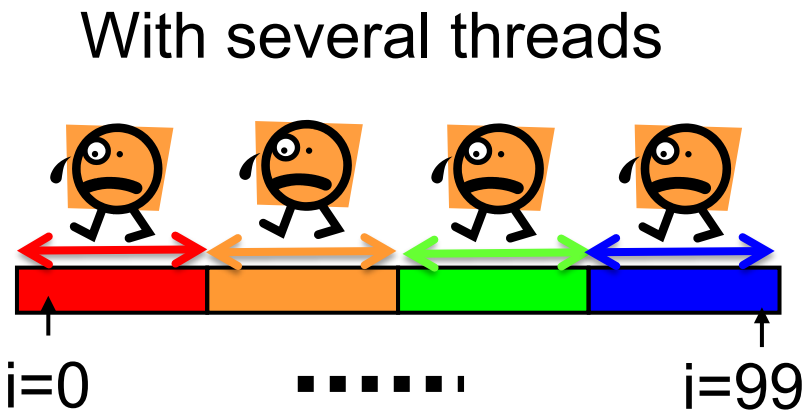
→ Computations in the loop are distributed among threads (work distribution)

- With 4 threads, each thread take 100/4=25 iterations → speed up!!
  - Indivisible cases are ok, such as 7 threads

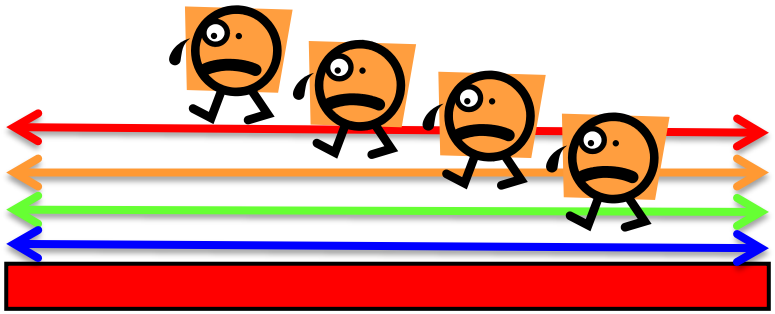
- Abbreviation: omp parallel + omp for = omp parallel for

Why "omp for" Reduces Execution Time





- 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 previous class, we tested /gs/hs1/tga-ppcomp/23/mm/ , which is sequential

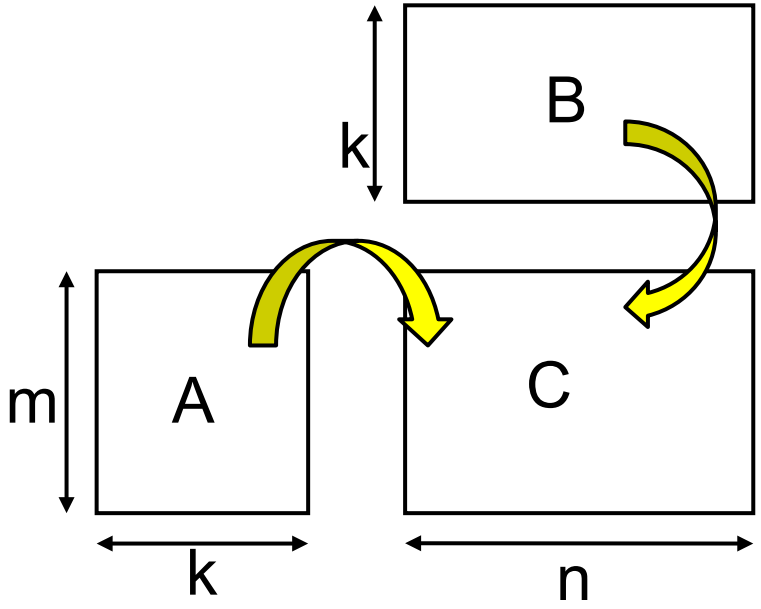
A: a (m × k) matrix

B: a (k × n) matrix

C: a (m × n) matrix

$$C \leftarrow A \ B$$

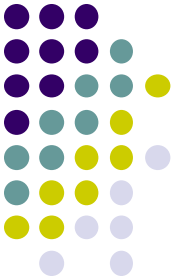
- This sample supports variable matrix sizes
- Execution: ./mm [m] [n] [k]



A parallel version is at /gs/hs1/tga-ppcomp/23/mm-omp/

- Please copy it to your home directory as usual

OpenMP Version of mm (mm-omp)

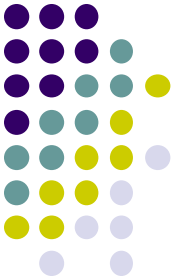


- matmul() function uses 3 loops
- Out of them, j loop is parallelized

```
#pragma omp parallel private(i,l)
#pragma omp for                    ← j loop is parallelized
   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];
         } }   }
```

  - "private" option is explained later

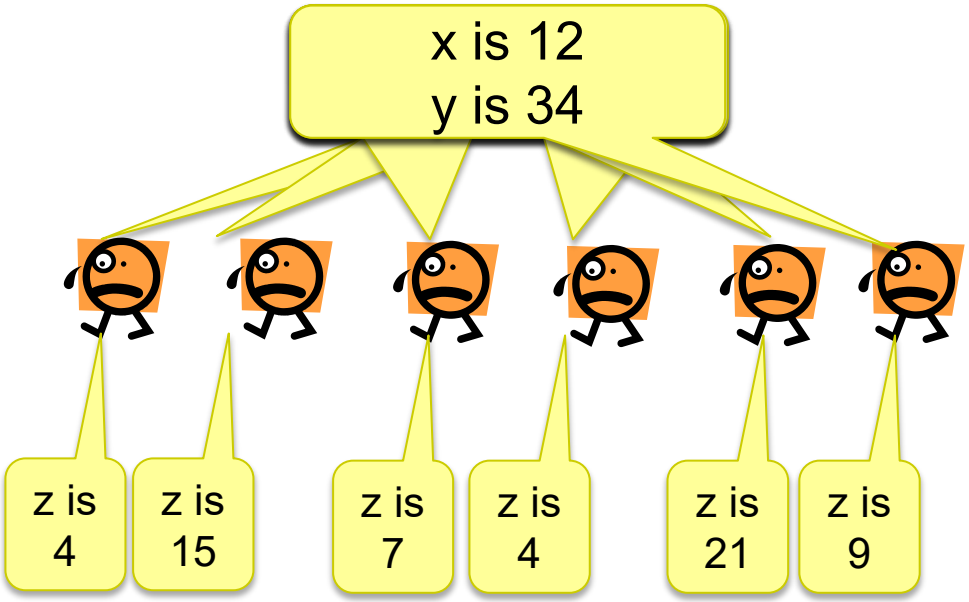
Shared Variables & Private Variables (1)



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

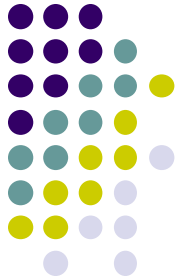


Shared ➔
Single instance for each x, y are shared by threads

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

```
{
    int s = 1000;
#pragma omp parallel
    {
        int i;
        i = func(s, omp_get_thread_num());
        printf( "%d¥n" , i);
    }
}
```

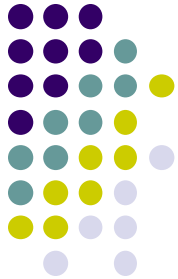
shared

private

```
int func(int a, int b)
{
    int rc = a+b;
    return rc;
}
```

private

Pitfall in Nested Loops (1)



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

```
  int i, j;
#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 j

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
j must be private

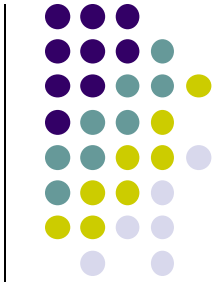
Pitfall in Nested Loops (2)

Two modifications (Either is ok)

```
  int i;
#pragma omp parallel for
  for (i = 0; i < m; i++) {
    int j;   // j is private
    for (j = 0; j < n; j++) {
       …
    } }
```

```
  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++) {
       …
    } }
```

OpenMP Version of mm (Again)

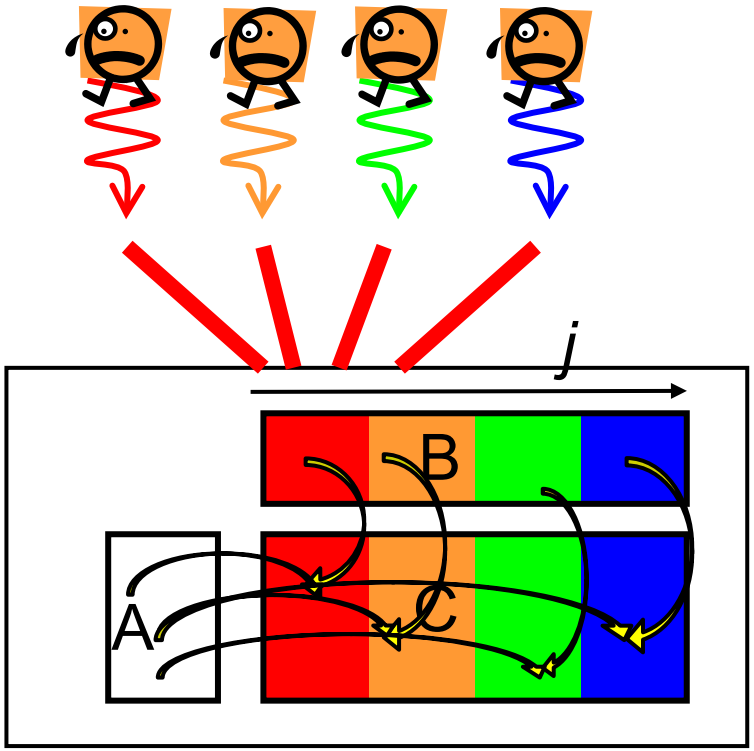


```
#pragma omp parallel private(i,l)
#pragma omp for
    for (j = 0; j < n; j++) {
        for (l = 0; l < k; l++) {
            for (i = 0; i < m; i++) {
                C[i+j*ldc] += A[i+l*lda] * B[l+j*ldb];
            } }   }
```

➔ i, l made private forcibly

In this sample, *j* loop is parallelized
➔ Each thread executes computations only for subset of [0, n)

How Arrays are Accessed in mm-omp

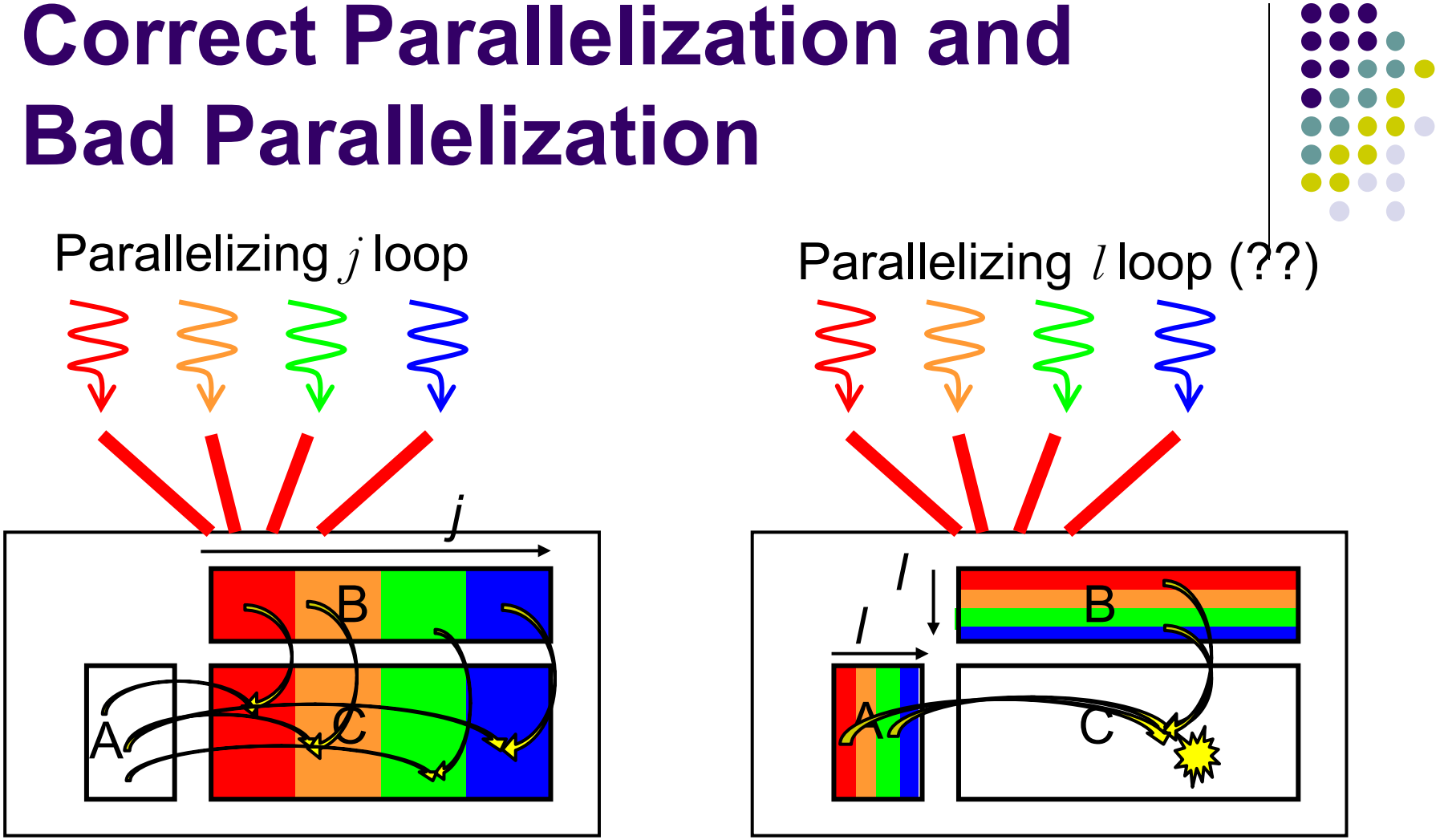


- It is programmers responsibility to make each thread does independent computation

j loop is parallelized
➔ Each thread executes computations only for subset of [0, n)

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

Correct Parallelization and Bad Parallelization



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

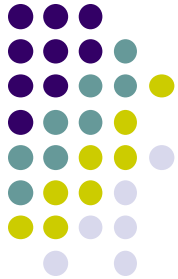
Similarly, parallelizing *i* loop is ok

Possible simultaneous write to same data

→ "Race condition" problem may occur.

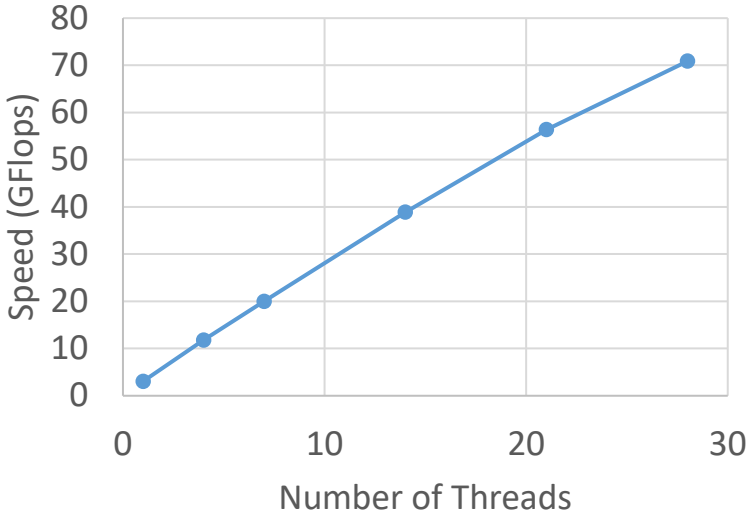
Answers may be wrong !!

Performance of mm-omp sample



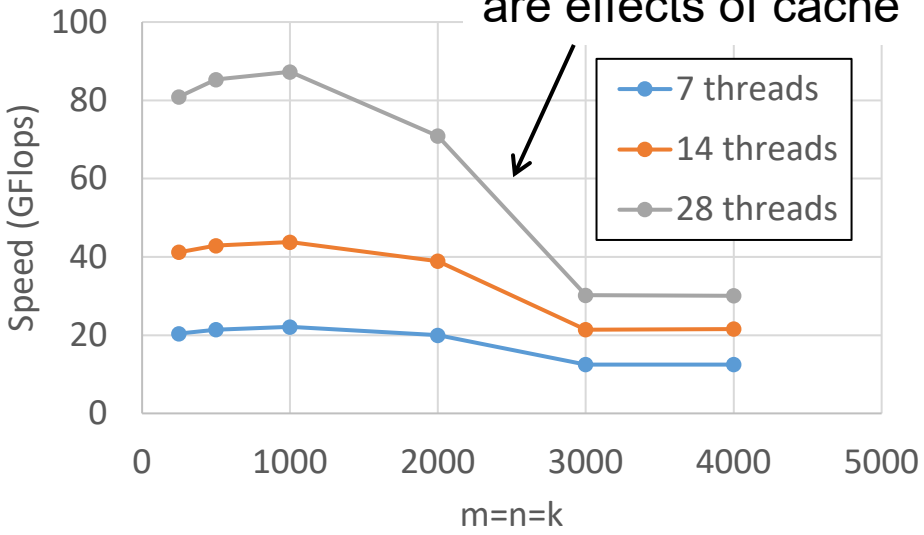
- On a TSUBAME3 f-node (28 cores)
- export OMP_PROC_BIND=SPREAD is done for stable performance
- Speed is (2mnk/t)

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



Varying m=n=k

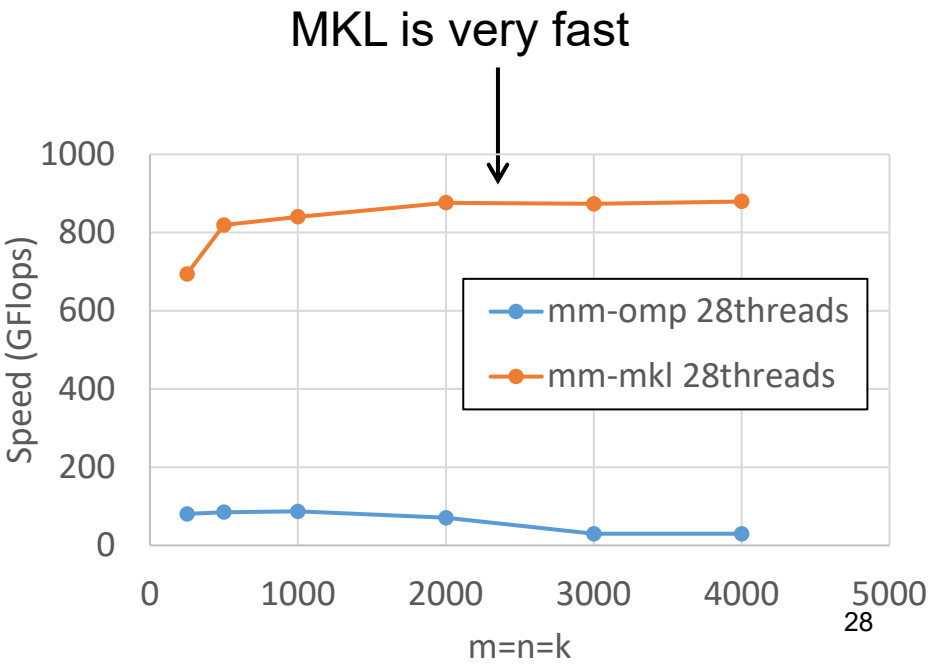
Should be constant "theoretically". There are effects of cache



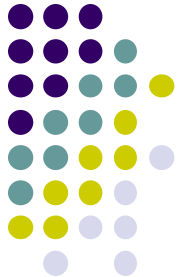
FYI: Using Optimized Libraries

- 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

```
cd ~/t3workspace
cp -r /gs/hs1/tga-ppcomp/23/mm-mkl  .
cd mm-mkl
module load intel
make
export OMP_NUM_THREADS=7
./mm 2000 2000 2000
```



FYI: Why are Fast Libraries Fast?



Such libraries use many optimizing techniques

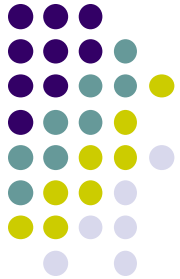
- Using multiple threads to use multiple cores

  ↑ 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

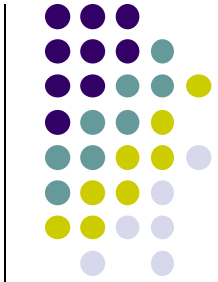
Today's Summary



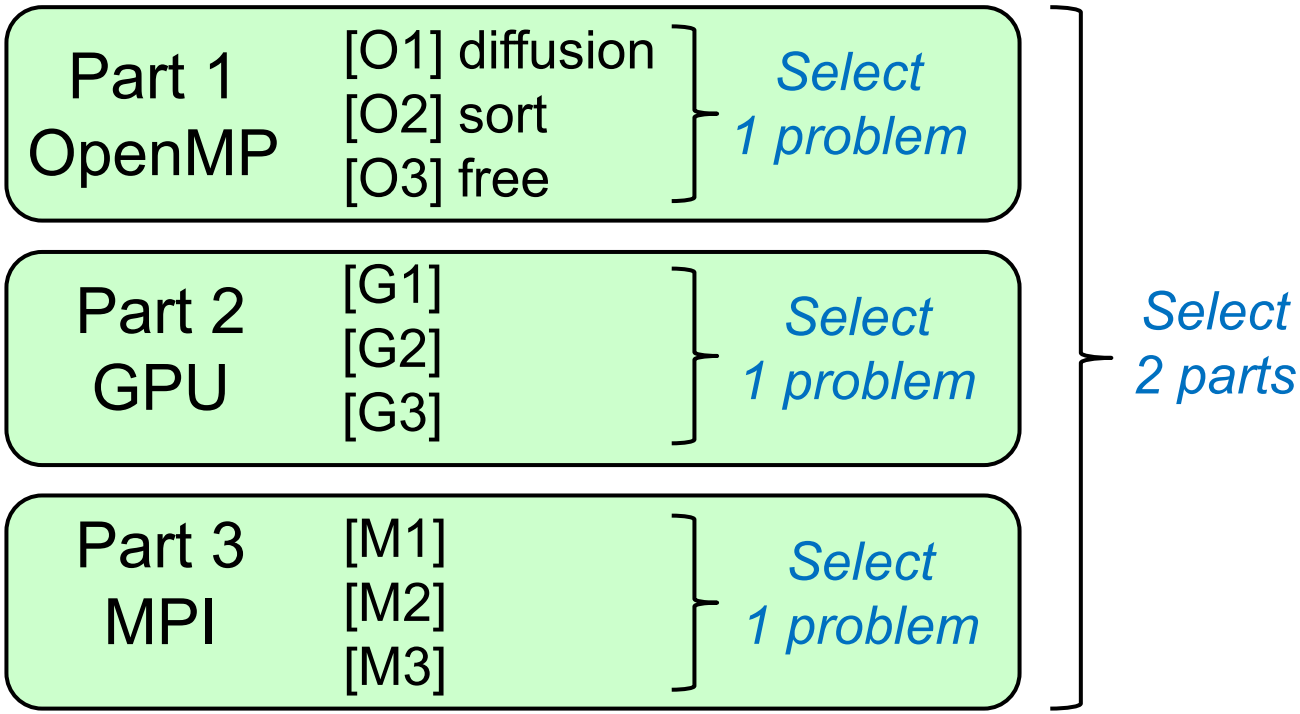
Introduction to OpenMP parallel programming

- 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

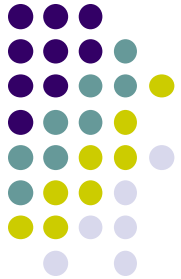
Assignments in this Course



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



Assignments in OpenMP Part (1)



Choose one of [O1]—[O3], and submit a report

Due date: May 11 (Thu)

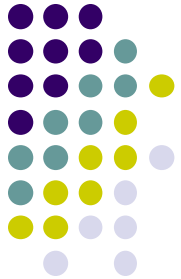
[O1] Parallelize “diffusion” sample program by OpenMP.

(/gs/hs1/tga-ppcomp/23/diffusion/ on TSUBAME)

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 (2)

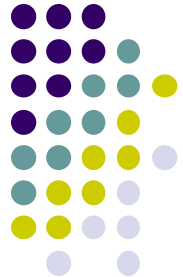


[O2] Parallelize “sort” sample program by OpenMP.
(/gs/hs1/tga-ppcomp/23/sort/ on TSUBAME)

Optional：

- Comparison with other algorithms than quick sort
  - Heap sort? Merge sort?

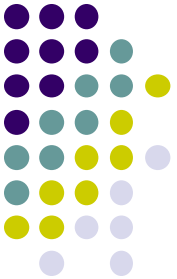
Assignments in OpenMP Part (3)



[O3] (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)

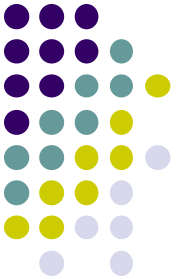


- Submit the followings via T2SCHOLA

  (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
- 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 a interactive nodes, 1 ≦ OMP_NUM_THREADS ≦ 14
    - 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

Next Class:

- Part1: OpenMP No. 2
  - diffusion：simple simulation of diffusion phenomena
    - Related to assignment [O1]