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

Part2: OpenMP (1)
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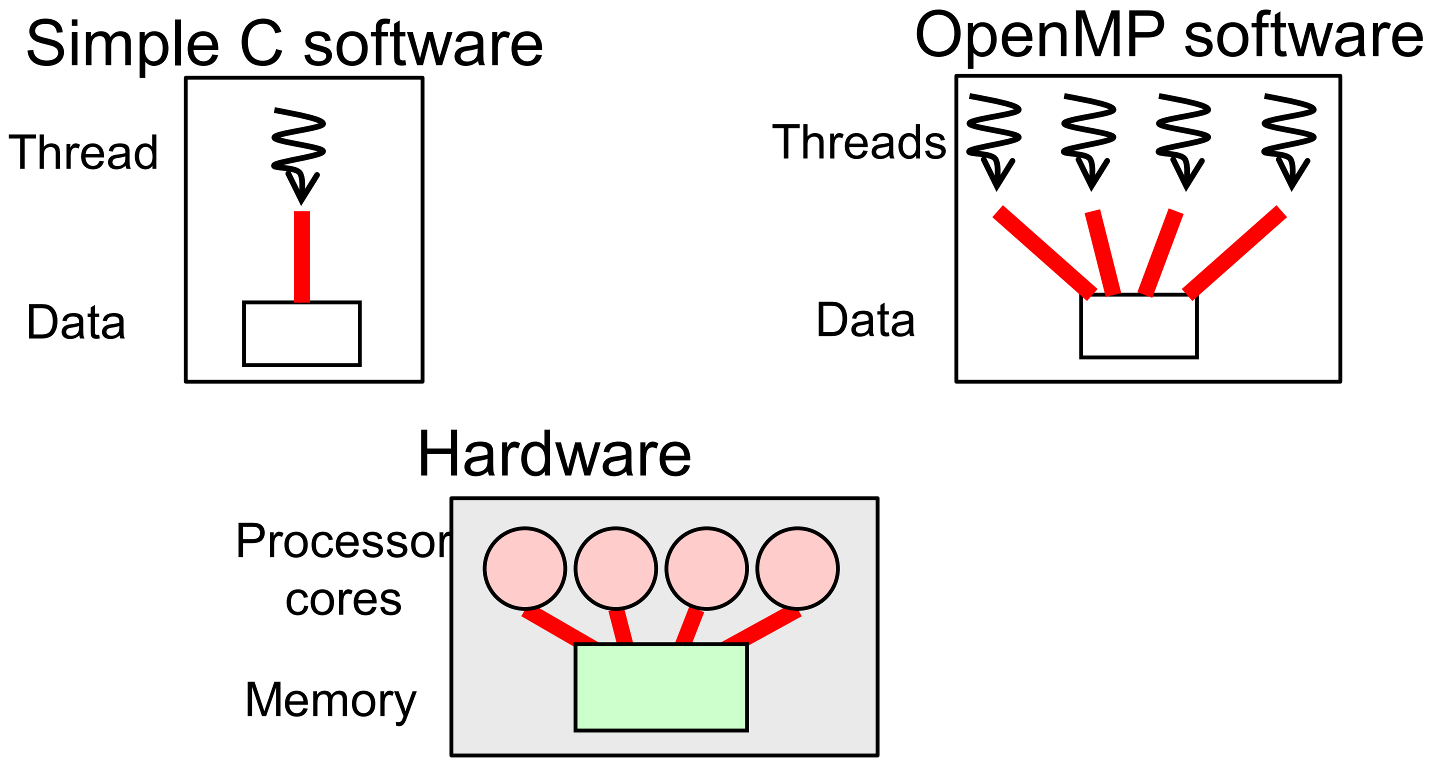
Overview of This Course

- 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
  - Threads can share data



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/22/ 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/22/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☹)

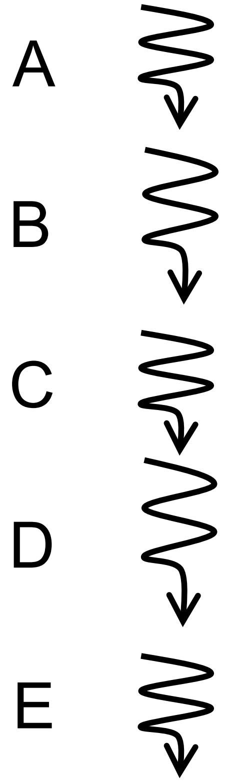
- gcc
  - -fopenmp option in compiling and linking
- NVIDIA HPC SDK (called PGI compiler)
  - module load nvhpc, and then use pgcc
  - -mp option in compiling and linking
- Intel compiler
  - module load intel, and then use icc
  - -openmp option in compiling and linking

Also see outputs of “make” in OpenMP sample directory

A Sequential Example

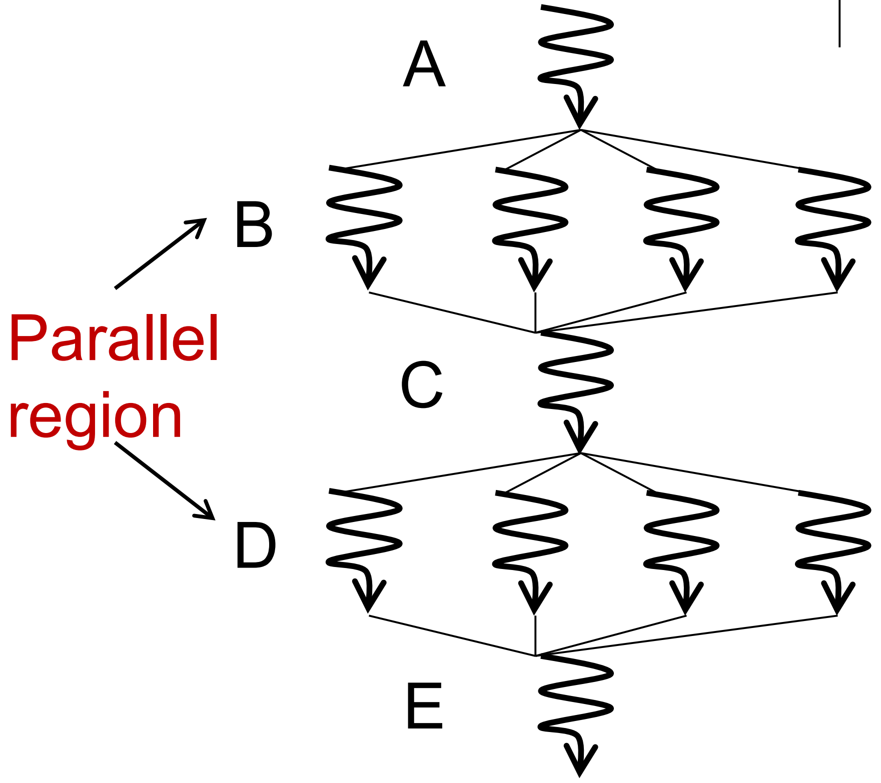
```
int main()
{
   A;

   {
         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

- Specify number of threads by OMP_NUM_THREADS environment variable (this is done out of program)
  - cf) export OMP_NUM_THREADS=7
    in command line
  - In default, number of cores (including HyperThreads) are used. On an interactive node, 7x2 = 14

- Obtain number of threads
  - cf) n = omp_get_num_threads();

- Obtain "my ID" of calling thread
  - cf) id = omp_get_thread_num();
    - 0 ≦ id < n (total number)

Outputs of hello-omp

Before the parallel region

```
Hello OpenMP World
I'm 8-th thread out of 14 threads
I'm 6-th thread out of 14 threads
I'm 9-th thread out of 14 threads
I'm 1-th thread out of 14 threads
I'm 0-th thread out of 14 threads
I'm 7-th thread out of 14 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

Executing a Sample with Various Number of Threads

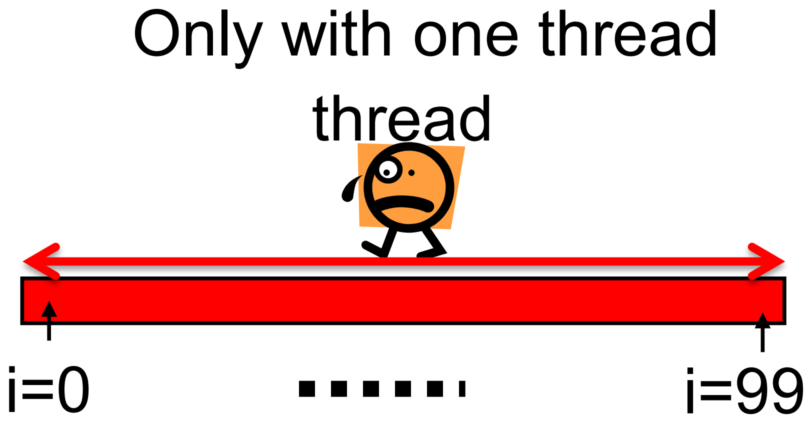
[make sure that there is an executable file "hello"]

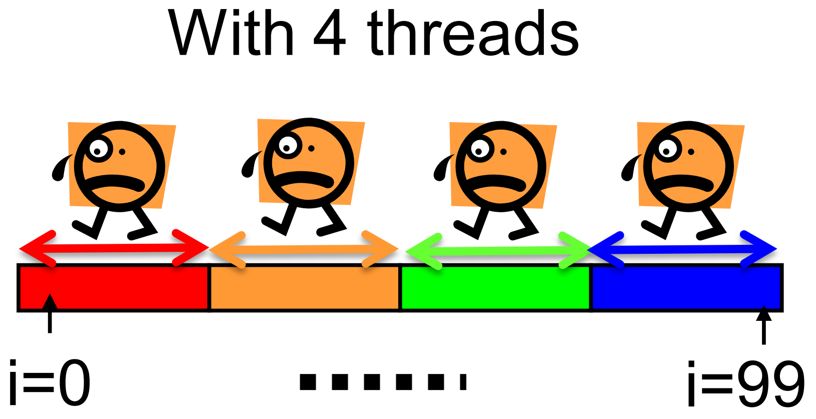
```
export OMP_NUM_THREADS=1
./hello

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





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; …

OpenMP has a syntax to do this smartly

#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

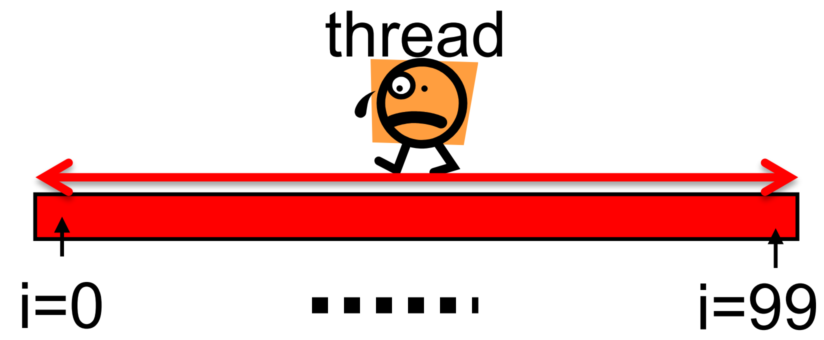
→ Computations in the loop are distributed among threads (work distribution)

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

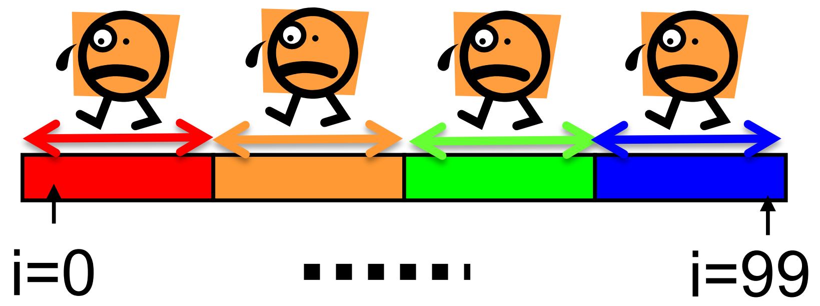
- Abbreviation: omp parallel + omp for = omp parallel for

Why "omp for" Reduces Execution Time

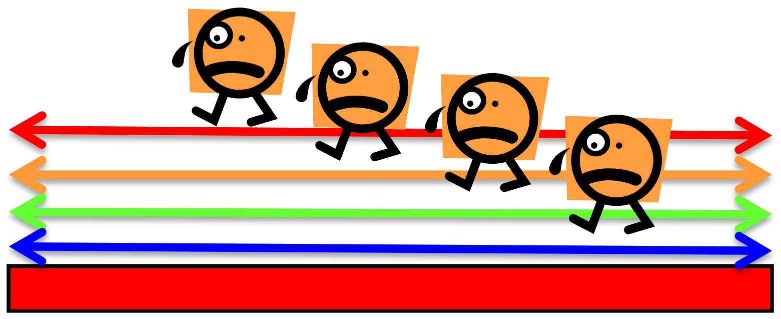
Only with one thread



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

Available at /gs/hs1/tga-ppcomp/22/mm/

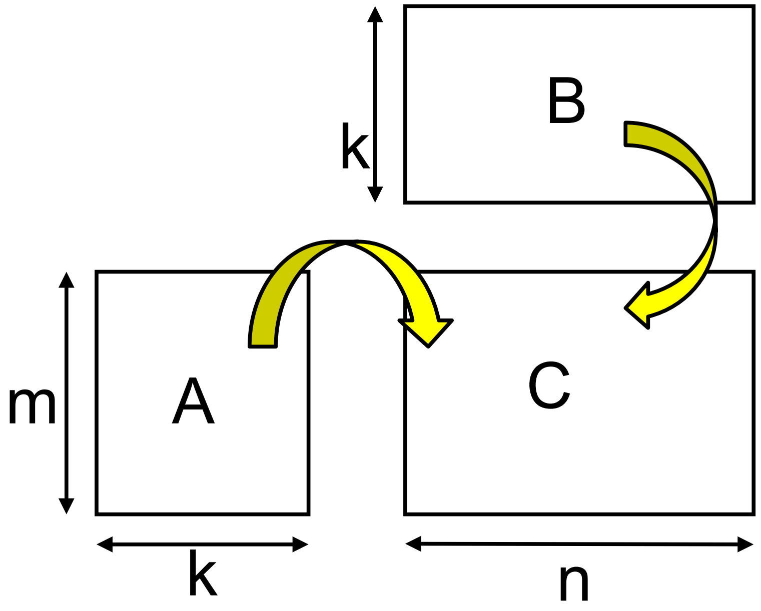
A: a $(m \times k)$ matrix

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]



```
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];
        } }  }
```

OpenMP Version of mm (mm-omp)

- There are 3 loops. Here, 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

In default, variables are classified as follows

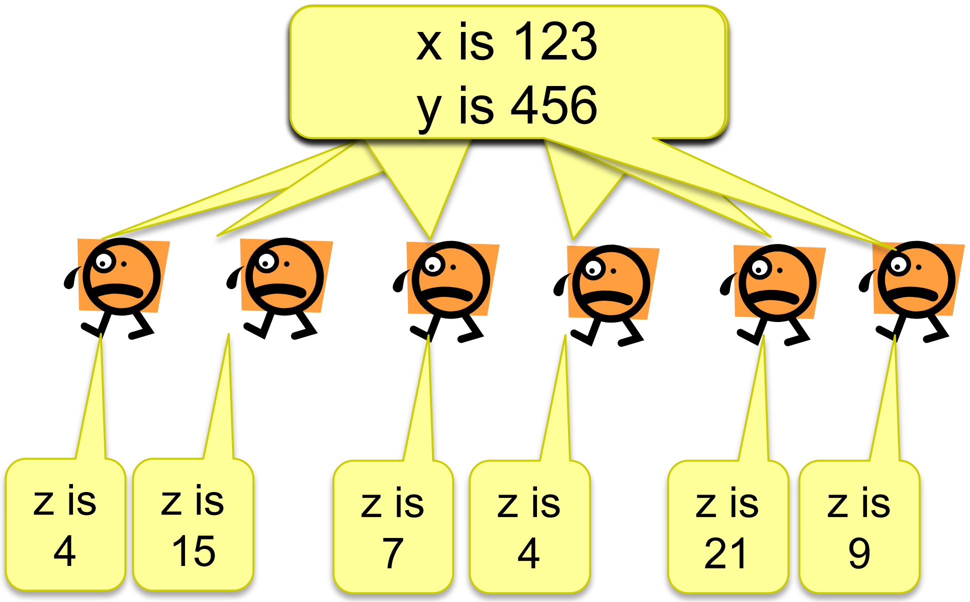
- Variables declared out of parallel region ⇒ Shared variables
- Global variables ⇒ Shared variables
- Variables declared inside parallel region ⇒ Private variables

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

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

Shared Variables & Private Variables (2)

We let *x*, *y* be shared, and *z* be private



Single instance for each x, y

Each thread has its own instance for z

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

Pitfall in Nested Loops (1)

- The following sample looks ok, but there is 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

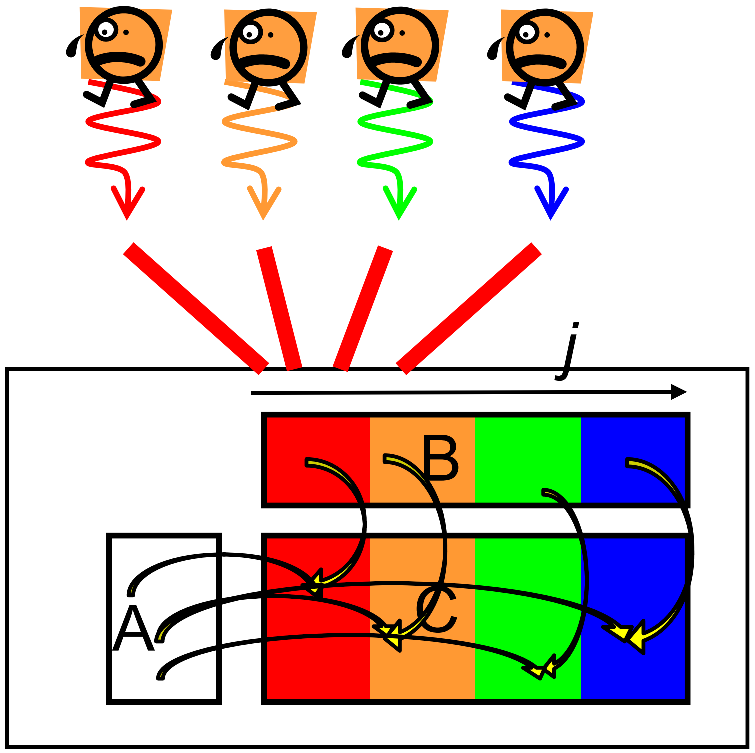
Pitfall in Nested Loops (2)

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++) {
      …
    } }
```

How Arrays are Accessed



- In mm sample, pointers A, B, C are global variables ➔ shared variables
- Since all threads see same variables of A, B, C, contents of arrays are also shared
- It is programmers responsibility to make each thread does independent computation

OpenMP Version of mm (Again)

- One of loops is parallelized

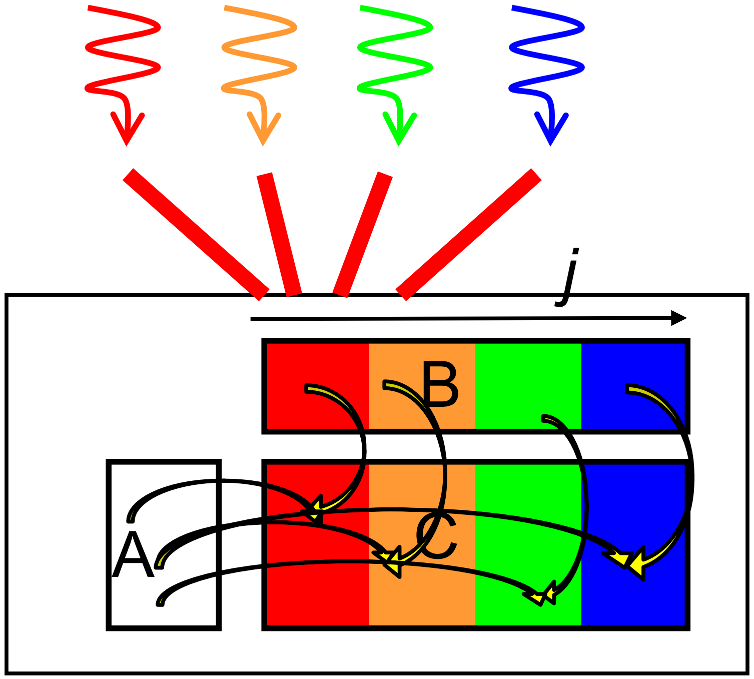
```
#pragma omp parallel private(i,l)
#pragma omp for
    for (j = 0; j < n; j++) {
        for (l = 0; l < k; l++) {
            for (i = 0; i < m; i++) {
                C[i+j*ldc] += A[i+l*lda] * B[l+j*ldb];
            } }  }
```

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

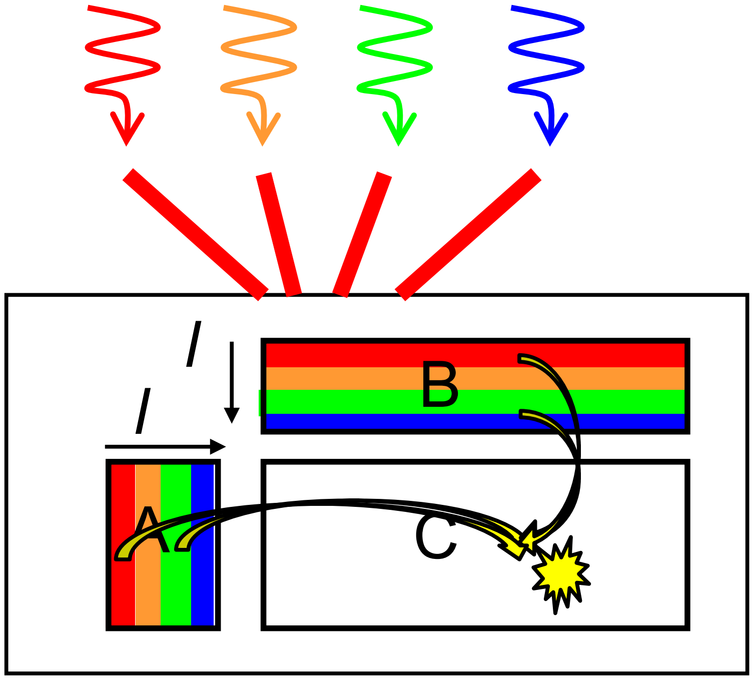
Parallelizing j loop



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 !!

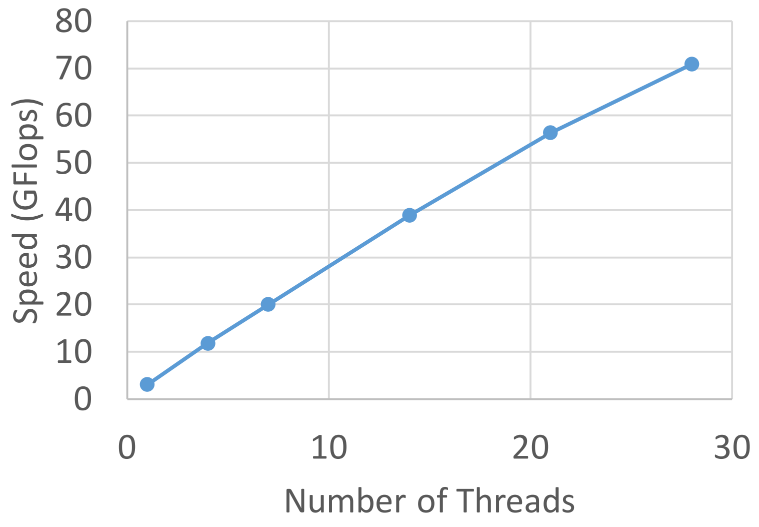
Performance of mm-omp sample

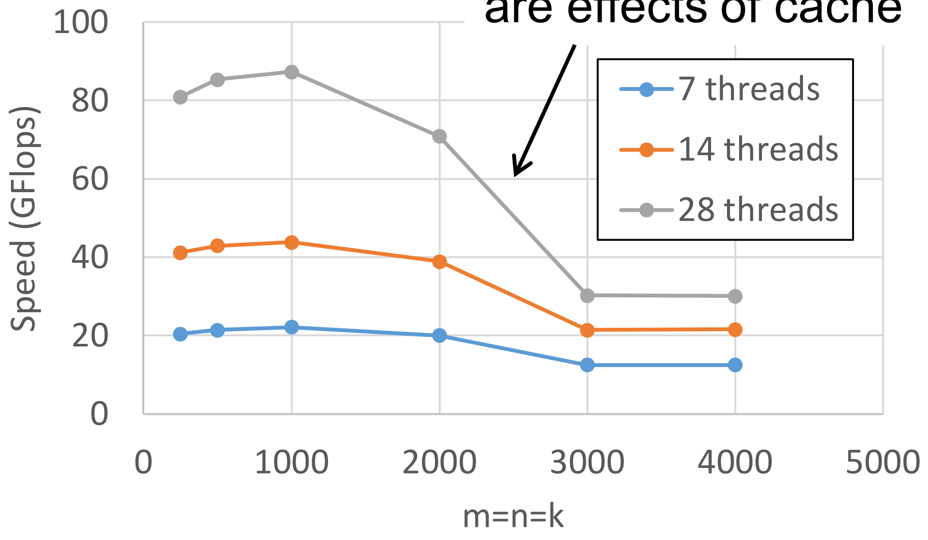
- On a TSUBAME3 f-node (28 cores)
- export OMP_PROC_BIND=SPREAD is done for stable performance
- Speed is (2mnk/t)

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

8 threads,
Varying m=n=k

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



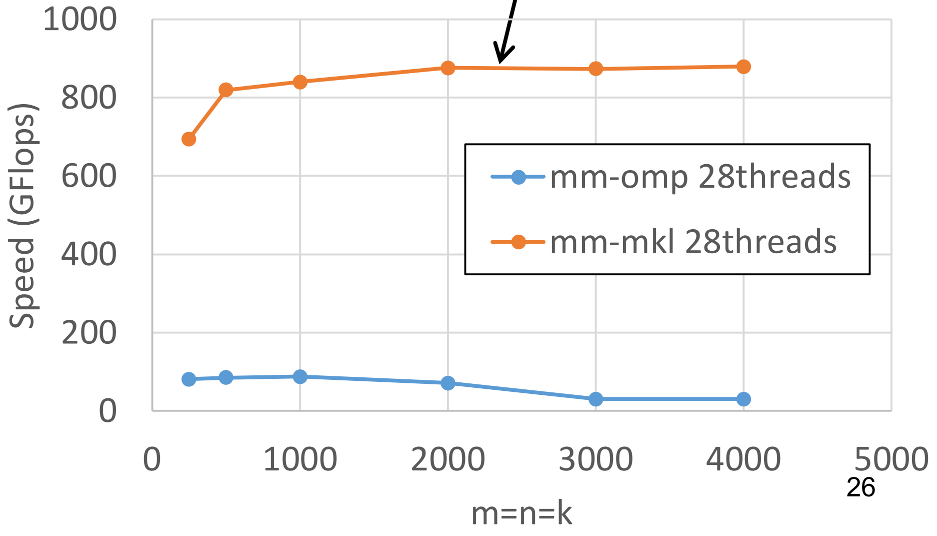


FYI: Optimized Library

- 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 Matrix multiply in MKL

```
cd ~/t3workspace
cp -r /gs/hs1/tga-ppcomp/22/mm-mkl  .
cd mm-mkl
module load intel
make
export OMP_NUM_THREADS=7
./mm 2000 2000 2000
```

MKL is very fast and stable
It uses SIMD, cache blocking, etc.



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

Part 1
OpenMP
[O1] diffusion
[O2] sort
[O3] free
Select 1 problem

Part 2
GPU
[G1]
[G2]
[G3]
Select 1 problem

Part 3
MPI
[M1]
[M2]
[M3]
Select 1 problem

Select 2 parts

Assignments in OpenMP Part (1)

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

Due date: May 12 (Thu)

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

(/gs/hs1/tga-ppcomp/22/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/22/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

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:

- Part1: OpenMP (2)
  - diffusion： simple simulation of diffusion phenomena
    - Related to assignment [O1]