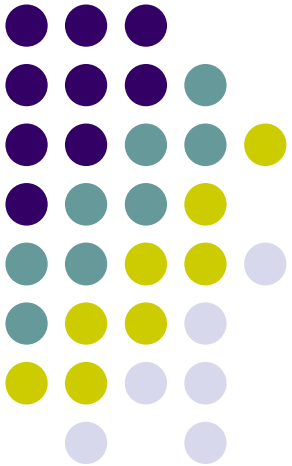
2018 Practical Parallel Computing (実践的並列コンピューティング) No. 3

Shared Memory Parallel Programming with OpenMP (1)



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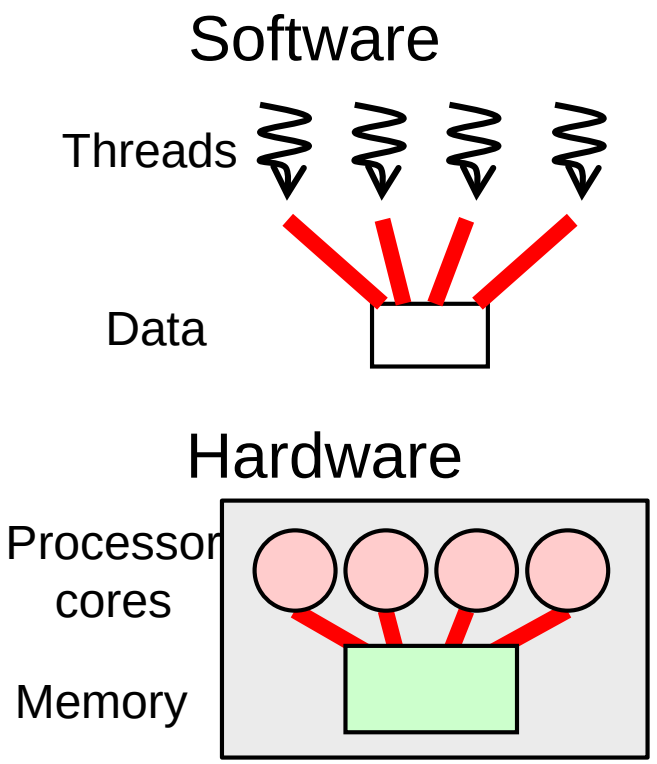
Features of OpenMP

- Parallel programming API based on shared memory model
  - Only one compute node can be used
  - On TSUBAME3.0, up to 28cores
- Extensions to C/C++/Fortran
  - Famous compilers support OpenMP!
  - You'll see much information on Web
- Directive syntaxes & library functions
  - Directives look like: #pragma omp ~~
  - (Simpler than MPI in Part2)
- Multiple threads work cooperatively
- Data are basically shared by threads
  - We can use thread-local (private) variables



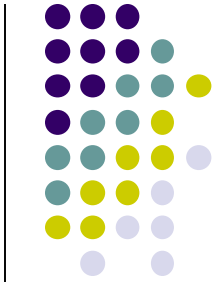
OpenMP Programs Look Like

```
   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



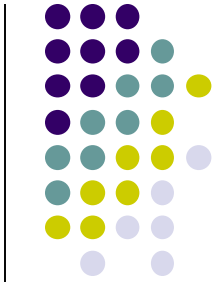
See ~endo-t-ac/ppcomp/18/ on TSUBAME

(1) Copy the following sub-directories to (anywhere in) your own home directory

- Pi (pi, pi-omp)
- Matrix multiply (mm, mm-omp)

(2) Executable binaries are generated by “make” command in each sub-directory

Executions of Samples



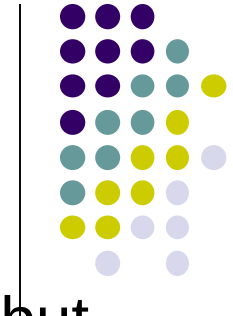
(3-1) Normal (sequential) versions：

- pi
  - ./pi 1000000
- mm
  - ./mm 500 500 500
- diffusion
  - ./diffusion

(3-2) OpenMP versions

- pi-omp
  - export OMP_NUM_THREADS=4 ← number of threads
  - ./pi 1000000
- mm
  - export OMP_NUM_THREADS=4
  - ./mm 500 500 500

Compiling OpenMP Programs



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

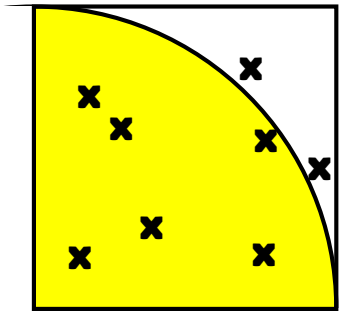
- gcc
  - -fopenmp option in compiling and linking
- PGI compiler
  - module load pgi, and then use pgcc
  - -mp option in compiling and linking
- Intel compiler
  - module load intel, and then use icc
  - -openmp option in compiling and linking

Also see outputs of “make” in OpenMP sample directory

“pi” sample

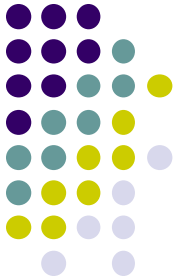
Estimate approximation of π (circumference/diameter) by Monte-Carlo method

- Sequential version in “pi”, OpenMP version in “pi-omp”
- Method
  - Select points in 1x1 square randomly
  - Let PR be probability that a point is included in quarter circle.
    4 x PR → π
- Execution : ./pi [n]
  - n: Number of point selection
- Compute complexity : O(n)



Note: This program is only for a simple sample. π is usually computed by different algorithms.

Submitting a Job to TSUBAME
~ in case of pi sample ~



- Sequential version
  - see pi directory
- OpenMP version
  - see pi-omp directory
  - in the case with 4 threads (4 processor cores)

pi/job.sh

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

./pi 100000000
```

resource type and count

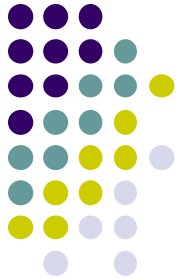
maximum run time

pi-omp/job.sh

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

export OMP_NUM_THREADS=4
./pi 100000000
```

- Job submission
  - qsub job.sh

Notes on Job Submission (1)

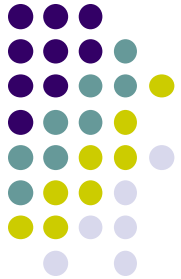


There are several notes since TSUBAME is a shared system

- Please specify resource type properly, according to the number of threads (CPU cores)
  - s_core: 1 core
  - q_core: 4 cores
  - q_node: 7 cores (+ 1GPU)
  - h_node: 14 cores (+ 2GPUs)
  - f_node: 28 nores (+ 4GPUs)

  For detail, see TSUBAME3.0 User's Guide (利用の手引き) Section 4.1

Notes on Job Submission

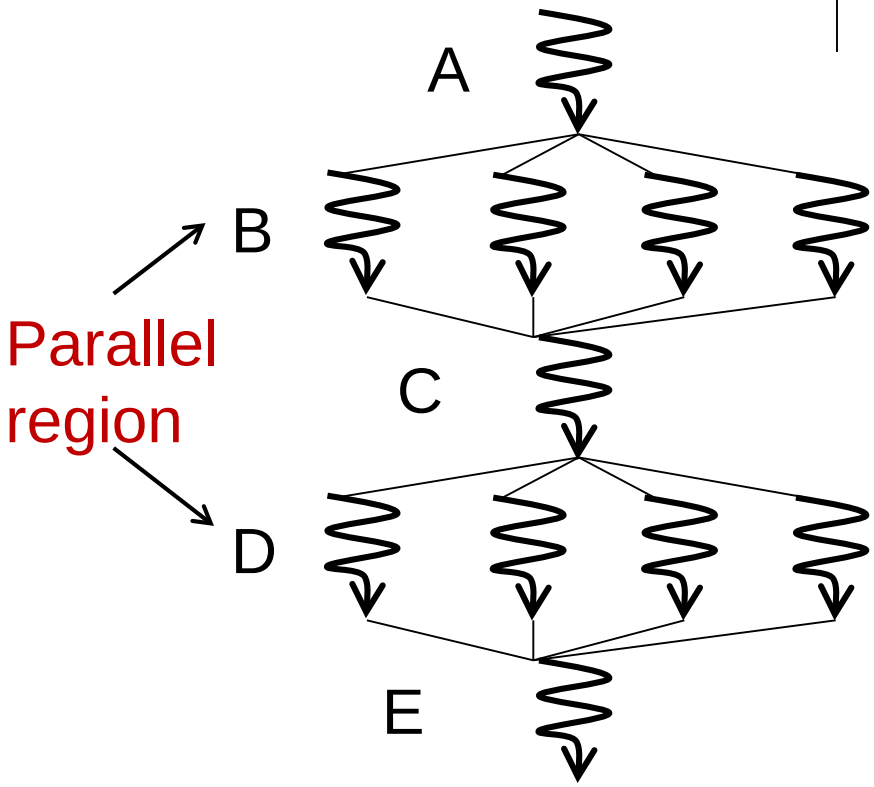


- Please specify maximum run time (h_rt) properly
  - If h_rt is larger than 0:10:00, you need to specify “TSUBAME group name” for accounting (charged/有料)

    qsub –g tga-ppcomp job.sh
  - Use tga-ppcomp group only for this lecture / tga-ppcompグループは、本授業の課題とそのテスト専用に使ってください
- Please do not execute CPU intensive programs on login nodes
  - It is OK to edit programs, compile programs, and submit jobs, and so on
  - “qrsh” may help you. See Section 4.3 in User’s Guide

Basic Parallelism in OpenMP: Parallel Region

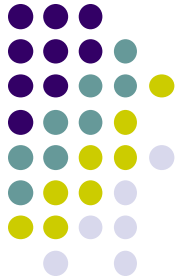
```
#include <omp.h>

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

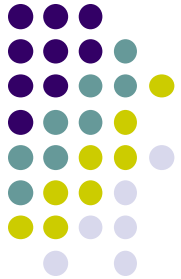
- Here a “block” is a region surrounded by braces {}
- Functions called from parallel region are also in parallel region

Number of Threads



- Specify number of threads by OMP_NUM_THREADS environment variable (out of program)
  - cf) export OMP_NUM_THREADS=4
    in command line
- 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)

#pragma omp for for Easy Parallel Programming



"for" loop with simple forms can parallelized easily

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

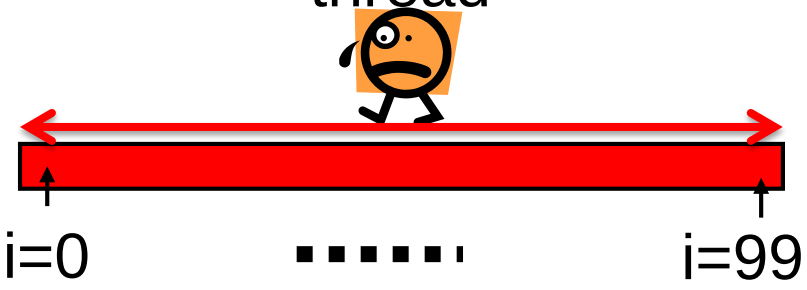
- "for" loop right after "omp for" is parallelized, with work distribution

- When this sample is executed with 4 threads, each thread take 100/4=25 iterations → speed up!!
  - Indivisible cases are ok, such as 7 threads

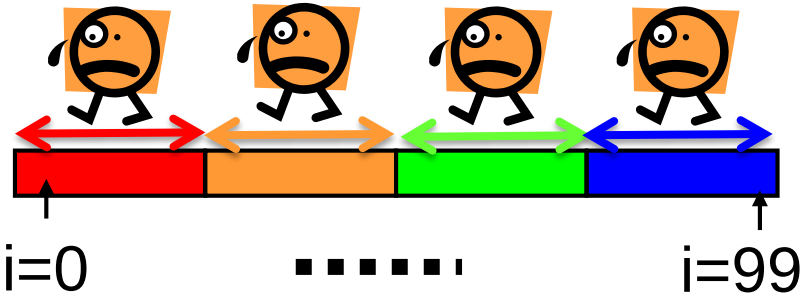
- Abbreviation: omp parallel + omp for = omp parallel for

Why “omp for” Reduces Execution Time

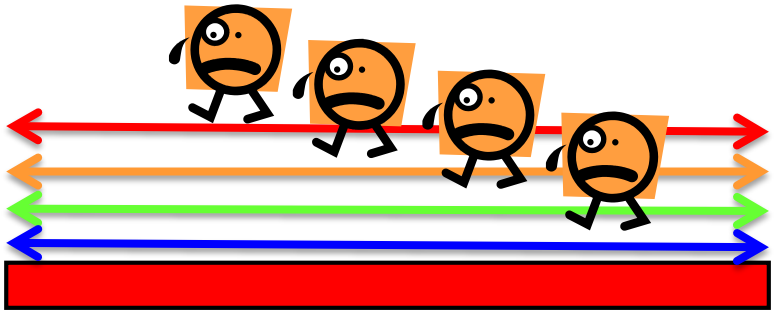
Without OpenMP thread



With “omp parallel” & “omp for”

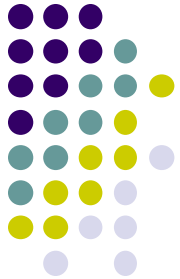


- What if we use “omp parallel”, but forget to write “omp for”?



Every thread would work for all iterations
→ No speed up ☹
→ Answer will be wrong ☹

When We Can Use “omp for”



- Loops with some (complex) forms cannot be supported, unfortunately ☹
- The target loop must be in the following form

```
#pragma omp for
  for (i = value; i op value; incr-part)
    body
```

“*op*” : <, >, <=, >=, etc.
“*incr-part*” : i++, i--, i+=c, i-=c, etc.

OK ☺: for (x = n; x >= 0; x-=4)
NG ☹: for (i = 0; test(i); i++)
NG ☹: for (p = head; p != NULL; p = p->next)

Advanced Topic on “omp for” (1): reduction

- Typical code pattern in for loop: Aggregate result of each iteration into a single variable, called reduction variable
  - cf) We add +1 to “count” variable in pi-omp sample
  - For such cases, “reduction” option is required

```
   int count = 0;
#pragma omp parallel
   {
#pragma omp for reduction (+:count)
     for (i = 0; i < 100; i++) {
        count += f(i);
     }
   }
```

Operator is one of +, -, *, &&, ||, etc

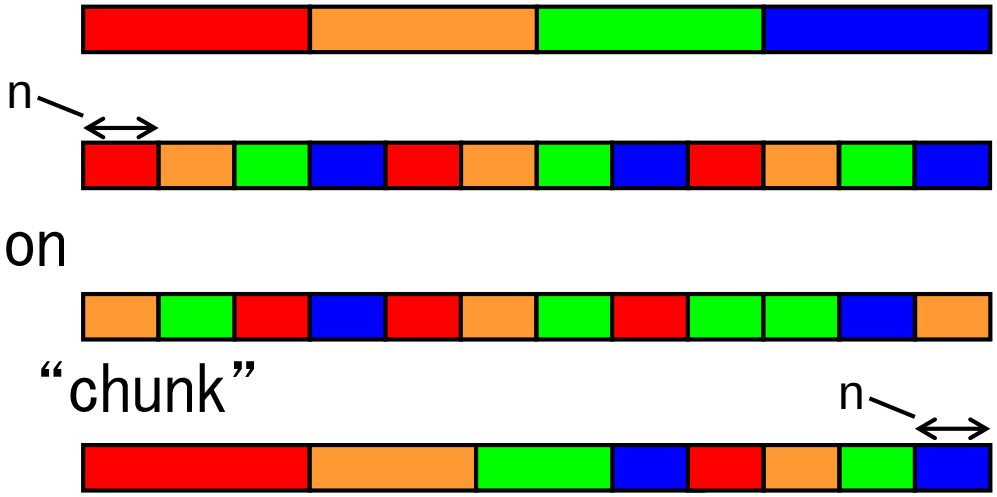
Name of reduction variable

If we forget to write “reduction” option → The answer would be wrong

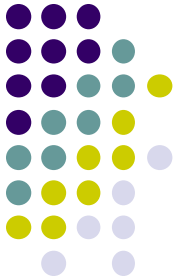
Advanced Topic on “omp for” (2): schedule

- Usually, each thread takes iterations uniformly
  - cf) 1000 iterations / 4 threads = 250 iteration per thread
- For some computations (execution times per iteration are varying), the default schedule may degrade performance
  `#pragma omp for schedule(･･･)` may improve

- `schedule(static)`
  uniform (default)
- `schedule(static, n)`
  block cyclic distribution
- `schedule(dynamic, n)`
  idle thread takes next “chunk”
- `schedule(guided, n)`
  “chunk” size gets smaller as the advance



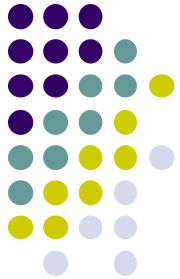
Time Measurement in Samples



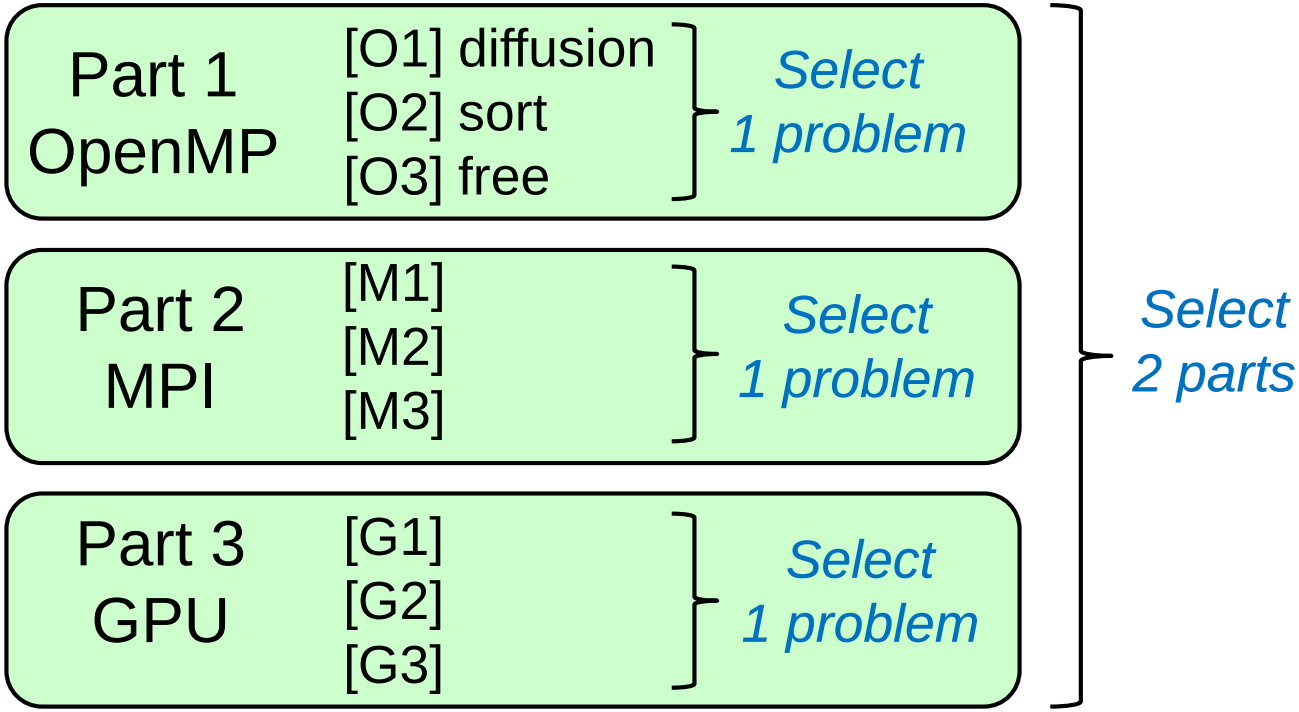
- gettimeofday() function is used
  - It provides wall-clock time, not CPU time
  - Time resolution is better than clock()

```
#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 */
}
```

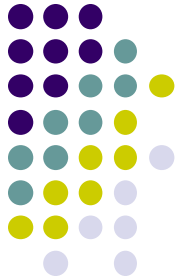
Assignments in this Course



- There is homework for each part. Submissions of reports for 2 parts are required
- Also attendances will be considered



Assignments in OpenMP Part (1)



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

Due date: May 7 (Monday)

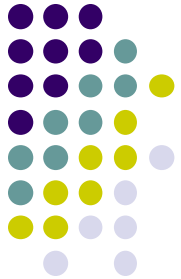
[O1] Parallelize “diffusion” sample program by OpenMP.

(~endo-t-ac/ppcomp/18/diffusion/ on TSUBAME)

Optional:

- Make array sizes variable parameters, which are specified by execution options. “malloc” will be needed.
- Improve performance further. Blocking, SIMD instructions, etc, may help.

Assignments in OpenMP Part (2)



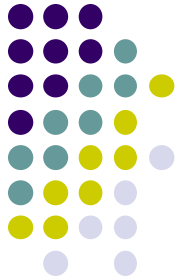
[O2] Parallelize “sort” sample program by OpenMP.

(~endo-t-ac/ppcomp/18/sort/ on TSUBAME)

Optional：

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

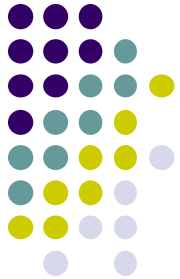
Assignments in OpenMP Part (3)



[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 Submission



- Submit the followings via OCW-i

  (1) A report document
  - A PDF or MS-Word file
  - 2 pages or more
  - in English or Japanese (日本語もok)

  (2) Source code files of your program
- Report 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 processor cores
    - With varying problem sizes
    - Discussion with your findings
    - Other machines than TSUBAME are ok, if available

Next Class:

- OpenMP(2)
  - mm: matrix multiply sample
  - diffusion : heat diffusion sample using stencil computation
    - Related to assignment [O1]