2019
Practical Parallel Computing
(実践的並列コンピューティング)
No. 4

Shared Memory Parallel Programming with OpenMP (2)

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“mm” sample: Matrix Multiply

Available at ~endo-t-ac/ppcomp/19/mm/

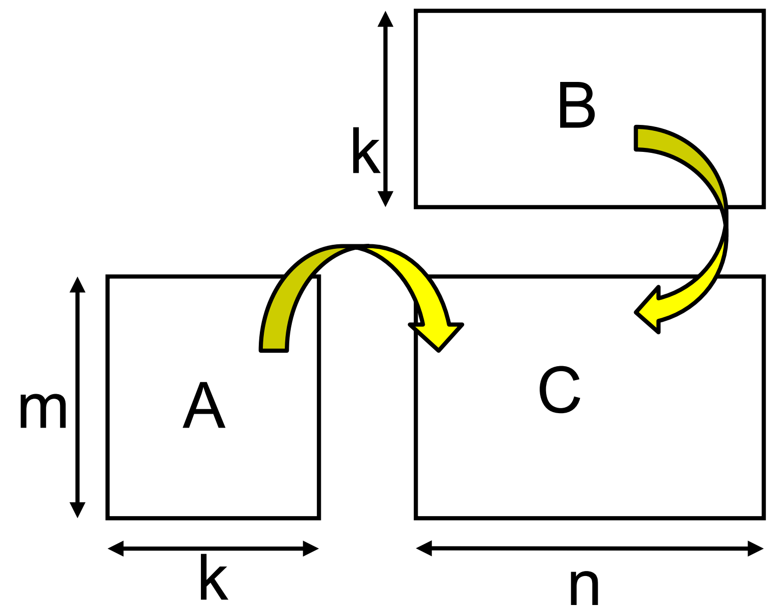
A: a (m × k) matrix, B: a (k × n) matrix

C: a (m × n) matrix

$C \leftarrow A \times B$

- Algorithm with a triple for loop
- Supports variable matrix size.
  - Each matrix is expressed as a 1D array by *column-major* format

- Execution: ./mm [m] [n] [k]



Matrix Multiply Algorithm

```
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) calculation

- [Q] What if loop order is changed?
  - IJL order in above. JLI order in mm sample
  - Number of operations does not change. But how is the speed?

Variable Length Arrays in (Classical) C Language

- int a[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

```
int a[5];

… a[i] can be used …
```

A variable length array

```
int *a;
a = (int *)malloc(sizeof(int)*n);

… a[i] can be used …

free(a);
```

array length (→ n)

※ Exceptionally, C99 specification includes variable length arrays

How We Do for Multiple Dimensional Arrays

int a[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

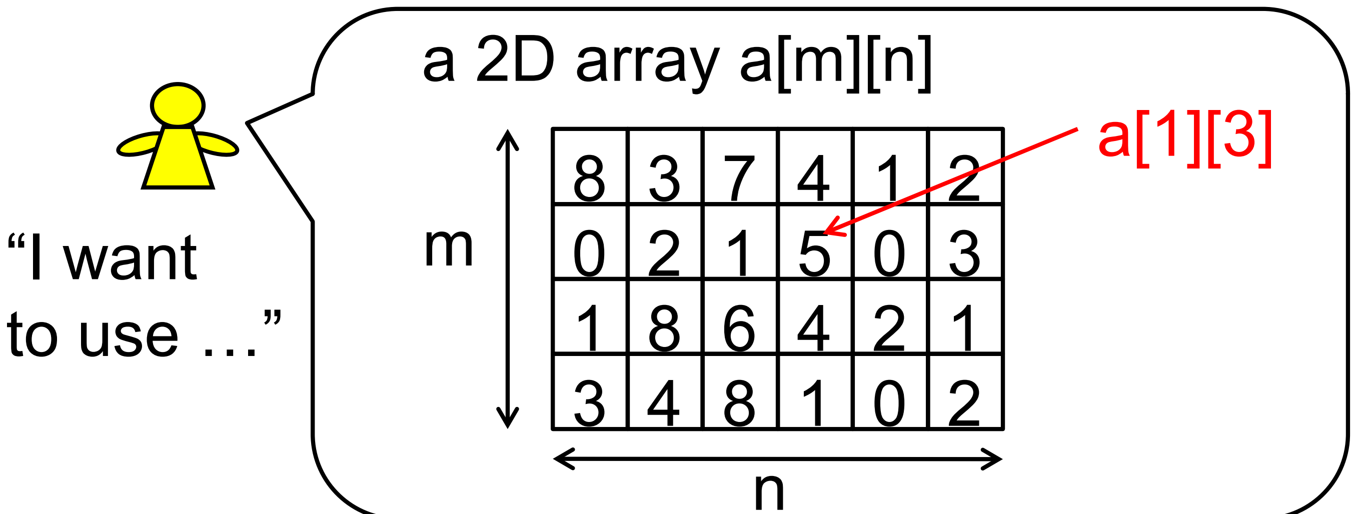
- We *malloc* m 1D arrays for every row (each has n length)
- We malloc 1D array of m length to store the above pointers

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

(mm sample uses this method)

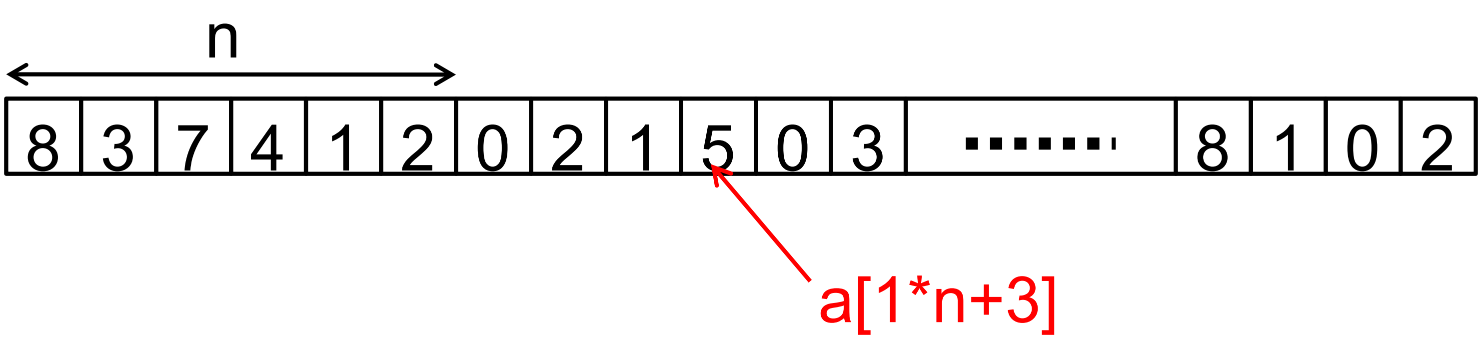
- To access an array element, we should use a[i*n+j] or a[i+j*m], instead of a[i][j]

Express a 2D array using a 1D array



Expressions in C language

int *a;   a = malloc(sizeof(int)*m*n);

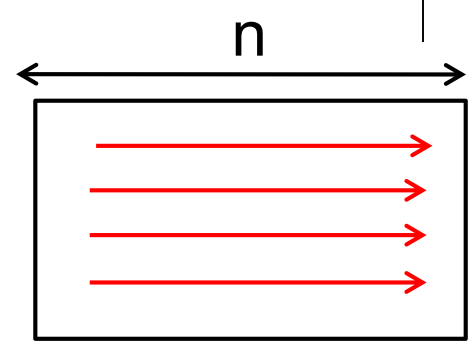


In this case, an element $a_{i,j}$ is a[i*n+j]

Two Data Formats

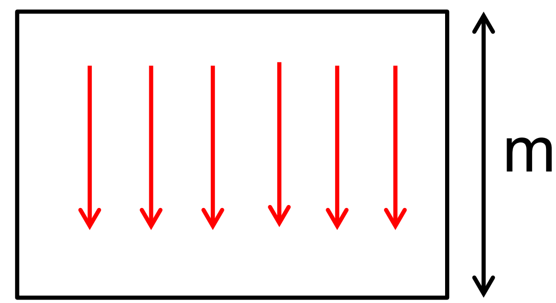
<u>Row major format</u>
- More natural for C programmers

$a_{i,j} \Rightarrow a[i*n+j]$



<u>Column major format</u>
- BLAS library
- mm sample

$a_{i,j} \Rightarrow a[i+j*m]$



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

[Q] Does the format affect the execution speed?

OpenMP Version of mm (mm-omp)

- One of loops is parallelized

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

What is “private” option for?

Shared Variables & Private Variables (1)

While OpenMP uses “shared memory model”, not all are shared

In default, variables are classified as follows

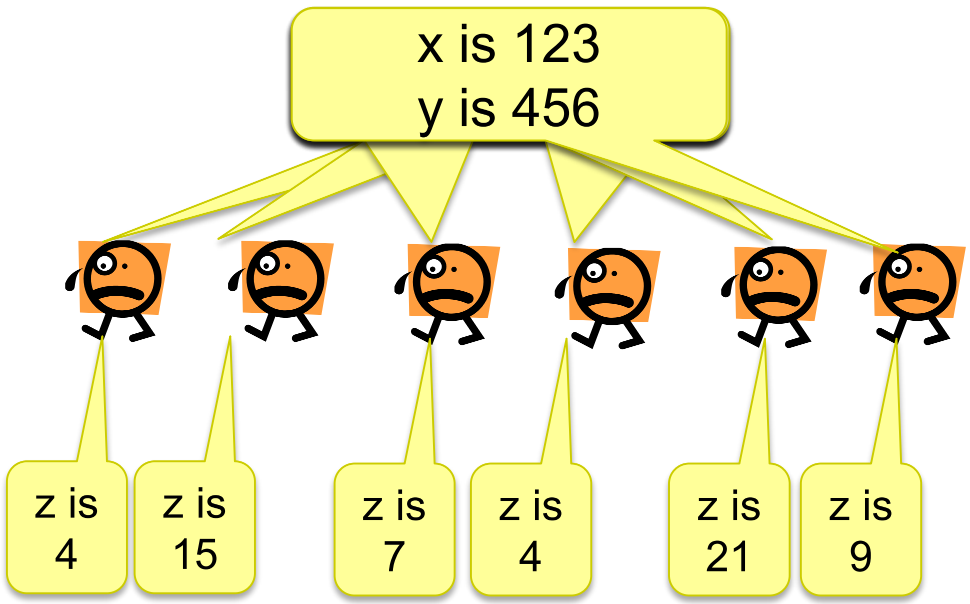
- Variables declared out of parallel region ⇒ Shared variables
- Variables declared inside parallel region ⇒ Private variables

```
{
    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)

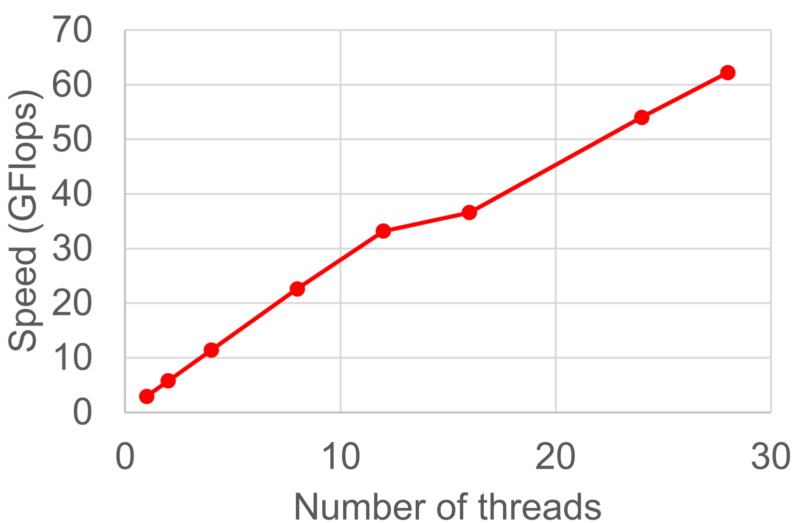
```
  int i;
#pragma omp parallel for
  for (i = 0; i < m; i++) {
    int j;    // j is private
    for (j = 0; j < n; j++) {
      ...
    } }
```

```
  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++) {
      ...
    } }
```

Performance of mm sample

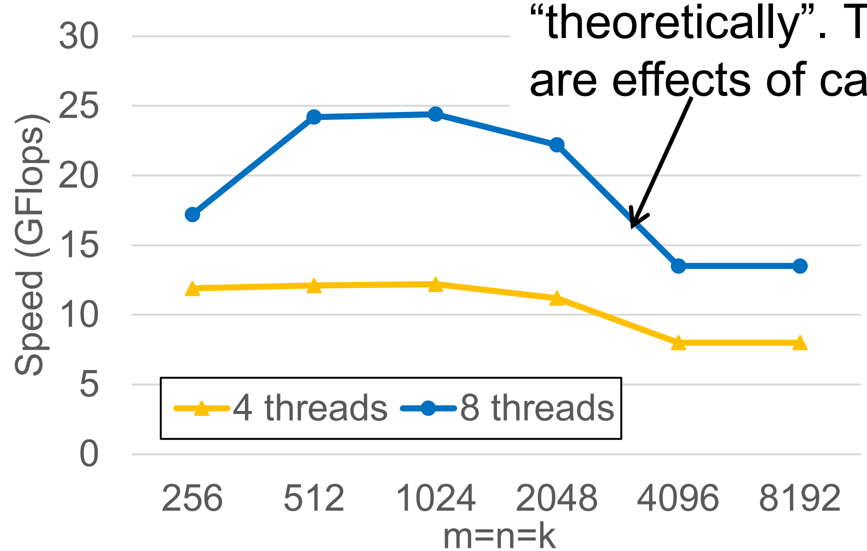
- A TSUBAME3 node (Xeon E5-2680 v4 x2 = 28core)
- Speed is (2mnk/t)

m=n=k=2048,
Varying # of threads



8 threads,
Varying m=n=k

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



OpenMP Version of mm (Again)

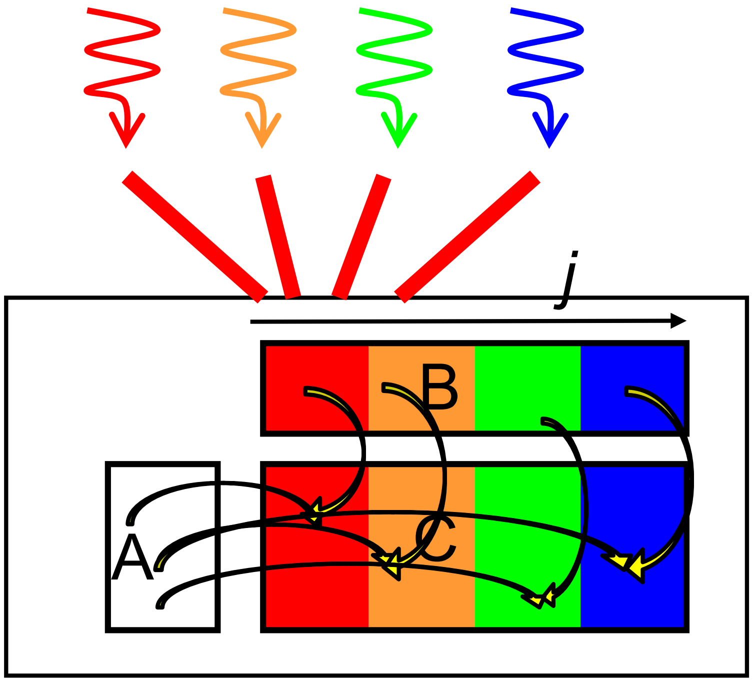
- One of loops is parallelized

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

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

How Multiple Threads Work

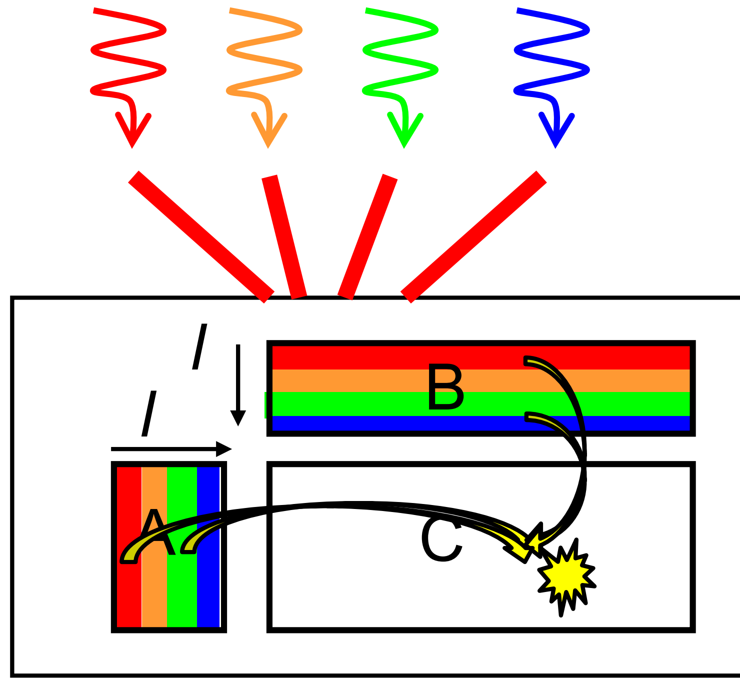
Parallelizing j loop



Simultaneous read
(in this case, A) is OK

Similarly, parallelizing
i loop is ok

Parallelizing l loop (??)



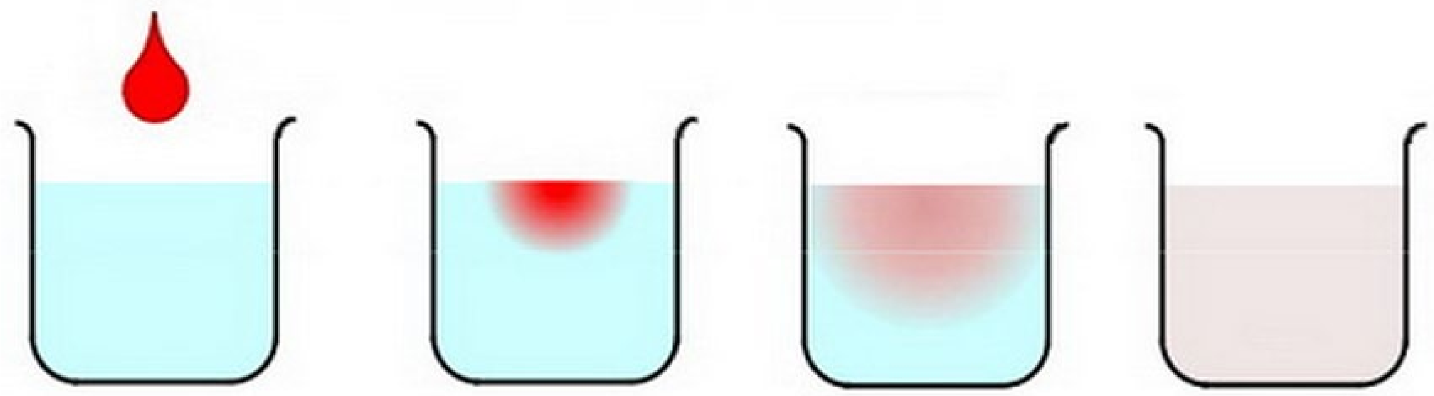
Possible simultaneous write
→ “Race condition” problem
may occur.

Answers may be wrong !!

“diffusion” Sample Program (1)

An example of diffusion phenomena:

- Pour a drop of ink into a water glass



The ink spreads gradually, and finally the density becomes uniform (Figure by Prof. T. Aoki)

- Density of ink in each point vary according to time → Simulated by computers
  - cf) Weather forecast compute wind speed, temperature, air pressure…

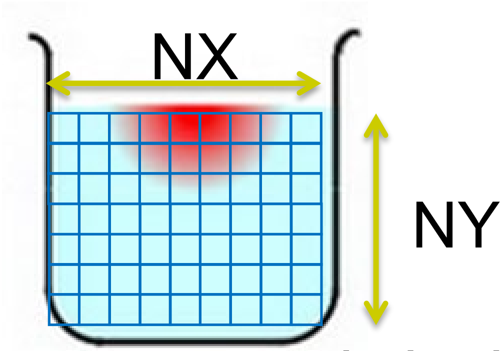
“diffusion” Sample Program (2)

Available at ~endo-t-ac/ppcomp/19/diffusion/

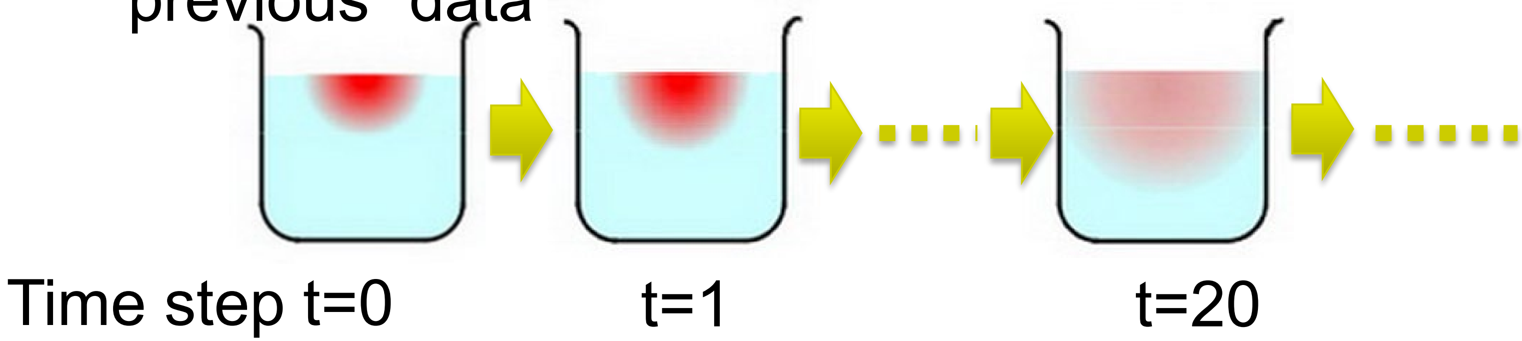
- Execution：./diffusion [nt]
- nt: Number of time steps
- nx, ny: Space grid size
  - nx=8192, ny=8192 (Fixed. See the code)
  - How can we make them variables? (See mm sample)
- Compute Complexity：O(nx × ny × nt)

Data Structures in diffusion

- Space to be simulated are divided into grids, and expressed by arrays (2D in this sample)

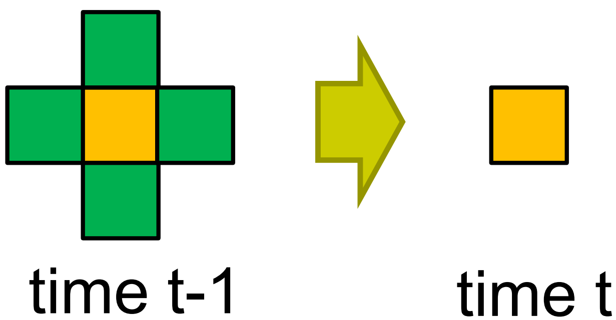


- Array elements are computed via timestep, by using "previous" data



Stencil Computations

- A data point (*x*,*y*) at time *t* is computed using following data at time *t-1* (previous data)
  - point (*x*,*y*)
  - "Neighbor" points of (*x*,*y*)



Points at boundary require special treatments

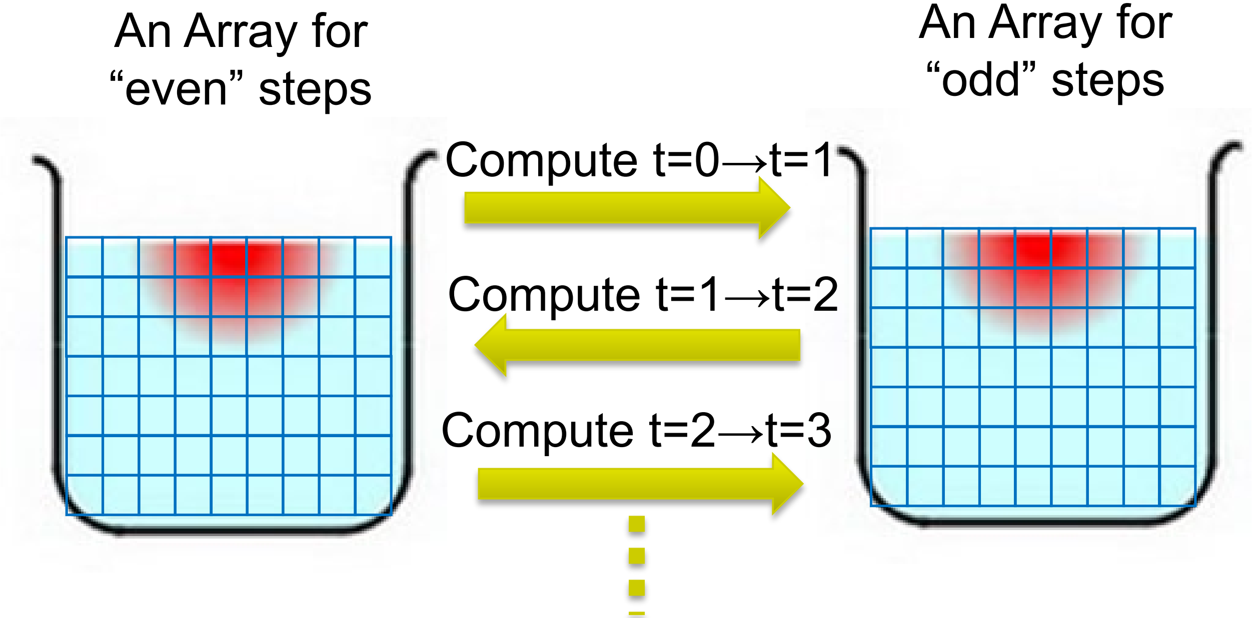
Original meanings of "stencil"

- Computations of similar type is called "stencil computation"
- The followings must be given beforehand
  - All data at time step 0 (Initial condition)
  - Data in "boundary" points for every time step (Boundary condition)

Double Buffering Technique

- A simple way is to make arrays for all time steps, but it consumes too much memory!

→ It is sufficient to have “current” array and “previous” array. “Double buffers” are used for many times



※ Sample program uses a global variables
float data[2][NY][NX];

How We Parallelize “diffusion” sample (Related to Assignment [O1])

- The program mainly uses “for” loops. So “omp parallel for” looks good.

- There are 3 (t, x, y) loops. Which should be parallelized?

[Hint] Parallelizing one of spatial (x, y) would be good. Spaces are divided into multiple threads

[Q] Parallelizing t loop is a not good idea. Why?

Assignments in OpenMP Part (Abstract)

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

Due date: May 9 (Thursday)

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

(~endo-t-ac/ppcomp/19/diffusion/ on TSUBAME)

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

(~endo-t-ac/ppcomp/19/sort/ on TSUBAME)

[O3] (Freestyle) Parallelize *any* program by OpenMP.

For more detail, please see No.3 slides or OCW-i.

Next Class:

- OpenMP(3)
  - "task parallelism" for programs with irregular structures
  - sort: Quick sort sample
    - Related to assignment [O2]

Information

Lecture

- Slides are uploaded in OCW
  - www.ocw.titech.ac.jp → search “2019 practical parallel computing”
- Assignments information/submission site are in OCW-i
  - Login portal.titech.ac.jp → OCW/OCW-i
- Inquiry
  - ppcomp@el.gsic.titech.ac.jp
- Sample programs
  - Login TSUBAME, and see ~endo-t-ac/ppcomp/19/ directory

TSUBAME

- Official web including Users guide
  - www.t3.gsic.titech.ac.jp
- Your account information
  - Login portal.titech.ac.jp → TSUBAME portal