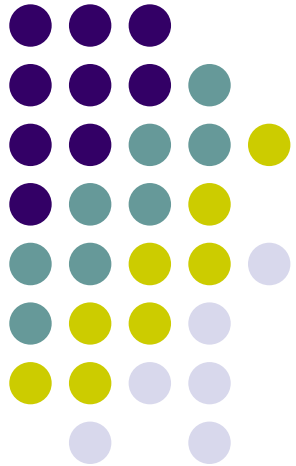
Practical Parallel Computing (実践的並列コンピューティング)

2025 Class No.8
[OpenACC Part] (2)
Discussion on Speed



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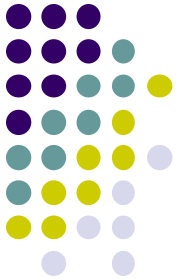
Overview of This Course



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

Note:
Modification to ppcomp-ex github

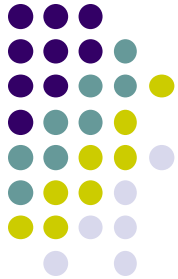
ppcomp-ex/acc/bsort has been missing, and I added it on github

Please update your ppcomp-ex directory

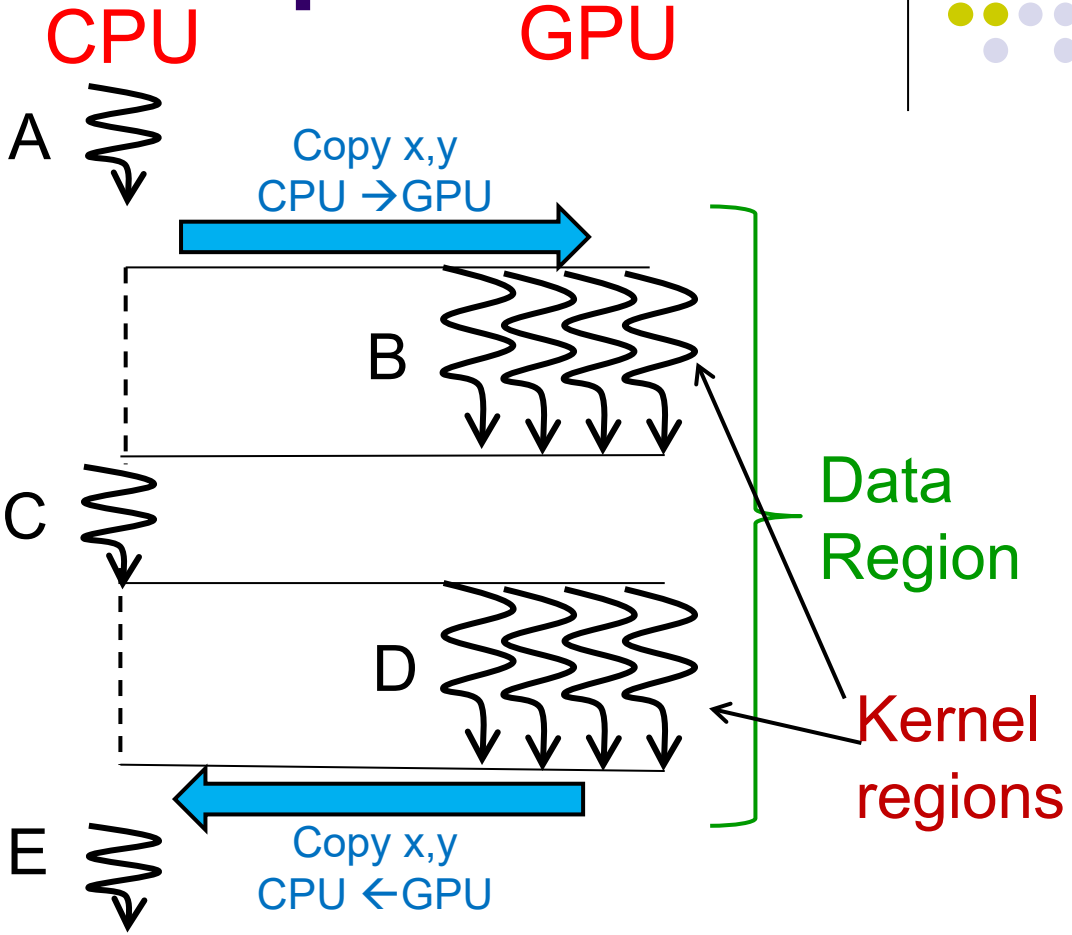
```
cd ppcomp-ex   // your ppcomp-ex directory
git pull
// ➔ acc/bsort/, cuda/sort, mpi/sortis copied
```

Thanks for cooperation

Review: Data Region and Kernel Region in OpenACC

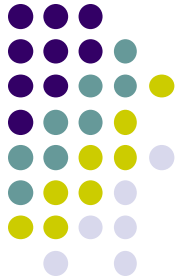


```
int main()
{
    A;
#pragma acc data copy(x,y)
    {
#pragma acc kernels
        {
            B;
        }
        C;
#pragma acc kernels
        D;
    }
    E;
}
```



- Data movement occurs at beginning and end of data region
- Data region may contain 1 or more kernel regions

Review: Loop Directive

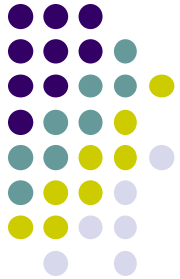


```
   int a[100], b[100], c[100];
   int i;
#pragma acc data copy(a,b,c)
#pragma acc kernels
#pragma acc loop independent
  for (i = 0; i < 100; i++) {
       a[i] = b[i]+c[i];
  }
```

- #pragma acc loop must be included in "acc kernels" or "acc parallel"
- Directly followed by "for" loop
  - The loop must have a loop counter, as in OpenMP
  - List/tree traversal is NG

- … loop independent: Iterations are done in parallel by multiple GPU threads
- … loop seq: Done sequentially. Not be parallelized
- … loop: Compiler decides

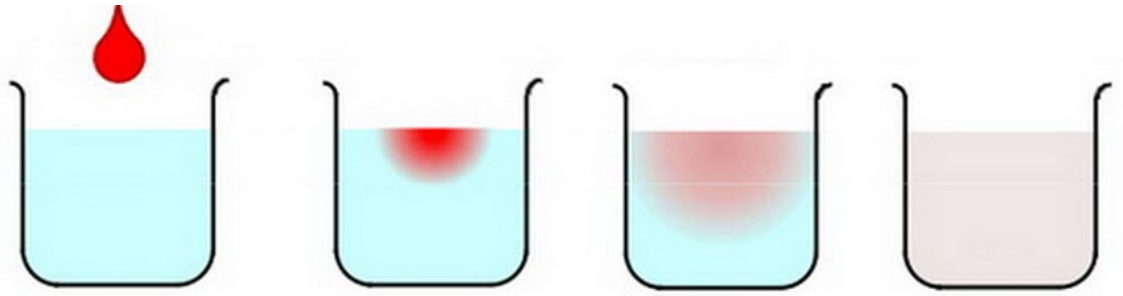
Notes on Assignment [A1][A2]



- You will need compiler options different from the diffusion directory for OpenACC
- You can use files in acc/diffusion or acc/bsort directory as basis
  - .c file is NOT parallelized
  - “Makefile” in these directories supports compiler options for OpenACC
  - Don’t forget “module load nvhpc” before “make”
    - The effect of module is valid until you ‘exit’ from the shell

“diffusion” Sample Program
Target of [A1], details are in ppcomp25-4

An example of diffusion phenomena:

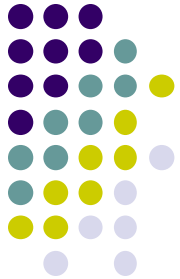


The ink spreads gradually, and finally the density becomes uniform (Figure by Prof. T. Aoki)

Base version: ppcomp-ex/base/diffusion/
You can use ppcomp-ex/acc/diffusion/

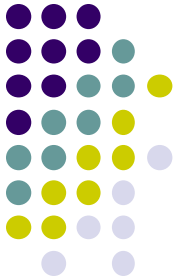
```
cd ppcomp-ex/acc/diffusion
module load nvhpc
make
./diffusion 20      // number of time steps
```

Consideration using OpenACC



- Where do we put #pragma acc loop independent ?
  - Which loops are parallelized?
- Where do we put #pragma acc kernels ?
  - It defines kernel region, executed on the GPU
  - Kernel region has to include “... acc loop”
- Where do we put #pragma acc data ?
  - It defines data region
  - Data touched by GPU must be on device memory
  - Too frequent data copy may decrease program speed

How Can We Parallelizing Diffusion?



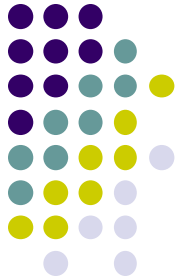
- x, y loops can be parallelized
  - We can use “#pragma acc loop” twice
- t loop cannot be parallelized

```
[Data transfer from CPU to GPU]
for (t = 0; t < nt; t++) {

  for (y = 1; y < NY-1; y++) {
    for (x = 1; x < NX-1; x++) {
          :
    }
  }
}
[Data transfer from GPU to CPU]
```

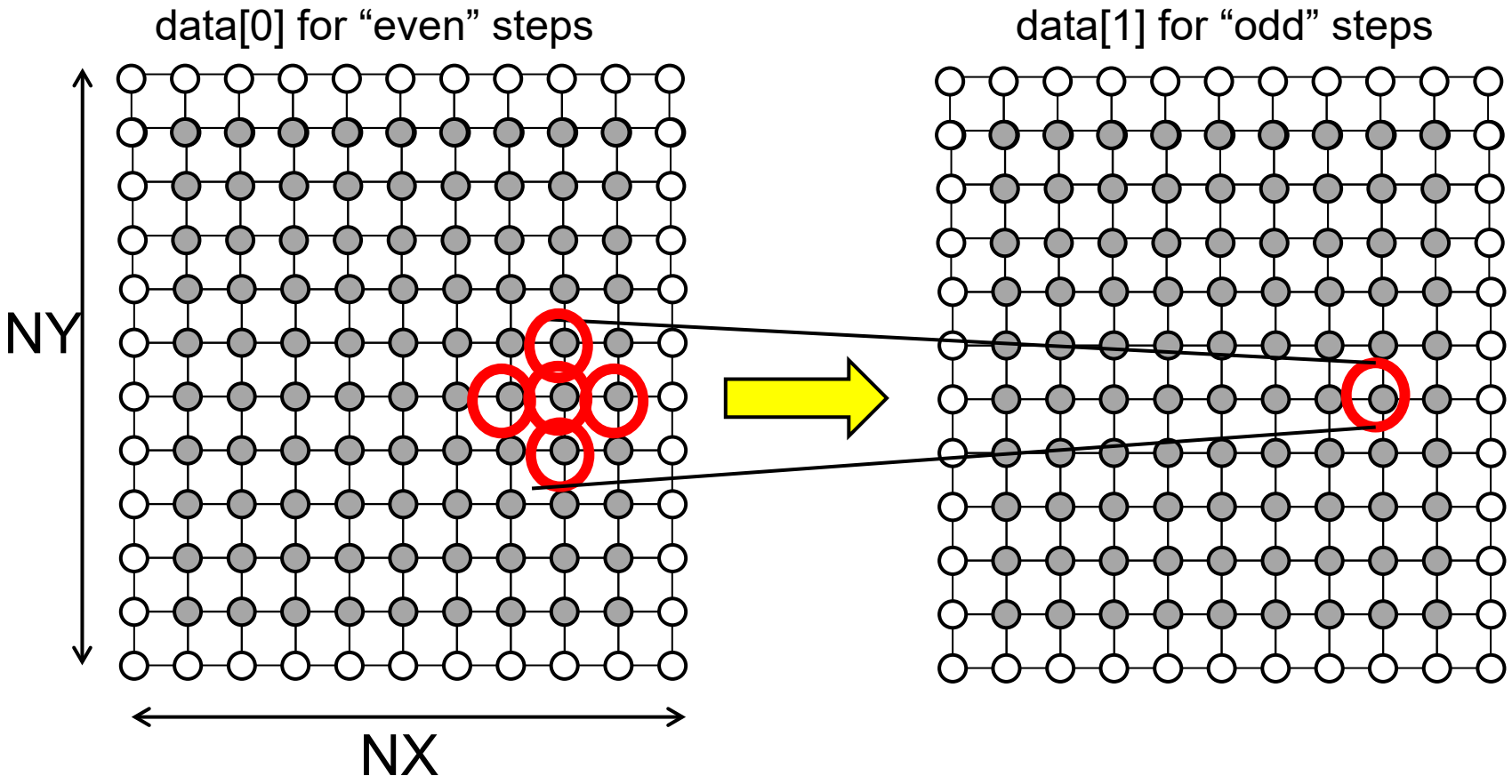
Specify kernel region by
#pragma acc kernels
Parallelize x, y loops by
#pragma acc loop ...

Specify data region by
#pragma acc data ...
➔ It’s better to transfer data *out of* t-loop

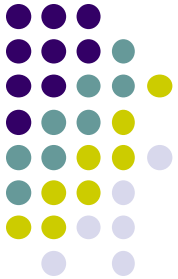
“diffusion” has Multi-Dimension Array



float data[2][NY][NX]; // 2 for double buffering



data Clause for Multi-Dimensional arrays



float A[2000][1000]; → an example of a 2-dimension array

#pragma acc data copy(A)

→ OK, all elements of A are copied

#pragma acc data copy(A[0:2000][0:1000])

→ OK, all elements of A are copied

#pragma acc data copy(A[500:600][0:1000])

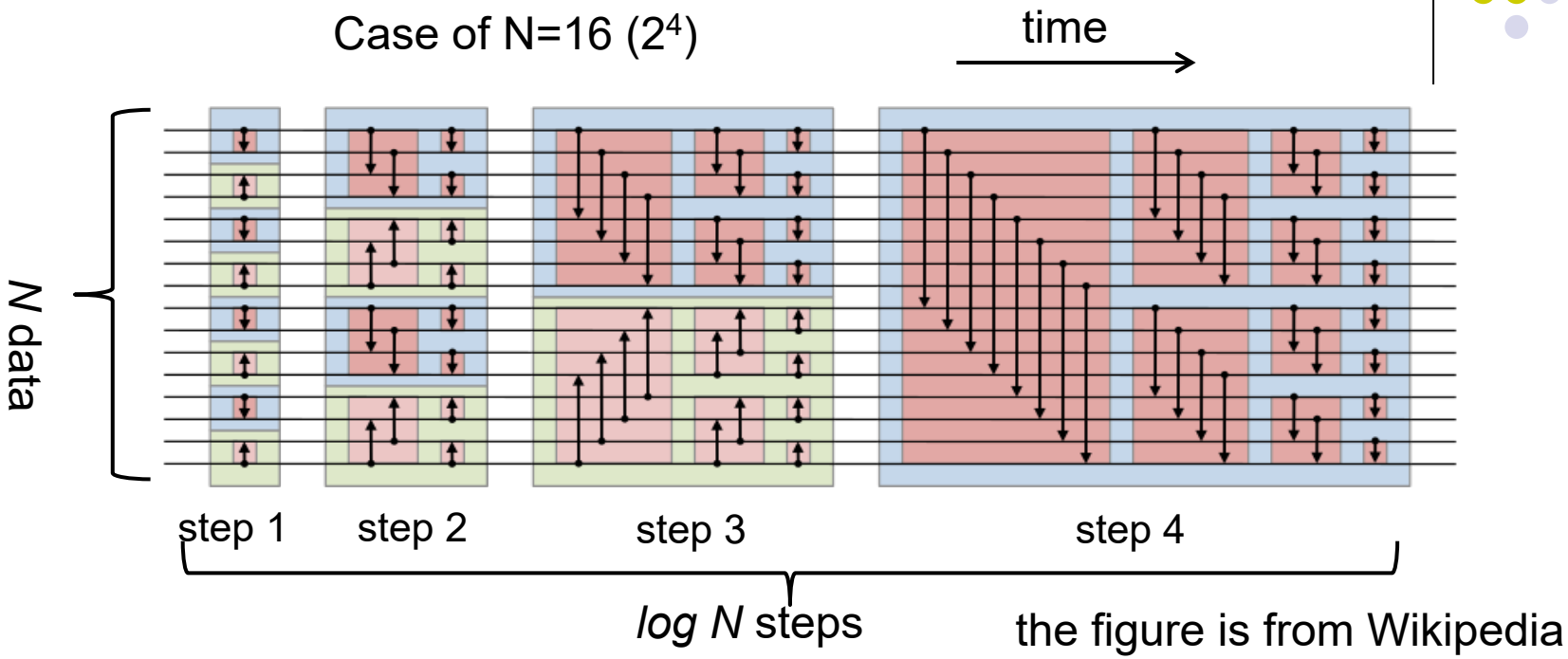
→ OK, rows[500,1100) are copied

#pragma acc data copy(A[0:2000][300:400])

→ Recently OK

“bsort” Sample Program

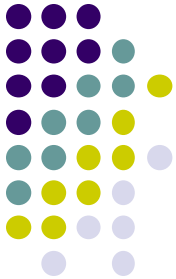
Target of [A2], details are in ppcomp25-4



Base version: ppcomp-ex/base/bsort/
You can use ppcomp-ex/acc/bsort/ (see notes in p.3)

```
cd ppcomp-ex/acc/bsort
module load nvhpc  // if not yet
make
./bsort 1000000 // number of elements to be sorted
```

How Can We Parallelizing bsort?



- k loops can be parallelized
- i, j loops cannot be parallelized

```
for (i = 1; (1<<i) <= N2; i++) { / step loop
  for (j = i-1; j >= 0; j--) { // sub-step loop
    :
    for (k = 0; k < N2; k++) {
        // compare 2 data and swap
    }
 }
}
```

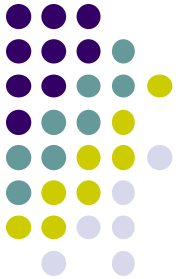
Specify kernel region by
#pragma acc kernels
Parallelize k loops by
#pragma acc loop ...

Next, where should the data region be?

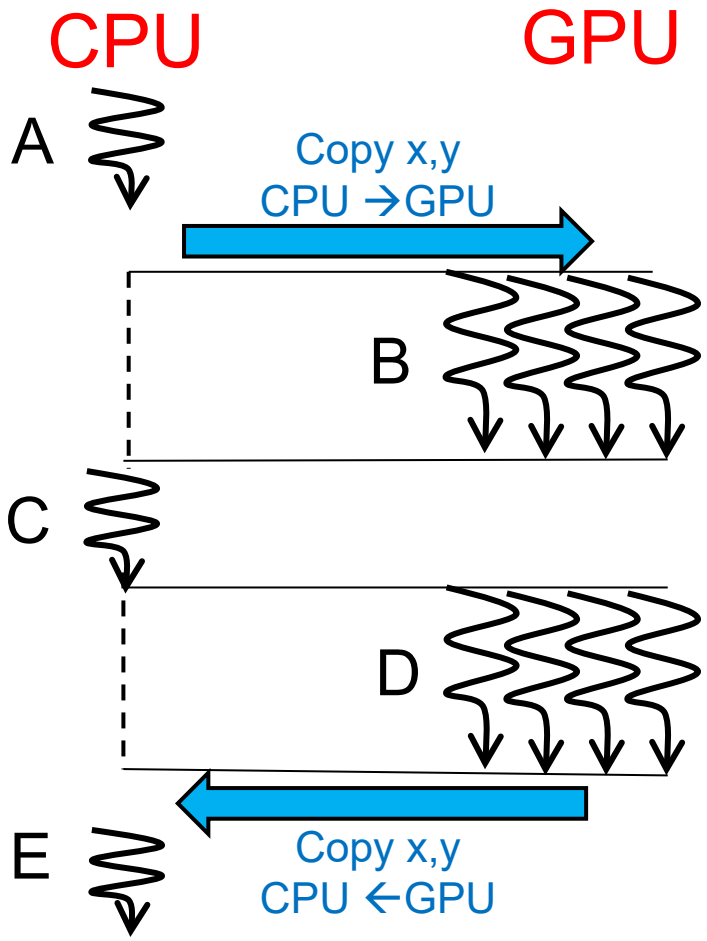
- Please consider reducing data copy cost

Data Transfer Costs in GPU Programming

Related to [A3], also [A1] [A2]



- In GPU programming, data transfer costs between CPU and GPU have impacts on speed
  - Program speed may be slower than expected ☹



from ppcomp25-7 slides

[A3] Evaluate speed of "acc/mm" sample in detail

ppcomp-ex/acc/mm/

- Use various matrices sizes
- Evaluate effects of data transfer cost
- Compare with CPU (OpenMP) version

Optional:

- To use different loop orders
- To change/improve the program
  - Cache blocking?

Speed of GPU Programs:
case of acc/mm

In mm-acc, speed in Gflops is computed by

$S = 2mnk / T_{total}$

T_{total} includes both computation time and transfer

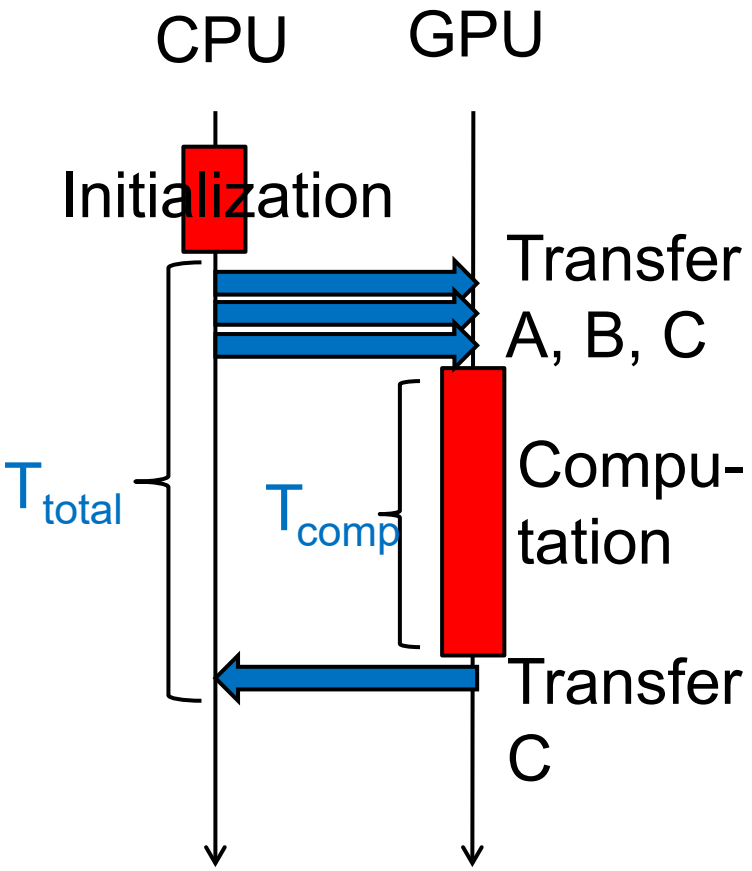
→ S counts slow-down by transfer

To see the effects, let's try another sample

ppcomp-ex/acc/mm-meas/

which outputs time for

- copyin (transfer A, B, C)
- computation
- copyout (transfer C)



In [A3], please evaluate effects of transfer costs

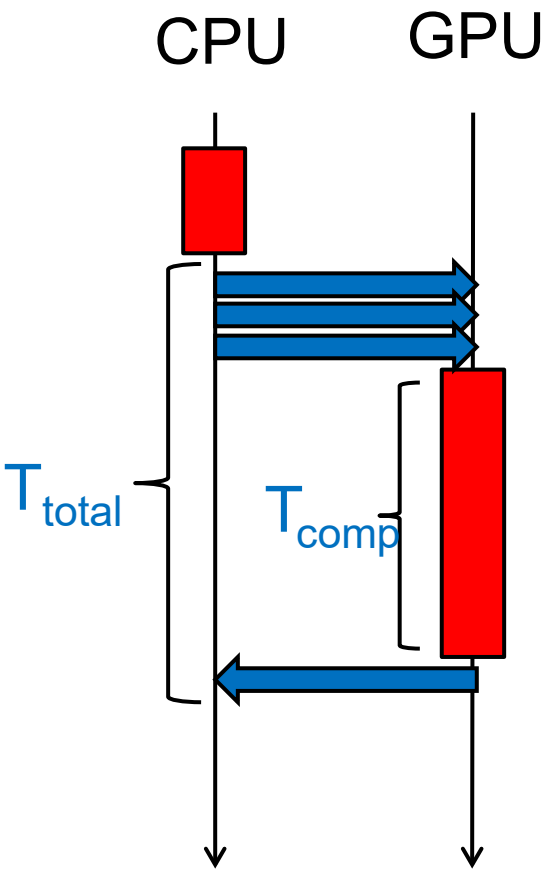
Measurement of Transfer Time

- Data transfer occurs at the beginning and the end of "data region"

```
// A,B,C are on CPU

#pragma acc data copyin(A,B) copy(C)
   {  // copyin (CPU->GPU) here

#pragma acc kernels
         {
            :
         }

   }  //copyout (GPU->CPU) here
```

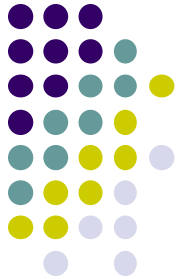
T_{total}

T_{comp}



See acc/mm-meas/mm.c
Also note that gettimeofday() must be called on CPU

Discussion on Data Transfer Costs



- Time for data transfer $T_{trans} \fallingdotseq M / B + L$
  - M: Data size in bytes
  - B: “Bandwidth” (speed)
  - L: “Latency” (if M is sufficiently large, we can ignore it)
- In a H100 GPU,
  - Theoretical bandwidth B is 64GB/s $(64 \times 10^9$ Bytes per second)
    - Actual transfer speed is slower than this value

Discussion on Computation and Transfer Costs

In mm-acc,

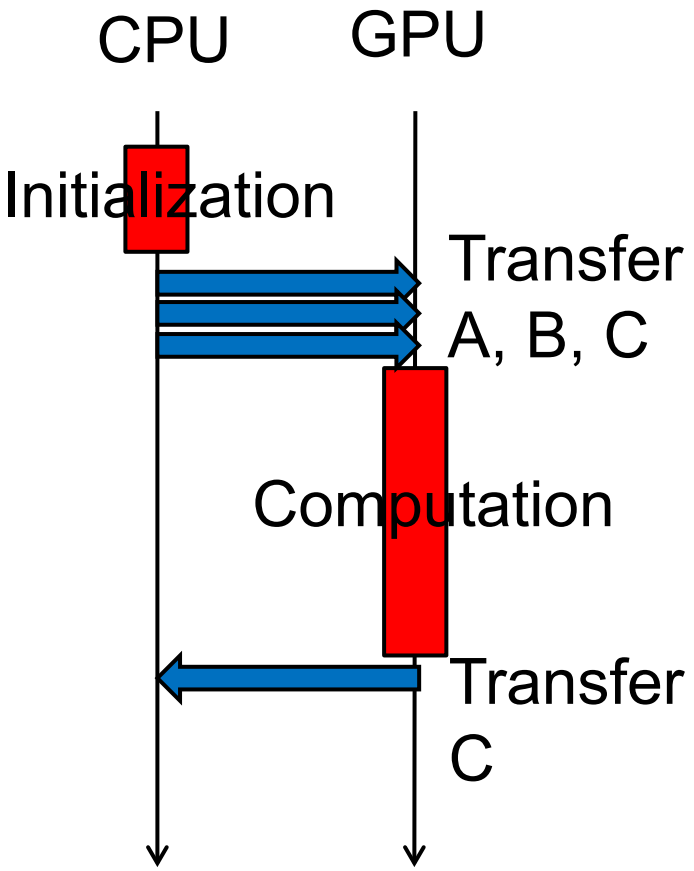
- Computation amount: 2mnk
- Data transfer amount:
  - A, B, C: CPU → GPU: 8(mk+kn+mn)
  - C: GPU → CPU: 8(mn)

sizeof(double) = 8

Observations:

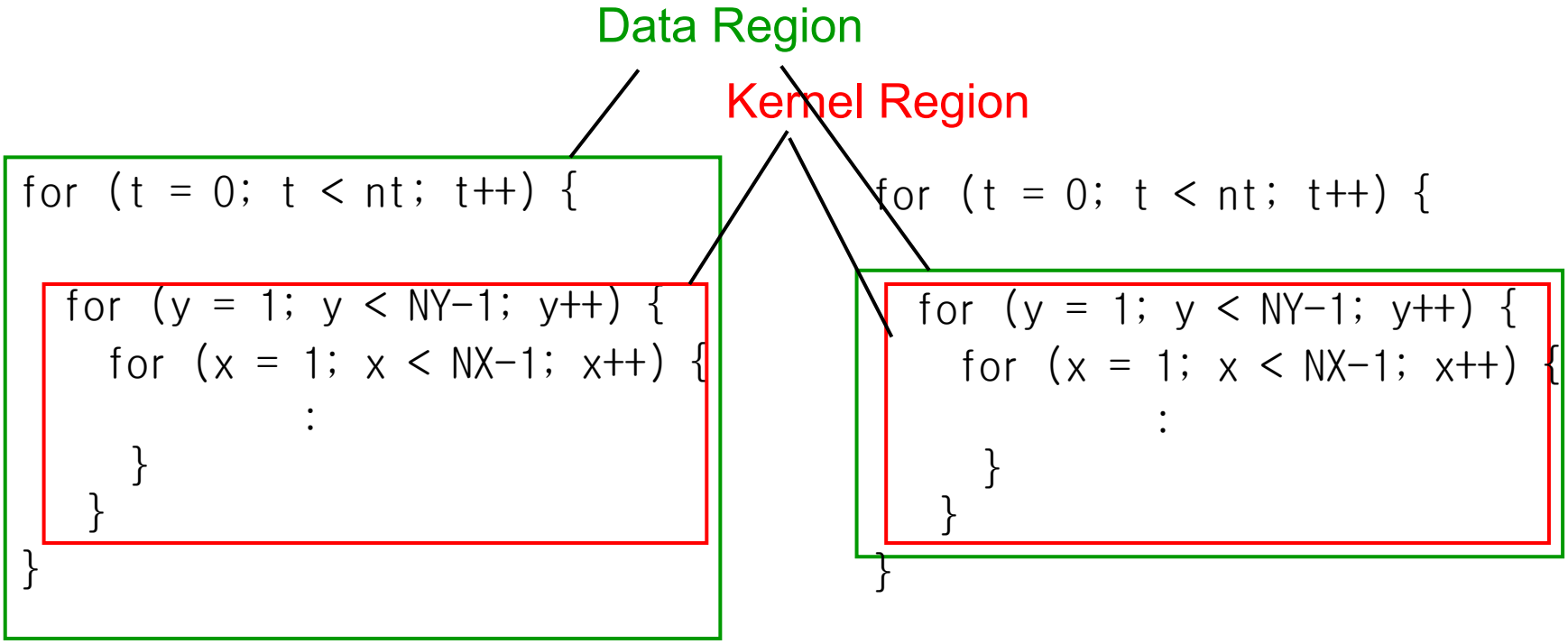
- We can compute actual transfer speed from $B \doteqdot M / T_{trans}$
  - L is ignored here
- Balance between computation and data transfer changes with different m, n, k

  When m, n, k are 2x:
  - Computation time is 8x
  - Transfer time is 4x



Discussion of data copy cost in diffusion [A1]

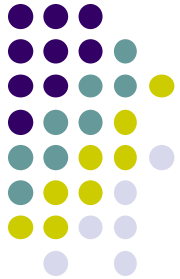
- Which is faster?



Computation: O(NX NY nt)
Data copy: O(NX NY)
➔ faster

Computation: O(NX NY nt)
Data copy: O(NX NY nt)

Note on OpenACC: Function Calls from GPU

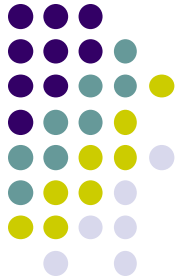


- Calling functions in kernel region is ok, but we need to be careful
  - "acc routine" directive is required by compiler to generate GPU code

```
int main()
{

#pragma acc kernels
   {

        … func(A[i]) …

   }

}
```

```
#pragma acc routine
int func(int arg)
{
    :
    :
    return …;
}
```

How about Library Functions?

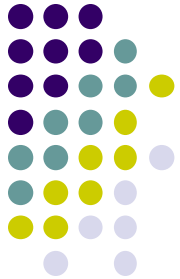


Inside kernel regions (#pragma acc kernel),

- Available library functions is very limited ☹
- We cannot use strlen(), memcpy(), fopen(), fflush()… ☹
- We cannot use gettimeofday() ☹

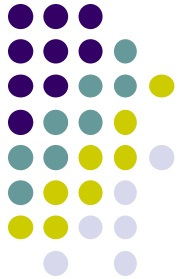
- Exceptionally, some mathematical functions are ok ☺
  - fabs, sqrt, fmax…
  - #include <math.h> is needed
- Recently, printf() in kernel regions is ok! ☺

Limitation of OpenACC (Some are Limitations of GPU)



- Task parallel program is not supported
  - like fib, qsort
  - Also CUDA is hard
- Mutual exclusion is not supported (generally)

  There are limited supports
  - OpenACC supports “acc loop reduction(...)” and “acc atomic”
  - CUDA supports atomic operations
- Hard to use some hardware features
  - Synchronize in thread block, SM’s shared memory, Tensor core...
  - CUDA can use



Assignments in OpenACC Part (1)

Choose one of [A1]—[A4], and submit a report

Due date: May 12 (Monday)

[A1] Parallelize “diffusion” sample program by OpenACC

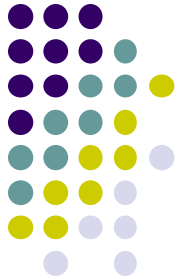
[A2] Parallelize “bsort” sample program by OpenACC

[A3] Evaluate speed of “acc/mm” sample in detail

[A4] (Freestyle) Parallelize *any* program by OpenACC

For more details, please see ppcomp25-7 slides

Next Part: CUDA Part



- Class #9
  - Introduction to CUDA, kernel functions
- Class #10
  - Characteristics of grid, thread blocks, threads
- Class #11
  - Performance improvement on GPU

- Schedule
  - Mon, May 5: No classes (national holiday)
  - Thu, May 8: Class #9, CUDA (1)