Practical Parallel Computing (実践的並列コンピューティング) 2021 No. 8

Part2: GPU (2)
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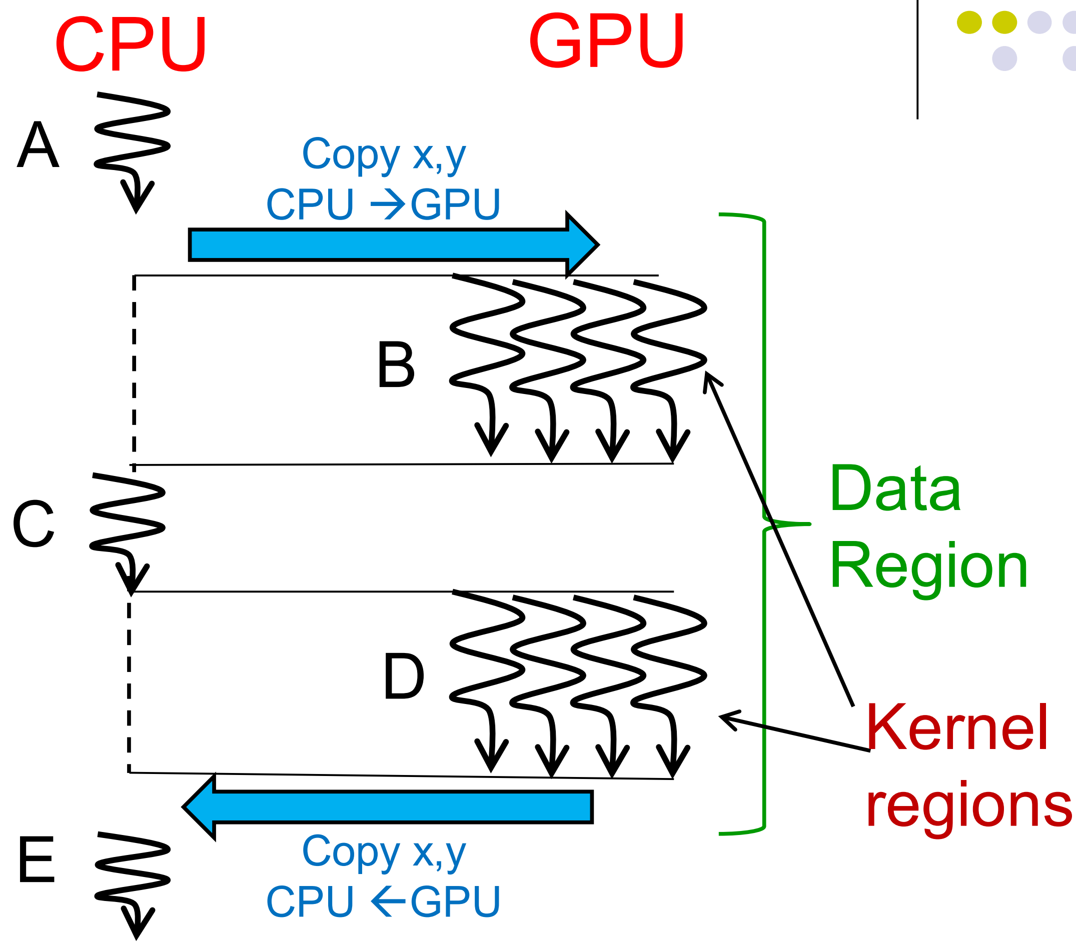
Overview of This Course

- Part 0: Introduction
  - 2 classes
- Part 1: OpenMP for shared memory programming
  - 4 classes
- Part 2: GPU programming
  - 4 classes ← We are here (2/4)
  - OpenACC (1.5 classes) and CUDA (2.5 classes)
- Part 3: MPI for distributed memory programming
  - 3 classes

Data Region and Kernel Region in OpenACC

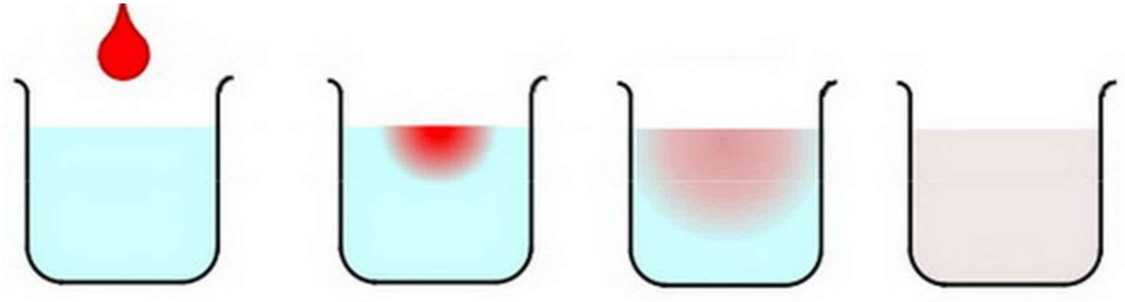
```
int main()
{
    A;
  #pragma acc data copy(x,y)
    {
  #pragma acc kernels
      {
          B;
      }
      C;
  #pragma acc kernels
      D;
    }
    E;
}
```



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

"diffusion" Sample Program
related to [G1]

An example of diffusion phenomena:

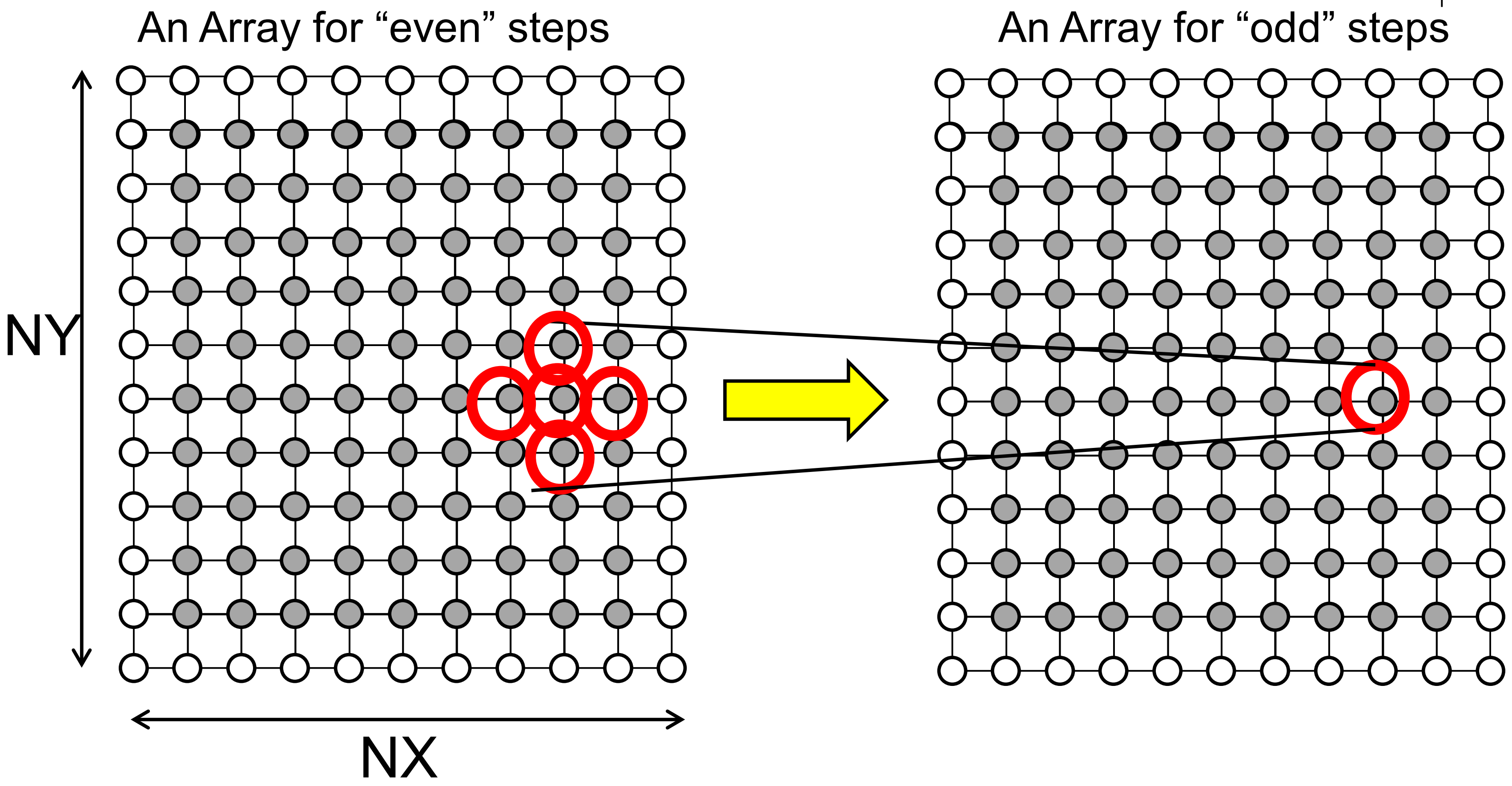


The ink spreads gradually, and finally the density becomes uniform (Figure by Prof. T. Aoki)

Available at /gs/hs1/tga-ppcomp/21/diffusion/

- Execution：./diffusion [nt]
  - nt: Number of time steps

Data Structure in “diffusion”



Consideration of Parallelizing Diffusion with OpenACC

related to [G1]

- 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]
```

Kernel region on GPU
Parallel x, y loops

It’s better to transfer data *out of* t-loop

data Clause for Multi-Dimensional arrays

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

…. data copy(A)

→ OK, all elements of A are copied

…. data copy(A[0:2000][0:1000])

→ OK, all elements of A are copied

…. data copy(A[500:600][0:1000])

→ OK, rows[500,1100) are copied

…. data copy(A[0:2000][300:400])

→ NG in current OpenACC

※ Currently, OpenACC does not support non-consecutive transfer

Notes on Assignment [G1] (1)

- You will need compiler options different from the diffusion directory for OpenACC
- You can use files in diffusion-acc directory as basis
  - /gs/hs1/tga-ppcomp/21/diffusion-acc/
  - “Makefile” in this directory supports compiler options for OpenACC
  - Don’t forget “module load nvhpc” before “make”

Notes on Assignment [G1] (2)

If you see compile error messages like:

```
 50, Accelerator restriction: call to 'fflush' with no acc
routine information
NVC++/x86-64 Linux 21.2-0: compilation completed with severe
errors
Makefile:16: recipe for target 'diffusion.o' failed
```

I/O functions (fflush(0) in this case) cannot be executed inside a kernel region

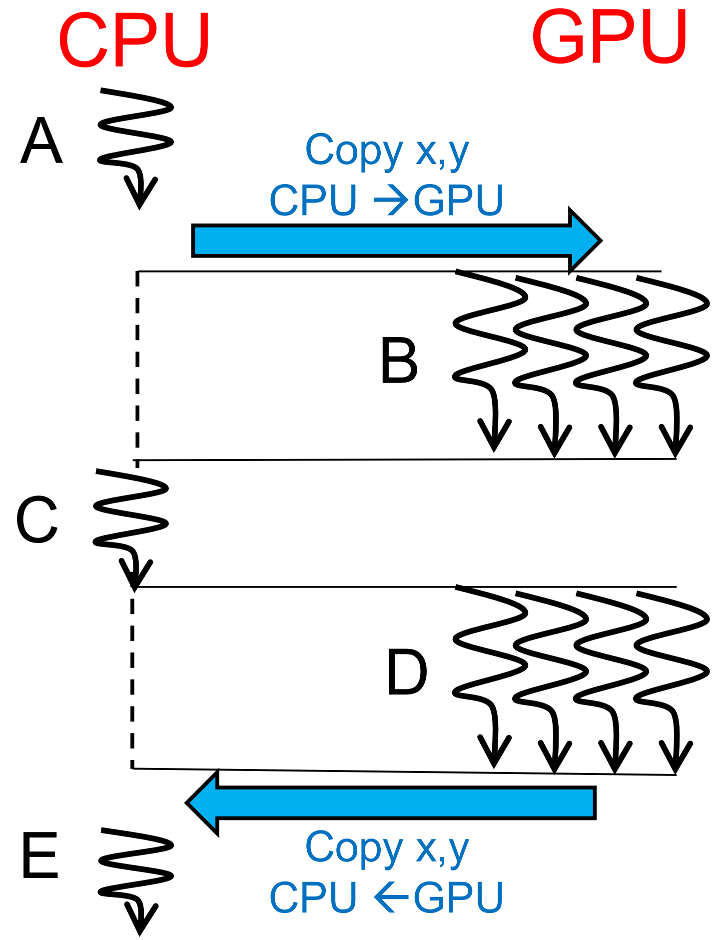
- Exceptionally, printf("…") is ok

In this case, please do either of

- Delete fflush(0) simply
- Consider to shorten the length of a kernel region

Data Transfer Costs in GPU Programming
Related to [G2]

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



Speed of GPU Programs:
case of mm-acc

In mm-acc, speed in Gflops is computed by

$$S = 2mnk / T_{total}$$

T_{total} includes both computation time and transfer

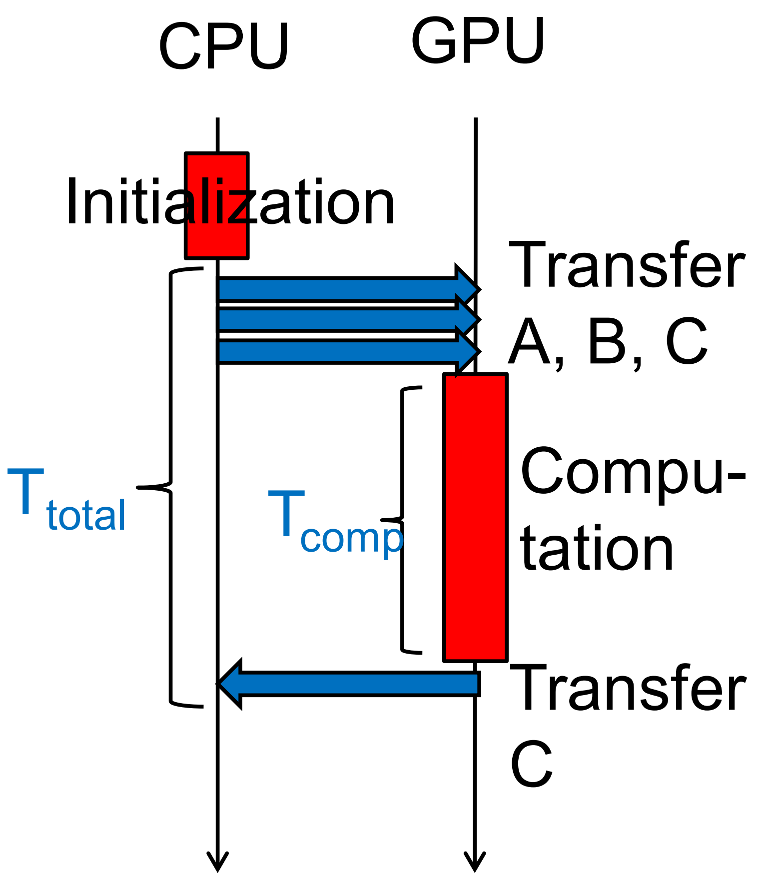
→ S counts slow-down by transfer

To see the effects, let's try another sample

/gs/hs1/tga-ppcomp/21/mm-meas-acc

which outputs time for

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



In [G2], please evaluate effects of transfer costs

Another Description Way for Copying Data

How can we measure transfer time?

- With "data" directive, "when we can copy" is restricted

→ We can copy data anytime by "acc enter data", "acc exit data" directives

```
// x,y are on CPU
#pragma acc data copy(x,y)
  {
    // x,y are on GPU
  }
// x,y are on CPU
```

⇒

```
// x,y are on CPU
#pragma acc enter data copyin(x,y)

  // x,y are on GPU

#pragma acc exit data copyout(x,y)
// x,y are on CPU
```

See differences between mm-acc/mm.c and mm-meas-acc/mm.c

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 P100 GPU,
  - Theoretical computation speed is 5.3TFlops
  - Theoretical bandwidth B is 16GB/s (2G double values per second)

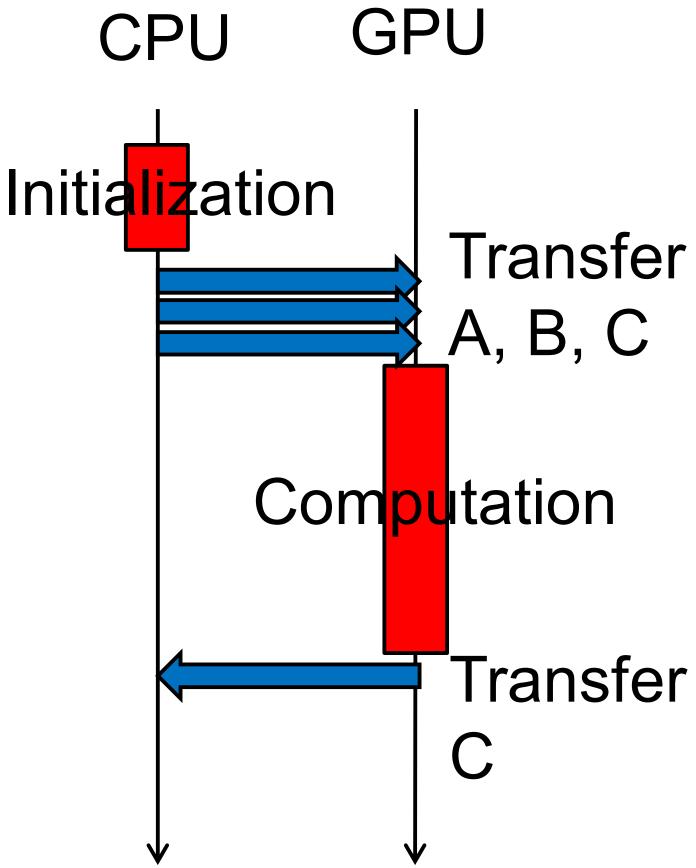
  → Transfer of values is much slower than computation ☹

Discussion on Computation and Transfer Costs

In mm-acc,

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

Transfer costs are relatively smaller with larger m, n, k



In diffusion-acc [G1], how can we reduce transfer costs?

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?

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

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

Now explanation of OpenACC is finished; we will go to CUDA

OpenACC and CUDA for GPUs

- OpenACC
  - C/Fortran + directives (#pragma acc …), Easier programming
  - NVIDIA HPC SDK compiler works
    - module load nvhpc
    - pgcc -acc … XXX.c
  - Basically for data parallel programs with for-loops

  → Only for limited types of algorithms ☹
- CUDA
  - Most popular and suitable for higher performance
  - Use “nvcc” command for compile
    - module load cuda
    - nvcc … XXX.cu

  Programming is harder, but more general

An OpenACC Program Look Like

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

   // After kernel region finishes,
   CPU can access to A[i],B[i]
```

Executed on GPU in parallel

A CUDA Program Look Like

Sample:
/gs/hs1/tga-ppcomp/21/add-cuda/

```
int A[100], B[100];
int *DA, *DB;
int i;
cudaMalloc(&DA, sizeof(int)*100);
cudaMalloc(&DB, sizeof(int)*100);
cudaMemcpy(DA,A,sizeof(int)*100,
    cudaMemcpyHostToDevice);
cudaMemcpy(DB,B,sizeof(int)*100,
    cudaMemcpyHostToDevice);

add<<<20, 5>>>(DA, DB);

cudaMemcpy(A,DA,sizeof(int)*100,
    cudaMemcpyDeviceToHost);
```

```
__global__ void add
   (int *DA, int *DB)
{
   int i = blockIdx.x*blockDim.x
         + threadIdx.x;
   DA[i] += DB[i];
}
```

Executed on GPU
(called a *kernel function*)

We have to separate code regions executed on CPU and GPU

Using add-cuda Sample

```
[make sure that you are at a interactive node (r7i7nX) ]
module purge    [If you have loaded nvhpc, delete it]
module load cuda        [Do once after login]
cd ~/t3workspace        [Example in web-only route]
cp -r /gs/hs1/tga-ppcomp/21/add-cuda  .
cd add-cuda
make
[An executable file "add" is created]
./add
```

※ [Standard route] A log-in node does not have a GPU

→ You can compile the sample there, but the program does not work!

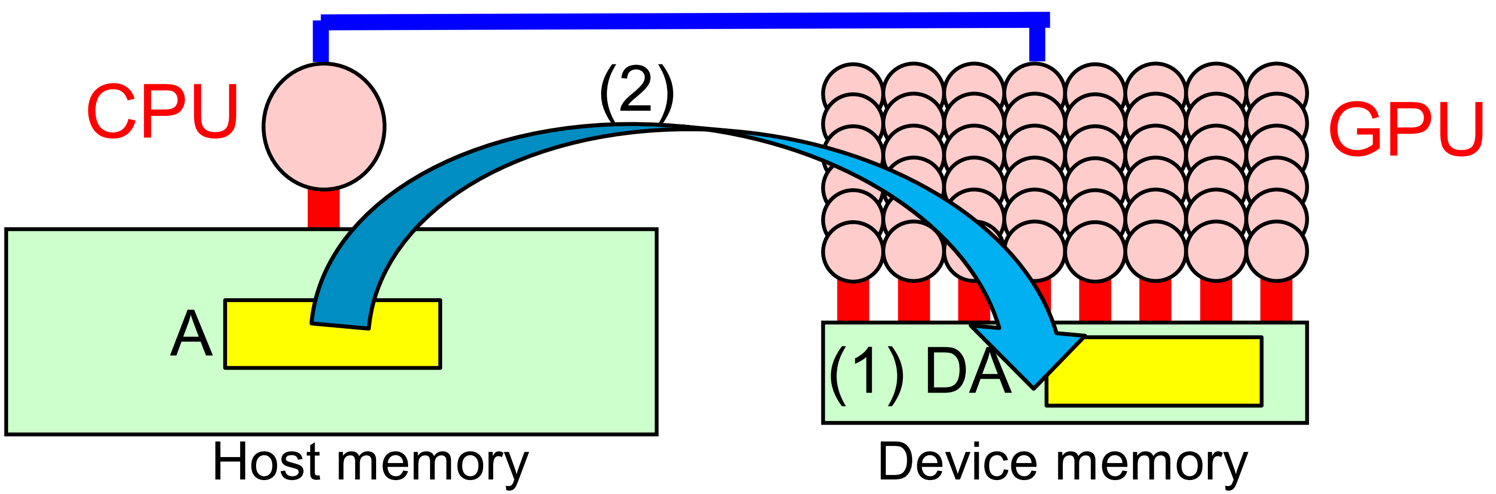
Preparing Data on Device Memory

(1) Allocate a region on device memory

cf) cudaMalloc((void**)&DA, *size*);

(2) Copy data from host to device

cf) cudaMemcpy(DA, A, *size*, cudaMemcpyDefault);



Note: cudaMalloc and cudaMemcpy must be called on CPU, NOT on GPU

Comparing OpenACC and CUDA

OpenACC

Both allocation and copy are done by acc data copyin

One variable name A may represent both

- A on host memory
- A on device memory

```
  int A[100];  ← on CPU
#pragma acc data copy(A)
#pragma acc kernels
 {
   … A[i] …
 }        ↖ on GPU
```

CUDA

cudaMalloc and cudaMemcpy are separated

Programmer have to prepare two pointers, such as A and DA

```
int A[100];
int *DA;
cudaMalloc(&DA, …);
cudaMemcpy(DA, A, …, …);
// Here CPU cannot access DA[i]

func<<<…, …>>>(DA, …);
```

Calling A GPU Kernel Function from CPU

- A region executed by GPU must be a distinct function
  - called a GPU kernel function

[CPU side]

```
func<<<20, 5>>>(…);
```

# of thread blocks

# of threads per block

In this case, 20x5=100 threads run on GPU

call

return

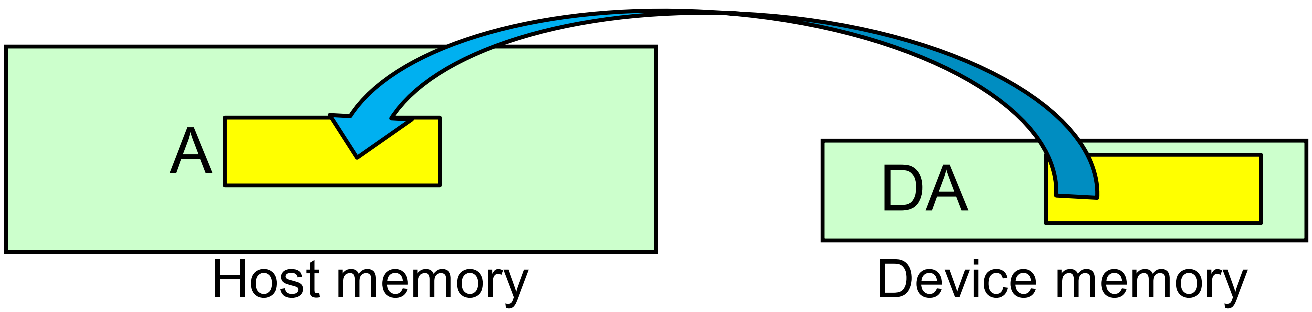
[GPU side]

```
__global__ void func(…)
{
      :
   return;
}
```

A GPU kernel function (called from CPU)

- needs __global__ keyword
- can take parameters
- can NOT return value; return type must be void

Copying Back Data from GPU



- Copy data using cudaMemcpy
  - cf) cudaMemcpy(A, DA, *size*, cudaMemcpyDefault);
  - 4th argument is one of
    - cudaMemcpyHostToDevice, cudaMemcpyDeviceToHost
    - cudaMemcpyDeviceToDevice, cudaMemcpyHostToHost
    - cudaMemcpyDefault ← Detect memory type automatically ☺
- When a memory area is unnecessary, free it
  - cf) cudaFree(DA);

Assignments in GPU Part (Abstract)

Choose one of [G1]—[G3], and submit a report

Due date: May 27 (Thursday)

[G1] Parallelize "diffusion" sample program by OpenACC or CUDA

[G2] Evaluate speed of "mm-acc" or "mm-cuda" in detail

[G3] (Freestyle) Parallelize *any* program by OpenACC or CUDA.

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
  - With varying problem sizes
  - Discussion with your findings
  - Other machines than TSUBAME are ok, if available

Next Class:

- GPU Programming (3) on May 13
  - Multi-threads on CUDA
- Also please note due date of OpenMP assignment is May 13