

Introduction to OpenACC

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Outline

- Introduction to GPU and OpenACC
- Basic syntax and the first OpenACC program: SAXPY
- Kernels vs. parallel directives
- An example: Laplace solver in OpenACC

The first try

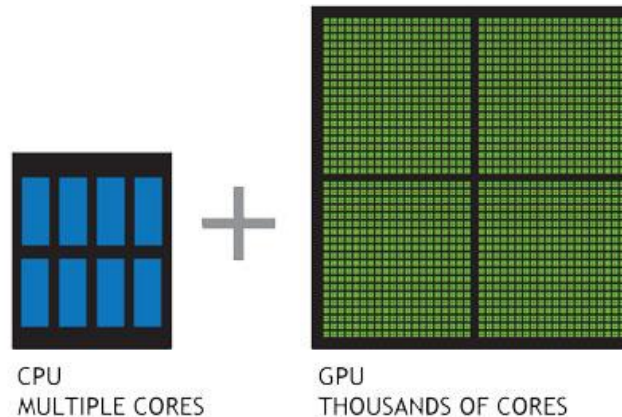
Data transfer between GPU and CPU/host

Data race and the reduction clause

- GPU and OpenACC task granularities

GPU and GPGPU

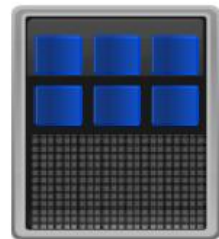
- Originally, graphics processing unit (GPU) is dedicated for manipulating computer graphics and image processing. Traditionally GPU is known as “video card”.
- GPU’s highly parallel structure makes it efficient for parallel programs. Nowadays GPUs are used for tasks that were formerly the domain of CPUs, such as scientific computation. This kind of GPU is called general-purpose GPU (GPGPU) .
- In many cases, a parallel program runs faster on GPU than on CPU. Note that a serial program runs slower on GPU than on CPU.
- The most popular type of GPU in the high-performance computing world is NVIDIA GPU. We will only focus on NVIDIA GPU here.



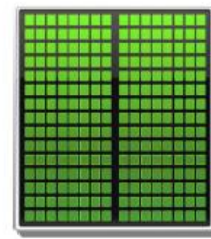
GPU is an accelerator

- GPU is a device on a CPU-based system. GPU is connected to CPU through PCI bus.
- Computer program can be parallelized and thus accelerated on GPU.
- CPU and GPU have separated memories. Data transfer between CPU and GPU is required in programming.

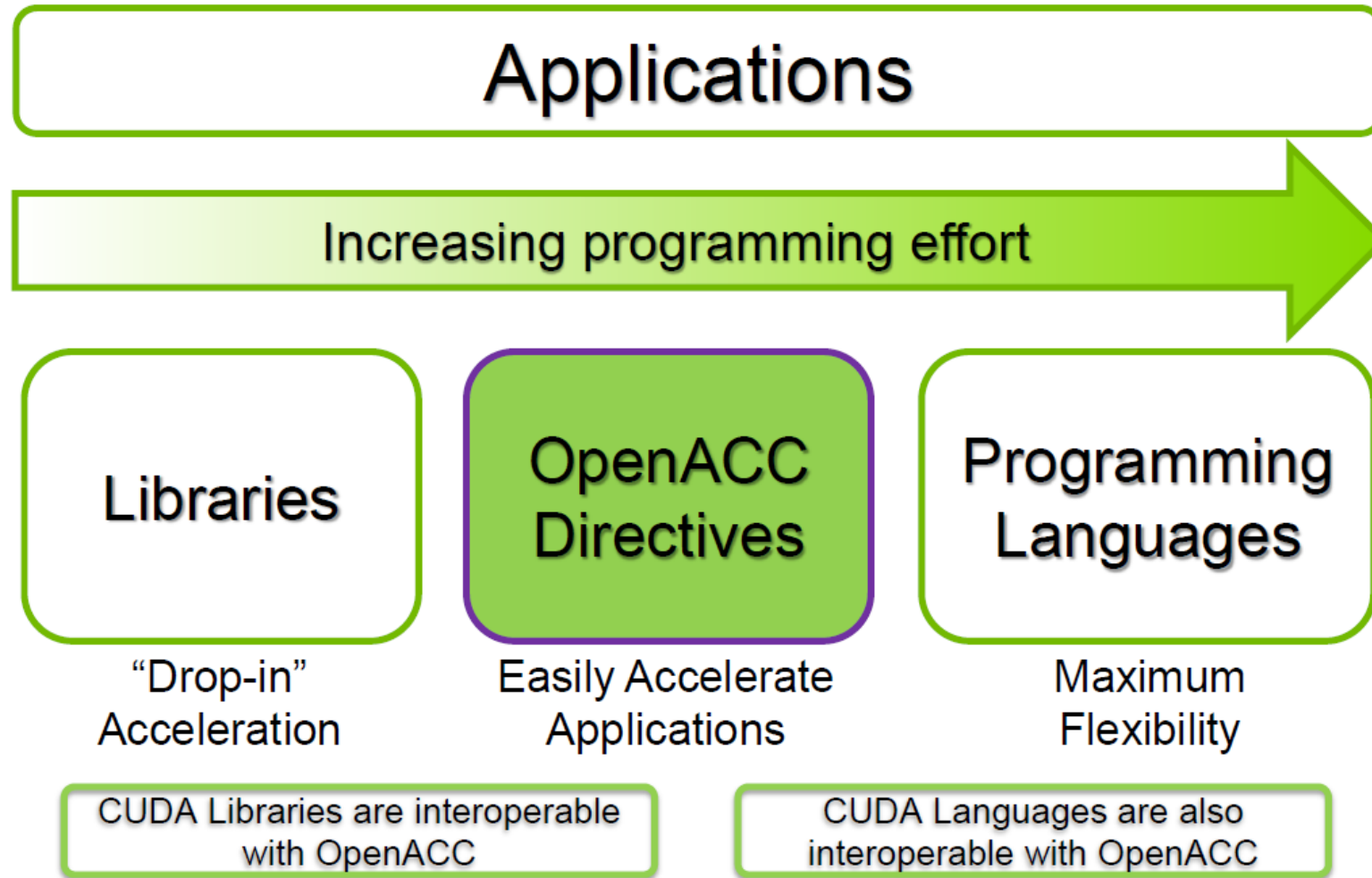
CPU



GPU



Three ways to accelerate applications on GPU



What is OpenACC

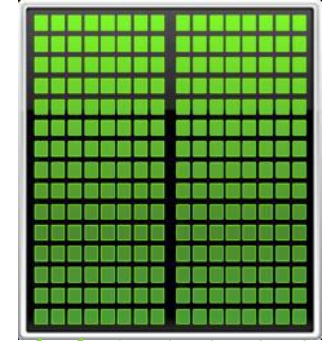
- OpenACC (for Open Accelerators) is a programming standard for parallel computing on accelerators (mostly on NIVIDIA GPU).
- It is designed to simplify GPU programming.
- The basic approach is to insert special comments (directives) into the code so as to offload computation onto GPUs and parallelize the code at the level of GPU (CUDA) cores.
- It is possible for programmers to create an efficient parallel OpenACC code with only minor modifications to a serial CPU code.

What are compiler directives?

- ❑ The directives tell the compiler or runtime to
 - ✓ Generate parallel code for GPU
 - ✓ Allocate GPU memory and copy input data
 - ✓ Execute parallel code on GPU
 - ✓ Copy output data to CPU and deallocate GPU memory
-
- ❑ The first OpenACC directive: **kernels**
 - ✓ ask the compiler to generate a GPU code
 - ✓ let the compiler determine safe parallelism and data transfer .

```
// ... serial code ...  
#pragma acc kernels  
for (int i= 0; i<n; i++) {  
    //... parallel code ...  
}  
  
// ... serial code ...
```

GPU



OpenACC Directive syntax

- C

`#pragma acc directive [clause [,] clause] ...]`...

often followed by a structured code block

- Fortran

`!$acc directive [clause [,] clause] ...]`...

often paired with a matching end directive surrounding a structured code block

`!$acc end directive`

The first OpenACC program: SAXPY

- Example: Compute $a*x + y$, where x and y are vectors, and a is a scalar.

C

```
int main(int argc, char **argv){
    int N=1000;
    float a = 3.0f;
    float x[N], y[N];
    for (int i = 0; i < N; ++i) {
        x[i] = 2.0f;
        y[i] = 1.0f;
    }
    #pragma acc kernels
    for (int i = 0; i < N; ++i) {
        y[i] = a * x[i] + y[i];
    }
}
```

Fortran

```
program main
    integer :: n=1000, i
    real :: a=3.0
    real, allocatable :: x(:), y(:)
    allocate(x(n),y(n))
    x(1:n)=2.0
    y(1:n)=1.0
    !$acc kernels
    do i=1,n
        y(i) = a * x(i) + y(i)
    enddo
    !$acc end kernels
end program main
```

Exercise 1: SAXPY

- 1) Login BU SCC and get an interactive session with GPU resources.
- 2) Provided a serial SAXPY code in C or Fortran, parallelize it using OpenACC directives.
- 3) Compile and run the SAXPY program.

Use OpenACC on BU SCC (1): Get GPU resources

- Login BU SCC

```
% ssh username@scc1.bu.edu
```

- Request an interactive session with one CPU core and one GPU:

```
% qssh -l gpus=1
```

- Load a PGI compiler:

```
% module load pgi/18.4
```

- Get GPU information

```
% pgaccelinfo
```

```
% nvidia-smi
```

Use OpenACC on BU SCC (2): Compile and Run

- On SCC, only the Portland Group compiler supports OpenACC
- Compile an OpenACC source code:

```
% pgcc -acc -Minfo=accel name.c -o exename
```

```
% pgf90 -acc -Minfo=accel name.f90 -o exename
```

- Note: the option **-Minfo=accel** is for printing useful information about accelerator region targeting.

- Run the executable:

```
% ./exename
```

Analysis of the compiling output

```
$ pgcc -acc -Minfo=accel saxpy_acc.c -o saxpy_acc
main:
  17, Generating copyin(x[:1000])
    Generating copy(y[:1000])
  19, Loop is parallelizable
    Accelerator kernel generated
    Generating Tesla code
  19, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
```

- ❑ Accelerator kernel is generated. The loop computation is offloaded to (Tesla) GPU and is parallelized.
- ❑ The keywords copy and copyin are related to data transfer. The keywords gang and vector are related to tasks granularity. We will cover these later.

Data dependency

- ❑ The loop is not parallelized if there is data dependency. For example,

```
#pragma acc kernels
for (int i = 0; i < N-1; i++) {
    x[i] = a * x[i+1];
}
```

- ❑ The compiling output:

```
.....
14, Loop carried dependence of x-> prevents parallelization
    Loop carried backward dependence of x-> prevents vectorization
Accelerator scalar kernel generated
    Loop carried backward dependence of x-> prevents vectorization
```

- ❑ The compiler creates a serial program, which runs slower on GPU than on CPU!

Pointer aliasing in C (1)

❑ An improper version of the SAXPY code (using pointers):

```
int N=1000;
float a = 3.0f;
float * x = (float*)malloc(N * sizeof(float));
float * y = (float*)malloc(N * sizeof(float));

for (int i = 0; i < N; ++i) {
    x[i] = 2.0f;
    y[i] = 1.0f;
}

#pragma acc kernels
for (int i = 0; i < N; ++i) {
    y[i] = a * x[i] + y[i];
}
```

- ✓ Pointer aliasing: Different pointers are allowed to access the same object. This may induce implicit data dependency in a loop.
- ✓ In this case, it is possible that the pointers x and y access to the same object. Potentially there is data dependency in the loop.

Pointer aliasing in C (2)

- ❑ The compiler refuses to parallelize the loop that is involved with pointer aliasing.
- ❑ Compiling output of the improper SAXPY code:

.....

20, Loop carried dependence of y-> prevents parallelization

Complex loop carried dependence of x-> prevents parallelization

Loop carried backward dependence of y-> prevents vectorization

Accelerator scalar kernel generated

Use *restrict* to avoid pointer aliasing

□ A proper version of the SAXPY code (using pointers):

```
int N=1000;
float a = 3.0f;
float *x = (float*)malloc(N * sizeof(float));
float * restrict y = (float*)malloc(N * sizeof(float));

for (int i = 0; i < N; ++i) {
    x[i] = 2.0f;
    y[i] = 1.0f;
}

#pragma acc kernels
for (int i = 0; i < N; ++i) {
    y[i] = a * x[i] + y[i];
}
```

- ✓ To avoid pointer aliasing, use the keyword *restrict*.
- ✓ *restrict* means: For the lifetime of the pointer *ptr*, only it or a value directly derived from it (such as *ptr + 1*) will be used to access the object to which it points.

Parallel directive (1)

- ❑ An improper version of SAXPY code (using *parallel* directive):

C

```
#pragma acc parallel
for (int i = 0; i < N; ++i) {
    y[i] = a * x[i] + y[i];
}
```

Fortran

```
!$acc parallel
do i=1,n
    y(i) = a*x(i)+y(i)
enddo
!$acc end parallel
```

- ✓ The *parallel* directive tells the compiler to create a parallel region. But differently from the *kernels* region, the code in the parallel region (the loop in this case) is executed (by all gangs) **redundantly**. There is no work sharing!

Parallel directive (2)

- ❑ A proper version of SAXPY code (using *parallel loop* directive):

C

```
#pragma acc parallel loop
for (int i = 0; i < N; ++i) {
    y[i] = a * x[i] + y[i];
}
```

Fortran

```
!$acc parallel loop
do i=1,n
    y(i) = a*x(i)+y(i)
enddo
!$acc end parallel loop
```

- ✓ It is necessary to add the keyword to *loop* to share the work (among gangs).
- ✓ In Fortran, the keyword *loop* can be replaced by *do*.
- ✓ In C, the keyword *loop* can be replaced by *for*.

kernels vs. parallel (1)

□ kernels

- More implicit.
- Gives the compiler more freedom to find and map parallelism.
- Compiler performs parallel analysis and parallelizes what it believes safe.

□ parallel

- More explicit.
- Requires analysis by programmer to ensure safe parallelism
- Straightforward path from OpenMP

kernels vs. parallel (2)

- Parallelize a code block with two loops:

kernels

```
#pragma acc kernels
{
  for (i=0; i<n; i++)
    a[i] = 3.0f*(float)(i+1);
  for (i=0; i<n; i++)
    b[i] = 2.0f*a[i];
}
```

- ✓ Generate two kernels
- ✓ There is an implicit barrier between the two loops: the second loop will start after the first loop ends.

parallel

```
#pragma acc parallel
{
  #pragma acc loop
  for (i=0; i<n; i++) a[i] = 3.0f*(float)(i+1);
  #pragma acc loop
  for (i=0; i<n; i++) b[i] = 2.0f*a[i];
}
```

- ✓ Generate one kernel
- ✓ There is no barrier between the two loops: the second loop may start before the first loop ends. (This is different from OpenMP).

Laplace Solver (1)

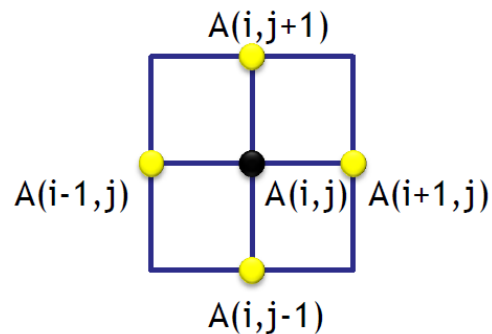
- Two-dimensional Laplace equation

$$\nabla^2 f(x, y) = 0$$

- Discretize the Laplacian with first-order differential method and express the solution as

$$A_{k+1}(i, j) = \frac{A_k(i-1, j) + A_k(i+1, j) + A_k(i, j-1) + A_k(i, j+1)}{4}$$

- The solution on one point is the average of its four neighbor points:



Laplace Solver (2)

- Use Jacobi iterative algorithm to obtain a convergent solution.
- **Jacobi iterative algorithm:**
 1. Give a trial solution A according to a provided initial condition.
 2. Compute a new solution, that is $A_{\text{new}}(i,j)$, based on the old values of the four neighbor points.
 3. Update the solution, i.e. $A=A_{\text{new}}$,
 4. Iterate steps 2 and 3 until converged, i.e. $\max(|A_{\text{new}}(i,j)-A(i,j)|) < \text{tolerance}$.
 5. Finally the converged solution is stored at A .

Laplace Solver (serial C)

```
while ( dt > MAX_TEMP_ERROR && iteration <= max_iterations ) {  
    for(i = 1; i <= ROWS; i++)  
        for(j = 1; j <= COLUMNS; j++) {  
            A_new[i][j] = 0.25 * (A[i+1][j] + A[i-1][j] + A[i][j+1] + A[i][j-1]);  
        }  
    dt = 0.0;  
    for(i = 1; i <= ROWS; i++)  
        for(j = 1; j <= COLUMNS; j++){  
            dt = fmax( fabs(A_new[i][j]-A[i][j]), dt);  
            A[i][j] = A_new[i][j];  
        }  
    iteration++;  
}
```

← A Loop for Jacobi iterations.

← Loops for computing a new solution

← Loops for updating the solution and finding the max error.

Laplace Solver (serial Fortran)

```
do while ( dt > max_temp_error .and. iteration <= max_iterations)
  do j=1,columns
    do i=1,rows
      A_new(i,j)=0.25*(A(i+1,j)+A(i-1,j)+ A(i,j+1)+A(i,j-1) )
    enddo
  enddo
  dt=0.0
  do j=1,columns
    do i=1,rows
      dt = max( abs(A_new(i,j) - A(i,j)), dt )
      A(i,j) = A_new(i,j)
    enddo
  enddo
  iteration = iteration+1
enddo
```

A Loop for Jacobi iterations.

Loops for computing a new solution

Loops for updating the solution and finding the max error.

Exercise 2: Laplace Solver in OpenACC

□ Provided a serial code (in C or Fortran) for solving the two-dimensional Laplace equation, parallelize it using OpenACC directives. Then compare the performance between the serial code and the OpenACC code.

- Hints:

1. Find the “hot spots”, the most time-consuming parts of the code. Usually they are loops.
2. Analyze parallelism. Which loops are parallelizable?
3. What directives should be used? Where to insert the directives?

Laplace Solver (OpenACC in C, version 1)

```
while ( dt > MAX_TEMP_ERROR && iteration <= max_iterations ) {  
    #pragma acc kernels  
    for(i = 1; i <= ROWS; i++)  
        for(j = 1; j <= COLUMNS; j++) {  
            A_new[i][j] = 0.25 * (A[i+1][j] + A[i-1][j] + A[i][j+1] + A[i][j-1]);  
        }  
    dt = 0.0;  
    #pragma acc kernels  
    for(i = 1; i <= ROWS; i++)  
        for(j = 1; j <= COLUMNS; j++){  
            dt = fmax( fabs(A_new[i][j]-A[i][j]), dt);  
            A[i][j] = A_new[i][j];  
        }  
    iteration++;  
}
```

← This loop is not parallelizable due to data dependency.

← These loops are parallelizable. Create a kernel region and ask the compiler to determine parallelism and data transfer.

← These loops are parallelizable. Create a kernel region and ask the compiler to determine parallelism and data transfer.

Laplace Solver (OpenACC in Fortran, version 1)

```
do while ( dt > max_temp_error .and. iteration <= max_iterations)
  !$acc kernels
  do j=1,columns
    do i=1,rows
      A_new(i,j)=0.25*(A(i+1,j)+A(i-1,j)+ A(i,j+1)+A(i,j-1) )
    enddo
  enddo
  !$acc end kernels
  dt=0.0
  !$acc kernels
  do j=1,columns
    do i=1,rows
      dt = max( abs(A_new(i,j) - A(i,j)), dt )
      A(i,j) = A_new(i,j)
    enddo
  enddo
  !$acc end kernels
  iteration = iteration+1
enddo
```

This loop is not parallelizable due to data dependency.

These loops are parallelizable. Create a kernel region and ask the compiler to parallelize it and transfer data.

These loops are parallelizable. Create a kernel region and ask the compiler to parallelize it and transfer data.

Analysis of performance (version 1)

- ❑ Compare the computation time (for 1000*1000 grids):
 - Serial code: **17.610445 seconds**.
 - OpenACC code (version 1): **48.796347 seconds**
- ✓ The OpenACC code is **much slower** than the serial code. What went wrong?
- ✓ We need to further analyze the parallelism and data transfer.

time(us): 25,860,945

61: compute region reached 3372 times

63: kernel launched 3372 times

grid: [32x250] block: [32x4]

device time(us): total=1,006,028 max=312 min=296 avg=298

elapsed time(us): total=1,149,681 max=862 min=337 avg=340

61: data region reached 6744 times

61: data copyin transfers: 3372

device time(us): total=4,570,063 max=1,378 min=1,353 avg=1,355

69: data copyout transfers: 3372

device time(us): total=4,217,959 max=1,987 min=1,248 avg=1,250

72: compute region reached 3372 times

74: kernel launched 3372 times

grid: [32x250] block: [32x4]

device time(us): total=1,143,160 max=342 min=325 avg=339

elapsed time(us): total=1,300,500 max=1,128 min=373 avg=385

74: reduction kernel launched 3372 times

grid: [1] block: [256]

device time(us): total=67,550 max=21 min=20 avg=20

elapsed time(us): total=146,840 max=436 min=42 avg=43

72: data region reached 6744 times

72: data copyin transfers: 6744

device time(us): total=9,567,773 max=1,648 min=1,346 avg=1,418

81: data copyout transfers: 3372

device time(us): total=5,176,980 max=1,553 min=1,534 avg=1,535

Profiling (version 1)

❑ export PGI_ACC_TIME=1
to activate profiling, then
run again.

- There are four data transfers between host(CPU) memory and GPU memory in every iteration of the outer while loop.
- The total time for data transfer is around **23.6 seconds**, which is much larger than the computing time around **2.5 seconds!**

Analysis of data transfer (version 1)

- These data transfers happen every iteration of the outer while loop!

```
while ( dt > MAX_TEMP_ERROR && iteration <= max_iterations ) {  
    #pragma acc kernels  
    for(i = 1; i <= ROWS; i++)  
        for(j = 1; j <= COLUMNS; j++) {  
            A_new[i][j] = 0.25 * (A[i+1][j] + A[i-1][j] + A[i][j+1] + A[i][j-1]);  
        }  
    dt = 0.0;  
    #pragma acc kernels  
    for(i = 1; i <= ROWS; i++)  
        for(j = 1; j <= COLUMNS; j++){  
            dt = fmax( fabs(A_new[i][j]-A[i][j]), dt);  
            A[i][j] = A_new[i][j];  
        }  
    iteration++;  
}
```

Copy in: A and A_new is copied from host to GPU.

Copy out: A and A_new is copied from GPU to host.

Copy in: A and A_new is copied from host to GPU.

Copy out: A and A_new is copied from GPU to host.

Data clauses

- ❑ **copy (list)**: Allocates memory on GPU and copies data from host to GPU when entering region and copies data to the host when exiting region.
 - ❑ **copyin(list)**: Allocates memory on GPU and copies data from host to GPU when entering region.
 - ❑ **copyout(list)**: Allocates memory on GPU and copies data to the host when exiting region.
 - ❑ **create(list)**: Allocates memory on GPU but does not copy.
 - ❑ **present(list)**: Data is already present on GPU.
- Syntax for C

```
#pragma acc data copy(a[0:size]) copyin(b[0:size]), copyout(c[0:size]) create(d[0:size]) present(d[0:size])
```
 - Syntax for Fortran

```
!$acc acc data copy(a(0:size)) copyin(b(0:size)), copyout(c(0:size)) create(d(0:size)) present(d(0:size))  
!$acc end data
```
 - If the compiler can determine the size of arrays, it is unnecessary to specify the size explicitly.

Laplace Solver (OpenACC in C , version 2)

```
#pragma acc data copy(A), create(A_new)
while ( dt > MAX_TEMP_ERROR && iteration <= max_iterations ) {
    #pragma acc kernels
    for(i = 1; i <= ROWS; i++)
        for(j = 1; j <= COLUMNS; j++) {
            A_new[i][j] = 0.25 * (A[i+1][j] + A[i-1][j] + A[i][j+1] + A[i][j-1]);
        }
    dt = 0.0;
    #pragma acc kernels
    for(i = 1; i <= ROWS; i++)
        for(j = 1; j <= COLUMNS; j++){
            dt = fmax( fabs(A_new[i][j]-A[i][j]), dt);
            A[i][j] = A_new[i][j];
        }
    iteration++;
}
```

Create a data region here. A is copied in before the while loop starts and is copied out after the while loop ends. A_new is allocated on GPU memory directly and is unnecessary to be copied to the host memory.

Create a kernel region here to parallelize the for loops, and there is no data transfer.

Create a kernel region here to parallelize the for loops, and there is very little data transfer.

Laplace Solver (OpenACC in Fortran , version 2)

```
!$acc data copy(A), create(A_new)
do while ( dt > max_temp_error .and. iteration <= max_iterations)
  !$acc kernels
  do j=1,columns
    do i=1,rows
      A_new(i,j)=0.25*(A(i+1,j)+A(i-1,j)+ A(i,j+1)+A(i,j-1) )
    enddo
  enddo
!$acc end kernels
dt=0.0
!$acc kernels
do j=1,columns
  do i=1,rows
    dt = max( abs(A_new(i,j) - A(i,j)), dt )
    A(i,j) = A_new(i,j)
  enddo
enddo
!$acc end kernels
iteration = iteration+1
enddo
```

Create a data region here. A is copied in before the while loop starts and is copied out after the while loop ends. A_new is allocated on GPU memory directly and is unnecessary to be copied to the host memory.

Create a kernel region here to parallelize the do loops, and there is no data transfer.

Create a kernel region here to parallelize the do loops, and there is very little data transfer.

time(us): 2,374,331

59: data region reached 2 times

59: data copyin transfers: 1

device time(us): total=1,564 max=1,564 min=1,564 avg=1,564

91: data copyout transfers: 1

device time(us): total=1,773 max=1,773 min=1,773 avg=1,773

63: compute region reached 3372 times

65: kernel launched 3372 times

grid: [32x250] block: [32x4]

device time(us): total=1,005,947 max=313 min=296 avg=298

elapsed time(us): total=1,102,391 max=946 min=324 avg=326

74: compute region reached 3372 times

74: data copyin transfers: 3372

device time(us): total=20,344 max=16 min=6 avg=6

76: kernel launched 3372 times

grid: [32x250] block: [32x4]

device time(us): total=1,150,552 max=344 min=327 avg=341

elapsed time(us): total=1,235,344 max=856 min=352 avg=366

76: reduction kernel launched 3372 times

grid: [1] block: [256]

device time(us): total=67,484 max=21 min=19 avg=20

elapsed time(us): total=151,147 max=358 min=43 avg=44

76: data copyout transfers: 3372

device time(us): total=68,104 max=46 min=17 avg=20

Profiling (version 2)

❑ export PGI_ACC_TIME=1
to activate profiling, then
run again.

- There are only 2 times data movement (of arrays) in total.
- There are data movements for the variable dt , but it is a scalar and thus the transfer processes cost very little time.
- The total time for data movement is around **0.09 second**, which is much smaller than the computing time (around **2.5 seconds**)!

Analysis of performance (version 2)

- ❑ Compare the computation time (for 1000*1000 grids):
 - Serial code: **17.610445 seconds**.
 - OpenACC code (version 1): **48.796347 seconds**
 - OpenACC code (version 2): **2.592581 seconds**

- ✓ The OpenACC code (version 2) is around **6.8 times faster** than the serial code.
Cheers!

- The speed-up would be even larger if the size of the problem increase.
- Note: The maximum size of GPU memory (typically 6 GB, 12 GB or 16 GB) is much smaller than regular CPU memory (e.g. 128 GB or 256 GB on BU SCC).

Reduction

- ❑ As we can see from the profiling results, a reduction kernel is created by the compiler.

What is reduction and why is it necessary?

- ❑ In the previous example, the variable *dt* can be modified by multiple workers (warps) simultaneously. This is called a **data race condition**. If data race happened, an incorrect result will be returned.
- ❑ To avoid data race, a reduction clause is required to protect the concerned variable.
- ❑ Fortunately, the compiler is smart enough to create a reduction kernel and avoid the data race automatically!

```
dt = 0.0;
#pragma acc kernels
for(i = 1; i <= ROWS; i++)
    for(j = 1; j <= COLUMNS; j++){
        dt = fmax( fabs(A_new[i][j]-A[i][j]), dt);
        A[i][j] = A_new[i][j];
    }
```

Laplace Solver (OpenACC in C , version 3)

```
#pragma acc data copy(A), create(A_new)
while ( dt > MAX_TEMP_ERROR && iteration <= max_iterations ) {
    #pragma acc parallel loops
    for(i = 1; i <= ROWS; i++)
        for(j = 1; j <= COLUMNS; j++) {
            A_new[i][j] = 0.25 * (A[i+1][j] + A[i-1][j] + A[i][j+1] + A[i][j-1]);
        }
    dt = 0.0;
    #pragma parallel loops reduction(max:dt)
    for(i = 1; i <= ROWS; i++)
        for(j = 1; j <= COLUMNS; j++){
            dt = fmax( fabs(A_new[i][j]-A[i][j]), dt);
            A[i][j] = A_new[i][j];
        }
    iteration++;
}
```

Create a data region here.

Create a parallel region here and parallelize the for loops.

Create a parallel region here and parallelize the for loops. Explicitly specify the reduction operator and variable.

Laplace Solver (OpenACC in Fortran , version 3)

```
!$acc data copy(A), create(A_new)
do while ( dt > max_temp_error .and. iteration <= max_iterations)
  !$acc parallel loop
  do j=1,columns
    do i=1,rows
      A_new(i,j)=0.25*(A(i+1,j)+A(i-1,j)+ A(i,j+1)+A(i,j-1) )
    enddo
  enddo
!$acc end parallel loop
dt=0.0
!$acc parallel loop reduction(max:dt)
do j=1,columns
  do i=1,rows
    dt = max( abs(A_new(i,j) - A(i,j)), dt )
    A(i,j) = A_new(i,j)
  enddo
enddo
!$acc end parallel loop
iteration = iteration+1
enddo
```

Create a data region here.

Create a parallel region here
and parallelize the do loops.

Create a parallel region here and
parallelize the do loops. Explicitly
specify the reduction operator
and variable.

Analysis of performance (version 3)

- ❑ Compare the computation time (for 1000*1000 grid):
 - Serial code: 17.610445 seconds.
 - OpenACC code (version 1): 48.796347 seconds
 - OpenACC code (version 2): 2.592581 seconds
 - OpenACC code (version 3): 2.259797 seconds
- ✓ Using **parallel** directive is a little faster than using **kernel** directive in this case (mostly due to different task granularities applied in the two cases).
- ✓ It is a good practice to explicitly specify reduction operators and variables.

NVIDIA GPU (CUDA) Task Granularity

- GPU device -- CUDA grids:
Kennels/grids are assigned to a device.
 - Streaming Multiprocessor (SM) -- CUDA thread blocks:
Blocks are assigned to a SM.
 - CUDA cores -- CUDA threads:
Threads are assigned to a core.
- ☐ Warp: a unit that consists 32 threads.
- ✓ Blocks are divided into warps.
 - ✓ The SM executes threads at warp granularity.



Kepler GK110 Full chip block diagram

OpenACC Task Granularity

- Gang --- block
- Worker – warp
- Vector – thread

☐ Syntax for C

```
#pragma acc kernels loop gang(n) worker(m) vector(k)
```

```
#pragma acc parallel loop num_gangs(n) num_workers(m) vector_length(k)
```

☐ Syntax for Fortran

```
!$acc kernels loop gang(n) worker(m) vector(k)
```

```
!$acc parallel loop num_gangs(n) num_workers(m) vector_length(k)
```

Appendix A: Submit a GPU job on SCC

- Submit a batch job:

```
% qsub job.sh
```

- A typical script for OpenACC jobs is like the following:

```
#!/bin/bash  
#$ -l gpus=1  
#$ -l h_rt=01:30:00  
#$ -P project_name  
#$ -N job_name  
./executable
```

Appendix B: More options for requesting GPU resources on SCC

- To request 4 CPU cores and 1 GPU
`-pe omp 4 -1 gpus=0.25`
- To request 12 CPU cores and 1 GPU
`-pe omp 12 -1 gpus=0.08`
- To request a GPU with compute capacity 3.5 or higher (including K40, P100, and V100)
`-1 gpus=1 -1 gpu_c=3.5`
- To request 4 CPU cores and 1 V100 GPU
`-pe omp 4 -1 gpus=0.25 -1 gpu_type=V100`

What is not covered

- Architecture of GPU
- Advanced OpenACC (vector, worker, gang, synchronization, etc)
- Using OpenACC with CUDA
- Using OpenACC with OpenMP (to use a few GPUs on one node)
- Using OpenACC with MPI (to use many GPUs on multiple nodes)

Further information

❑ OpenACC official website: <http://www.openacc.org/node/1>

❑ Help

help@scc.bu.edu

shaohao@bu.edu