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 faster on CPU than on GPU.

• 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 accelerated on GPU.
- CPU and GPU has separated memories. Data transfer between CPU and GPU is required for programming.
Three ways to accelerate applications on GPU

Applications

Increasing programming effort

Libraries
“Drop-in” Acceleration
CUDA Libraries are interoperable with OpenACC

OpenACC Directives
Easily Accelerate Applications
CUDA Languages are also interoperable with OpenACC

Programming Languages
Maximum Flexibility
What is OpenACC

- OpenACC (for Open Accelerators) is a programming standard for parallel computing on accelerators (mostly on NIVDIA 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 ...
```
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 $a \times x + y$, where $x$ and $y$ are vectors, and $a$ is a scalar.

**C**

```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**

```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
```
Using OpenACC on BU SCC (1): Get GPU resources

• Login BU SCC
  \texttt{\% ssh username@sccl.bu.edu}

• Request an interactive session with one CPU core and one GPU:
  \texttt{\% qlogin -l gpus=1}

• Use the newest PGI compiler:
  \texttt{\% module switch pgi/13.5 pgi/16.5}

• Get GPU information
  \texttt{\% pgaccelinfo}
  \texttt{\% nvidia-smi}
Using 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`
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 code.
Analysis of the compiling output

$ pgcc -acc -Minfo=accel saxpy_array.c -o saxpy_array
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 involved with data transfer. The keywords gang and vector are involved with tasks granularity. We will mention these later.
The loop is not parallelized if there is data dependency. For example,

```c
#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!
An improper version of the SAXPY code (using pointers):

```c
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 the same object. Potentially there is data dependency in the loop.
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):

```c
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 \textit{parallel} directive):

\begin{verbatim}
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
\end{verbatim}

- The \textit{parallel} directive tells the compiler to create a parallel region. But differently from the \textit{kernels} region, the code in the parallel region (the loop in this case) is executed (by all gangs) \textbf{redundantly}. There is no work sharing (among gangs)!
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
!$acc parallel loop
do i=1,n
    y(i) = a*x(i)+y(i)
endo
!$acc end parallel loop
```

- It is necessary to add the keyword to loop share the works (among gangs).
- In Fortran, the keyword loop can be replaced by do here.
- 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
Parallelize a code block with two loops:

### kernels

```c
#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

```c
#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 only depends on the four neighbor points:
Laplace Solver (2)

- Use Jacobi iterative algorithm to obtain a convergent solution.

- **Jacobi iterative algorithm:**
  1. Give a trial solution $A$ depending on 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 $A$. 
while ( dt > MAX_TEMP_ERROR && iteration <= max_iterations ) {
    for(i = 1; i <= ROWS; i++)
        for(j = 1; j <= COLUMNS; j++) {
        }
    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++;
}
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
```
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++) {
        }
    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++;
}
Laplace Solver (OpenACC in Fortran, version 1)

```fortran
!$acc kernels
do while ( dt > max_temp_error .and. iteration <= max_iterations)
  A_new(i,j) = 0.25*(A(i+1,j)+A(i-1,j)+A(i,j+1)+A(i,j-1))
enddo
enddo
!$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 determine parallelism and data transfer.

These loops are parallelizable. Create a kernel region and ask the compiler to determine parallelism and data transfer.
Analysis of performance (version 1)

- Compare the computation time (for 1000*1000 grid):
  - 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.
There are four times data transfer 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**!

- export PGI_ACC_TIME=1 to activate profiling, then run again.
Analysis of data transfer (version 1)

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

```c
while ( dt > MAX_TEMP_ERROR && iteration <= max_iterations ) {
    #pragma acc kernels
    for(i = 1; i <= ROWS; i++)
        for(j = 1; j <= COLUMNS; j++) {
        }
    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
  ```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
  ```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 it explicitly.
Laplace Solver (OpenACC in C, version 2)

```c
#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++) {
        }
    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, but there is no data transfer.

Create a kernel region here to parallelize the for loops, but there is no data transfer.
Laplace Solver (OpenACC in Fortran, version 2)

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, but there is no data transfer.

Create a kernel region here to parallelize the do loops, but there is no data transfer.
There are only 2 times data movement (of arrays) in total.

- There are data movements for the variable $dt$, but it is not an array 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)!

export PGI_ACC_TIME=1 to activate profiling, then run again.
Analysis of performance (version 2)

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

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.
- The maximum size of GPU memory (typically 6 GB or 12 GB) is much smaller than regular CPU memory (e.g. 128 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!

```c
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];
    }
```
#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++) {
        }
    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++;
}
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
       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).
- It is a good habit 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 of 32 threads.
  - Blocks are divided into warps.
  - The SM executes threads at warp granularity.
  - The warp size can be changed in the future.
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:
  
  ```bash
  #!/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 (e.g. for budge node)
  -pe omp 12 -1 gpus=0.08

- To request a whole budge node (12 CPU cores and 8 GPUs)
  -pe omp 12 -1 gpus=0.6

- To request 2 nodes with 12 CPU cores and 8 GPUs on each node
  -pe mpi_12_tasks_per_node 24 -1 gpus=0.6

- To request 1 node with 2 K40 GPUs
  -pe omp 16 -1 gpus=0.125 -1 gpu_type=K40m
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](http://www.openacc.org/node/1)

- Help
  - help@scc.bu.edu
  - shaohao@bu.edu