GPU Computing with OpenACC Directives

A Very Simple Exercise: SAXPY

SAXPY in C

```
void saxpy(int n,
           float a,
           float *x,
           float *restrict y)
{
#pragma acc kernels
  for (int i = 0; i < n; ++i)
    y[i] = a*x[i] + y[i];
}

...
// Perform SAXPY on 1M elements
saxpy(1<<20, 2.0, x, y);
...
```

SAXPY in Fortran

```
subroutine saxpy(n, a, x, y)
  real :: x(:), y(:), a
  integer :: n, i
$!acc kernels
  do i=1,n
    y(i) = a*x(i)+y(i)
  enddo
$!acc end kernels
end subroutine saxpy

...
$ Perform SAXPY on 1M elements
call saxpy(2**20, 2.0, x_d, y_d)
...
```

Directive Syntax

- Fortran

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

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

  `!$acc end directive`

- C

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

  Often followed by a structured code block

`kernels`: Your first OpenACC Directive

Each loop executed as a separate *kernel* on the GPU.

```
!$acc kernels
    do i=1,n
       a(i) = 0.0
       b(i) = 1.0
       c(i) = 2.0
    end do

    do i=1,n
       a(i) = b(i) + c(i)
    end do
!$acc end kernels
```

kernel 1

kernel 2

Kernel:
A parallel function that runs on the GPU

Kernels Construct

Fortran

```
!$acc kernels [clause …]
    structured block
!$acc end kernels
```

C

```
#pragma acc kernels [clause …]
    { structured block }
```

Clauses

```
if( condition )
async( expression )
```

Also, any data clause (more later)

Compile and run

- C:

```
pgcc -acc -ta=nvidia -Minfo=accel -o saxpy_acc saxpy.c
```

- Fortran:

```
pgf90 -acc -ta=nvidia -Minfo=accel -o saxpy_acc saxpy.f90
```

- Compiler output:

```
pgcc -acc -Minfo=accel -ta=nvidia -o saxpy_acc saxpy.c
saxpy:
      8, Generating copyin(x[:n-1])
         Generating copy(y[:n-1])
         Generating compute capability 1.0 binary
         Generating compute capability 2.0 binary
      9, Loop is parallelizable
         Accelerator kernel generated
          9, #pragma acc loop worker, vector(256) /* blockIdx.x threadIdx.x */
             CC 1.0 : 4 registers; 52 shared, 4 constant, 0 local memory bytes; 100% occupancy
             CC 2.0 : 8 registers; 4 shared, 64 constant, 0 local memory bytes; 100% occupancy
```

© NVIDIA 2013

First Attempt: OpenACC C

```
while ( error > tol && iter < iter_max ) {
  error=0.0;

#pragma acc kernels
  for( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {

      Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                           A[j-1][i] + A[j+1][i]);

      error = max(error, abs(Anew[j][i] - A[j][i]);
    }
  }

#pragma acc kernels
  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }

  iter++;
}
```

Execute GPU kernel for loop nest

Execute GPU kernel for loop nest

First Attempt: OpenACC Fortran

```
do while ( err > tol .and. iter < iter_max )
  err=0._fp_kind

!$acc kernels
  do j=1,m
    do i=1,n

      Anew(i,j) = .25_fp_kind * (A(i+1, j  ) + A(i-1, j  ) + &
                                 A(i  , j-1) + A(i  , j+1))

      err = max(err, Anew(i,j) - A(i,j))
    end do
  end do
!$acc end kernels

!$acc kernels
  do j=1,m-2
    do i=1,n-2
      A(i,j) = Anew(i,j)
    end do
  end do
!$acc end kernels
  iter = iter +1
end do
```

Generate GPU kernel for loop nest

Generate GPU kernel for loop nest

First Attempt: Compiler output (C)

```
pgcc  -acc -ta=nvidia -Minfo=accel -o laplace2d_acc laplace2d.c
main:
     57, Generating copyin(A[:4095][:4095])
         Generating copyout(Anew[1:4094][1:4094])
         Generating compute capability 1.3 binary
         Generating compute capability 2.0 binary
     58, Loop is parallelizable
     60, Loop is parallelizable
         Accelerator kernel generated
         58, #pragma acc loop worker, vector(16) /* blockIdx.y threadIdx.y */
         60, #pragma acc loop worker, vector(16) /* blockIdx.x threadIdx.x */
             Cached references to size [18x18] block of 'A'
             CC 1.3 : 17 registers; 2656 shared, 40 constant, 0 local memory bytes; 75% occupancy
             CC 2.0 : 18 registers; 2600 shared, 80 constant, 0 local memory bytes; 100% occupancy
         64, Max reduction generated for error
     69, Generating copyout(A[1:4094][1:4094])
         Generating copyin(Anew[1:4094][1:4094])
         Generating compute capability 1.3 binary
         Generating compute capability 2.0 binary
     70, Loop is parallelizable
     72, Loop is parallelizable
         Accelerator kernel generated
         70, #pragma acc loop worker, vector(16) /* blockIdx.y threadIdx.y */
         72, #pragma acc loop worker, vector(16) /* blockIdx.x threadIdx.x */
             CC 1.3 : 8 registers; 48 shared, 8 constant, 0 local memory bytes; 100% occupancy
             CC 2.0 : 10 registers; 8 shared, 56 constant, 0 local memory bytes; 100% occupancy
```

© NVIDIA 2013

First Attempt: Performance

CPU: Intel Xeon X5680
6 Cores @ 3.33GHz

GPU: NVIDIA Tesla M2070

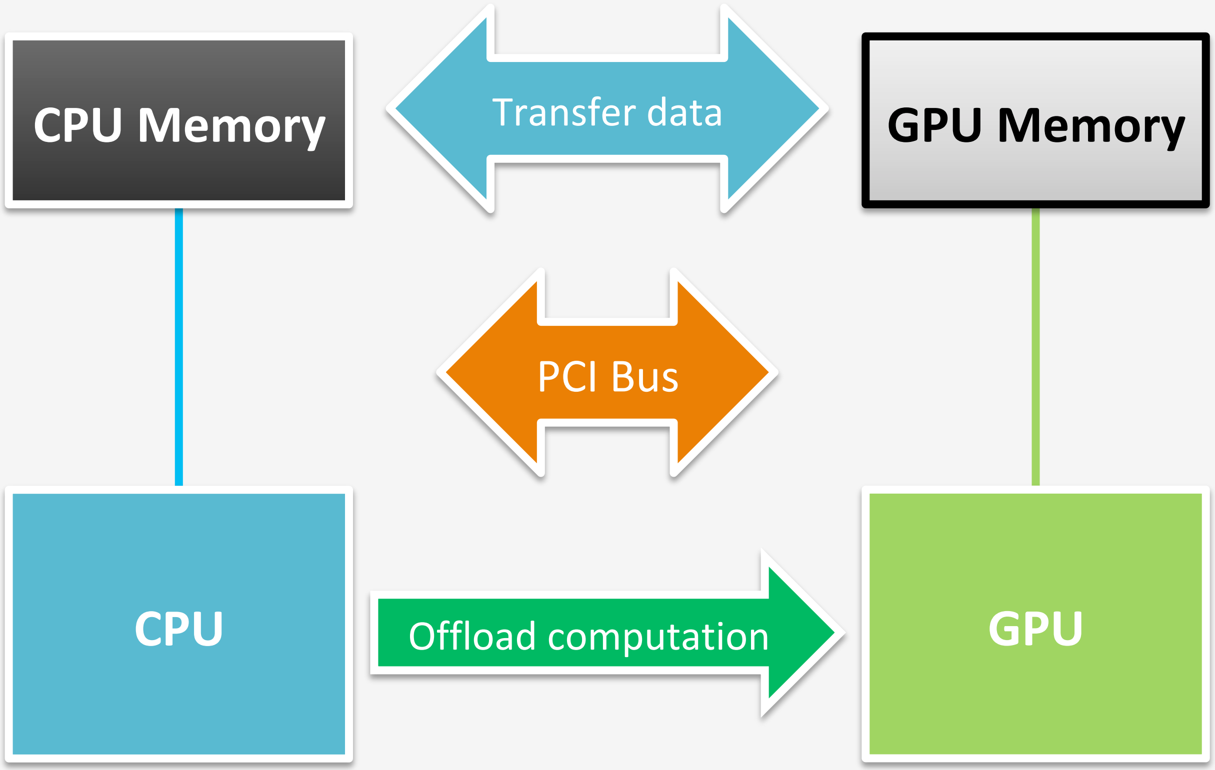
Execution	Time (s)	Speedup
CPU 1 OpenMP thread	69.80	--
CPU 2 OpenMP threads	44.76	1.56x
CPU 4 OpenMP threads	39.59	1.76x
CPU 6 OpenMP threads	39.71	1.76x
OpenACC GPU	162.16	0.24x FAIL

Speedup vs. 1 CPU core

Speedup vs. 6 CPU cores

© NVIDIA 2013

Basic Concepts



For efficiency, decouple data movement and compute off-load

© NVIDIA 2013

Excessive Data Transfers

```
while ( error > tol && iter < iter_max )
{
  error=0.0;
```

A, Anew resident on host

Copy

```
#pragma acc kernels
```

A, Anew resident on accelerator

These copies happen every iteration of the outer while loop!*

```
  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++) {
      Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                           A[j-1][i] + A[j+1][i]);
      error = max(error, abs(Anew[j][i] - A[j][i]);
    }
  }
```

A, Anew resident on accelerator

Copy

A, Anew resident on host

```
    ...
}
```

*Note: there are two #pragma acc kernels, so there are 4 copies per while loop iteration!

© NVIDIA 2013

Data Management

Data Construct

Fortran

```
!$acc data [clause …]
    structured block
!$acc end data
```

C

```
#pragma acc data [clause …]
    { structured block }
```

General Clauses

```
if( condition )
async( expression )
```

Manage data movement. Data regions may be nested.

© NVIDIA 2013

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 from another containing data region.

and `present_or_copy[in|out]`, `present_or_create`, `deviceptr`.

© NVIDIA 2013

Array Shaping

- Compiler sometimes cannot determine size of arrays
  - Must specify explicitly using data clauses and array “shape”

- C

```
#pragma acc data copyin(a[0:size-1]), copyout(b[s/4:3*s/4])
```

- Fortran

```
!$pragma acc data copyin(a(1:size)), copyout(b(s/4:3*s/4))
```

- Note: data clauses can be used on `data`, `kernels` or `parallel`

© NVIDIA 2013

Update Construct

Fortran

```
!$acc update [clause …]
```

C

```
#pragma acc update [clause …]
```

Clauses

```
host( list )
device( list )
```

```
if( expression )
async( expression )
```

Used to update existing data after it has changed in its corresponding copy (e.g. update device copy after host copy changes)

Move data from GPU to host, or host to GPU.
Data movement can be conditional, and asynchronous.

© NVIDIA 2013

Second Attempt: OpenACC C

```
#pragma acc data copy(A), create(Anew)
while ( error > tol && iter < iter_max ) {
  error=0.0;

#pragma acc kernels
  for( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {

      Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                           A[j-1][i] + A[j+1][i]);

      error = max(error, abs(Anew[j][i] - A[j][i]);
    }
  }

#pragma acc kernels
  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }

  iter++;
}
```

Copy A in at beginning of loop, out at end. Allocate Anew on accelerator

© NVIDIA 2013

Second Attempt: OpenACC Fortran

```
!$acc data copy(A), create(Anew)
do while ( err > tol .and. iter < iter_max )
  err=0._fp_kind

!$acc kernels
  do j=1,m
    do i=1,n

      Anew(i,j) = .25_fp_kind * (A(i+1, j  ) + A(i-1, j  ) + &
                                 A(i  , j-1) + A(i  , j+1))

      err = max(err, Anew(i,j) - A(i,j))
    end do
  end do
!$acc end kernels

  ...

iter = iter +1
end do
!$acc end data
```

Copy A in at beginning of loop, out at end. Allocate Anew on accelerator

© NVIDIA 2013

Second Attempt: Performance

CPU: Intel Xeon X5680
6 Cores @ 3.33GHz

GPU: NVIDIA Tesla M2070

Execution	Time (s)	Speedup
CPU 1 OpenMP thread	69.80	--
CPU 2 OpenMP threads	44.76	1.56x
CPU 4 OpenMP threads	39.59	1.76x
CPU 6 OpenMP threads	39.71	1.76x
OpenACC GPU	13.65	2.9x

Speedup vs. 1 CPU core

Speedup vs. 6 CPU cores

Note: same code runs in 9.78s on NVIDIA Tesla M2090 GPU

© NVIDIA 2013

Further speedups

- OpenACC gives us more detailed control over parallelization
  - Via gang, worker, and vector clauses

- By understanding more about OpenACC execution model and GPU hardware organization, we can get higher speedups on this code

- By understanding bottlenecks in the code via profiling, we can reorganize the code for higher performance

© NVIDIA 2013

Finding Parallelism in your code

- (Nested) for loops are best for parallelization
- Large loop counts needed to offset GPU/memcpy overhead
- Iterations of loops must be <u>independent</u> of each other
- Compiler must be able to figure out sizes of data regions
  - Can use directives to explicitly control sizes
- Pointer arithmetic should be avoided if possible
  - Use subscripted arrays, rather than pointer-indexed arrays.
- Function calls within accelerated region must be inlineable.

© NVIDIA 2013

Tips and Tricks

- (PGI) Use time option to learn where time is being spent
  `-ta=nvidia,time`
- Eliminate pointer arithmetic
- Inline function calls in directives regions
  (PGI): `-inline` or `-inline,levels(<N>)`
- Use contiguous memory for multi-dimensional arrays
- Use data regions to avoid excessive memory transfers

OpenACC Learning Resources

- OpenACC info, specification, FAQ, samples, and more
  - http://openacc.org
- PGI OpenACC resources
  - http://www.pgroup.com/resources/accel.htm

COMPLETE OPENACC API

Kernels Construct

Fortran

```
!$acc kernels [clause …]
    structured block
!$acc end kernels
```

C

```
#pragma acc kernels [clause …]
    { structured block }
```

Clauses

```
if( condition )
async( expression )
```

Also any data clause

© NVIDIA 2013

Kernels Construct

Each loop executed as a separate kernel on the GPU.

```
!$acc kernels
    do i=1,n
       a(i) = 0.0
       b(i) = 1.0                  kernel 1
       c(i) = 2.0
    end do

    do i=1,n
       a(i) = b(i) + c(i)          kernel 2
    end do
!$acc end kernels
```

© NVIDIA 2013

Parallel Construct

Fortran

```
!$acc parallel [clause …]
    structured block
!$acc end parallel
```

C

```
#pragma acc parallel [clause …]
    { structured block }
```

Clauses

```
if( condition )
async( expression )
num_gangs( expression )
num_workers( expression )
vector_length( expression )
```

```
private( list )
firstprivate( list )
reduction( operator:list )
```

Also any data clause

© NVIDIA 2013

Parallel Clauses

`num_gangs ( expression )`	Controls how many parallel gangs are created (CUDA `gridDim`).
`num_workers ( expression )`	Controls how many workers are created in each gang (CUDA `blockDim`).
`vector_length ( list )`	Controls vector length of each worker (SIMD execution).
`private( list )`	A copy of each variable in list is allocated to each gang.
`firstprivate ( list )`	`private` variables initialized from host.
`reduction( operator:list )`	`private` variables combined across gangs.

© NVIDIA 2013

Loop Construct

Fortran

```
!$acc loop [clause …]
    loop
!$acc end loop
```

C

```
#pragma acc loop [clause …]
    { loop }
```

Combined directives

```
!$acc parallel loop [clause …]
!$acc kernels loop [clause …]
```

```
!$acc parallel loop [clause
…]
!$acc kernels loop [clause …]
```

Detailed control of the parallel execution of the following loop.

© NVIDIA 2013

Loop Clauses

`collapse( n )`	Applies directive to the following `n` nested loops.
`seq`	Executes the loop sequentially on the GPU.
`private( list )`	A copy of each variable in list is created for each iteration of the loop.
`reduction( operator:list )`	`private` variables combined across iterations.

© NVIDIA 2013

Loop Clauses Inside parallel Region

`gang`	Shares iterations across the gangs of the parallel region.
`worker`	Shares iterations across the workers of the gang.
`vector`	Execute the iterations in SIMD mode.

© NVIDIA 2013

Loop Clauses Inside kernels Region

`gang [( num_gangs )]`	Shares iterations across across at most *num_gangs* gangs.
`worker [( num_workers )]`	Shares iterations across at most *num_workers* of a single gang.
`vector [( vector_length )]`	Execute the iterations in SIMD mode with maximum *vector_length*.
`independent`	Specify that the loop iterations are independent.

© NVIDIA 2013

OTHER SYNTAX

© NVIDIA 2013

Other Directives

`cache` construct	Cache data in software managed data cache (CUDA shared memory).
`host_data` construct	Makes the address of device data available on the host.
`wait` directive	Waits for asynchronous GPU activity to complete.
`declare` directive	Specify that data is to allocated in device memory for the duration of an implicit data region created during the execution of a subprogram.

© NVIDIA 2013

Runtime Library Routines

Fortran

```
use openacc
#include "openacc_lib.h"

acc_get_num_devices
acc_set_device_type
acc_get_device_type
acc_set_device_num
acc_get_device_num
acc_async_test
acc_async_test_all
```

C

```
#include "openacc.h"

acc_async_wait
acc_async_wait_all
acc_shutdown
acc_on_device
acc_malloc
acc_free
```

© NVIDIA 2013

Environment and Conditional Compilation

`ACC_DEVICE` *`device`*	Specifies which device type to connect to.
`ACC_DEVICE_NUM num`	Specifies which device number to connect to.
`_OPENACC`	Preprocessor directive for conditional compilation. Set to OpenACC version

© NVIDIA 2013