GPU programming



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OpenACC introduction

- express parallelism
- optimize data movements
- practical examples





3 Ways to Accelerate Applications

Applications

Libraries

OpenACC Directives

Programming Languages

"Drop-in"
Acceleration

Easily Accelerate Applications

Maximum Flexibility

Portability

Performance



OpenACC Friendly Disclaimer

OpenACC Directives

Easily Accelerate Applications

OpenACC does not make GPU programming easy. (...)

GPU programming and parallel programming is not easy. It cannot be made easy. However, GPU programming need not be difficult, and certainly can be made straightforward, once you know how to program and know enough about the GPU architecture to optimize your algorithms and data structures to make effective use of the GPU for computing. OpenACC is designed to fill that role.

(Michael Wolfe, The Portland Group)



OpenACC History

- OpenACC is a high-level specification with compiler directives for expressing parallelism for accelerators.
 - Portable to a wide range of accelerators.
 - One specification for Multiple Vendors and Multiple Devices
- OpenACC specification was released in November 2011.
 - Original members: CAPS, Cray, NVIDIA, Portland Group
- OpenACC 2.0 was released in June 2013
 - More functionality
 - Improve portability
- OpenACC 2.5 in November 2015
- OpenACC had more than 10 member organizations



Directive Based Approach

- Directives are added to serial source code
 - Manage loop parallelization
 - Manage data transfer between CPU and GPU memory
- Directives are formatted as comments
 - They don't interfere with serial execution
- Maintaines portability of original code

- Works with C/C++ or Fortran
 - Can be combined with explicit CUDA C/Fortran usage



OpenACC - Simple, Powerful, Portable

CPU Optimized for Serial Tasks GPU Accelerator Optimized for Parallel Tasks

1. Simple:

- Simple compiler directives
- Directives are the easy path to accelerate compute intensive applications
- Compiler parallelizes code

2. Open:

 OpenACC is an open GPU directives standard, making GPU programming straightforward and portable across parallel and multicore processors

3. Portable:

Works on many-core GPUs and multi-core CPUs

4. Powerful:

 GPU Directives allow complete access to the massive parallel power of a GPU



Directive Syntax

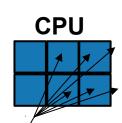
" C/C++
#pragma acc directive [clause [,] clause] ...]
Often followed by a structured code block

Fortran

```
!$acc directive [clause [,] clause] ...]
Often paired with a matching end directive
surrounding a structured code block
!$acc end directive
```



Familiar to OpenMP Programmers

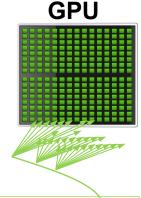


OpenMP

```
main() {
  double pi = 0.0; long i;

#pragma omp parallel for reduction(+:pi)
  for (i=0; i<N; i++)
  {
    double t = (double)((i+0.05)/N);
    pi += 4.0/(1.0+t*t);
  }

printf("pi = %f\n", pi/N);
}</pre>
```



OpenACC

```
main() {
   double pi = 0.0; long i;

#pragma acc parallel loop reduction(+:pi)
   for (i=0; i<N; i++)
   {
      double t = (double)((i+0.05)/N);
      pi += 4.0/(1.0+t*t);
   }

printf("pi = %f\n", pi/N);
}</pre>
```



OpenACC Info & Vendors

- http://www.openacc-standard.org
- Novelty in OpenACC 2.0 are significant
 - OpenACC 1.0 maybe not very mature...
- Some changes are inspired by the development of CUDA programming model
 - but the standard is not limited to NVIDIA GPUs: one of its pros is the interoperability between platforms
- Standard implementation
 - CRAY provides full OpenACC 2.0 support in CCE 8.2
 - PGI support to OpenACC 2.0 is almost complete
 - GNU implementation effort ongoing (there is a partial implementation in the 5.1 release)
- We will focus on PGI compiler
 - 30 days trial license useful for testing
- PGI:
 - all-in-one compiler, easy usage
 - sometimes the compiler tries to help you...
 - but also a constraint on the compiler to use



Porting to OpenACC

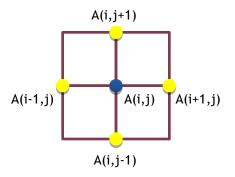
- 1. Identify available parallelism
- 2. Express parallelism
- 3. Express data movement
- 4. Optimize loop performance



Example: Jacobi Iteration

- Iteratively converges to correct value (e.g. Temperature), by computing new values at each point from the average of neighboring points.
 - Common, useful algorithm
 - Example: Solve Laplace equation in 2D:

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



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



Jacobi Iteration: C/C++ Code

```
while ( error > tol && iter < iter max ) {</pre>
  error=0.0;
  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]);
  for ( int j = 1; j < n-1; j++) {
    for ( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
  iter++;
```

- 1. Iterate until converged
- 2. Iterate across matrix elements
- 3. Calculate new value from neighbors
- 4. Compute max error for convergence
- 5. Swap input/output arrays



Jacobi Iteration: Fortran Code

```
do while ( err > tol .and. iter < iter max )
 err=0. fp kind
 do j=1,m
   do i=1,n
    Anew(i,j) = .25 * (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
 do j=1,m-2
   do i=1,n-2
     A(i,j) = Anew(i,j)
   end do
 end do
  iter = iter +1
end do
```

- 1. Iterate until converged
- 2. Iterate across matrix elements
- 3. Calculate new value from neighbors
- 4. Compute max error for convergence
- 5. Swap input/output arrays



1. Identify parallelism

```
while ( error > tol && iter < iter max ) {</pre>
  error=0.0;
  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]);
  for ( int j = 1; j < n-1; j++) {
    for ( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
  }
  iter++;
```

Data dependency between iterations

Independent loop iterations

Independent loop iterations



parallel construct

- Programmer identifies a block of code suitable for parallelization
- and guarantees that no dependency occurs across iterations
- Compiler generates parallel instructions for that loop
 - e.g., a parallel CUDA kernel for a GPU

```
#pragma acc parallel loop
for (int j=1;j<n-1;j++) {
    for (int i=1;i<n-1;i++) {
        A[j][i] = B[j][i] + C[j][i]
    }
}</pre>
```



kernels construct

The kemels construct expresses that a region m ay contain parallelism and the compiler determines what can be safely parallelized

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

cond do

cond do

cond do

cond do

kernel 1

kernel 2

kernel 2

cond do

kernel 2
```

 The compiler identifies 2 parallel loops and generate 2 kernels



parallel VS kernels

parallel

- Requires analysis by programmer to ensure safe parallelism
- Straightforward path from OpenMP
- Mandatory to fully control the different levels of parallelism
- Implicit barrier at the end of the parallel region

kernels

- Compiler performs parallel analysis and parallelizes what it believes safe
- Can cover larger area of code with a single directive
- Please, write clean codes and add directives to help the compiler
- Implicit barrier at the end and between each loop



C tip: the restrict keyword

Declaration of intent given by the programmer to the compiler

Applied to a pointer, e.g.

float *restrict ptr

Meaning: "for the lifetime of 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"

- Limits the effects of pointer aliasing
- OpenACC compilers often require restrict to determine independence between the iterations of a loop
 - Crucial when adopting kernels directive, but also for other optimizations
 - Note: if the programmer violates the declaration, the behavior is undefined



SAXPY example code

- Use restrict to help the compiler when adopting kernels
 - Apply a loop directive
- Be careful: restrict is C99 but not C++ standard

```
int main(int argc, char **argv)
 int N = 1 << 20; // 1 million floats
 if (argc > 1)
   N = atoi(arqv[1]);
  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;
   v[i] = 1.0f;
  saxpy(N, 3.0f, x, y);
  return 0;
```



100p construcut

- Applies to a loop which must immediately follow this directive
- Describes:
 - type of parallelism
 - loop-private variables, arrays, and reduction operations
- We already encountered it combined with the parallel directive
 - combining kernels and loop is also possible but limits the capability of kernels construct (i.e. extending to wide regions of code)

```
C/C++
#pragma acc loop [clause ...]
{ for block }

Fortran
!$acc loop [clause ...]
{ do block }
```



independent clause

- In a kernels construct, the independent loop clause helps the compiler in guaranteeing that the iterations of the loop are independent with each other
- E.g., consider m>n

```
#pragma acc kernels
#pragma acc loop independent
for(int i;i<n;i++)
    c[i] = 2.*c[m+i];</pre>
```

 In parallel construct the independent clause is implied on all loop directives without a seq clause



seq and collapse

- The seq clause specifies that the associated loops have to be executed sequentially on the accelerator
- Beware: the loop directive applies to the immediately following loop

- collapse(<n_loops>) clause allows for extending loop to tightly nested loops
 - but the compiler may decide to collapse loops anyway, check the report!



Loop reductions

- The reduction clause on a loop specifies a reduction operator on one or more scalar variables
 - For each variable, a private copy is created for each thread executing the associated loops
 - At the end of the loop, the values for each thread are combined using the reduction clause
- Reductions may be defined even at parallel level (advanced topic)
- Common operators are supported:

```
+ * max min && || ....
```



```
while ( error > tol && iter < iter max ) {</pre>
  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]);
  for ( int j = 1; j < n-1; j++) {
    for ( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
  iter++;
```



```
do while ( err > tol .and. iter < iter max )
 err=0. fp kind
!$acc kernels
 do j=1,m
   do i=1,n
    Anew(i,j) = .25 * (A(i+1,j)) + A(i-1,j) + &
                        A(i, j-1) + A(i, j+1)
      err = max(err, Anew(i,j) - A(i,j))
   end do
  end do
 do j=1,m-2
   do i=1,n-2
     A(i,j) = Anew(i,j)
   end do
 end do
!$acc end kernels
  iter = iter +1
end do
```



```
while ( error > tol && iter < iter max ) {</pre>
  error=0.0;
#pragma acc parallel loop reduction(max:error)
  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 parallel loop
  for ( int j = 1; j < n-1; j++) {
    for ( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
  iter++;
```



```
do while (err > tol .and. iter < iter max)
 err=0. fp kind
!$acc parallel loop reduction(max:error)
 do j=1,m
   do i=1,n
    Anew(i,j) = .25 * (A(i+1,j) + A(i-1,j) + &
                       A(i, j-1) + A(i, j+1)
     err = max(err, Anew(i,j) - A(i,j))
   end do
 end do
!$acc end parallel loop
!$acc parallel loop
 do j=1,m-2
   do i=1,n-2
     A(i,j) = Anew(i,j)
   end do
 end do
!$acc end parallel loop
 iter = iter +1
end do
```



Compiling and running (PGI)

pgcc -acc -ta=tesla -Minfo=all -acc=noautopar -o laplace2d.x laplace2d.c

```
main:
     34, Loop not vectorized: may not be beneficial
         Unrolled inner loop 4 times
         Generated 3 prefetches in scalar loop
     44, Loop not vectorized/parallelized: potential early exits
     48, Generating copyout (Anew[1:4094][1:4094])
         Generating copyin(A[:][:])
         Generating copyout(A[1:4094][1:4094])
     50, Loop is parallelizable
     51, Loop is parallelizable
         Accelerator kernel generated
         Generating Tesla code
         50, #pragma acc loop gang, vector(4) /* blockIdx.y threadIdx.y */
         51, #pragma acc loop gang, vector(32) /* blockIdx.x threadIdx.x */
         54, Max reduction generated for error
     58, Loop is parallelizable
     59, Loop is parallelizable
         Accelerator kernel generated
         Generating Tesla code
         58, #pragma acc loop gang, vector(4) /* blockIdx.y threadIdx.y */
         59, #pragma acc loop gang, vector(32) /* blockIdx.x threadIdx.x */
```

For the hands-on, compile using the makefile and run by typing

```
$ make pgi
$ ./laplace2d N (N is the GPU number to use, 0 1 2 ...)
```



Laplace 2D

Compile serial code for reference

Accelerate serial code with OpenACC

- Use kernels construct
- Use parallel construct
- Performance





Selecting the device

- Device selection can be achieved by OpenACC runtime library routines
 - device type: acc_device_cuda/acc_device_nvidia for PGI
 - GPUs are numbered starting from 0 (PGI)

```
#ifdef OPENACC
   int mygpu, myrealgpu, num devices;
   acc device t my device type = acc device nvidia;
   if (argc == 1) mygpu = 0; else mygpu = atoi(argv[1]);
   acc set device type (my device type);
   num devices = acc get num devices(my device type) ;
   fprintf(stderr, "Number of devices available: %d \n ", num devices);
   acc set device num(mygpu, my device type);
   fprintf(stderr, "Trying to use GPU: %d \n", mygpu);
  mvrealqpu = acc get device num(my_device_type);
   fprintf(stderr, "Actually I am using GPU: %d \n", myrealgpu);
#endif
```



Performance

Execution	Time (s) - PGI
CPU 1 OpenMP thread	22.5
CPU 2 OpenMP threads	11.5
CPU 4 OpenMP threads	6.5
CPU 8 OpenMP threads	3.9
CPU 16 OpenMP threads	2.5
OpenACC GPU	9.2

2 eight-core Intel(R) Xeon(R) CPU E5-2687W @ 3.10GHz GPU Nvidia Tesla K80 PCI-e 3.0

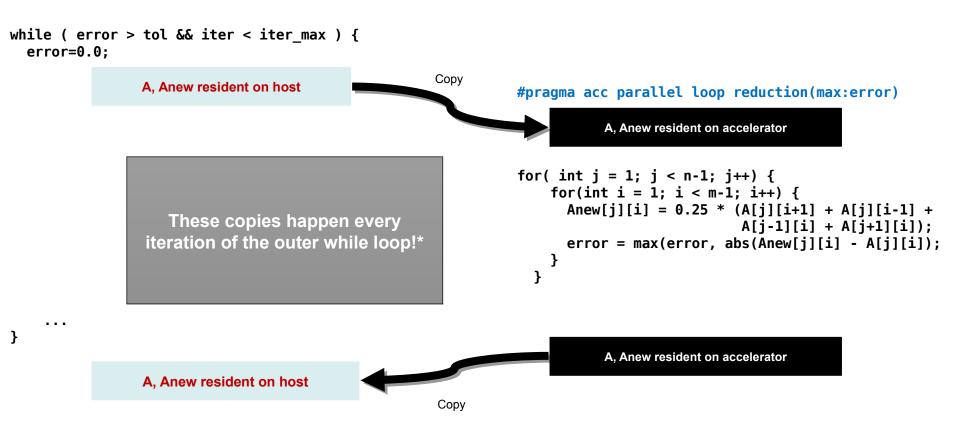


What is going wrong?

```
Accelerator Kernel Timing data
      laplace2d.c
        main
          69: region entered 1000 times
              time(us): total=77524918 init=240 region=77524678
                         kernels=4422961 data=66464916
4.4 seconds
                                                                          66.5 seconds
              w/o init: total=77524678 max=83398 min=72025 avg=77524
              72: kernel launched 1000 times
                  grid: [256x256] block: [16x16]
                  time(us): total=4422961 max=4543 min=4345 avg=4422
      laplace2d.c
        main
          57: region entered 1000 times
              time(us): total=82135902 init=216 region=82135686
                         kernels=8346306 data=66775717
8.3 seconds
                                                                          66.8 seconds
              w/o init: total=82135686 max=159083 min=76575 avg=82135
              60: kernel launched 1000 times
                  grid: [256x256] block: [16x16]
                   time(us): total=8201000 max=8297 min=8187 avg=8201
              64: kernel launched 1000 times
                  grid: [1] block: [256]
                  time(us): total=145306 max=242 min=143 avg=145
      acc init.c
        acc init
          29: region entered 1 time
                                                            Huge Data Transfer Bottleneck!
              time(us): init=158248
                                                                Computation: 12.7 seconds
                                                              Data movement: 133.3 seconds
```



Excessive data transfers



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



data construct

```
C/C++

#pragma acc data [clause ...]

{ structured block }
```

Fortran

!\$acc data [clause ...]
structured block
!\$acc end data

- Manages explicitely data movements
- Crucial to handle GPU data persistence
- Allows for decoupling the scope of GPU variables from that of the accelerated regions
- May be nested
- Data clauses define different possible behaviours
 - the usage is similar to that of data clauses in parallel regions



data clauses

```
Allocates memory on GPU and copies data from host to
copy ( list )
                    GPU when entering region and copies data to the host
                    when exiting region.
                    Allocates memory on GPU and copies data from host to
copyin (list)
                    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.
```



Array shaping

- The compiler sometimes cannot determine the sizes of arrays
 - you must specify them by using data clauses and array "shape"
 - you may need just a section of an array
 - sub-array syntax is allowed, in Fortran it is language-native
- C/C++
 #pragma acc data copyin(a[1:size]), copyout(b[s/4:3*s/4+1])
- Fortran!\$pragma acc data copyin(a(1:size)), copyout(b(s/4:s))
- Data clauses can be used on data, kernels or parallel



Laplace 2D

- Use data construct
- Performance





```
#pragma acc data copy(A), create(Anew)
while ( error > tol && iter < iter max ) {</pre>
  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]);
  for ( int j = 1; j < n-1; j++) {
    for ( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
  iter++;
```



```
!$acc data copy(A), create(Anew)
do while ( err > tol .and. iter < iter max )
 err=0. fp kind
!$acc kernels
 do j=1,m
   do i=1,n
    Anew(i,j) = .25 * (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
 do j=1,m-2
   do i=1,n-2
     A(i,j) = Anew(i,j)
   end do
 end do
!$acc end kernels
 iter = iter +1
end do
!$acc end data
```



```
#pragma acc data copy(A), create(Anew)
while ( error > tol && iter < iter max ) {</pre>
  error=0.0;
#pragma acc parallel loop reduction(max:error)
  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 parallel loop
  for ( int j = 1; j < n-1; j++) {
    for ( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
  iter++;
```



```
!$acc data copy(A), create(Anew)
do while ( err > tol .and. iter < iter max )
 err=0. fp kind
!$acc parallel loop reduction(max:error)
 do j=1,m
   do i=1,n
    Anew(i,j) = .25 * (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
!$acc end parallel loop
!$acc parallel loop
 do j=1,m-2
   do i=1,n-2
     A(i,j) = Anew(i,j)
   end do
 end do
!$acc end parallel loop
 iter = iter +1
end do
!$acc end data
```



Performance

Execution	Time (s) - PGI
CPU 1 OpenMP thread	22.5
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CPU 16 OpenMP threads	2.5
OpenACC GPU	0.6

2 eight-core Intel(R) Xeon(R) CPU E5-2687W @ 3.10GHz GPU Nvidia Tesla K80 PCI-e 3.0



4. Optimize loop performance

```
#pragma acc data copy(A), create(Anew)
while ( error > tol && iter < iter max ) {</pre>
  error=0.0;
#pragma acc parallel loop collapse(2) reduction(max:error)
  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 parallel loop collapse(2)
  for ( int j = 1; j < n-1; j++) {
    for ( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
  iter++;
```



4. Optimize loop performance

```
!$acc data copy(A), create(Anew)
do while ( err > tol .and. iter < iter max )
 err=0. fp kind
!$acc parallel loop collapse(2) reduction(max:error)
 do j=1,m
   do i=1,n
    Anew(i,j) = .25 * (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
!$acc end parallel loop
!$acc parallel loop collapse(2)
 do j=1,m-2
   do i=1,n-2
     A(i,j) = Anew(i,j)
   end do
 end do
!$acc end parallel loop
 iter = iter +1
end do
!$acc end data
```



4. Optimize loop performance

```
#pragma acc data copy(A), create(Anew)
while ( error > tol && iter < iter max ) {</pre>
  error=0.0;
#pragma acc kernels loop gang(32), vector(16)
  for ( int j = 1; j < n-1; j++) {
#pragma acc loop gang(16), vector(32)
    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 loop gang(16), vector(32)
  for ( int j = 1; j < n-1; j++) {
#pragma acc loop
    for ( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
  iter++;
```



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