# GPU Computing with OpenACC Directives



#### **GPUs Reaching Broader Set of Developers**





Time





# **OpenACC Directives**





Your original Fortran or C code

### Familiar to OpenMP Programmers





#### **OpenACC** Open Programming Standard for Parallel Computing

"OpenACC will enable programmers to easily develop portable applications that maximize the performance and power efficiency benefits of the hybrid CPU/GPU architecture of Titan."

--Buddy Bland, Titan Project Director, Oak Ridge National Lab

"OpenACC is a technically impressive initiative brought together by members of the OpenMP Working Group on Accelerators, as well as many others. We look forward to releasing a version of this proposal in the next release of OpenMP."

--Michael Wong, CEO OpenMP Directives Board

















#### **OpenACC** The Standard for GPU Directives



- Easy: Directives are the easy path to accelerate compute intensive applications
- Open: OpenACC is an open GPU directives standard, making GPU programming straightforward and portable across parallel and multi-core processors

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



### High-level, with low-level access



Compiler directives to specify parallel regions in C, C++, Fortran

- OpenACC compilers offload parallel regions from host to accelerator
- Portable across OSes, host CPUs, accelerators, and compilers
- Create high-level heterogeneous programs
  - Without explicit accelerator initialization,
  - Without explicit data or program transfers between host and accelerator
- Programming model allows programmers to start simple
  - Enhance with additional guidance for compiler on loop mappings, data location, and other performance details
- Compatible with other GPU languages and libraries
  - Interoperate between CUDA C/Fortran and GPU libraries
  - e.g. CUFFT, CUBLAS, CUSPARSE, etc.

### **Directives: Easy & Powerful**



Real-Time Object Detection

Global Manufacturer of Navigation Systems



#### Valuation of Stock Portfolios using Monte Carlo

Global Technology Consulting Company



#### Interaction of Solvents and Biomolecules

University of Texas at San Antonio



#### 5x in 40 Hours2x in 4 Hours5x in 8 Hours

Optimizing code with directives is quite easy, especially compared to CPU threads or writing CUDA kernels. The most important thing is avoiding restructuring of existing code for production applications.

-- Developer at the Global Manufacturer of Navigation Systems

#### Small Effort. Real Impact.



Large Oil Company

3x in 7 days

Solving billions of equations iteratively for oil production at world's largest petroleum reservoirs UNIVERSITY of HOUSTON CULLEN COLLEGE OF ENGINEERING

Univ. of Houston Prof. M.A. Kayali

20x in 2 days

Studying magnetic systems for innovations in magnetic storage media and memory, field sensors, and biomagnetism



Uni. Of Melbourne Prof. Kerry Black 65x in 2 days

Better understand complex reasons by lifecycles of snapper fish in Port Phillip Bay



Ufa State Aviation Prof. Arthur Yuldashev 7x in 4 Weeks

Generating stochastic geological models of oilfield reservoirs with borehole data



#### GAMESS-UK

Dr. Wilkinson, Prof. Naidoo

10x

Used for various fields such as investigating biofuel production and molecular sensors.

\* Achieved using the PGI Accelerator Compiler

### Focus on Exposing Parallelism



# With Directives, tuning work focuses on *exposing parallelism*, which makes codes inherently better

#### Example: Application tuning work using directives for new Titan system at ORNL

#### S3D

Research more efficient combustion with nextgeneration fuels



- Tuning top 3 kernels (90% of runtime)
- 3 to 6x faster on CPU+GPU vs. CPU+CPU
- But also improved all-CPU version by 50%



#### CAM-SE

Answer questions about specific climate change adaptation and mitigation scenarios

- Tuning top key kernel (50% of runtime)
- 6.5x faster on CPU+GPU vs. CPU+CPU
- Improved performance of CPU version by 100%

### **OpenACC Specification and Website**



Full OpenACC 1.0 Specification available online

#### http://www.openacc-standard.org

- Quick reference card also available
- Beta implementations available now from PGI, Cray, and CAPS

#### The OpenACC<sup>™</sup> API QUICK REFERENCE GUIDE

The OpenACC Application Program Interface describes a collection of compiler directives to specify loops and regions of code in standard C, C++ and Fortran to be offloaded from a host CPU to an attached accelerator, providing portability across operating systems, host CPUs and accelerators.

Most OpenACC directives apply to the immediately following structured block or loop; a structured block is a single statement or a compound statement (C or C++) or a sequence of statements (Fortran) with a single entry point at the top and a single exit at the bottom.



# Start Now with OpenACC Directives



# Sign up for a free trial of the directives compiler now!

#### Free trial license to PGI Accelerator

#### Tools for quick ramp

#### www.nvidia.com/gpudirectives





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GPU COMPUTING SOLUTIONS	Accelerate )	Your Scientifi	ic Code wit	h OpenA(	CC
Main What is GPU Computing?	The Open St	andard for G	iPU Accelei	ator Dire	ctives
Why Choose Tesla Industry Software Solutions Tesla Workstation Solutions Tesla Data Center Solutions Tesla Bio Workbench Where to Buy Contact US Sign up for Tesla Alerts Fermi GPU Computing Architecture	Thousands of cores w Based on the <u>OpenACC</u> way to accelerate your you can accelerate your code and the compiler of your code to the GP directive hint can acce you can get started an #include <=tdo.h> #define N 10000 int main(void) { double pi = 0.0 #pragma acc rec	<pre>vorking for you. _ standard, GPU directi' scientific or industrial ur code by simply insert will automatically map U. Here's an example o elerate the calculation of d see results in the sam Of; long i; pion for</pre>	ves are the easy, pr code. With GPU din ing compiler hints ir compute-intensive f how easy a single if pi. With GPU diren ne afternoon.	oven ectives, ito your portions ctives,	I have written mic (written in Fortran properties of two a dimensional magne directives approach port my existing co perform my compu- which resulted in a speedup (more than computation." Lear Professor M. Amin University of Houst
SOFTWARE AND HARDWARE INFO	for (i=0; i <n; td="" {<=""><td>i++)</td><td></td><td></td><td></td></n;>	i++)			
Tesla Product Literature Tesla Software Features Software Development Tools CUDA Training and Consulting	<pre>double t= (     pi +=4.0/(1     printf("pi=%f\n     return 0; }</pre>	<pre>(double) ((i+0.5)/N); 1.0+t*t); n",pi/N);</pre>			'The PGI compiler : just how powerful software we are wr times faster on the are very pleased an
Services GPU Cloud Computing Service Providers OpenACC GPU Directives	By starting with a free working on the techno directives standard. O	e, 30-day trial of PGI dir logy that is the foundat	ectives today, you a tion of the OpenACC	are :	future uses. It's like supercomputer." <u>Le</u> Dr. Kerry Black

#### A Very Simple Exercise: SAXPY SAXPY in C SAX



#### SAXPY in Fortran

```
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];
}</pre>
```

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

. . .

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



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



#### **Kernels Construct**



Fortran !\$acc kernels [clause ...] structured block !\$acc end kernels

L
#pragma acc kernels [clause ...]
{ structured block }

#### Clauses

if( condition )
async( expression )
Also, any data clause (more later)

# 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
  - Otherwise the compiler can't parallelize loops that access ptr
  - Note: if programmer violates the declaration, behavior is undefined

### Complete SAXPY example code





### 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:

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



```
Jacobi Iteration C Code
while ( error > tol && iter < iter_max ) {</pre>
                                                                            Iterate until converged
   error=0.0;
   for( int j = 1; j < n-1; j++) {</pre>
                                                                             Iterate across matrix
     for(int i = 1; i < m-1; i++) {</pre>
                                                                                  elements
                                                                          Calculate new value from
       Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                             A[j-1][i] + A[j+1][i]);
                                                                                  neighbors
                                                                            Compute max error for
       error = max(error, abs(Anew[j][i] - A[j][i]);
                                                                                convergence
    3
   }
  for( int j = 1; j < n-1; j++) {</pre>
    for( int i = 1; i < m-1; i++ ) {</pre>
                                                                          Swap input/output arrays
       <u>A[j][</u>i] = Anew[j][i];
     }
   }
   iter++;
}
```

NVIDIA



# OpenMP C Code

}

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

```
#pragma omp parallel for shared(m, n, Anew, A)
  for( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {</pre>
      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 omp parallel for shared(m, n, Anew, A)
  for( int j = 1; j < n-1; j++) {</pre>
    for( int i = 1; i < m-1; i++ ) {</pre>
      A[j][i] = Anew[j][i];
    }
  }
  iter++;
```





Parallelize loop across CPU threads



Parallelize loop across CPU threads

## **OpenMP Fortran Code**



Parallelize loop across

**CPU threads** 

Parallelize loop across

**CPU** threads

do while ( err > tol .and. iter < iter\_max )
 err=0.\_fp\_kind</pre>

end do

```
!$omp parallel do shared(m,n,Anew,A) reduction(max:err)
 do j=1,m
   do i=1.n
     Anew(i,j) = .25_{fp}kind * (A(i+1, j) + A(i-1, j) + \&
                                A(i , j-1) + A(i , j+1))
     err = max(err, Anew(i,j) - A(i,j))
   end do
 end do
!$omp parallel do shared(m,n,Anew,A)
 do j=1,m-2
   do i=1,n-2
    A(i,j) = Anew(i,j)
   end do
 end do
 iter = iter + 1
```

### Exercises: General Instructions (compiling)

- Exercises are in "exercises/openacc" directory in your home directory
  - Solutions are in "exercise\_solutions/openacc" directory
- To compile, use one of the provided makefiles
   C:
   > make

Fortran:

> make -f Makefile\_f90

Remember these compiler flags: -acc -ta=nvidia -Minfo=accel

### Exercises: General Instructions (running)



To run, use qsub with one of the provided job files

- > qsub laplace\_acc.job
- > qstat # prints qsub status

Output is placed in <a>laplace\_acc.job.o<job#></a> when finished.

#### OpenACC job file looks like this

#!/bin/csh
#PBS -1 walltime=3:00
./laplace2d\_acc

#### The OpenMP version specifies number of cores to use

#!/bin/csh
#PBS -1 walltime=3:00
setenv OMP\_NUM\_THREADS 6
./laplace2d\_omp



Edit this to control the number of cores to use

### GPU startup overhead



If no other GPU process running, GPU driver may be swapped out

- Linux specific
- Starting it up can take 1-2 seconds

#### Two options

- Run nvidia-smi in persistence mode (requires root permissions)
- Run "nvidia-smi -q -l 30" in the background
- If your running time is off by ~2 seconds from results in these slides, suspect this
  - Nvidia-smi should be running in persistent mode for these exercises



Task: use acc kernels to parallelize the Jacobi loop nests

Edit laplace2D.c or laplace2D.f90 (your choice)

- In the 001-laplace2D-kernels directory
- Add directives where it helps
- Figure out the proper compilation command (similar to SAXPY example)
  - Compile both with and without OpenACC parallelization
  - Optionally compile with OpenMP (original code has OpenMP directives)
- Run OpenACC version with laplace\_acc, OpenMP with laplace\_omp
- Q: can you get a speedup with just kernels directives?
  - Versus 1 CPU core? Versus 6 CPU cores?

### Exercise 1 Solution: OpenACC C

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

```
#pragma acc kerners
for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
        A[j][i] = Anew[j][i];
    }
    }
    iter++;
}_____</pre>
```



Execute GPU kernel for loop nest



Execute GPU kernel for loop nest



```
Exercise 1 Solution: OpenACC Fortran
                                                                                  do while ( err > tol .and. iter < iter_max )</pre>
 err=0._fp_kind
                                                                  Generate GPU kernel for
!$acc kernels
                                                                        loop nest
 do j=1,m
   do i=1.n
     Anew(i,j) = .25_{fp}kind * (A(i+1, j) + A(i-1, j) + \&
                              A(i, j-1) + A(i, j+1))
     err = max(err, Anew(i,j) - A(i,j))
   end do
 end do
!$acc end kernels
                                                                  Generate GPU kernel for
!$acc kernels
                                                                        loop nest
 do j=1,m-2
   do i=1, n-2
    A(i,j) = Anew(i,j)
   end do
 end do
!$acc end kernels
 iter = iter + 1
end do
```

### Exercise 1 Solution: C Makefile



```
CC = pgcc
CCFLAGS =
ACCFLAGS = -acc -ta=nvidia, -Minfo=accel
OMPFLAGS = -fast -mp -Minfo
```

BIN = laplace2d\_omp laplace2d\_acc

all: \$(BIN)

```
laplace2d_acc: laplace2d.c
    $(CC) $(CCFLAGS) $(ACCFLAGS) -0 $@ $<</pre>
```

laplace2d\_omp: laplace2d.c
 \$(CC) \$(CCFLAGS) \$(OMPFLAGS) -0 \$@ \$<</pre>

clean:

\$(RM) \$(BIN)

### **Exercise 1 Solution: Fortran Makefile**



```
F90 = pgf90
CCFLAGS =
ACCFLAGS = -acc -ta=nvidia, -Minfo=accel
OMPFLAGS = -fast -mp -Minfo
```

BIN = laplace2d\_f90\_omp laplace2d\_f90\_acc

all: \$(BIN)

```
laplace2d_f90_acc: laplace2d.f90
    $(F90) $(CCFLAGS) $(ACCFLAGS) -0 $@ $<</pre>
```

laplace2d\_f90\_omp: laplace2d.f90
 \$(F90) \$(CCFLAGS) \$(OMPFLAGS) -o \$@ \$<</pre>

clean:

\$(RM) \$(BIN)

### Exercise 1: 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

#### **Exercise 1: Performance**

CPU: Intel Xeon X5690 6 Cores @ 3.47GHz



#### GPU: NVIDIA Tesla M2090

Execution (4096x4096)	Time (s)	Speedup
CPU 1 OpenMP thread	105.6	
CPU 2 OpenMP threads	62.5	1.69x
CPU 4 OpenMP threads	43.3	2.44x
CPU 6 OpenMP threads	41.2	2.56x
OpenACC GPU	180.0	0.23x FAIL

Speedup vs. 1 CPU core

Speedup vs. 6 CPU cores

### What went wrong?



#### Add -ta=nvidia, time to compiler command line



#### **Basic Concepts**





For efficiency, decouple data movement and compute off-load

#### **Excessive Data Transfers**





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

![](_page_38_Picture_0.jpeg)

#### DATA MANAGEMENT

#### Data Construct

![](_page_39_Picture_1.jpeg)

#### Fortran

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

#### С

#### #pragma acc data [clause ...] { structured block }

#### **General Clauses**

if( condition )
async( expression )

Manage data movement. Data regions may be nested.

#### Data Clauses

![](_page_40_Picture_1.jpeg)

**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.

### Array Shaping

![](_page_41_Picture_1.jpeg)

Compiler sometimes cannot determine size of arrays

Must specify explicitly using data clauses and array "shape"

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

#### Fortran

• C

!\$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

### **Update Construct**

![](_page_42_Picture_1.jpeg)

Fortran !\$acc update [clause ...]

#pragma acc update [clause ...]

oression )

#### Clauses

host( list )	if( expression )
device( list )	async( expressio

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.

#### **Exercise 2: Jacobi Data Directives**

![](_page_43_Picture_1.jpeg)

- Task: use acc data to minimize transfers in the Jacobi example
- Start from given laplace2D.c or laplace2D.f90 (your choice)
  - In the 002-laplace2d-data directory
  - Add directives where it helps (hint: [do] while loop)
- Q: What speedup can you get with data + kernels directives?
  - Versus 1 CPU core? Versus 6 CPU cores?

### Exercise 2 Solution: OpenACC C

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

```
#pragma acc kernels
  for( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {</pre>
      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]);
   3
  }
#pragma acc kernels
  for( int j = 1; j < n-1; j++) {</pre>
    for( int i = 1; i < m-1; i++ ) {</pre>
      A[j][i] = Anew[j][i];
    }
  }
  iter++;
```

![](_page_44_Picture_3.jpeg)

### Exercise 2 Solution: OpenACC Fortran

![](_page_45_Picture_1.jpeg)

![](_page_45_Figure_2.jpeg)

!\$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

![](_page_45_Picture_8.jpeg)

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

#### **Exercise 2: Performance**

CPU: Intel Xeon X5690 6 Cores @ 3.47GHz

![](_page_46_Picture_2.jpeg)

#### GPU: NVIDIA Tesla M2090

Execution	Time (s)	Speedup
CPU 1 OpenMP thread	105.6	
CPU 2 OpenMP threads	62.5	1.69x
CPU 4 OpenMP threads	43.3	2.44x
CPU 6 OpenMP threads	41.2	2.56x
OpenACC GPU	10.50	3.92x

Speedup vs. 1 CPU core

Speedup vs. 6 CPU cores

#### **Further speedups**

![](_page_47_Picture_1.jpeg)

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

Will tackle these in later exercises

### Finding Parallelism in your code

![](_page_48_Picture_1.jpeg)

- (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
  - To help compiler: restrict keyword (C), independent clause
- 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.

### **Tips and Tricks**

![](_page_49_Picture_1.jpeg)

- (PGI) Use time option to learn where time is being spent
  - -ta=nvidia,<mark>time</mark>
- 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
- Conditional compilation with \_OPENACC macro

### **OpenACC Learning Resources**

![](_page_50_Picture_1.jpeg)

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