GPU Computing with OpenACC Directives

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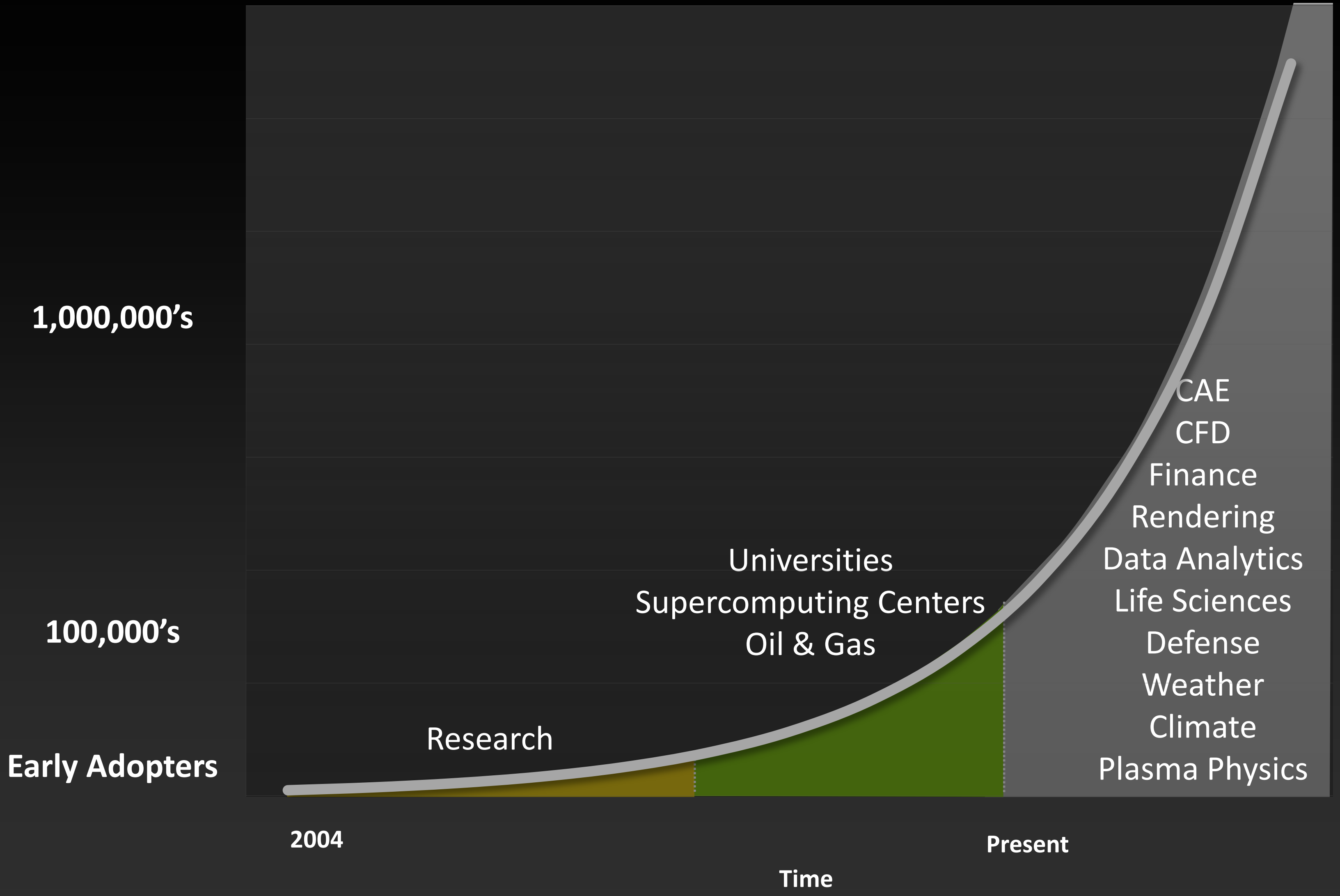
NVIDIA Corporation

GPUs Reaching Broader Set of Developers

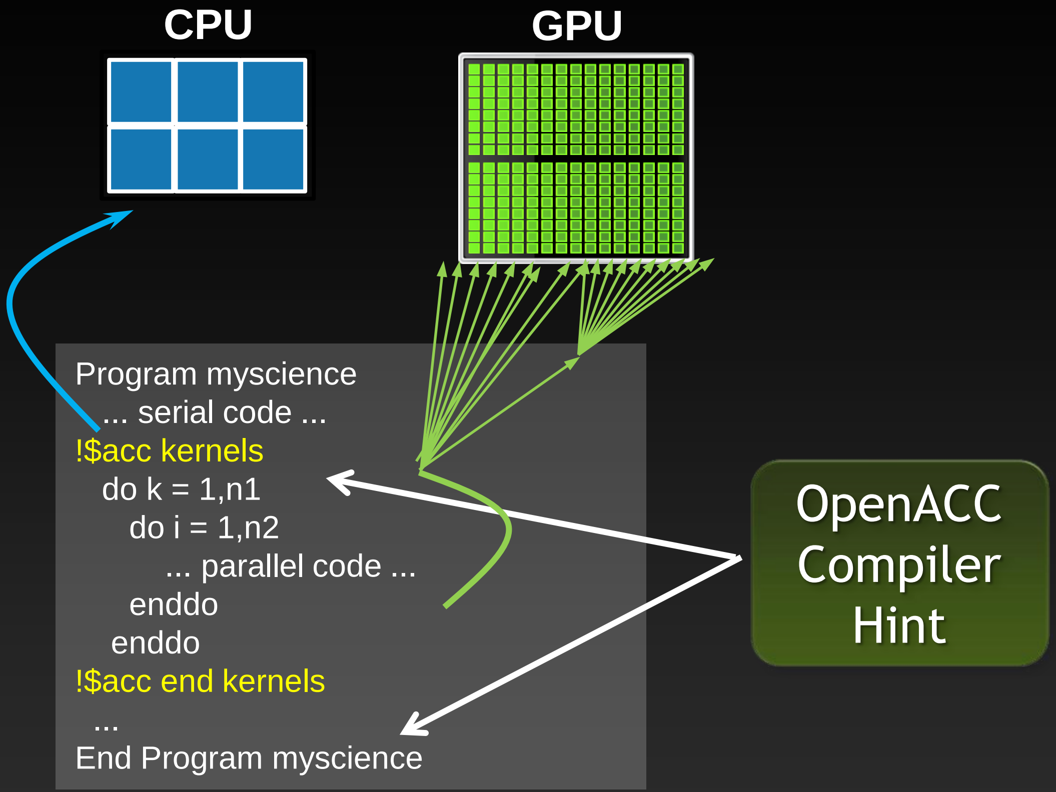


3 Ways to Accelerate Applications

Applications

Libraries	OpenACC Directives	Programming Languages
"Drop-in" Acceleration	Easily Accelerate Applications	Maximum Flexibility

OpenACC Directives



```
Program myscience
 ... serial code ...
!$acc kernels
  do k = 1,n1
    do i = 1,n2
      ... parallel code ...
    enddo
  enddo
!$acc end kernels
 ...
End Program myscience
```

Your original Fortran or C code

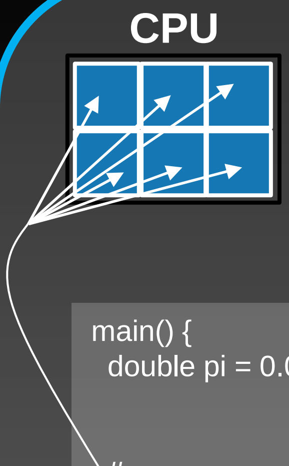
Simple Compiler hints

Compiler Parallelizes code

Works on many-core GPUs & multicore CPUs

Familiar to OpenMP Programmers

OpenMP

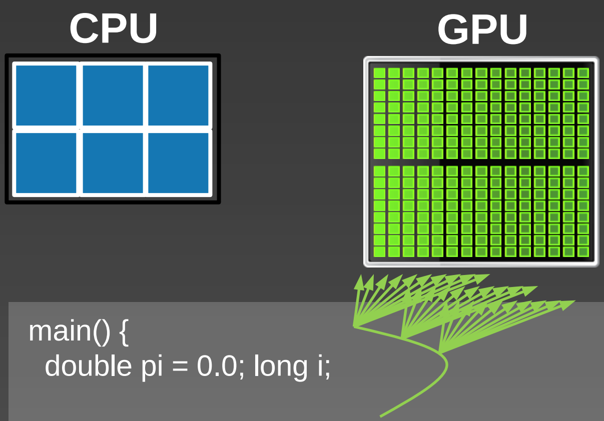


```
main() {
  double pi = 0.0; long i;


  #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);
}
```

OpenACC



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

  #pragma acc kernels
  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);
}
```

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 Standard - Founding Members

NVIDIA. CRAY THE SUPERCOMPUTER COMPANY PGI CAPS

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

OpenACC®
DIRECTIVES FOR ACCELERATORS

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

5x in 40 Hours

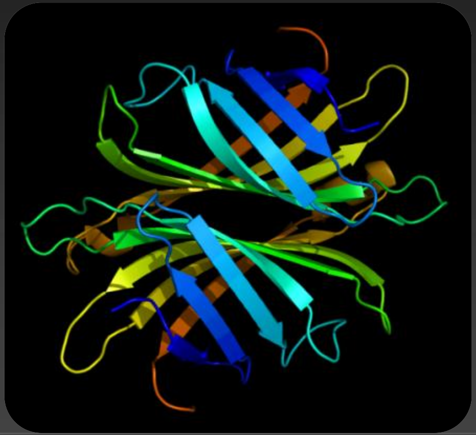
Valuation of Stock Portfolios using Monte Carlo

Global Technology Consulting Company

2x in 4 Hours

Interaction of Solvents and Biomolecules

University of Texas at San Antonio



5x 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	**Univ. of Houston**	**Uni. Of Melbourne**	**Ufa State Aviation**	**GAMESS-UK**
	Prof. M.A. Kayali	Prof. Kerry Black	Prof. Arthur Yuldashev	Dr. Wilkinson, Prof. Naidoo
3x in 7 days	20x in 2 days	65x in 2 days	7x in 4 Weeks	10x
Solving billions of equations iteratively for oil production at world’s largest petroleum reservoirs	Studying magnetic systems for innovations in magnetic storage media and memory, field sensors, and biomagnetism	Better understand complex reasons by lifecycles of snapper fish in Port Phillip Bay	Generating stochastic geological models of oilfield reservoirs with borehole data	Used for various fields such as investigating biofuel production and molecular sensors.

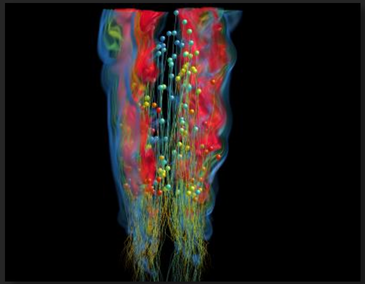
* Achieved using the PGI Accelerator Compiler

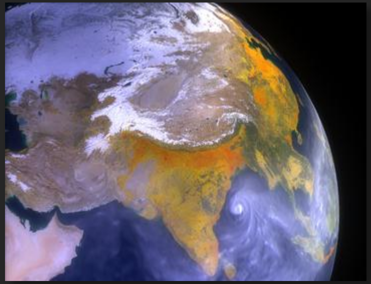
Focus on Exposing Parallelism

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 next-generation fuels





CAM-SE
Answer questions about specific climate change adaptation and mitigation scenarios

- 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%

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

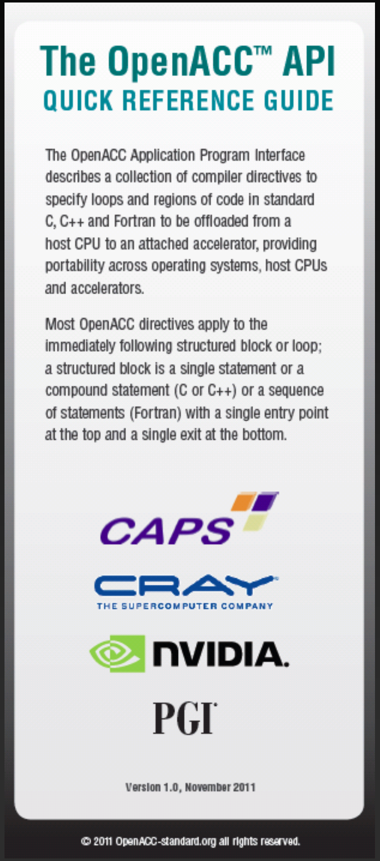
OpenACC Specification and Website

- Full OpenACC 2.0 Specification available online

  http://www.openacc-standard.org

- Quick reference card also available

- Compilers available now from PGI, Cray, and CAPS


The OpenACC™ 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.

CAPS
CRAY THE SUPERCOMPUTER COMPANY
NVIDIA.
PGI

Version 1.0, November 2011

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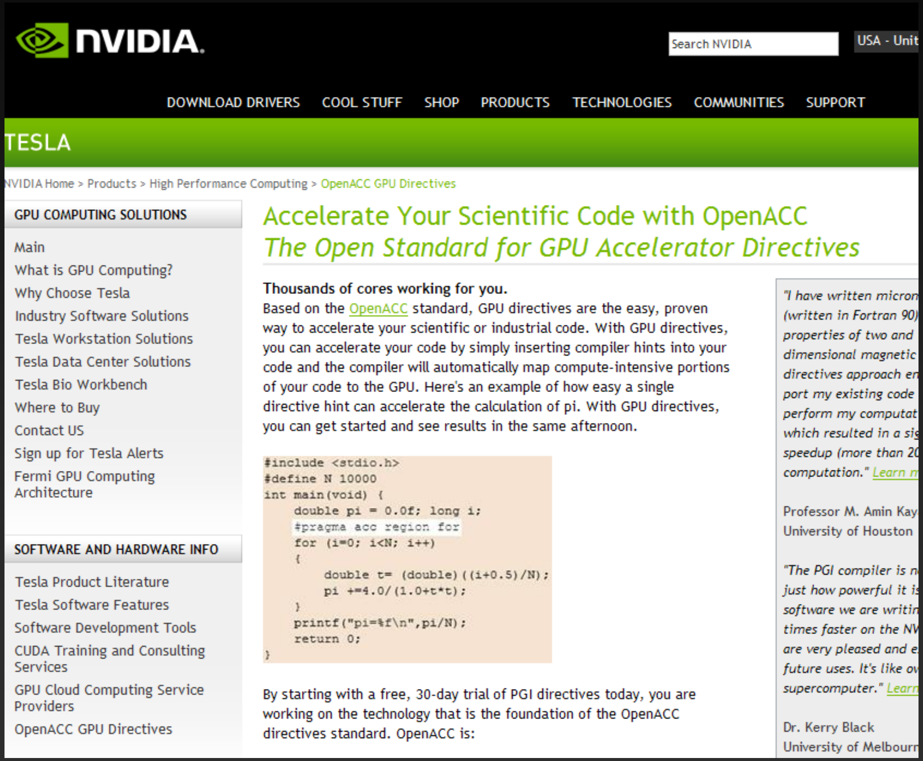
Start Now with OpenACC Directives

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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Accelerate Your Scientific Code with OpenACC

The Open Standard for GPU Accelerator Directives

Thousands of cores working for you.

Based on the OpenACC standard, GPU directives are the easy, proven way to accelerate your scientific or industrial code. With GPU directives, you can accelerate your code by simply inserting compiler hints into your code and the compiler will automatically map compute-intensive portions of your code to the GPU. Here's an example of how easy a single directive hint can accelerate the calculation of pi. With GPU directives, you can get started and see results in the same afternoon.

```
#include <stdio.h>
#define N 10000
int main(void) {
    double pi = 0.0f; long i;
    #pragma acc region for
    for (i=0; i<N; i++)
    {
        double t= (double)((i+0.5)/N);
        pi +=4.0/(1.0+t*t);
    }
    printf("pi=%f\n",pi/N);
    return 0;
}
```

By starting with a free, 30-day trial of PGI directives today, you are working on the technology that is the foundation of the OpenACC directives standard. OpenACC is:

"I have written micron
(written in Fortran 90)
properties of two and
dimensional magnetic
directives approach en
port my existing code
perform my computat
which resulted in a sig
speedup (more than 20
computation." Learn m

Professor M. Amin Kay
University of Houston

"The PGI compiler is n
just how powerful it is
software we are writin
times faster on the NV
are very pleased and e
future uses. It's like ov
supercomputer." Learn

Dr. Kerry Black
University of Melbourn

NVIDIA.

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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)

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

http://en.wikipedia.org/wiki/Restrict

Complete SAXPY example code

- Trivial first example
  - Apply a loop directive
  - Learn compiler commands

```
#include <stdlib.h>

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];
}
```

*restrict:
"I promise y does not alias x"

```
int main(int argc, char **argv)
{
  int N = 1<<20; // 1 million floats

  if (argc > 1)
    N = atoi(argv[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;
    y[i] = 1.0f;
  }

  saxpy(N, 3.0f, x, y);

  return 0;
}
```

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
```

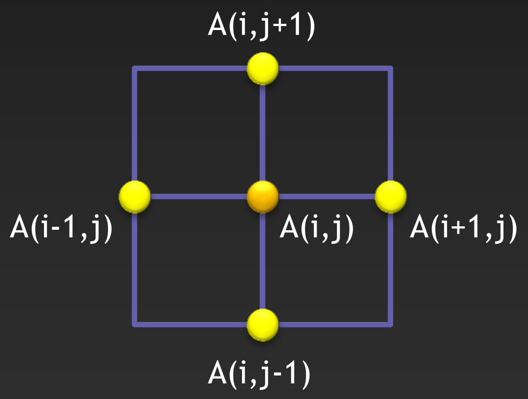
- Compiler output:

```
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
```

grid example

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 Code

```
while ( error > tol && iter < iter_max ) {
  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++;
}
```

Iterate until converged

Iterate across matrix elements

Calculate new value from neighbors

Compute max error for convergence

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_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

  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
```

Iterate until converged

Iterate across matrix elements

Calculate new value from neighbors

Compute max error for convergence

Swap input/output arrays

OpenMP C Code

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

#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++) {

      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++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }

  iter++;
}
```

Parallelize loop across CPU threads

Parallelize loop across CPU threads

OpenMP Fortran Code

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

!$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
end do
```

Parallelize loop across CPU threads

Parallelize loop across CPU threads

Exercises: General Instructions (compiling)

- Exercises are in “exercises” directory in your home directory
  - Solutions are in “solutions” directory

- To compile, use one of the provided makefiles

```
> cd exercises/001-laplace2D-kernels
```

C:

```
> make
```

Fortran:

```
> make -f Makefile_f90
```

- Remember these compiler flags:

```
-acc -ta=nvidia,cuda5.5,cc3.5 -Minfo=accel
```

Exercises: General Instructions (running)

To run, use one of the provided job files

- ➢ `qsub myjob_acc – to run the OpenACC version`
- ➢ `Qsub myjob_omp – to run the OMP version (build it first!)`

```
> ./chk          # prints your job(s) status
```

Output is placed in openacc_001_....o<job#> when finished.

OpenACC job file looks like this

```
#PBS -l walltime=1:00
./laplace2d_acc
```

The OpenMP version specifies number of cores to use

```
#PBS -l walltime=1:00
export OMP_NUM_THREADS 6
./laplace2d_omp
```

Edit this to control the number of cores to use

Exercise 1: Jacobi Kernels

- Task: use `acc kernels` to parallelize the Jacobi loop nests

- Edit laplace2d.c
- In the `001-laplace2D-kernels` directory
  - Add directives where it helps
  - Figure out the proper compilation command (similar to SAXPY example)
    - Compile with OpenACC parallelization (make laplace2d_acc)
    - Optionally compile with OpenMP (original code has OpenMP directives)
  - Run OpenACC with qsub myjob_acc, OpenMP with qsub myjob_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;

#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

Exercise 1 Solution: 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

Exercise 1 Solution: C Makefile

```
CC       = pgcc
CCFLAGS  =
ACCFLAGS = -acc -ta=nvidia,cuda5.5,cc3.5 -Minfo=accel
OMPFLAGS = -fast -mp -Minfo

BIN =  laplace2d_omp laplace2d_acc

all: $(BIN)

laplace2d_acc: laplace2d.c
        $(CC) $(CCFLAGS) $(ACCFLAGS) -o $@ $<

laplace2d_omp: laplace2d.c
        $(CC) $(CCFLAGS) $(OMPFLAGS) -o $@ $<

clean:
        $(RM) $(BIN)
```

Exercise 1 Solution: Fortran Makefile

```
F90       = pgf90
CCFLAGS   =
ACCFLAGS = -acc -ta=nvidia,cuda5.5,cc3.5 -Minfo=accel
OMPFLAGS = -fast -mp -Minfo

BIN =  laplace2d_f90_omp laplace2d_f90_acc

all: $(BIN)

laplace2d_f90_acc: laplace2d.f90
        $(F90) $(CCFLAGS) $(ACCFLAGS) -o $@ $<

laplace2d_f90_omp: laplace2d.f90
        $(F90) $(CCFLAGS) $(OMPFLAGS) -o $@ $<

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 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

What went wrong?

- Add PGI_ACC_TIME=1 to execution command line

```
e.g.: PGI_ACC_TIME=1 ./laplace2d_acc
Accelerator Kernel Timing data
/usr/users/6/harrism/openacc-workshop/solutions/001-laplace2D-kernels/laplace2d.c
  main
    69: region entered 1000 times
        time(us): total=77524918 init=240 region=77524678
                  kernels=4422961 data=66464916
        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
/usr/users/6/harrism/openacc-workshop/solutions/001-laplace2D-kernels/laplace2d.c
  main
    57: region entered 1000 times
        time(us): total=82135902 init=216 region=82135686
                  kernels=8346306 data=66775717
        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
        time(us): init=158248
```

4.4 seconds

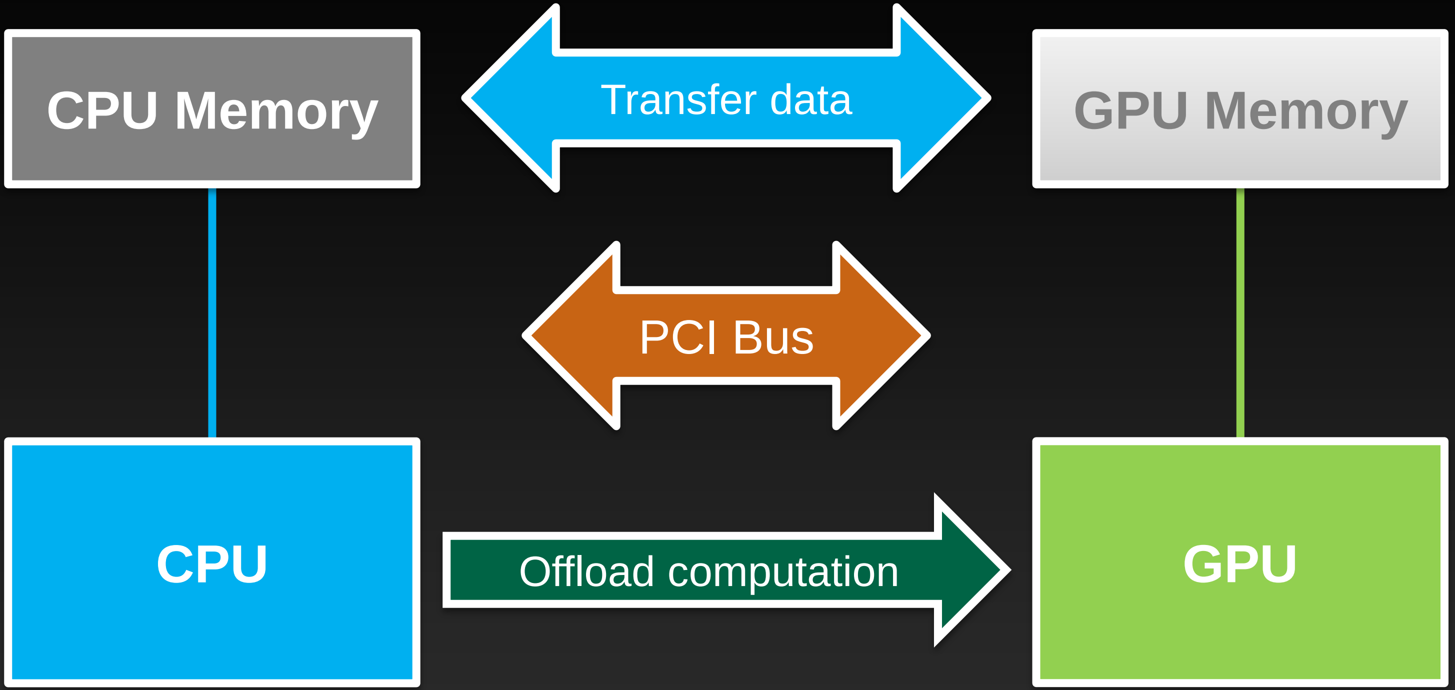
66.5 seconds

8.3 seconds

66.8 seconds

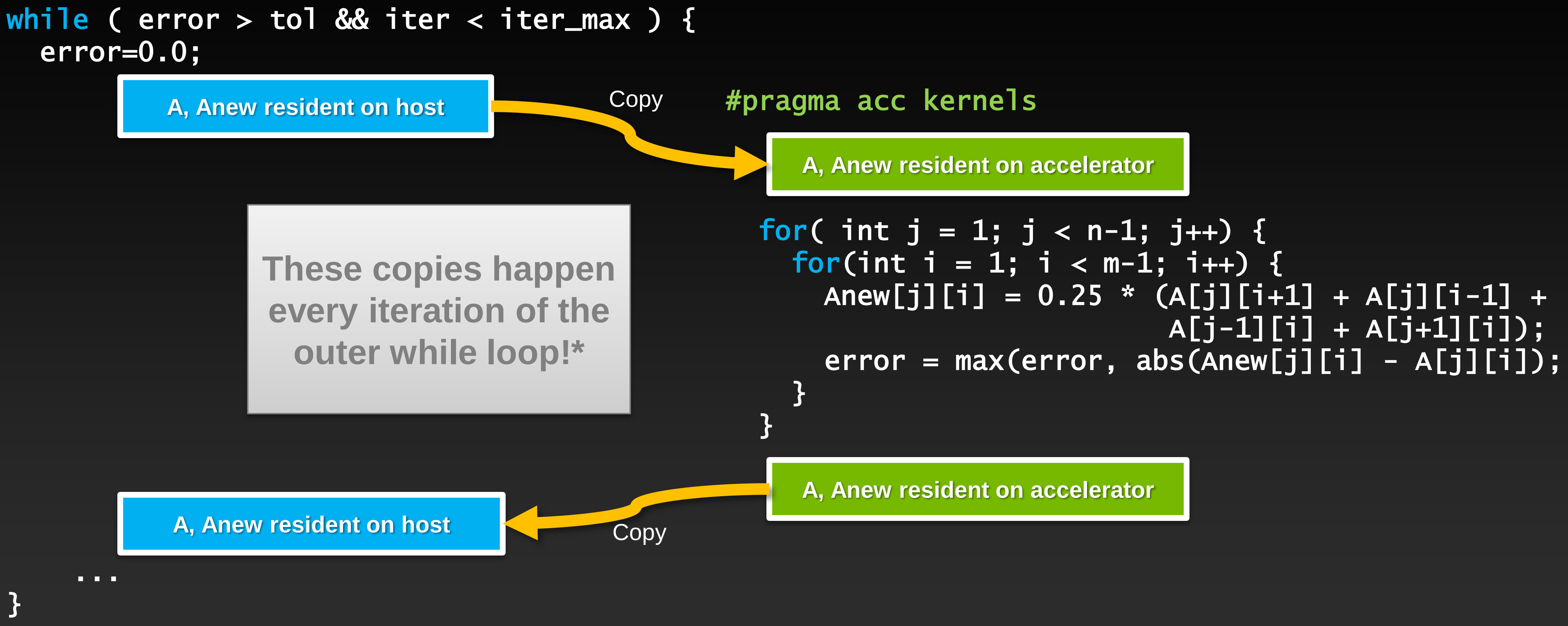
Huge Data Transfer Bottleneck!
Computation: 12.7 seconds
Data movement: 133.3 seconds

Basic Concepts



For efficiency, decouple data movement and compute off-load

Excessive Data Transfers



```
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]);
                                                  }
                                                }

      ...
}
```

A, Anew resident on host
Copy
A, Anew resident on accelerator
A, Anew resident on accelerator
Copy
A, Anew resident on host

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

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

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.

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`.

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`

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.

Exercise 2: Jacobi Data Directives

- 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;

#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

Exercise 2 Solution: 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

Exercise 2: 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

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

- Will tackle these in later exercises

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
  - 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

- (PGI) Use time option to learn where time is being spent
  - PGI_ACC_TIME=1
- 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

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

Complete OpenACC API

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 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

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
```

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

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.

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.

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.

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.

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.

Other Syntax

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.

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
```

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

Thank you