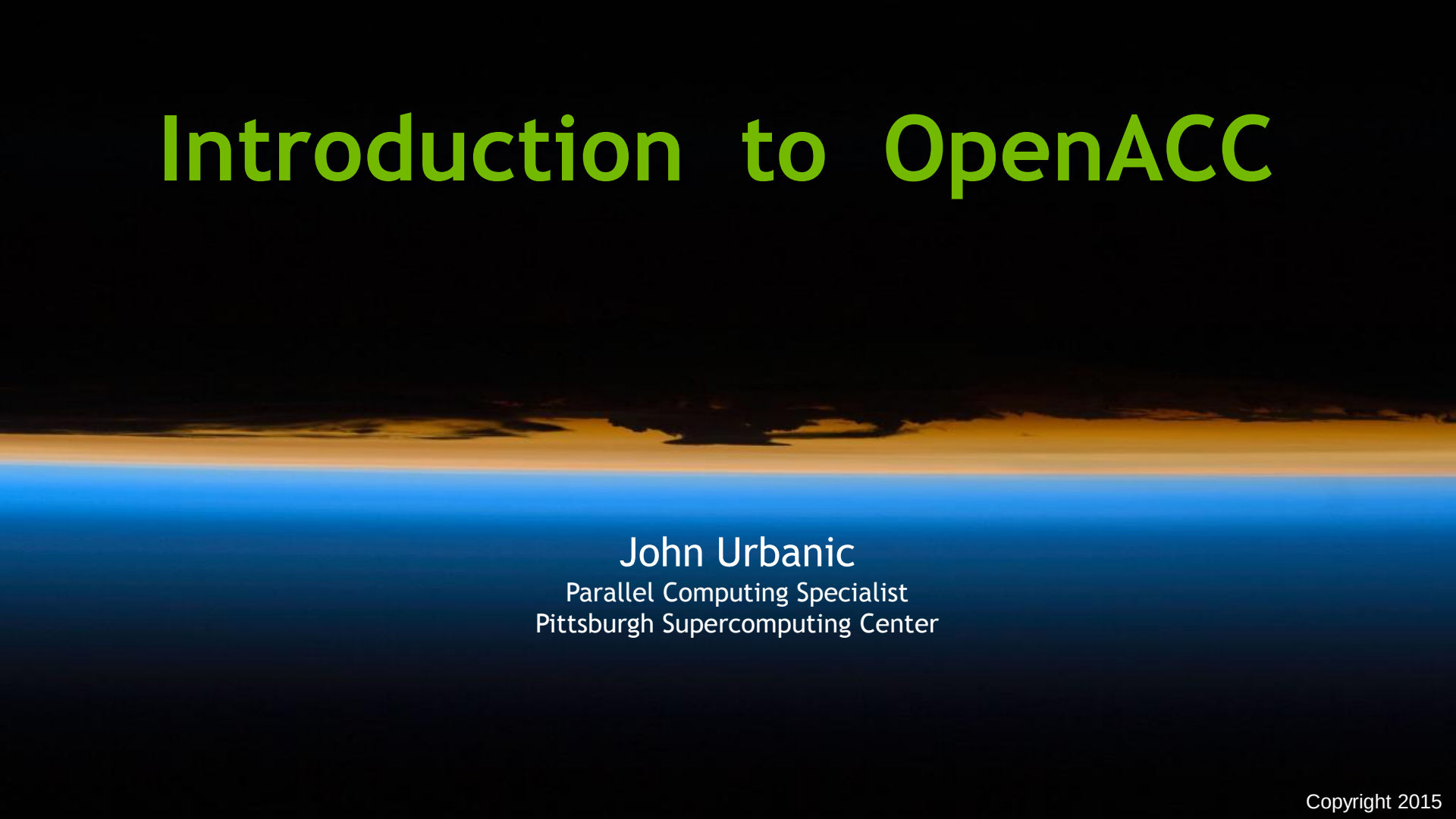
# Introduction to OpenACC



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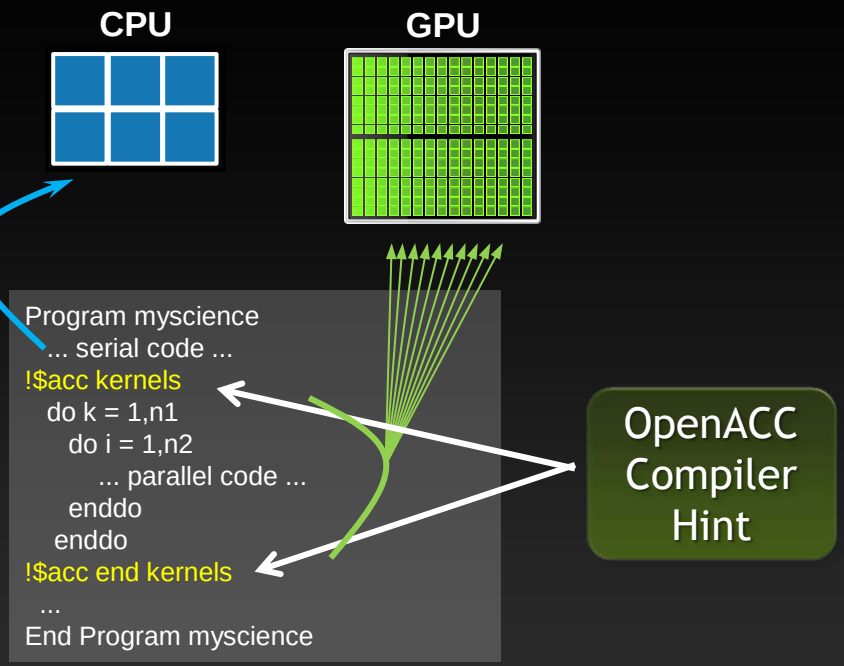
# What is OpenACC?

*It is a directive based standard to allow developers to take advantage of accelerators such as GPUs from NVIDIA and AMD, Intel's Xeon Phi, FPGAs, and even DSP chips.*

# Directives




Your original
Fortran or C code

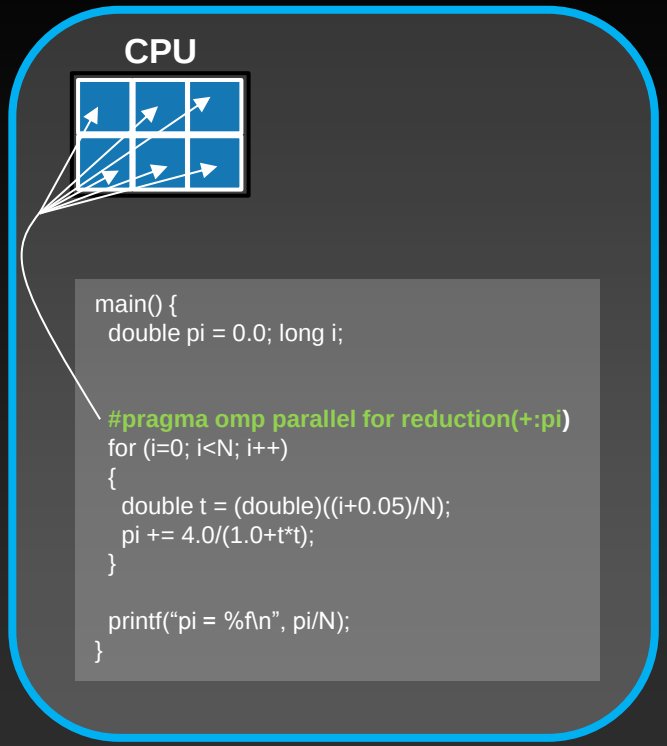
Simple compiler hints from coder.

Compiler generates parallel threaded code.

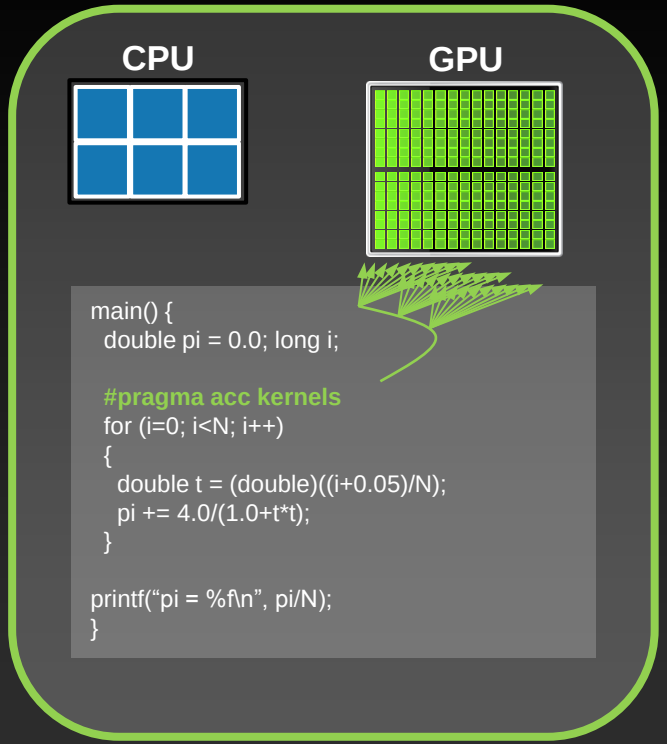
Ignorant compiler just sees some comments.

# Familiar to OpenMP Programmers

**OpenMP**

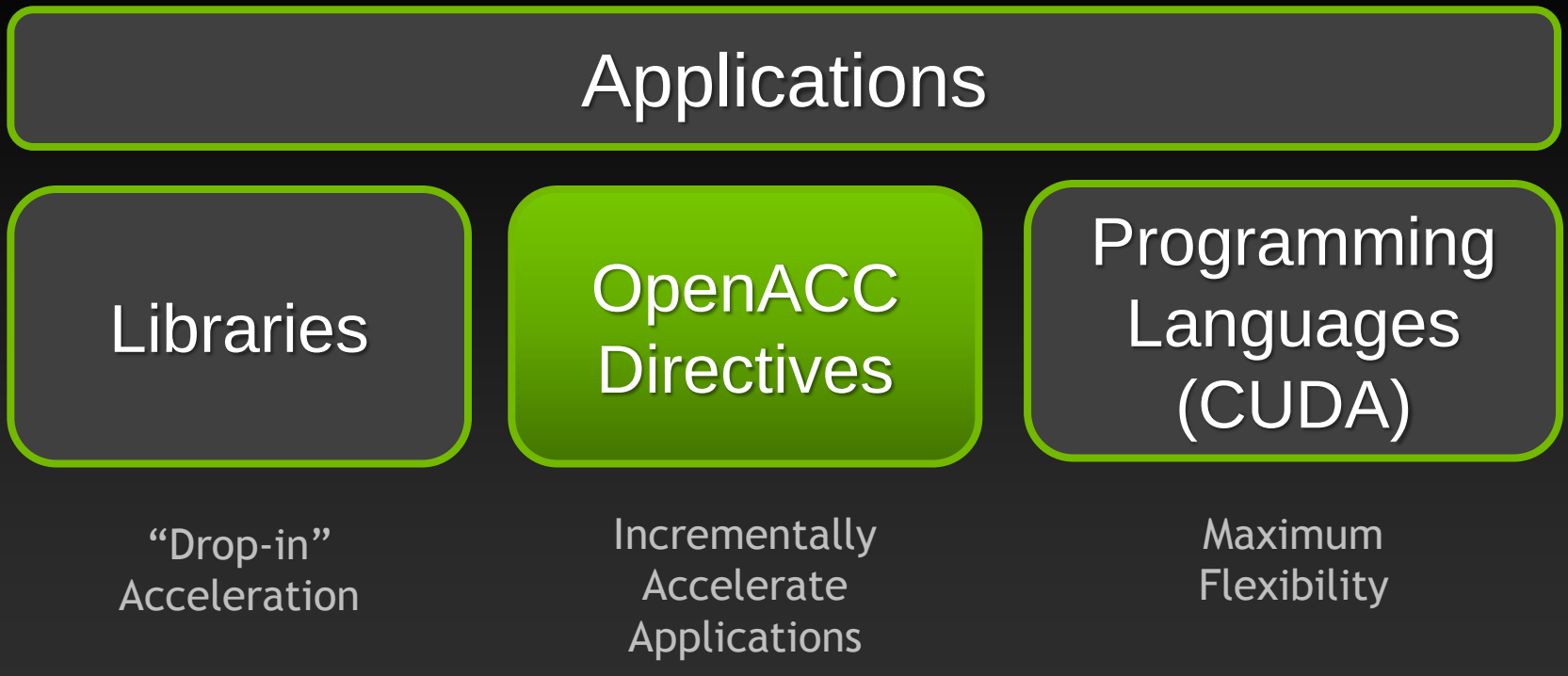



**OpenACC**




More on this later!

# How Else Would We Accelerate Applications?



# Key Advantages Of This Approach

- High-level. No involvement of OpenCL, CUDA, etc.
- Single source. No forking off a separate GPU code. Compile the same program for accelerators or serial, non-GPU programmers can play along.
- Efficient. Experience shows very favorable comparison to low-level implementations of same algorithms.
- Performance portable. Supports GPU accelerators and co-processors from multiple vendors, current and future versions.
- Incremental. Developers can port and tune parts of their application as resources and profiling dictates. No wholesale rewrite required. Which can be *quick*.

# A Few Cases

Reading DNA nucleotide sequences

*Shanghai JiaoTong University*

4 directives

16x faster

Designing circuits for quantum computing

*UIST, Macedonia*

1 week

40x faster

Extracting image features in real-time

*Aselsan*

3 directives

4.1x faster

HydroC- Galaxy Formation

*PRACE Benchmark Code, CAPS*

1 week

3x faster

Real-time Derivative Valuation

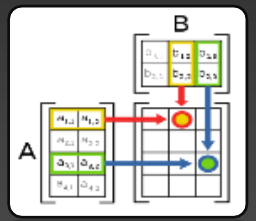
*Opel Blue, Ltd*


Few hours

70x faster

Matrix Matrix Multiply

*Independent Research Scientist*




4 directives

6.4x faster

# A Champion Case

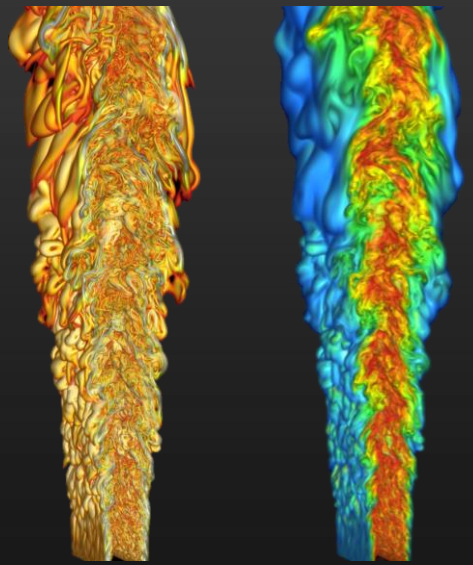
## 4x Faster

| Jaguar | Titan |
| --- | --- |
| 42 days | 10 days |

Modified <1%
Lines of Code

15 PF! One of fastest simulations ever!

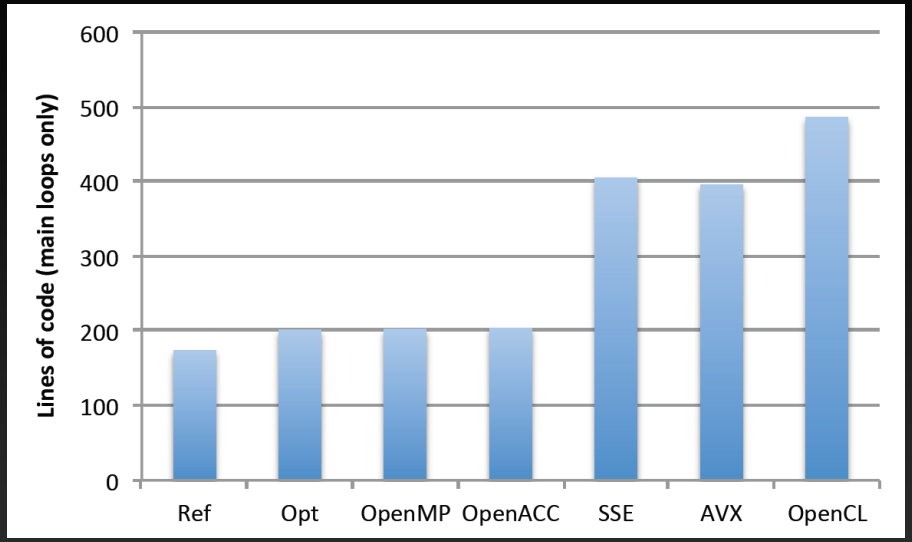
Design alternative fuels with up to 50% higher efficiency

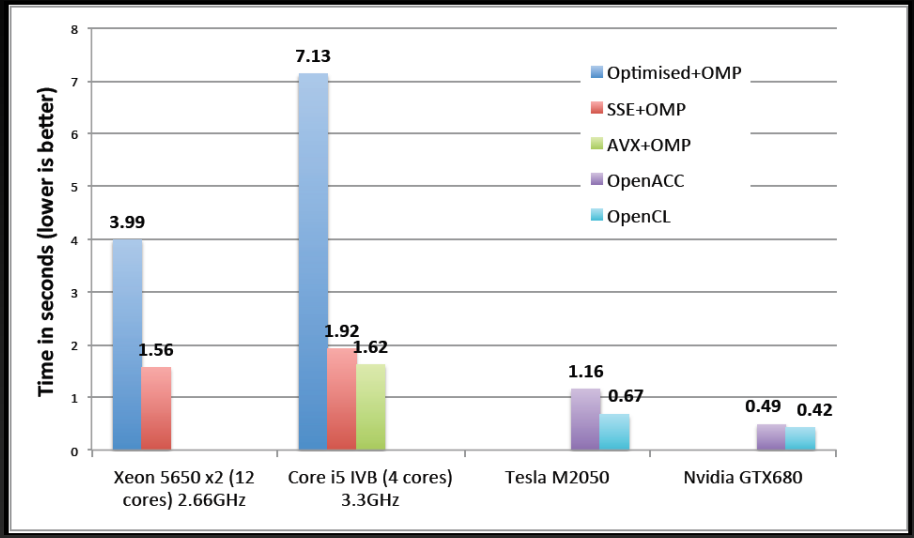


**S3D: Fuel Combustion**

# Comparison to Alternatives

## Lattice-Boltzmann Example



# Broad Accelerator Support

- Xeon Phi support already in CAPS.  Demonstrated and soon to be release for PGI.
- AMD line of accelerated processing  units (APUs) as well as the AMD line of discrete GPUs for preliminary PGI support.
- Carma – a hybrid platform based on ARM Cortex-A9 quad core and  an NVIDIA Quadro® 1000M GPU.
- NVIDIA…

# NVIDIA Rules

or writes the rules. They have been the foremost supporter of GPU computing for much of the past decade, and have earned the focus of this workshop. We are using NVIDIA GPUs as our platform and our touchstone because:

- They are proven
- Well understood
- Best bang for buck if you want to buy an accelerator
- Excellent support by vendor and community
- It is the basis for our leading edge platform, Keeneland
- It will not be going obsolete any time soon
- NVIDIA recently acquired PGI. That gave us a slight preference for the PGI compiler over the Cray one. Both are available on Blue Waters.

# True Standard

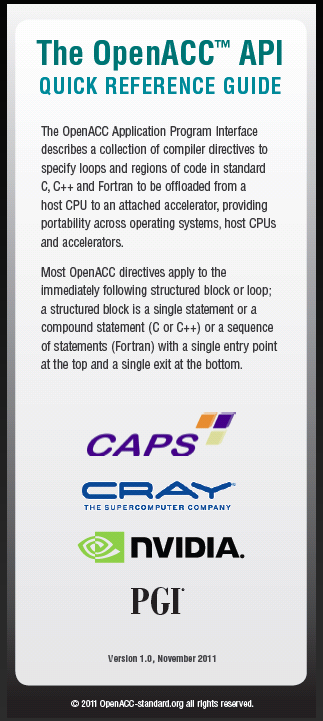
- Full OpenACC 1.0 and 2.0 Specifications available online

  http://www.openacc-standard.org

- Quick reference card also available

- Implementations available now from PGI, Cray, and CAPS.

- GCC version of OpenACC in 4.9x and standard in 5.0 (official release early April).



# A Simple Example: 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];
}

...
// Somewhere in main
// call 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


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

# kernels: Our first OpenACC Directive

We request that each loop execute as a separate *kernel* on the GPU. This is an incredibly powerful directive.

```
!$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 routine to run on the GPU

# General Directive Syntax and Scope

Fortran

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

C

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

I may indent the directives at the natural code indentation level for readability. It is a common practice to always start them in the first column (ala #define/#ifdef). Either is fine with C or Fortran 90 compilers.

# Complete SAXPY Example Code

```
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;
}
```

```
#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];
}
```

"I promise y is not aliased by Anything else (esp. x)" (more later)

# Compile and Run

- C: `cc -acc -Minfo=accel saxpy.c`
- Fortran: `ftn -acc -Minfo=accel saxpy.f90`

Compiler Output

```
cc -acc -Minfo=accel 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
```

- Run: `aprun -n1 a.out`

# Compare: Partial CUDA C SAXPY Code

## Just the subroutine

```
__global__ void saxpy_kernel( float a, float* x, float* y, int n ){
  int i;
  i = blockIdx.x*blockDim.x + threadIdx.x;
  if( i <= n ) x[i] = a*x[i] + y[i];
}

void saxpy( float a, float* x, float* y, int n ){
  float *xd, *yd;
  cudaMalloc( (void**)&xd, n*sizeof(float) );
  cudaMalloc( (void**)&yd, n*sizeof(float) ); cudaMemcpy( xd, x, n*sizeof(float),
                    cudaMemcpyHostToDevice );
  cudaMemcpy( yd, y, n*sizeof(float),
                    cudaMemcpyHostToDevice );
  saxpy_kernel<<< (n+31)/32, 32 >>>( a, xd, yd, n );
  cudaMemcpy( x, xd, n*sizeof(float),
                    cudaMemcpyDeviceToHost );
  cudaFree( xd ); cudaFree( yd );
}
```

# Compare: Partial CUDA Fortran SAXPY Code

## Just the subroutine

```
module kmod
 use cudafor
contains
 attributes(global) subroutine saxpy_kernel(A,X,Y,N)
  real(4), device :: A, X(N), Y(N)
  integer, value :: N
  integer :: i
  i = (blockidx%x-1)*blockdim%x + threadidx%x
  if( i <= N ) X(i) = A*X(i) + Y(i)
 end subroutine
end module

 subroutine saxpy( A, X, Y, N )
  use kmod
  real(4) :: A, X(N), Y(N)
  integer :: N
  real(4), device, allocatable, dimension(:):: &
                Xd, Yd
  allocate( Xd(N), Yd(N) )
  Xd = X(1:N)
  Yd = Y(1:N)
  call saxpy_kernel<<<(N+31)/32,32>>>(A, Xd, Yd, N)
  X(1:N) = Xd
  deallocate( Xd, Yd )
 end subroutine
```

# Again: Complete SAXPY Example Code

## Main Code

```
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;
}
```

## Entire Subroutine

```
#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];
}
```

# Big Difference!

- With CUDA, we changed the structure of the old code. Non-CUDA programmers can't understand new code. It is not even ANSI standard code.
- We have separate sections for the host code, and the GPU code. Different flow of code. Serial path now gone forever.
- Where did these "32's" and other mystery variables come from? This is a clue that we have some hardware details to deal with here.
- Exact same situation as assembly used to be. How much hand-assembled code is still being written in HPC now that compilers have gotten so efficient?

# This looks easy! Too easy…

- If it is this simple, why don't we just throw ***kernel*** in front of every loop?
- Better yet, why doesn't the compiler do this for me?

The answer is that there are two general issues that prevent the compiler from being able to just automatically parallelize every loop.

- Data Dependencies in Loops
- Data Movement

The compiler needs your higher level perspective (in the form of directive hints) to get correct results, and reasonable performance.

# Data Dependencies

Most directive based parallelization consists of splitting up big do/for loops into independent chunks that the many processors can work on simultaneously.

Take, for example, a simple for loop like this:

```
for(index=0, index<1000000,index++)
        Array[index] = 4 * Array[index];
```

When run on 1000 processors, it will execute something like this…

# No Data Dependency

Processor 1

```
for(index=0, index<999,index++)
   Array[index] = 4*Array[index];
```

Processor 2

```
for(index=1000, index<1999,index++)
   Array[index] = 4*Array[index];
```

Processor 3

```
for(index=2000, index<2999,index++)
   Array[index] = 4*Array[index];
```

Processor 4

```
for(index=3000, index<3999,index++)
   Array[index] = 4*Array[index];
```

Processor 5

```
for(index=4000, index<4999,index++)
   Array[index] = 4*Array[index];
```

# Data Dependency

But what if the loops are not entirely independent?

Take, for example, a similar loop like this:

```
for(index=1, index<1000000,index++)
        Array[index] = 4 * Array[index] – Array[index-1];
```

This is perfectly valid serial code.

# Data Dependency

Now Processor 2, in trying to calculate its first iteration…

```
for(index=1000, index<1999,index++)
      Array[1000] = 4 * Array[1000] – Array[999];
```

needs the result of Processor 1's last iteration. If we want the correct ("same as serial") result, we need to wait until processor 1 finishes. Likewise for processors 3, 4, …

# Data Dependencies

That is a data dependency. If the compiler even ***suspects*** that there is a data dependency, it will, for the sake of correctness, refuse to parallelize that loop.

```
11, Loop carried dependence of 'Array' prevents parallelization
    Loop carried backward dependence of 'Array' prevents vectorization
```

As large, complex loops are quite common in HPC, especially around the most important parts of your code, the compiler will often balk most when you most need a kernel to be generated. What can you do?

# Data Dependencies

- Rearrange your code to make it more obvious to the compiler that there is not really a data dependency.
- Eliminate a real dependency by changing your code.
  - There is a common bag of tricks developed for this as this issue goes back 40 years in HPC. Many are quite trivial to apply.
  - The compilers have gradually been learning these themselves.
- Override the compiler's judgment (`independent` clause) at the risk of invalid results. Misuse of `restrict` has similar consequences.

# C Detail: the `restrict` keyword

- Standard C (as of C99).
- Important for optimization of serial as well as OpenACC and OpenMP code.
- Promise given by the programmer to the compiler for a pointer

```
float *restrict ptr
```

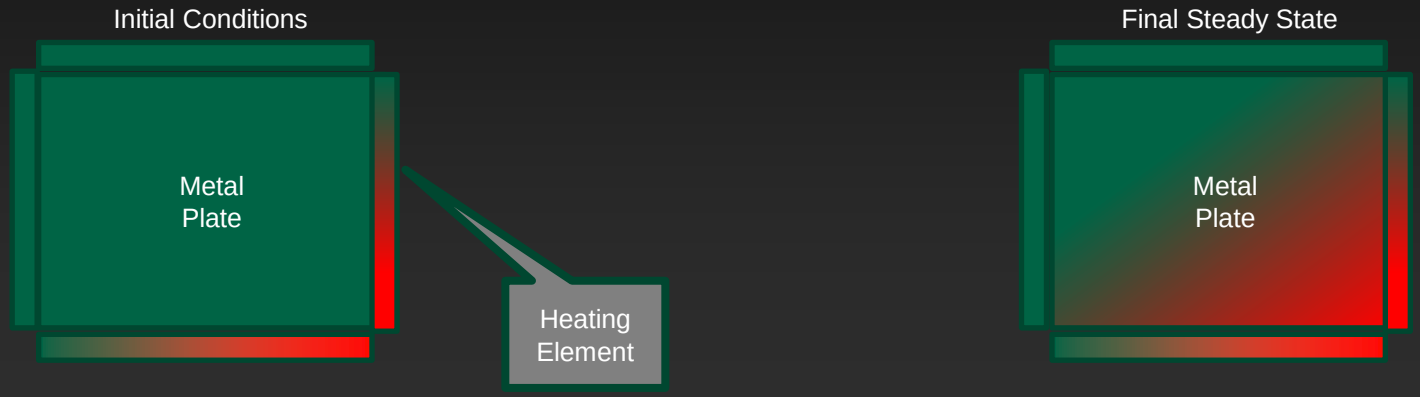
  Meaning: "for the lifetime of `ptr`, only it or a value directly derived from it (such as `ptr + 1`) will be used to access the object to which it points"

- 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

# Our Foundation Exercise: Laplace Solver

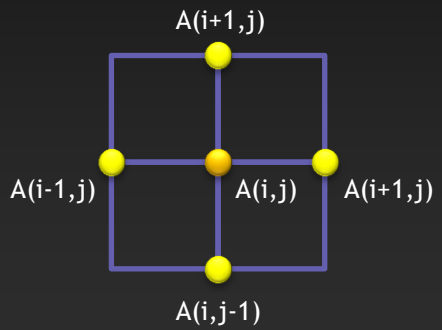
- I've been using this for MPI, OpenMP and now OpenACC. It is a great simulation problem, not rigged for OpenACC.
- In this most basic form, it solves the Laplace equation: $\nabla^2 f(x, y) = 0$
- The Laplace Equation applies to many physical problems, including:
  - Electrostatics
  - Fluid Flow
  - Temperature

- For temperature, it is the Steady State Heat Equation:



# Exercise Foundation: Jacobi Iteration

- The Laplace equation on a grid states that each grid point is the average of it's neighbors.
- We can iteratively converge to that state by repeatedly computing new values at each point from the average of neighboring points.
- We just keep doing this until the difference from one pass to the next is small enough for us to tolerate.




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

# Serial Code Implementation

```
for(i = 1; i <= ROWS; i++) {
     for(j = 1; j <= COLUMNS; j++) {
          Temperature[i][j] = 0.25 * (Temperature_last[i+1][j] + Temperature_last[i-1][j] +
                                      Temperature_last[i][j+1] + Temperature_last[i][j-1]);
     }
}
```

```
do j=1,columns
     do i=1,rows
          temperature(i,j)= 0.25 * (temperature_last(i+1,j)+temperature_last(i-1,j) + &
                                    temperature_last(i,j+1)+temperature_last(i,j-1) )
     enddo
enddo
```

# Serial C Code (kernel)

```
while ( dt > MAX_TEMP_ERROR && iteration <= max_iterations ) {

     for(i = 1; i <= ROWS; i++) {
          for(j = 1; j <= COLUMNS; j++) {
               Temperature[i][j] = 0.25 * (Temperature_last[i+1][j] + Temperature_last[i-1][j] +
                                           Temperature_last[i][j+1] + Temperature_last[i][j-1]);
          }
     }

     dt = 0.0;

     for(i = 1; i <= ROWS; i++){
          for(j = 1; j <= COLUMNS; j++){
               dt = fmax( fabs(Temperature[i][j]-Temperature_last[i][j]), dt);
               Temperature_last[i][j] = Temperature[i][j];
          }
     }

     if((iteration % 100) == 0) {
          track_progress(iteration);
     }

     iteration++;

}
```

Done?

Calculate

Update temp array and find max change

Output

# Serial C Code Subroutines

```
void initialize(){

    int i,j;

    for(i = 0; i <= ROWS+1; i++){
        for (j = 0; j <= COLUMNS+1; j++){
            Temperature_last[i][j] = 0.0;
        }
    }

    // these boundary conditions never change throughout run

    // set left side to 0 and right to a linear increase
    for(i = 0; i <= ROWS+1; i++) {
        Temperature_last[i][0] = 0.0;
        Temperature_last[i][COLUMNS+1] = (100.0/ROWS)*i;
    }

    // set top to 0 and bottom to linear increase
    for(j = 0; j <= COLUMNS+1; j++) {
        Temperature_last[0][j] = 0.0;
        Temperature_last[ROWS+1][j] = (100.0/COLUMNS)*j;
    }
}
```

BCs could run from 0 to ROWS+1 or from 1 to ROWS. We chose the former.

```
void track_progress(int iteration) {

  int i;

  printf("-- Iteration: %d --\n", iteration);
  for(i = ROWS-5; i <= ROWS; i++) {
     printf("[%d,%d]: %5.2f ", i, i,Temperature[i][i]);
  }
  printf("\n");
}
```

# Whole C Code

```
#include <stdlib.h>
#include <stdio.h>
#include <math.h>
#include <sys/time.h>

// size of plate
#define COLUMNS    1000
#define ROWS       1000

// largest permitted change in temp (This value takes about 3400 steps)
#define MAX_TEMP_ERROR 0.01

double Temperature[ROWS+2][COLUMNS+2];      // temperature grid
double Temperature_last[ROWS+2][COLUMNS+2]; // temperature grid from last iteration

//   helper routines
void initialize();
void track_progress(int iter);

int main(int argc, char *argv[]) {

    int i, j;                                            // grid indexes
    int max_iterations;                                  // number of iterations
    int iteration=1;                                     // current iteration
    double dt=100;                                       // largest change in t
    struct timeval start_time, stop_time, elapsed_time;  // timers

    printf("Maximum iterations [100-4000]?\n");
    scanf("%d", &max_iterations);

    gettimeofday(&start_time,NULL); // Unix timer

    initialize();                   // initialize Temp_last including boundary conditions

    // do until error is minimal or until max steps
    while ( dt > MAX_TEMP_ERROR && iteration <= max_iterations ) {

        // main calculation: average my four neighbors
        for(i = 1; i <= ROWS; i++) {
            for(j = 1; j <= COLUMNS; j++) {
                Temperature[i][j] = 0.25 * (Temperature_last[i+1][j] + Temperature_last[i-1][j] +
                                            Temperature_last[i][j+1] + Temperature_last[i][j-1]);
            }
        }

        dt = 0.0; // reset largest temperature change

        // copy grid to old grid for next iteration and find latest dt
        for(i = 1; i <= ROWS; i++){
            for(j = 1; j <= COLUMNS; j++){
              dt = fmax( fabs(Temperature[i][j]-Temperature_last[i][j]), dt);
              Temperature_last[i][j] = Temperature[i][j];
            }
        }

        // periodically print test values
        if((iteration % 100) == 0) {
            track_progress(iteration);
        }

        iteration++;
    }

    gettimeofday(&stop_time,NULL);
    timersub(&stop_time, &start_time, &elapsed_time); // Unix time subtract routine

    printf("\nMax error at iteration %d was %f\n", iteration-1, dt);
    printf("Total time was %f seconds.\n", elapsed_time.tv_sec+elapsed_time.tv_usec/1000000.0);

}

// initialize plate and boundary conditions
// Temp_last is used to to start first iteration
void initialize(){

    int i,j;

    for(i = 0; i <= ROWS+1; i++){
        for (j = 0; j <= COLUMNS+1; j++){
            Temperature_last[i][j] = 0.0;
        }
    }

    // these boundary conditions never change throughout run

    // set left side to 0 and right to a linear increase
    for(i = 0; i <= ROWS+1; i++) {
        Temperature_last[i][0] = 0.0;
        Temperature_last[i][COLUMNS+1] = (100.0/ROWS)*i;
    }

    // set top to 0 and bottom to linear increase
    for(j = 0; j <= COLUMNS+1; j++) {
        Temperature_last[0][j] = 0.0;
        Temperature_last[ROWS+1][j] = (100.0/COLUMNS)*j;
    }
}

// print diagonal in bottom right corner where most action is
void track_progress(int iteration) {

    int i;

    printf("---------- Iteration number: %d ------------\n", iteration);
    for(i = ROWS-5; i <= ROWS; i++) {
        printf("[%d,%d]: %5.2f  ", i, i, Temperature[i][i]);
    }
    printf("\n");
}
```

# Serial Fortran Code (kernel)

```
do while ( dt > max_temp_error .and. iteration <= max_iterations)

  do j=1,columns
     do i=1,rows
        temperature(i,j)=0.25*(temperature_last(i+1,j)+temperature_last(i-1,j)+ &
                               temperature_last(i,j+1)+temperature_last(i,j-1) )
     enddo
  enddo

  dt=0.0

  do j=1,columns
     do i=1,rows
        dt = max( abs(temperature(i,j) - temperature_last(i,j)), dt )
        temperature_last(i,j) = temperature(i,j)
     enddo
  enddo

  if( mod(iteration,100).eq.0 ) then
     call track_progress(temperature, iteration)
  endif

  iteration = iteration+1

enddo
```

Done?

Calculate

Update temp array and find max change

Output

# Serial Fortran Code Subroutines

```
subroutine initialize( temperature_last )
      implicit none

      integer, parameter             :: columns=1000
      integer, parameter             :: rows=1000
      integer                        :: i,j

      double precision, dimension(0:rows+1,0:columns+1) :: temperature_last

      temperature_last = 0.0

      !these boundary conditions never change throughout run

      !set left side to 0 and right to linear increase
      do i=0,rows+1
         temperature_last(i,0) = 0.0
         temperature_last(i,columns+1) = (100.0/rows) * i
      enddo

      !set top to 0 and bottom to linear increase
      do j=0,columns+1
         temperature_last(0,j) = 0.0
         temperature_last(rows+1,j) = ((100.0)/columns) * j
      enddo

end subroutine initialize
```

```
subroutine track_progress(temperature, iteration)
      implicit none

      integer, parameter             :: columns=1000
      integer, parameter             :: rows=1000
      integer                        :: i,iteration

      double precision, dimension(0:rows+1,0:columns+1) :: temperature

      print *, '---------- Iteration number: ', iteration, ' ---------------'
      do i=5,0,-1
         write (*,'("("i4,",",i4,"):",f6.2,"  ")',advance='no'), &
                  rows-i,columns-i,temperature(rows-i,columns-i)
      enddo
      print *
```

# Whole Fortran Code

```
program serial
      implicit none

      !Size of plate
      integer, parameter             :: columns=1000
      integer, parameter             :: rows=1000
      double precision, parameter    :: max_temp_error=0.01

      integer                        :: i, j, max_iterations, iteration=1
      double precision               :: dt=100.0
      real                           :: start_time, stop_time

      double precision, dimension(0:rows+1,0:columns+1) :: temperature, temperature_last

      print*, 'Maximum iterations [100-4000]?'
      read*,   max_iterations

      call cpu_time(start_time)      !Fortran timer

      call initialize(temperature_last)

      !do until error is minimal or until maximum steps
      do while ( dt > max_temp_error .and. iteration <= max_iterations)

         do j=1,columns
            do i=1,rows
               temperature(i,j)=0.25*(temperature_last(i+1,j)+temperature_last(i-1,j)+ &
                                      temperature_last(i,j+1)+temperature_last(i,j-1) )
            enddo
         enddo

         dt=0.0

         !copy grid to old grid for next iteration and find max change
         do j=1,columns
            do i=1,rows
               dt = max( abs(temperature(i,j) - temperature_last(i,j)), dt )
               temperature_last(i,j) = temperature(i,j)
            enddo
         enddo

         !periodically print test values
         if( mod(iteration,100).eq.0 ) then
            call track_progress(temperature, iteration)
         endif

         iteration = iteration+1

      enddo

      call cpu_time(stop_time)

      print*, 'Max error at iteration ', iteration-1, ' was ',dt
      print*, 'Total time was ',stop_time-start_time, ' seconds.'

end program serial
```

```
! initialize plate and boundery conditions
! temp_last is used to to start first iteration
subroutine initialize( temperature_last )
      implicit none

      integer, parameter             :: columns=1000
      integer, parameter             :: rows=1000
      integer                        :: i,j

      double precision, dimension(0:rows+1,0:columns+1) :: temperature_last

      temperature_last = 0.0

      !these boundary conditions never change throughout run

      !set left side to 0 and right to linear increase
      do i=0,rows+1
         temperature_last(i,0) = 0.0
         temperature_last(i,columns+1) = (100.0/rows) * i
      enddo

      !set top to 0 and bottom to linear increase
      do j=0,columns+1
         temperature_last(0,j) = 0.0
         temperature_last(rows+1,j) = ((100.0)/columns) * j
      enddo

end subroutine initialize

!print diagonal in bottom corner where most action is
subroutine track_progress(temperature, iteration)
      implicit none

      integer, parameter             :: columns=1000
      integer, parameter             :: rows=1000
      integer                        :: i,iteration

      double precision, dimension(0:rows+1,0:columns+1) :: temperature

      print *, '---------- Iteration number: ', iteration, ' ---------------'
      do i=5,0,-1
         write (*,'("("i4,",",i4,"):",f6.2,"  ")',advance='no'), &
                    rows-i,columns-i,temperature(rows-i,columns-i)
      enddo
      print *
end subroutine track_progress
```

# Exercises: General Instructions for Compiling

- Exercises are in the “Exercises/Laplace” directory in your home directory
- Solutions are in the “Laplace/Solutions” subdirectory
- To compile

```
cc -acc laplace.c
ftn -acc laplace.f90
```

- This will generate the executable a.out

# Exercises: Very useful compiler option

Adding -Minfo=accel to your compile command will give you some very useful information about how well the compiler was able to honor your OpenACC directives.

```
instr009@h2ologin2:~/Test> cc -acc -Minfo=accel laplace_bad_acc.c
main:
     71, Generating present_or_copyout(Temperature[1:1000][1:1000])
         Generating present_or_copyin(Temperature_old[0:][0:])
         Generating NVIDIA code
         Generating compute capability 1.3 binary
         Generating compute capability 2.0 binary
         Generating compute capability 3.0 binary
     72, Loop is parallelizable
     73, Loop is parallelizable
         Accelerator kernel generated
         72, #pragma acc loop gang /* blockIdx.y */
         73, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
     82, Generating present_or_copyin(Temperature[1:1000][1:1000])
         Generating present_or_copy(Temperature_old[1:1000][1:1000])
         Generating NVIDIA code
         Generating compute capability 1.3 binary
         Generating compute capability 2.0 binary
         Generating compute capability 3.0 binary
     83, Loop is parallelizable
     84, Loop is parallelizable
         Accelerator kernel generated
         83, #pragma acc loop gang /* blockIdx.y */
         84, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
     85, Max reduction generated for dt
```

# Exercises: General Instructions for Running

Make sure you are in an interactive session - with idev - if you aren't already. The command prompt is your clue.

To run, use aprun:

```
instr003@nid25357:~> aprun -n1 a.out
```

You can compare against the serial code you are starting with to see what performance gains you achieve. You can compile the serial version without any extra flags (just cc or ftn), but run it as per the above. Rename your a.out's to avoid confusion.

# Exercise 1: Using kernels to parallelize the main loops

## (About 45 minutes)

**Q: Can you get a speedup with just the kernels directives?**

1. Edit *laplace_serial.c*/f90
   1. Maybe copy your intended OpenACC version to *laplace_acc.c* to start
   2. Add directives where it helps

2. Compile with OpenACC parallelization
   1. cc -acc -Minfo=accel laplace_acc.c or
      ftn -acc -Minfo=accel laplace_acc.f90
   2. Look at your compiler output to make sure you are having an effect

3. Run
   1. aprun -n1 a.out (Try 4000 iterations if you want a solution that converges to current tolerance)
   2. Serial version for baseline time
   3. Your OpenACC version for performance difference

# Exercise 1 C Solution

```
while ( dt > MAX_TEMP_ERROR && iteration <= max_iterations ) {

    #pragma acc kernels
    for(i = 1; i <= ROWS; i++) {
        for(j = 1; j <= COLUMNS; j++) {
            Temperature[i][j] = 0.25 * (Temperature_last[i+1][j] + Temperature_last[i-1][j] +
                                        Temperature_last[i][j+1] + Temperature_last[i][j-1]);
        }
    }

    dt = 0.0; // reset largest temperature change

    #pragma acc kernels
    for(i = 1; i <= ROWS; i++){
        for(j = 1; j <= COLUMNS; j++){
            dt = fmax( fabs(Temperature[i][j]-Temperature_last[i][j]), dt);
            Temperature_last[i][j] = Temperature[i][j];
        }
    }

    if((iteration % 100) == 0) {
        track_progress(iteration);
    }

    iteration++;
}
```

Generate a GPU kernel

Generate a GPU kernel

# Exercise 1 Fortran Solution

```
do while ( dt > max_temp_error .and. iteration <= max_iterations)

    !$acc kernels
    do j=1,columns
       do i=1,rows
          temperature(i,j)=0.25*(temperature_last(i+1,j)+temperature_last(i-1,j)+ &
                                 temperature_last(i,j+1)+temperature_last(i,j-1) )
       enddo
    enddo
    !$acc end kernels

    dt=0.0

    !$acc kernels
    do j=1,columns
       do i=1,rows
          dt = max( abs(temperature(i,j) - temperature_last(i,j)), dt )
          temperature_last(i,j) = temperature(i,j)
       enddo
    enddo
    !$acc end kernels

    if( mod(iteration,100).eq.0 ) then
       call track_progress(temperature, iteration)
    endif

    iteration = iteration+1

enddo
```

Generate a GPU kernel

Generate a GPU kernel

# Exercise 1: Compiler output (C)

```
instr009@h2ologin2:~/Update> cc -acc -Minfo=accel laplace_bad_acc.c
main:
     62, Generating present_or_copyout(Temperature[1:1000][1:1000])
         Generating present_or_copyin(Temperature_last[0:][0:])
         Generating NVIDIA code
         Generating compute capability 1.3 binary
         Generating compute capability 2.0 binary
         Generating compute capability 3.0 binary
     63, Loop is parallelizable
     64, Loop is parallelizable
         Accelerator kernel generated
         63, #pragma acc loop gang /* blockIdx.y */
         64, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
     73, Generating present_or_copyin(Temperature[1:1000][1:1000])
         Generating present_or_copy(Temperature_last[1:1000][1:1000])
         Generating NVIDIA code
         Generating compute capability 1.3 binary
         Generating compute capability 2.0 binary
         Generating compute capability 3.0 binary
     74, Loop is parallelizable
     75, Loop is parallelizable
         Accelerator kernel generated
         74, #pragma acc loop gang /* blockIdx.y */
         75, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
     76, Max reduction generated for dt
```

Compiler was able to parallelize

Compiler was able to parallelize

# Exercise 1: Performance

## 3372 steps to convergence

| Execution | Time (s) | Speedup |
|---|---|---|
| CPU Serial (C) | 36 | -- |
| CPU 2 OpenMP threads | 24 | 1.5x |
| CPU 4 OpenMP threads | 15 | 2.4x |
| CPU 8 OpenMP threads | 9.8 | 3.7x |
| CPU 16 OpenMP threads | 5.0 | 7.2 |
| OpenACC GPU | 64 | 0.6x (0.08 vs. 16 CPU) |

**CPU: AMD 6276 Interlagos**
**8 Cores @ 2.3+GHz**
**GPU: NVIDIA GK110 Kepler**

# What's with the OpenMP?

- We can compare our GPU results to the best the multi-core XEON CPUs can do.

- If you are familiar with OpenMP, or even if you are not, you can compile and run the OpenMP enabled versions in your OpenMP directory as:

```
cc -mp=nonuma laplace_omp.c     or    ftn -mp=nonuma laplace_omp.f90
```

then to run on 8 threads do:

```
export OMP_NUM_THREADS=8
aprun -n 1 -d 8 a.out
```

# What went wrong?

`export PGI_ACC_TIME=1` to activate profiling and run again:

```
Accelerator Kernel Timing data
/mnt/a/u/training/instr009/Update/laplace_bad_acc.c
  main  NVIDIA  devicenum=0
    time(us): 22,902,870
    62: compute region reached 3372 times
        62: data copyin reached 3372 times
             device time(us): total=4,561,531 max=1,362 min=1,350 avg=1,352
        64: kernel launched 3372 times
            grid: [8x1000]  block: [128]
             device time(us): total=441,105 max=268 min=129 avg=130
            elapsed time(us): total=487,585 max=282 min=141 avg=144
        70: data copyout reached 3372 times
             device time(us): total=4,063,246 max=1,230 min=1,202 avg=1,204
    73: compute region reached 3372 times
        73: data copyin reached 6744 times
             device time(us): total=9,135,367 max=1,428 min=1,346 avg=1,354
        75: kernel launched 3372 times
            grid: [8x1000]  block: [128]
             device time(us): total=546,820 max=296 min=155 avg=162
            elapsed time(us): total=593,424 max=309 min=171 avg=175
        75: reduction kernel launched 3372 times
            grid: [1]  block: [256]
             device time(us): total=91,638 max=161 min=25 avg=27
            elapsed time(us): total=136,871 max=174 min=38 avg=40
        82: data copyout reached 3372 times
             device time(us): total=4,063,163 max=1,259 min=1,202 avg=1,204
```

4.5 seconds

0.5 seconds

4.0 seconds

9.1 seconds

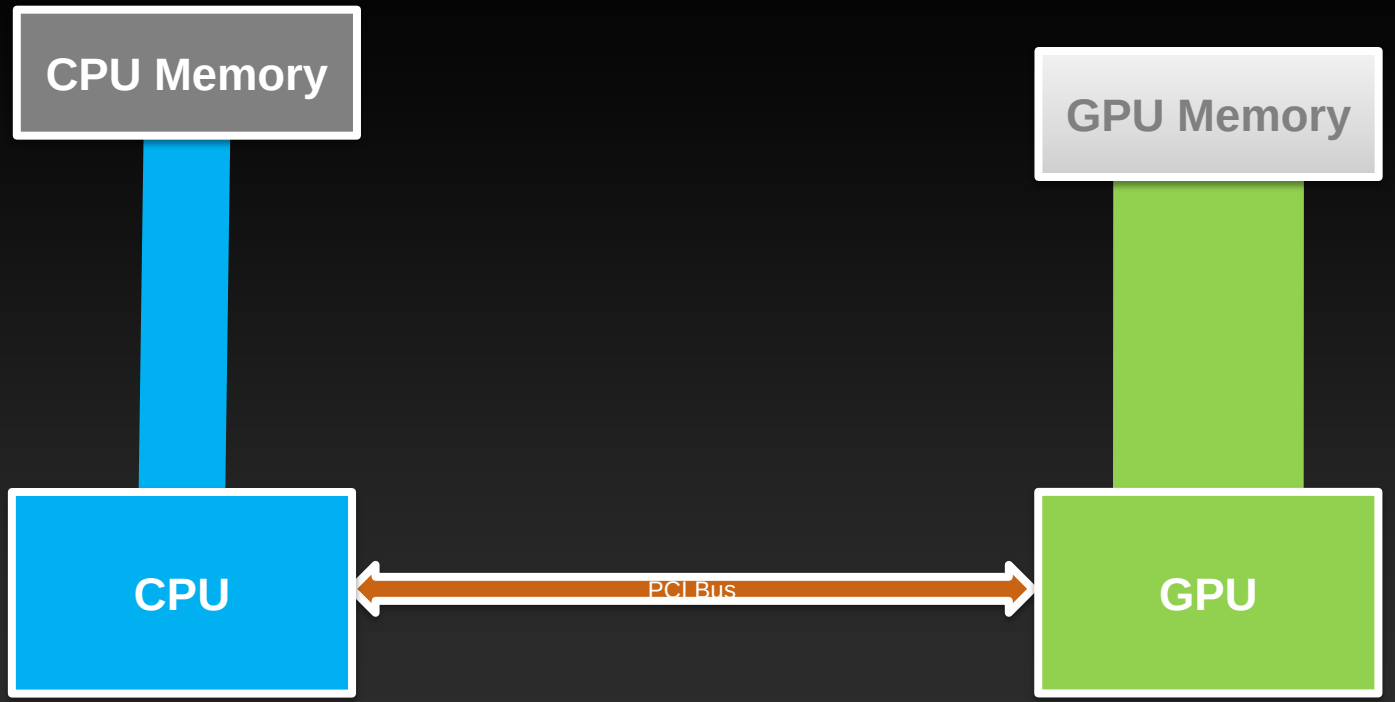
0.6 seconds

0.1 seconds

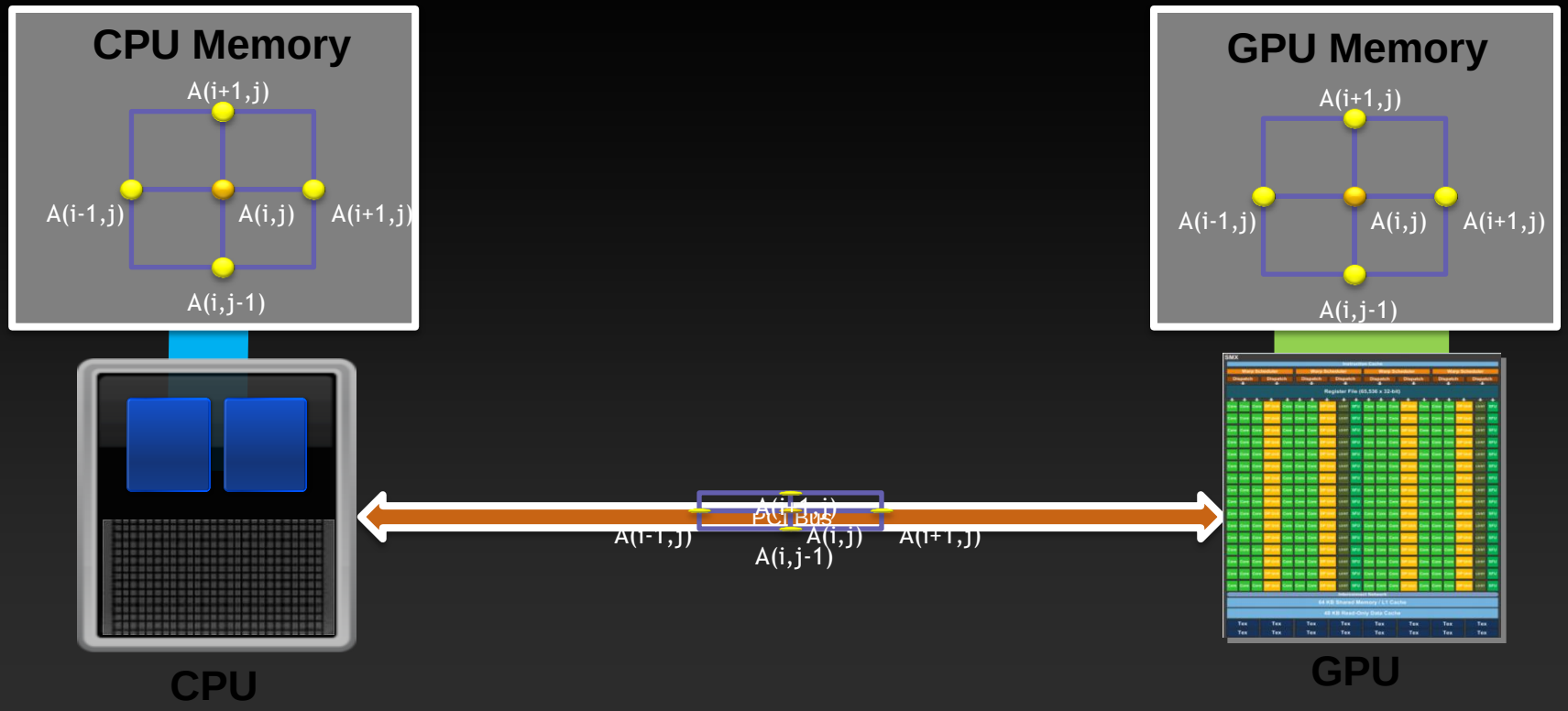
4.0 seconds

# Basic Concept

## Simplified, but sadly true



# Multiple Times Each Iteration



# Excessive Data Transfers

```
while ( dt > MAX_TEMP_ERROR && iteration <= max_iterations ) {
```

Temperature, Temperature_old resident on host

Temperature, Temperature_old resident on device

```
#pragma acc kernels
for(i = 1; i <= ROWS; i++) {
   for(j = 1; j <= COLUMNS; j++) {
       Temperature[i][j] = 0.25 * (Temperature_old[i+1][j] + …
   }
}
```

Temperature, Temperature_old resident on device

Temperature, Temperature_old resident on host

4 copies happen every iteration of the outer while loop!

```
dt = 0.0;
```

Temperature, Temperature_old resident on host

Temperature, Temperature_old resident on device

```
#pragma acc kernels
for(i = 1; i <= ROWS; i++) {
   for(j = 1; j <= COLUMNS; j++) {
       Temperature[i][j] = 0.25 * (Temperature_old[i+1][j] + …
```

Temperature, Temperature_old resident on device

Temperature, Temperature_old resident on host

```
}
```

# Data Management

The First, Most Important, and possibly Only OpenACC Optimization

# First, about that “reduction”

```
while ( dt > MAX_TEMP_ERROR && iteration <= max_iterations ) {
     #pragma acc kernels
     for(i = 1; i <= ROWS; i++) {
          for(j = 1; j <= COLUMNS; j++) {
               Temperature[i][j] = 0.25 * (Temperature_last[i+1][j] + Temperature_last[i-1][j] +
                                           Temperature_last[i][j+1] + Temperature_last[i][j-1]);
          }
     }

     dt = 0.0;

     #pragma acc kernels loop reduction (max:dt)
     for(i = 1; i <= ROWS; i++){
          for(j = 1; j <= COLUMNS; j++){
               dt = fmax( fabs(Temperature[i][j]-Temperature_last[i][j]), dt);
               Temperature_last[i][j] = Temperature[i][j];
          }
     }

     .
     .
     iteration++;
}
```

This will be combined with (intelligently) initialized parallel copies at end.

This explicitly declares the reduction.

Exiting this loop, each processor has a different idea of what the max dt is.

That the compiler recognizes this and does a reduction is a wonderful thing. Indeed, we can get too sophisticated for it to happen automatically.

# Data Construct Syntax and Scope

## Fortran

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

## C

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

# 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.

Principal use: For many important data structures in your code, this is a logical default to input, modify and return the data.

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

Principal use: Think of this like an array that you would use as just an input to a subroutine.

`copyout( list )` — Allocates memory on GPU and copies data to the host when exiting region.

Principal use: A result that isn't overwriting the input data structure.

`create( list )` — Allocates memory on GPU but does not copy.

Principal use: Temporary arrays.

# Present Data Clauses

The "present" data clauses are used when the data is already present because of a containing data region.

`present( list )`

Data is already present on GPU from another containing data region.

Principal use: You are calling this routine from inside a routine that already has a data clause.

`present_or_copy`
`present_or_copyin`
`present_or_copyout`
`present_or_create`

You can't be positive that the data is present from a surrounding data region.

Principal use: A subroutine that may or may not be called from within a data region or for multi-threaded codes so that only one thread migrates data.

# Array Shaping

- Compilers sometimes cannot determine the size of arrays, so we must specify explicitly using data clauses with an array “shape”. The compiler will let you know if you need to do this. Sometimes, you will want to for your own efficiency reasons.

- C

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

- Fortran

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

- Fortran uses start:end and C uses start:length
- Data clauses can be used on `data`, `kernels` or `parallel`

# Compiler will (increasingly) often make a good guess…

```
int main(int argc, char *argv[]) {

  int i;
  double A[2000], B[1000], C[1000];

  #pragma acc kernels
  for (i=0; i<1000; i++){

    A[i] = 4 * i;
    B[i] = B[i] + 2;
    C[i] = A[i] + 2 * B[i];

  }
}
```

Smarter

Smartest

```
pgcc -acc -Minfo=accel loops.c
main:
   6, Generating present_or_copyout(C[:])
      Generating present_or_copy(B[:])
      Generating present_or_copyout(A[:1000])
      Generating NVIDIA code
   7, Loop is parallelizable
      Accelerator kernel generated
```

# Data Regions Have Real Consequences

## *Simplest Kernel*

```
int main(int argc, char** argv){

float A[1000];



    #pragma acc kernels
    for( int iter = 1; iter < 1000 ; iter++){
      A[iter] = 1.0;
    }

    A[10] = 2.0;


  printf("A[10] = %f", A[10]);
}
```

A[] Copied To GPU

A[] Copied To Host

Runs On Host

*Output:*

A[10] = 2.0

## *With Global Data Region*

```
int main(int argc, char** argv){

float A[1000];

 #pragma acc data copy(A)
  {

    #pragma acc kernels
    for( int iter = 1; iter < 1000 ; iter++){
      A[iter] = 1.0;
    }

    A[10] = 2.0;

  }

  printf("A[10] = %f", A[10]);
}
```

A[] Copied To GPU

Still Runs On Host

A[] Copied To Host

*Output:*

A[10] = 1.0

# Data Regions Are Different Than Compute Regions

Compute Region

```
int main(int argc, char** argv){

float A[1000];

#pragma acc data copy(A)
 {

    #pragma acc kernels
    for( int iter = 1; iter < 1000 ; iter++){
      A[iter] = 1.0;
    }

    A[10] = 2.0;

  }

  printf("A[10] = %f", A[10]);
}
```

Data Region

*Output:*

A[10] = 1.0

# Data Movement Decisions

- Much like loop data dependencies, sometime the compiler needs your human intelligence to make high-level decisions about data movement. Otherwise, it must remain conservative - sometimes at great cost.

- You must think about when data truly needs to migrate, and see if that is better than the default.

- Besides the scope based data clauses, there are OpenACC options to let us manage data movement more intensely or asynchronously. We could manage the above behavior with the `update` construct:

Fortran :
```
!$acc update [host(), device(), …]
```

C:
```
#pragma acc update [host(), device(), …]
```

Ex: `#pragma acc update host(Temp_array)  //Gets host a current copy`

# Exercise 2: Use acc `data` to minimize transfers

(about 40 minutes)

**Q: What speedup can you get with data + kernels directives?**

- Start with your Exercise 1 solution or grab laplace_bad_acc.c/f90 from the Solutions subdirectory. This is just the solution of the last exercise.

- Add *data* directives where it helps.
  - Think: when *should* I move data between host and GPU? Think how you would do it by hand, then determine which data clauses will implement that plan.
  - Hint: you may find it helpful to ignore the output at first and just concentrate on getting the solution to converge quickly (at 3372 steps). Then worry about *updating* the printout.

# Exercise 2 C Solution

```
#pragma acc data copy(Temperature_last), create(Temperature)
while ( dt > MAX_TEMP_ERROR && iteration <= max_iterations ) {

    // main calculation: average my four neighbors
    #pragma acc kernels
    for(i = 1; i <= ROWS; i++) {
        for(j = 1; j <= COLUMNS; j++) {
            Temperature[i][j] = 0.25 * (Temperature_last[i+1][j] + Temperature_last[i-1][j] +
                                        Temperature_last[i][j+1] + Temperature_last[i][j-1]);
        }
    }

    dt = 0.0; // reset largest temperature change

    // copy grid to old grid for next iteration and find latest dt
    #pragma acc kernels
    for(i = 1; i <= ROWS; i++){
        for(j = 1; j <= COLUMNS; j++){
          dt = fmax( fabs(Temperature[i][j]-Temperature_last[i][j]), dt);
          Temperature_last[i][j] = Temperature[i][j];
        }
    }

    // periodically print test values
    if((iteration % 100) == 0) {
        #pragma acc update host(Temperature)
        track_progress(iteration);
    }

    iteration++;
}
```

No data movement in this block.

Except once in a while here.

# Exercise 2 Fortran Solution

```
!$acc data copy(temperature_last), create(temperature)
do while ( dt > max_temp_error .and. iteration <= max_iterations)

   !$acc kernels
   do j=1,columns
      do i=1,rows
         temperature(i,j)=0.25*(temperature_last(i+1,j)+temperature_last(i-1,j)+ &
                                temperature_last(i,j+1)+temperature_last(i,j-1) )
      enddo
   enddo
   !$acc end kernels

   dt=0.0

   !copy grid to old grid for next iteration and find max change
   !$acc kernels
   do j=1,columns
      do i=1,rows
         dt = max( abs(temperature(i,j) - temperature_last(i,j)), dt )
         temperature_last(i,j) = temperature(i,j)
      enddo
   enddo
   !$acc end kernels

   !periodically print test values
   if( mod(iteration,100).eq.0 ) then
      !$acc update host(temperature)
      call track_progress(temperature, iteration)
   endif

   iteration = iteration+1

enddo
!$acc end data
```

Keep these on GPI

Extra efficient:

!$acc update host(temperature(columns-5:columns,rows-5:rows))

Except bring back a copy here

# Exercise 2: Performance

## 3372 steps to convergence

| Execution | Time (s) | Speedup |
|---|---|---|
| CPU Serial (C) | 36 | -- |
| CPU 2 OpenMP threads | 24 | 1.5x |
| CPU 4 OpenMP threads | 15 | 2.4x |
| CPU 8 OpenMP threads | 9.8 | 3.7x |
| CPU 16 OpenMP threads | 5.0 | 7.2 |
| OpenACC GPU | 1.7 | 21x (3X vs. 16 CPU) |

**CPU: AMD 6276 Interlagos**
**8 Cores @ 2.3+GHz**
**GPU: NVIDIA GK110 Kepler**

# Further speedups

- OpenACC gives us even 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
- But you have already gained most of any potential speedup, and you did it with a few lines of directives!

# General Principles: Finding Parallelism In Code

- Nested for/do loops are best for parallelization
  - Large loop counts are best
- Iterations of loops must be independent of each other
  - To help compiler: `restrict` keyword (C), `independent` clause
  - Use subscripted arrays, rather than pointer-indexed arrays (C)
- Data regions should avoid wasted transfers
  - If applicable, could use directives to explicitly control sizes
- Various other annoying things can interfere with accelerated regions
  - IO
  - Limitations on function calls and nested parallelism (relaxed much in 2.0)

# Is OpenACC Living Up To My Claims?

- High-level. No involvement of OpenCL, CUDA, etc.
- Single source. No forking off a separate GPU code. Compile the same program for accelerators or serial, non-GPU programmers can play along.
- Efficient. Experience show very favorable comparison to low-level implementations of same algorithms. **kernels** is magical!
- Performance portable. Supports GPU accelerators and co-processors from multiple vendors, current and future versions.
- Incremental. Developers can port and tune parts of their application as resources and profiling dictates. No wholesale rewrite required. Which can be *quick*.