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

Simple compiler hints from coder.

Compiler generates parallel threaded code.

Ignorant compiler just sees some comments.

Your original Fortran or C code
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 = %fn", pi/N);
}
How Else Would We Accelerate Applications?

Applications

Libraries

“Drop-in” Acceleration

OpenACC Directives

Incrementally Accelerate Applications

Programming Languages (CUDA)

Maximum Flexibility
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.
True Standard

- Full OpenACC specifications (now on 3.0) available online
  
  http://www.openacc-standard.org

- Quick reference card also available and useful

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

- GCC version of OpenACC started in 5.x, but use 10.x

- Best free option is very probably PGI Community version:
  
  http://www.pgroup.com/products/community.htm
Serious Adoption

NEW PLATFORMS

Sunway TaihuLight
Built around OpenACC

GROWING COMMUNITY

- 6,000+ enabled developers
- Hackathons constantly
- Diverse online community

PORTING SUCCESS

- Five of 13 CAAR codes using OpenACC
- Gaussian ported to Tesla with OpenACC
- FLUENT using OpenACC in R18 production release
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** 42 days  
**Titan** 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**
A Simple Example: SAXPY

**SAXPY in C**

```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**

```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.

```fortran
!$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:**
A parallel routine to run on the GPU
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

```c
#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];
}

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;
}
```

“I promise y is not aliased by Anything else (esp. x)”
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
  ```c
  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
Compile and Run

- C: \texttt{pgcc -acc -Minfo=accel saxpy.c}
- Fortran: \texttt{pgf90 -acc -Minfo=accel saxpy.f90}

Compiler Output

\begin{verbatim}
pgcc -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
     Generating Tesla code
     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
\end{verbatim}

- Run: \texttt{a.out}
Compare: Partial CUDA C SAXPY Code
Just the subroutine

```c
__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 );
}
```
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

```c
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

```c
#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 numbers 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:

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

When run on 1000 processors, it will execute something like this...
for(index=0, index<999,index++)
Array[index] = 4*Array[index];

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

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

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

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:

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

This is perfectly valid serial code.
Data Dependency

Now Processor 1, in trying to calculate its first iteration...

```c
for(index=1000; index<1999; index++)
    String[1000] = 4 * String[1000] - String[999];
```

needs the result of Processor 0’s last iteration. If we want the correct (“same as serial”) result, we need to wait until processor 0 finishes. Likewise for processors 2, 3, ...
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 with *kernels*.

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.
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:
The Laplace equation on a grid states that each grid point is the average of its 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.

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

Serial C Code (kernel)

Calculate

Update temp array and find max change

Output

Done?
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;
    }
}

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");
}

BCs could run from 0 to ROWS+1 or from 1 to ROWS. We chose the former.
```c
#include <stdlib.h>
#include <stdio.h>
#include <math.h>
#include <sys/time.h>

#define COLUMNS    1000
#define ROWS       1000

#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

void initialize();                   // initialize Temp_last including boundary conditions
void track_progress(int iter);      // print test values periodically

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
    // 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]);
            }
        }
        // copy grid to old grid for next iteration and find latest change
        for(i = 1; i <= ROWS; i++){
            for(j = 1; j <= COLUMNS; j++){
                Temperature_last[i][j] = Temperature[i][j];
                // these boundary conditions never change throughout run
                if(i == 1) Temperature_last[i][j] = 0.0;
                if(i == ROWS) Temperature_last[i][j] = (100.0/ROWS)*i;
                if(j == 1) Temperature_last[i][j] = 0.0;
                if(j == COLUMNS) Temperature_last[i][j] = (100.0/COLUMNS)*j;
            }
        }
        // print test values periodically
        if((iteration % 100) == 0) {
            track_progress(iteration);
        }
        iteration++;
    }
    gettimeofday(&stop_time,NULL);
    timersub(&stop_time, &start_time, &elapsed_time); // Unix time subtract routine
    printf("Max 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 start first iteration
void initialize(){
    int i,j;
    for(i = 0; i <= ROWS+1; i++) { // grid indexes
        for (j = 0; j <= COLUMNS+1; j++) {
            Temperature_last[i][j] = 0.0;
        }
    }
    // these boundary conditions never change throughout run
    for(i = 0; i <= ROWS+1; i++) { // set left side to 0 and right to a linear increase
        Temperature_last[i][0] = 0.0;
        Temperature_last[i][COLUMNS+1] = (100.0/ROWS)*i;
    }
    for(j = 0; j <= COLUMNS+1; j++) { // set top to 0 and bottom to linear increase
        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");
}
```

Whole C Code

gmtimeofday(&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 start first iteration
void initialize(){
    int i,j;
    for(i = 0; i <= ROWS+1; i++) { // grid indexes
        for (j = 0; j <= COLUMNS+1; j++) {
            Temperature_last[i][j] = 0.0;
        }
    }
    // these boundary conditions never change throughout run
    for(i = 0; i <= ROWS+1; i++) { // set left side to 0 and right to a linear increase
        Temperature_last[i][0] = 0.0;
        Temperature_last[i][COLUMNS+1] = (100.0/ROWS)*i;
    }
    for(j = 0; j <= COLUMNS+1; j++) { // set top to 0 and bottom to linear increase
        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");
```
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
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

  temperature = initial temperature

  ! these boundary conditions never change throughout run
  ! set left side to 0 and right to linear increase
  do i=0,rows+1
    temperature(0,i) = 0.0
    temperature(rows+1,i) = (100.0/rows) * i
  enddo

  ! set top to 0 and bottom to linear increase
  do j=0,columns+1
    temperature(j,0) = 0.0
    temperature(j,columns+1) = ((100.0)/columns) * j
  enddo
end subroutine track_progress
program serial
implicit none
!
! Size of plate
integer, parameter :: columns=1000
integer, parameter :: rows=1000
!
! Precisions, parameters
integer :: i,j, max_iterations, iteration=1
integer :: dt=100.0
real :: start_time, stop_time
!
! Parameters for error calculation
double precision, dimension(0:rows+1,0:columns+1) :: temperature, temperature_last
!
print*, 'Maximum iterations $[100$-$4000]?$'
read*, max_iterations
!
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Exercises: General Instructions for Compiling

- Exercises are in the “Exercises/OpenACC” directory in your home directory

- Solutions are in the “Solutions” subdirectory

- To compile
  - `pgcc -acc laplace.c`
  - `pgf90 -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.

```
[urbanic@gpu017 Solutions]$ pgcc -acc -Minfo=accel laplace_acc.c
main:
  59, Generating create(Temperature[:][:]) [if not already present]
  Generating copy(Temperature_last[:][:]) [if not already present]
  64, Loop is parallelizable
  65, Loop is parallelizable
    Generating Tesla code
    64, #pragma acc loop gang, vector(4) /* blockIdx.y threadIdx.y */
    65, #pragma acc loop gang, vector(32) /* blockIdx.x threadIdx.x */
  75, Loop is parallelizable
  76, Loop is parallelizable
    Generating Tesla code
    75, #pragma acc loop gang, vector(4) /* blockIdx.y threadIdx.y */
    76, #pragma acc loop gang, vector(32) /* blockIdx.x threadIdx.x */
    77, Generating implicit reduction(max:dt)
  85, Generating update self(Temperature[:][:])
```
Special Instructions for Running on the GPUs (during this workshop)

As mentioned, on Bridges2 you generally only have to use the queueing system when you want to. However, as we have hundreds of you wanting quick turnaround, we will have to use it today.

Once you have an a.out that you want to run, you should use the simple job that we have already created (in Exercises/OpenACC) for you to run:

```
fred@bridges2-login011$ sbatch gpu.job
```
Output From Your Batch Job

The machine will tell you it submitted a batch job, and you can await your output, while it will come back in a file with the corresponding number as a name:

```
slurm-138555.out
```

As everything we are doing this afternoon only requires a few minutes at most (and usually just seconds), you could just sit there and wait for the file to magically appear. At which point you can “more” it or review it with your editor.
Changing Things Up

If you get impatient, or want to see what the machine is up to, you can look at the situation with `squeue`.

You might wonder what happened to the interaction count that the user is prompted for. I stuck a reasonable default (4000 iterations) into the job file. You can edit it if you want to. The whole job file is just a few lines.

Congratulations, you are now a Batch System veteran. Welcome to supercomputing.
Exercise 1: Using kernels to parallelize the main loops
(About 20 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. `pgcc -acc -Minfo=accel laplace_acc.c` or
      `pgf90 -acc -Minfo=accel laplace_acc.f90`
   2. Look at your compiler output to make sure you are having an effect

3. Run
   1. `sbatch gpu.job` (Leave it at 4000 iterations if you want a solution that converges to current tolerance)
   2. Look at output in file that returns (something like `slurm-138555.out`)
   3. Compare the serial and your OpenACC version for performance difference
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++;
}
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
Exercise 1: Compiler output (C)

[urbanic@gpu017 Solutions]$ pgcc -acc -Minfo=accel laplace_acc.c

main:
59, Generating create(Temperature[:][:]) [if not already present]
   Generating copy(Temperature_last[:][:]) [if not already present]
64, Loop is parallelizable
65, Loop is parallelizable
   Generating Tesla code
   64, #pragma acc loop gang, vector(4) /* blockIdx.y threadIdx.y */
   65, #pragma acc loop gang, vector(32) /* blockIdx.x threadIdx.x */
75, Loop is parallelizable
76, Loop is parallelizable
   Generating Tesla code
   75, #pragma acc loop gang, vector(4) /* blockIdx.y threadIdx.y */
   76, #pragma acc loop gang, vector(32) /* blockIdx.x threadIdx.x */
77, Generating implicit reduction(max:dt)
85, Generating update self(Temperature[:][:]):

Compiler was able to parallelize
Compiler was able to parallelize
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
    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++;
}
## Exercise 1: Performance

3372 steps to convergence

<table>
<thead>
<tr>
<th>Execution</th>
<th>Time (s)</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU Serial</td>
<td>20.8</td>
<td>--</td>
</tr>
<tr>
<td>CPU 2 OpenMP threads</td>
<td>9.6</td>
<td>2.1</td>
</tr>
<tr>
<td>CPU 4 OpenMP threads</td>
<td>4.8</td>
<td>4.3</td>
</tr>
<tr>
<td>CPU 8 OpenMP threads</td>
<td>2.7</td>
<td>7.7</td>
</tr>
<tr>
<td>CPU 16 OpenMP threads</td>
<td>1.4</td>
<td>14.8</td>
</tr>
<tr>
<td>CPU 28 OpenMP threads</td>
<td>0.9</td>
<td>23.1</td>
</tr>
<tr>
<td>OpenACC GPU</td>
<td>31.1</td>
<td>0.6x</td>
</tr>
</tbody>
</table>

Using PGI 20.11 on a V100
What’s with the OpenMP?

- We can compare our GPU results to the **best** the multi-core 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:

  ```
  pgcc -mp laplace_omp.c  or  pgf90 -mp laplace_omp.f90
  ```

  then to run on 8 threads do:

  ```
  export OMP_NUM_THREADS=8
  a.out
  ```

- Note that you probably only have 8 real cores if you are still on a GPU node. Do something like “interact -n28” if you want a full node of cores.
What went wrong?

export PGI_ACC_TIME=1 to activate profiling and run again:

Accelerator Kernel Timing data
/home/urbanic/latex/laplace_bad_acc.c
main NVIDIA devicenum=0
time(us): 12,095,531
  62: compute region reached 3372 times
  64: kernel launched 3372 times
      grid: [32x250] block: [32x4]
      device time(us): total=127,989 max=48 min=37 avg=37
      elapsed time(us): total=241,221 max=1,407 min=61 avg=71
  62: data region reached 6744 times
  62: data copyin transfers: 3372
      device time(us): total=2,446,765 max=972 min=712 avg=725
  70: data copyout transfers: 3372
      device time(us): total=2,098,635 max=835 min=616 avg=622
  73: compute region reached 3372 times
  73: data copyin transfers: 3372
      device time(us): total=32,465 max=97 min=6 avg=9
  75: kernel launched 3372 times
      grid: [32x250] block: [32x4]
      device time(us): total=179,342 max=63 min=52 avg=53
      elapsed time(us): total=294,686 max=407 min=76 avg=87
  75: reduction kernel launched 3372 times
      grid: [1] block: [256]
      device time(us): total=50,490 max=23 min=14 avg=14
      elapsed time(us): total=137,910 max=549 min=34 avg=40
  75: data copyout transfers: 3372
      device time(us): total=60,080 max=266 min=13 avg=17
  73: data region reached 6744 times
  73: data copyin transfers: 6744
      device time(us): total=5,004,411 max=1,005 min=716 avg=743
  82: data copyout transfers: 3372
      device time(us): total=7,095,354 max=854 min=616 avg=621
Basic Concept
Simplified, but sadly true

All bandwidths one-direction.
Multiple Times Each Iteration

CPU Memory

- A(i-1,j)
- A(i,j)
- A(i+1,j)
- A(i,j-1)

GPU Memory

- A(i-1,j)
- A(i,j)
- A(i+1,j)
- A(i,j-1)

CPU

GPU
Excessive Data Transfers

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

    Temperature, Temperature_old resident on host

    #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

    #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

    dt = 0.0;

    Temperature, Temperature_old resident on host

    #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

    #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

}
Data Management

The First, Most Important, and Possibly Only OpenACC Optimization
Scoped Data Construct Syntax

Fortran

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

C

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

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SUPERCOMPUTING
CENTER
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.
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

#define 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
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];
    }
}

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**

```c
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;
}
```

**Output:**

```
A[10] = 2.0
```

**With Global Data Region**

```c
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;
    #pragma acc data copy(A)
    {
        #pragma acc kernels
        for( int iter = 1; iter < 1000 ; iter++){
            A[iter] = 1.0;
        }
        A[10] = 2.0;
    }
}
```

**Output:**

```
A[10] = 1.0
```
```c
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;
    }
}
```

**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)  //Get host a copy from device
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.
#pragma acc data copy(Temperature_last, 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++;
}
#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++;
}
Slightly better still solution

```c
#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[ROWS-4:5][COLUMNS-4:5])
        track_progress(iteration);
    }

    iteration++;
}
```

Only need corner elements.
!$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
## Exercise 2: Performance

3372 steps to convergence

<table>
<thead>
<tr>
<th>Execution</th>
<th>Time (s)</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU Serial</td>
<td>20.8</td>
<td>--</td>
</tr>
<tr>
<td>CPU 2 OpenMP threads</td>
<td>9.6</td>
<td>2.1</td>
</tr>
<tr>
<td>CPU 4 OpenMP threads</td>
<td>4.8</td>
<td>4.3</td>
</tr>
<tr>
<td>CPU 8 OpenMP threads</td>
<td>2.7</td>
<td>7.7</td>
</tr>
<tr>
<td>CPU 16 OpenMP threads</td>
<td>1.4</td>
<td>14.8</td>
</tr>
<tr>
<td>CPU 28 OpenMP threads</td>
<td>0.9</td>
<td>23.1</td>
</tr>
<tr>
<td>OpenACC GPU</td>
<td>0.64</td>
<td>32.5</td>
</tr>
</tbody>
</table>
OpenACC or OpenMP?

Don’t draw any grand conclusions yet. We have gotten impressive speedups from both approaches. But our problem size is pretty small. Our main data structure is:

$$1000 \times 1000 = 1\text{M elements} = 8\text{MB of memory}$$

We have 2 of these (temperature and temperature_last) so we are using roughly 16 MB of memory. Not very large. When divided over cores it gets even smaller and can easily fit into cache.

The algorithm is realistic, but the problem size is tiny and hence the memory bandwidth stress is very low.
We can easily scale this problem up, so why don’t I? Because it is nice to have exercises that finish in a few minutes or less.

We scale this up to 10K x 10K (1.6 GB problem size) for the hybrid challenge. These numbers start to look a little more realistic. But the serial code takes over 30 minutes to finish. That would have gotten us off to a slow start!

<table>
<thead>
<tr>
<th>Execution</th>
<th>Time (s)</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU Serial</td>
<td>2187</td>
<td>--</td>
</tr>
<tr>
<td>CPU 16 OpenMP threads</td>
<td>183</td>
<td>12</td>
</tr>
<tr>
<td>CPU 28 OpenMP threads</td>
<td>162</td>
<td>13.5</td>
</tr>
<tr>
<td>OpenACC</td>
<td>103</td>
<td>21</td>
</tr>
</tbody>
</table>

10K x 10K Problem Size
Latest Happenings In Data Management

**Unified Memory**
- Unified address space allows us to pretend we have shared memory
- Skip data management, hope it works, and then optimize if necessary
- For dynamically allocated memory can eliminate need for pointer clauses

**NVLink**
- One route around PCI bus (with multiple GPUs)
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!
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 shows 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.
In Conclusion...

OpenMP

OpenACC

MPI