What is OpenMP?

It is a directive based standard to allow programmers to develop threaded parallel codes on shared memory computers.
Directives

Simple compiler hints from coder.

Compiler generates parallel threaded code.

Ignorant compiler just sees some comments.

Your original Fortran or C code

Program myscience
  ... serial code ...

!$omp parallel do
  do k = 1,n1
  do i = 1,n2
    ... parallel code ...
  enddo
  enddo

!$omp end parallel do
...

End Program myscience
Directives: an awesome idea whose time has arrived.

**OpenMP**

```c
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**

```c
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);
}
```
Key Advantages Of This Approach

- High-level. No involvement of pthreads or hardware specifics.

- Single source. No forking off a separate GPU code. Compile the same program for multi-core or serial, non-parallel programmers can play along.

- Efficient. Very favorable comparison to pthreads.

- Performance portable. Easily scales to different configurations.

- Incremental. Developers can port and tune parts of their application as resources and profiling dictates. No wholesale rewrite required. Which can be quick.
Broad Compiler Support (For 3.x)

- GCC
- MS Visual Studio
- Intel
- IBM
- PGI
- Cray
A True Standard With A History

OpenMP.org: specs and forums and useful links

- POSIX threads

- 1997 OpenMP 1.0
- 1998 OpenMP 2.0
- 2005 OpenMP 2.5 (Combined C/C++/Fortran)
- 2008 OpenMP 3.0
- 2011 OpenMP 3.1
- 2013 OpenMP 4.0 (Accelerators)
- 2018 OpenMP 5.0
Hello World

Hello World in C

```c
int main(int argc, char** argv){
    #pragma omp parallel
    { printf("Hello world.\n");
    }
}
```

Hello World in Fortran

```fortran
program hello
    !$OMP PARALLEL
    print *,"Hello World."
    !$OMP END PARALLEL
    stop
    end
```

Output with OMP_NUM_THREADS=4

Hello World.  
Hello World. 
Hello World. 
Hello World. 

---

*Hello World*
This is how these directives integrate into code:

Fortran

```fortran
!$omp parallel [clause ...]
  !$omp structured block
!$omp end parallel
```

C

```c
#pragma omp parallel [clause ...]
{
  structured block
}
```

Clause: optional modifiers
Which we shall discuss

I will 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.
```c
#include <pthread.h>
#include <stdio.h>
#define NUM_THREADS 4

void *PrintHello(void *threadid)
{
    printf("Hello World.\n");
    pthread_exit(NULL);
}

int main (int argc, char *argv[])
{
    pthread_t threads[NUM_THREADS];
    int rc;
    long t;
    for(t=0; t<NUM_THREADS; t++){
        rc = pthread_create(&threads[t], NULL, PrintHello, (void *)t);
        if(rc){
            exit(-1);
        }
    }
    pthread_exit(NULL);
}
```
Big Difference!

- With pthreads, we changed the structure of the original code. Non-threading programmers can’t understand new code.

- We have separate sections for the original flow, and the threaded code. Serial path now gone forever.

- This only gets worse as we do more with the code.

- 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?
Thread vs. Process

Two Processes

A[0] = 10;
B[4][Y] = 20;
Y = Y + 1;
for (i=1; i<100; i++) {
  A[i] = A[i-1];
}
Y = 0;
B[0][0] = 30;
A[0] = 30;

Two Threads

A[0] = 10;
B[4][Y] = 20;
Y = Y + 1;
for (i=1; i<100; i++) {
  A[i] = A[i-1];
}
Y = 0;
B[0][0] = 30;
A[0] = 30;
General Thread Capability

- Master
- Thread
- Spawned Threads
- Thread Killed
Typical Desktop Application Threading

Open Browser Tabs (Spawn Thread)

Close Browser Tab (Kill Thread)
Typical Game Threading

Game Physics

Synchronization

Rendering

AI
HPC Application Threading

A[0] = 10;

i = i+1;

for(...) {
    B[100][100]
}

if (y=4) {

print X

for(...) {
    X[1000][10...

for or do loop

works on big array

for or do loop

works on big array
HPC Use of OpenMP

- This last fact means that we will emphasize the capabilities of OpenMP with a different focus than non-HPC programmers.
- We will focus on getting our kernels to parallelize well.
- We will be most concerned with dependencies, and not deadlocks and race conditions which confound other OpenMP applications.
- This is very different from the generic approach you are likely to see elsewhere. The “encyclopedic” version can obscure how easy it is to get started with common loops.
This looks easy! Too easy...

- Why don’t we just throw `parallel for/do` (the OpenMP command for this purpose) in front of every loop?

- Better yet, why doesn’t the compiler do this for me?

The answer is that there are several general issues that would generate incorrect results or program hangs if we don’t recognize them:

  - Data Dependencies
  - Data Races
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:

```plaintext
for(index=0; index<10000; index++)
    Array[index] = 4 * Array[index];
```

When run on 10 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];

...
But what if the loops are not entirely independent?

Take, for example, a similar loop like this:

```c
for(index=1; index<10000; index++)
    Array[index] = 4 * Array[index] - Array[index-1];
```

This is perfectly valid serial code.
Now Processor 1, in trying to calculate its first iteration,

\[
\text{for}(\text{index}=1000; \text{index}<1999; \text{index}++)
\]

\[
\text{Array}[1000] = 4 \times \text{Array}[1000] - \text{Array}[999];
\]

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, ...
How about this distributed across those same 10 processors?

```c
for (index=1; index<10000; index++){
    Array[index] = Array[index]+1
    X = Array[index];
}
```

There is no obvious dependence between iterations, but $X$ may not get set to $Array[9999]$ as it would in the serial execution. Any one of the PEs may get the “final word”. Versions of this crop up and are called Output Dependencies.
Recognizing and Eliminating Data Dependencies

Recognize dependencies by looking for:
- A dependence between iterations. Often visible due to use of differing indices.
- Is the variable written and also read?
- Any non-indexed (scaler) variables that are written to by index dependent variables.
- You may get compiler warnings, and you may not.

Can these be overcome?
- Sometimes a simple rearrangement of the code will suffice. There is a common bag of tricks developed for this as this issue goes back 40 years in HPC (for vectorized computers). Many are quite trivial to apply.
- We will now learn about OpenMP capabilities that will make some of these disappear.
- Sometimes they are fundamental to the algorithm and there is no answer other than rewrite completely or leave as serial.

But you must catch these!
Loops with Shared Variables

Most serious loops have other variables besides an array or two. The sharing of these variables introduces some potential issues. Here is a toy problem with a scalar that is written to.

```c
float height[1000], width[1000], cost_of_paint[1000];
float area, price_per_gallon = 20.00, coverage = 20.5;

for (index=0; index<1000; index++){
    area = height[index] * width[index];
    cost_of_paint[index] = area * price_per_gallon / coverage;
}
```

C Version

```fortran
real*8 height(1000), width(1000), cost_of_paint(1000)
real*8 area, price_per_gallon, coverage

do index=1,1000
    area = height(index) * width(index)
    cost_of_paint(index) = area * price_per_gallon / coverage
end do
```

Fortran Version
Applying Some OpenMP

A quick dab of OpenMP would start like this:

```
#pragma omp parallel for
for (index=0; index<1000; index++){
    area = height[index] * width[index];
    cost_of_paint[index] = area * price_per_gallon / coverage;
}
```

We are requesting that this for/do loop be executed in parallel on the available processors. This might be considered the most basic OpenMP construct.
We may as well follow through and see how we would compile and run this. We are using PGI compilers here. Others are very similar (-fopenmp, -omp). Likewise, if you are using a different command shell, you may do “setenv OMP_NUM_THREADS 8”.

Fortran:

```bash
pgf90 -mp paintcost.f
export OMP_NUM_THREADS=8
a.out
```

A few items to remember, but we will appreciate the flexibility these parameters afford us as we get more sophisticated with our optimization.

C:

```bash
pgcc -mp paintcost.c
export OMP_NUM_THREADS=8
a.out
```
Something is wrong.

If we ran this code we would find that sometimes our results differ from the serial code (and are simply wrong). The reason is that we have a shared variable that is getting overwritten by all of the threads.

```c
#pragma omp parallel for
for (index=0; index<1000; index++){
    area = height[index] * width[index];
    cost_of_paint[index] = area * price_per_gallon / coverage;
}
```

Between it’s assignment and use there are (7 here) other threads accessing and changing it. This is obviously not what we want.
Shared Variables

For (index=0; index<1000; index++){
    area = height[index] * width[index];
    cost_of_paint[index] = area * price;
}

With Two Threads

By default variables are shared in OpenMP. Exceptions include index variables and variables declared inside parallel regions (C/C++). More later.
What We Want

For the index = 0 to 1000, calculate the area as `area = height[index] * width[index]`; and the cost of paint as `cost_of_paint[index] = area * price...` with two threads.

We can accomplish this with the `private` clause.
Apply the private clause and we have a working loop:

```
#pragma omp parallel for private(area)
for (index=0; index<1000; index++){
    area = height[index] * width[index];
    cost_of_paint[index] = area * price_per_gallon / coverage;
}
```

Fortran Version

```
!$omp parallel do private(area)
do index=1,1000
    area = height(index) * width(index)
    cost_of_paint(index) = area * price_per_gallon / coverage
end do
!$omp end parallel do
```

There are several ways we might wish these controlled variables to behave. Let’s look at the related data-sharing clauses. private is the most common by far.
Other Data Sharing Clauses

**shared(list)**  
This is the default (with the exception of index and locally declared variables. You might use this clause for clarification purposes.

**firstprivate(list)**  
This will initialize the privates with the value from the master thread.  
*Otherwise, this does not happen!*

**lastprivate(list)**  
This will copy out the last thread value into the master thread copy.  
*Otherwise, this does not happen!*  
Available in for/do loop or section only, not available where “last iteration” isn’t clearly defined.

**default(list)**  
You can change the default type to some of the others.

**threadprivate(list)**  
Define at global level and these privates will be available in every parallel region. Use with `copyin()` to initialize values from master thread. Can think of these as on heap, while privates are on stack.
What is automatically private?

The default rules for sharing (which you should never be shy about redundantly designating with clauses) have a few subtleties.

- Default is **shared**, except for...
- local variables in any called subroutine, unless using `static` (C) or `save` (Fortran)
- loop index variable
- inner loop index variables in Fortran, but not in C.
- variables declared within the block (for C).

These last two points make the C99 loop syntax quite convenient:

```c
#pragma omp parallel for
for ( int i = 0; i <= n; i++ ){
    for ( int j = 0; j<= m; j++ ){
        Array[i][j] = Array[i][j]+1
    }
}
```
The parallel for/do loop is common enough that we want to make sure we really understand what is going on.

In general (well beyond OpenMP reasons), you want your innermost loop to index over adjacent items in memory. This is opposite for Fortran and C. In C this last index changes fastest. We can collapse nested loops with a `collapse(n)` clause.
Let's see what we can do with a simple program that counts prime numbers.

C Version

```c
#include <stdlib.h>
#include <stdio.h>

int main ( int argc, char *argv[] )
{
    int n = 500000;
    int not_primes=0;
    int i,j;

    for ( i = 2; i <= n; i++ )
    {
        for ( j = 2; j < i; j++ )
        {
            if ( i % j == 0 )
            {
                not_primes++;
                break;
            }
        }
    }

    printf("Primes: %d\n", n - not_primes);
}
```

Fortran Version

```fortran
program primes
    integer n, not_primes, i, j
    n = 500000
    not_primes=0
    do i = 2,n
        do j = 2,i-1
            if (mod(i,j) == 0) then
                not_primes = not_primes + 1
                exit
            end if
        end do
    end do
    print *, 'Primes: ', n - not_primes
end program
```
Prime Counter

The most obvious thing is to parallelize the main loop.

C Version

```c
#pragma omp parallel for private (j)
for ( i = 2; i <= n; i++ ){
    for ( j = 2; j < i; j++ ){
        if ( i % j == 0 ){
            not_primes++;
            break;
        }
    }
}
```

Fortran Version

```fortran
!$omp parallel do
    do i = 2,n
        do j = 2,i-1
            if (mod(i,j) == 0) then
                not_primes = not_primes + 1
                exit
            end if
        end do
    end do
!$omp end parallel do
```

If we run this code on multiple threads, we will find that we get inconsistent results. What is going on?
The problem here is a shared variable (not_primes) that is being written to by many threads.

The statement `not_primes = not_primes + 1` may look “atomic”, but in reality it requires the processor to first read, then update, then write the variable into memory. While this is happening, another thread may be writing its own (now obsolete) update. In this case, some of the additions to `not_primes` may be overwritten and ignored.

Will **private** fix this? Private variables aren’t subject to data races, and we will end up with multiple valid `not_prime` subtotals. The question then becomes, how do we sum these up into the real total we are looking for?

It is common to have a private variable that has to live on after the loop. This requires us to **reduce** these private copies back to a single scaler.
Reductions

Reductions are private variables that must be reduced to a single value eventually.

C Version

```c
#pragma omp parallel for private (j) \
    reduction(+: not_primes)
for ( i = 2; i <= n; i++ ){
    for ( j = 2; j < i; j++ ){
        if ( i % j == 0 ){
            not_primes++;
            break;
        }
    }
}
```

Fortran Version

```fortran
!$omp parallel do reduction(+:not_primes)
    do i = 2,n
        do j = 2,i-1
            if (mod(i,j) == 0) then
                not_primes = not_primes + 1
                exit
            end if
        end do
    end do
$omp end parallel do
```

At the end of the parallel region (the do/for loop), the private reduction variables will get combined using the operation we specified. Here, it is sum (+).
Reductions

In addition to sum, we have a number of other options. You will find sum, min and max to be the most common. Note that the private variable copies are all initialized to the values specified.

<table>
<thead>
<tr>
<th>Operation</th>
<th>Initialization</th>
</tr>
</thead>
<tbody>
<tr>
<td>+</td>
<td>0</td>
</tr>
<tr>
<td>max</td>
<td>least number possible</td>
</tr>
<tr>
<td>min</td>
<td>largest number possible</td>
</tr>
<tr>
<td>-</td>
<td>0</td>
</tr>
<tr>
<td>Bit (&amp;,</td>
<td>, ^, iand, ior)</td>
</tr>
<tr>
<td>Logical (&amp;&amp;,</td>
<td></td>
</tr>
</tbody>
</table>
A few notes before we leave (for now):

- The OpenMP standard forbids branching out of parallel do/for loops. Since the outside loop is the threaded one (that is how it works), our break/exit statement for the inside loop are OK.

- You can verify the output at primes.utm.edu/nthprime/index.php#piofx Note that we count 1 as prime. They do not.
Our Foundation Exercise: Laplace Solver

- We will also use this for MPI and OpenACC. It is a great simulation problem, not rigged for OpenMP.
- 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:

![Initial Conditions](Metal Plate) ![Final Steady State](Metal Plate)
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]);
    }
}

while j = 1,columns do
    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
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 Subroutines

```c
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.
```
#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++) {
                Temperature_last[i][j] = Temperature[i][j];
                Temperature_last[i][j] = Temperature[i][j];
            }
        }

        // periodically print test values
        if((iteration % 100) == 0) {
            track_progress(iteration);
        }
        iteration++;
    }
    gettimeofday(&stop_time,NULL);
    timer(sub(&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 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 = 0; i <= ROWS-5; i++) {
        for(j = 0; j <= COLUMNS-5; j++) {
            printf("\%d,\%d: \%5.2f  ", i, j, Temperature[i][j]);
        }
    }
    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
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 *

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 = max(abs(temperature(1,j) - temperature_last(1,j)), dt )
      temperature_last(1,j) = temperature(1,j)
  enddo

  !do until error is minimal or until maximum steps
  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

  !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 )
      enddo
  enddo

  !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 = max(abs(temperature(1,j) - temperature_last(1,j)), dt )
      temperature_last(1,j) = temperature(1,j)
  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
Exercise 1: Use OpenMP to parallelize the Jacobi loops
(About 45 minutes)

1) Log onto a node requesting all the cores (28 on a regular Bridges node).

   > interact -n 28

2) Edit laplace_serial.c or laplace_serial.f90 (your choice) and add directives where it helps.

3) Run your code on various numbers of cores (such as 8, per below) and see what kind of speedup you achieve.

   > pgcc -mp laplace_omp.c or pgf90 -mp laplace_omp.f90
   > export OMP_NUM_THREADS=8
   > a.out
On some platforms the universal Fortran cpu_time() function will report aggregate CPU time. You can divide your answer by the number of threads to get an effective answer. Or, you can take this opportunity to start using some of the useful OpenMP run time library - namely omp_get_time().

C:
#include <omp.h>
double start_time = omp_get_wtime();
...
double end_time = omp_get_wtime();

Fortran:
use omp_lib
double precision :: start_time, stop_time
start_time = omp_get_wtime()
...
end_time = omp_get_wtime()
while ( dt > MAX_TEMP_ERROR && iteration <= max_iterations ) {
    #pragma omp parallel for private(i,j)
    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 omp parallel for reduction(max:dt) private(i,j)
    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++;
}
Exercise 1 Fortran Solution

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

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

dt=0.0

!$omp parallel do reduction(max:dt)
do j=1,columns
  do i=1,rows
    dt = max( abs(temperature(i,j) - temperature_last(i,j)), dt )
    temperature_last(i,j) = temperature(i,j)
  enddo
enddo
!$omp end parallel do

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

iteration = iteration+1
enddo
For the solution in the Laplace directory, we found this kind of scaling when running to convergence at 3372 iterations.

<table>
<thead>
<tr>
<th>Threads</th>
<th>C (s)</th>
<th>Fortran (s)</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>18.7</td>
<td>18.7</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>9.4</td>
<td>9.4</td>
<td>1.99</td>
</tr>
<tr>
<td>4</td>
<td>4.7</td>
<td>4.7</td>
<td>3.98</td>
</tr>
<tr>
<td>8</td>
<td>2.5</td>
<td>2.5</td>
<td>7.48</td>
</tr>
<tr>
<td>16</td>
<td>1.4</td>
<td>1.4</td>
<td>13.4</td>
</tr>
<tr>
<td>28</td>
<td>0.89</td>
<td>0.86</td>
<td>21.5</td>
</tr>
</tbody>
</table>

The larger version of this problem that we use for the hybrid programming example (10K x 10K) continues to scale nicely on Bridges 12TB memory nodes to hundreds of cores!

Codes were compiled with no extra flags, and there was some minor variability.
Time for a breather.

Congratulations, you have now mastered the OpenMP parallel for/do loop. That is a pretty solid basis for using OpenMP. To recap, you just have to keep an eye out for:

- Dependencies
- Data races

and know how to deal with them using:

- Private variables
- Reductions
Different Work Sharing Constructs

Master
Thread
parallel for/do
parallel for/do
parallel for/do

What we have been doing

What we could do (less overhead, no idle cores, finer control, more flexible algorithms)
Number of Threads in a Parallel Region

In order of precedence:

**IF clause** Logical value determines if this region is parallel or serial.

**NUM_THREADS clause** Set this to specify how many threads in this region.

**omp_set_num_threads()** A library API to set the threads.

**OMP_NUM_THREADS** The environment variable we have been using.

Default Often the number of cores on the node.

There is also, depending on the compute environment, the possibility of dynamic thread counts. There are a few library APIs to deal with that.
Fortran 90 has data parallel constructs that map very well to threads. You can declare a workshare region and OpenMP will do the right thing for:

- FORALL
- WHERE
- Array assignments

```fortran
PROGRAM WORKSHARE
  INTEGER N, I, J
  PARAMETER (N=100)
  REAL AA(N,N), BB(N,N), CC(N,N), DD(N,N)
  .
  .
  !$OMP PARALLEL SHARED(AA,BB,CC,DD,FIRST,LAST)
  .
  .
  !$OMP WORKSHARE
  CC = AA * BB
  DD = AA + BB
  FIRST = CC(1,1) + DD(1,1)
  LAST = CC(N,N) + DD(N,N)
  !$OMP END WORKSHARE
  .
  .
  !$OMP END PARALLEL
END
```
Each section will be processed by one thread. The number of sections can be greater or less than the number of threads available - in which case threads will do more than one section or skip, respectively.
Both for/do loops run concurrently. Still same results as serial here.
And for ultimate flexibility: Tasks

Any thread can spin off tasks. And, any thread can pick up a task. They will all wait for completion at the end of the region.
Fibonacci Tasks

```c
#include <stdio.h>
#include <omp.h>

int main()
{
    int n = 10;

    #pragma omp parallel shared(n)
    {
        #pragma omp single
        printf("fib(%d) = %d\n", n, fib(n));
    }
}
```

```c
int fib(int n)
{
    int i, j;

    if (n<2)
        return n;
    else {

        #pragma omp task shared(i) firstprivate(n)
        i=fib(n-1);

        #pragma omp task shared(j) firstprivate(n)
        j=fib(n-2);

        #pragma omp taskwait
        return i+j;
    }
}
```

Our tasks are spinning off tasks recursively! The threads will eventually pick them all off. This example is a little too clever.
Tasks have some additional directives and clauses.

- **taskwait** (wait for completion of child tasks, should almost always use)
- **taskgroup** (wait on child & descendants)
- **taskyield** (can suspend for another task, avoid deadlock)
- **final** (no more task creation after this level)
- **untied** (can change thread dynamically)
- **mergable** (can merge data with enclosing region)
- **depend** (list variable dependencies between tasks [in/out/inout] This provides a way to order workflow.)

We won’t go into them further, because you only need to know they exist in case you are developing a sophisticated HPC applications that needs these. This capability is useful for:

- Graphs
- Any kind of pointer chasing
Parallel Region with C

```c
#pragma omp parallel shared(t, t_old) private(i,j, iter) firstprivate(niter)
for(iter = 1; iter <= niter; iter++) {

    #pragma omp for
    for(i = 1; i <= NR; i++) {
        for(j = 1; j <= NC; j++) {
            t[i][j] = 0.25 * (t_old[i+1][j] + t_old[i-1][j] +
                              t_old[i][j+1] + t_old[i][j-1]);
        }
    }

dt = 0.0;

    #pragma omp for reduction(max:dt)
    for(i = 1; i <= NR; i++){
        for(j = 1; j <= NC; j++){
            dt = fmax(fabs(t[i][j]-t_old[i][j]), dt);
            t_old[i][j] = t[i][j];
        }
    }
    if((iter % 100) == 0) {
        print_trace(iter);
    }
}
```

This is a simpler loop than our actual exercise two's condition while loop.

Working example in slide notes below is not that complicated, but we will skip it for the nonce.
Parallel Region with Fortran

$omp parallel shared(T, Told) private(i,j,iter) firstprivate(niter)
  do iter=1,niter
    !$omp do
    do j=1,NC
      do i=1,NR
        $T(i,j) = 0.25 * ( Told(i+1,j)+Told(i-1,j)+$
        $Told(i,j+1)+Told(i,j-1) )$
      $enddo$
      $enddo$
    !$omp end do
  $do$
  dt = 0
  !$omp do reduction(max:dt)
  do j=1,NC
    do i=1,NR
      dt = max( abs(t(i,j) - told(i,j)), dt )$
      Told(i,j) = T(i,j)$
    $enddo$
    $enddo$
  !$omp end do
  if( mod(iter,100).eq.0 ) then
    call print_trace(t, iter)$
  endif
  $enddo$
$omp end parallel
Thread control.

If we did this, we would get correct results, but we would also find that our output is a mess.

How many iterations [100-1000]? 1000
----------- Iteration number: 100 -----------
[995,995]: 63.33 [996,996]: 72.67 [997,997]: 81.40 [998,998]: 88.97 [999,999]: 94.86 [1000,1000]: 98.67

----------- Iteration number: 100 -----------
[995,995]: 63.33 [996,996]: 72.67 [997,997]: 81.40 [998,998]: 88.97

----------- Iteration number: 100 -----------
[995,995]: 63.33 [996,996]: 72.67

All of our threads are doing output. We only want the master thread to do this. This is where we find the rich set of thread control tools available to us in OpenMP.
The Master directive will only allow the region to be executed by the master thread. Other threads skip. By skip we mean race ahead - to the next iteration. We really should have an "omp barrier" after this or threads could already be altering t as we are writing it out. Life in parallel regions can get tricky!
Barrier

A barrier is executed by all threads only at:

- A **barrier** command
- Entry to and exit from a parallel region
- **Exit only** from a worksharing command (like do/for)
- Except if we use the **nowait** clause

There are no barriers for any other constructs including **master** and **critical**!
Now we are using OpenMP runtime library routines, and not directives. We would have to use ifdef if we wanted to preserve the serial version. Also, we should include a barrier somewhere here as well.
### Other Synchronization Directives & Clauses

<table>
<thead>
<tr>
<th>Directive</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>single</strong></td>
<td>Like Master, but any thread will do. Has a <code>copyprivate</code> clause that can be used to copy its private values to all other threads.</td>
</tr>
<tr>
<td><strong>critical</strong></td>
<td>Only one thread at a time can go through this section. Can be named or unnamed (only one thread in <em>all</em> unnamed regions).</td>
</tr>
<tr>
<td><strong>atomic</strong></td>
<td>Eliminates data race on this one specific, simple statement. More efficient than <code>critical</code>.</td>
</tr>
<tr>
<td><strong>ordered</strong></td>
<td>Forces serial order on loops.</td>
</tr>
<tr>
<td><strong>nowait</strong></td>
<td>This clause will eliminate implied barriers on certain directives.</td>
</tr>
<tr>
<td><strong>flush</strong></td>
<td>Even cache coherent architectures need this to eliminate possibility of register storage issues. Tricky, but important <em>iff</em> you get tricky. We will return to this.</td>
</tr>
</tbody>
</table>
As we have started to get away from the simplicity of the do/for loop and pursue the freedom of parallel regions and individual thread control, we have started to encounter subtle pitfalls.

So, you may be relieved to know that we have covered almost all of the OpenMP directives at this point. However, there are a few more run-time library routines to mention...
## Run-time Library Routines

<table>
<thead>
<tr>
<th>Routine</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>OMP_SET_NUM_THREADS</td>
<td>Sets the number of threads that will be used in the next parallel region.</td>
</tr>
<tr>
<td>OMP_GET_NUM_THREADS</td>
<td>Returns the number of threads that are currently in the team executing the parallel region from which it is called.</td>
</tr>
<tr>
<td>OMP_GET_MAX_THREADS</td>
<td>Returns the maximum value that can be returned by a call to the OMP_GET_NUM_THREADS function.</td>
</tr>
<tr>
<td>OMP_GET_THREAD_NUM</td>
<td>Returns the thread number of the thread, within the team, making this call.</td>
</tr>
<tr>
<td>OMP_GET_THREAD_LIMIT</td>
<td>Returns the maximum number of OpenMP threads available to a program.</td>
</tr>
<tr>
<td>OMP_GET_NUM_PROCS</td>
<td>Returns the number of processors that are available to the program.</td>
</tr>
<tr>
<td>OMP_IN_PARALLEL</td>
<td>Used to determine if the section of code which is executing is parallel or not.</td>
</tr>
<tr>
<td>OMP_SET_DYNAMIC</td>
<td>Enables or disables dynamic adjustment of the number of threads available for execution of parallel regions.</td>
</tr>
<tr>
<td>OMP_GET_DYNAMIC</td>
<td>Used to determine if dynamic thread adjustment is enabled or not.</td>
</tr>
<tr>
<td>OMP_SET_NESTED</td>
<td>Used to enable or disable nested parallelism.</td>
</tr>
<tr>
<td>OMP_GET_NESTED</td>
<td>Used to determine if nested parallelism is enabled or not.</td>
</tr>
<tr>
<td>OMP_SET_SCHEDULE</td>
<td>Sets the loop scheduling policy when “runtime” is used as the schedule kind in the OpenMP directive.</td>
</tr>
<tr>
<td>OMP_GET_SCHEDULE</td>
<td>Returns the loop scheduling policy when “runtime” is used as the schedule kind in the OpenMP directive.</td>
</tr>
<tr>
<td>OMP_SET_MAX_ACTIVE_LEVELS</td>
<td>Sets the maximum number of nested parallel regions.</td>
</tr>
<tr>
<td>OMP_GET_MAX_ACTIVE_LEVELS</td>
<td>Returns the maximum number of nested parallel regions.</td>
</tr>
<tr>
<td>OMP_GET_LEVEL</td>
<td>Returns the current level of nested parallel regions.</td>
</tr>
<tr>
<td>OMP_GET_ANCESTOR_THREAD_NUM</td>
<td>Returns, for a given nested level of the current thread, the thread number of ancestor thread.</td>
</tr>
<tr>
<td>OMP_GET_TEAM_SIZE</td>
<td>Returns, for a given nested level of the current thread, the size of the thread team.</td>
</tr>
<tr>
<td>OMP_GET_ACTIVE_LEVEL</td>
<td>Returns the number of nested, active parallel regions enclosing the task that contains the call.</td>
</tr>
<tr>
<td>OMP_IN_FINAL</td>
<td>Returns true if the routine is executed in the final task region; otherwise it returns false.</td>
</tr>
<tr>
<td>OMP_INIT_LOCK</td>
<td>Initializes a lock associated with the lock variable.</td>
</tr>
<tr>
<td>OMP_DESTROY_LOCK</td>
<td>Disassociates the given lock variable from any locks.</td>
</tr>
<tr>
<td>OMP_SET_LOCK</td>
<td>Acquires ownership of a lock.</td>
</tr>
<tr>
<td>OMP_UNSET_LOCK</td>
<td>Releases a lock.</td>
</tr>
<tr>
<td>OMP_TEST_LOCK</td>
<td>Attempts to set a lock, but does not block if the lock is unavailable.</td>
</tr>
<tr>
<td>OMP_INIT_NEST_LOCK</td>
<td>Initializes a nested lock associated with the lock variable.</td>
</tr>
<tr>
<td>OMP_DESTROY_NEST_LOCK</td>
<td>Disassociates the given nested lock variable from any locks.</td>
</tr>
<tr>
<td>OMP_SET_NEST_LOCK</td>
<td>Acquires ownership of a nested lock.</td>
</tr>
<tr>
<td>OMP_UNSET_NEST_LOCK</td>
<td>Releases a nested lock.</td>
</tr>
<tr>
<td>OMP_TEST_NEST_LOCK</td>
<td>Attempts to set a nested lock, but does not block if the lock is unavailable.</td>
</tr>
</tbody>
</table>
#include <stdio.h>
#include <omp.h>

omp_lock_t my_lock;

int main() {
    omp_init_lock(&my_lock);

    #pragma omp parallel
    {
        int tid = omp_get_thread_num();
        int i;

        omp_set_lock(&my_lock);

        for (i = 0; i < 5; ++i) {
            printf("Thread %d - in locked region\n", tid);
        }

        printf("Thread %d - ending locked region\n", tid);

        omp_unset_lock(&my_lock);
    }

    omp_destroy_lock(&my_lock);
}

This could have been done with just an omp critical!
Pthreads like flexibility

We now have the ability to start coding just about any kind of thread flow we can imagine. And we can start creating all kinds of subtle and non-repeatable bugs. This is normally where we start the fun of cataloging all of the ways we can get into trouble:

- Race conditions
- Deadlocks
- Livelocks
- Missing flush

<table>
<thead>
<tr>
<th></th>
<th>Thread A</th>
<th>Thread B</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lock(USB Drive)</td>
<td>Lock(File)</td>
<td>Lock(USB Drive)</td>
</tr>
<tr>
<td>Lock(File)</td>
<td>Lock(File)</td>
<td>Copy(File)</td>
</tr>
<tr>
<td>Copy(File)</td>
<td>Unlock(File)</td>
<td>Unlock(USB Drive)</td>
</tr>
<tr>
<td>Unlock(File)</td>
<td>Unlock(USB Drive)</td>
<td>Unlock(File)</td>
</tr>
</tbody>
</table>

Deadlock

So, what are the benefits of these paradigms? Efficiency
If you start delving into these capabilities, you need to understand the flush command. Even shared memory machines have cache issues and compiler instruction reordering that can cause shared values to get out of sync if you insist on reading and writing shared variables from different threads (like rolling your own locks or mutexes). You can rectify these problems with:

- implicit barriers (as mentioned previously)
- barrier (incurs synchronization penalty)
- flush (no sync)

If you think you are wandering into this territory, the best reference for examples and warnings is:

OpenMP Application Program Interface
http://openmp.org/mp-documents/OpenMP_Examples_4.0.1.pdf
Complexity vs. Efficiency

How much you will gain in efficiency by using these more flexible (dangerous) routines depends upon your algorithm. How asynchronous can it be?

The general question is, how much time are threads spending at barriers? If you can’t tell, profiling will.
We do have a way of greatly affecting the thread scheduling while still using do/for loops. That is to use the `schedule` clause.

Let’s think about what happens with our prime number program if the loop iterations are just evenly distributed across our processors. Some of our iterations/threads will finish much earlier than others.
Scheduling Options

**static, n**  
Divides iterations evenly amongst threads. You can optionally specify the chunk size to use.

**dynamic, n**  
As a thread finishes, it is assigned another. Default chunk size is 1.

**guided, n**  
Block size will decrease with each new assignment to account for remaining iterations at that time. Chunk size specifies minimum (and defaults to 1).

**runtime**  
Decided at runtime by OMP_SCHEDULE variable.

**auto**  
Let the compiler/runtime decide.
Exercise 2: Improving Prime Number
(About 30 minutes)

Speed up the prime number count just using the scheduling options you have available.

1) Start with the prime_serial.c/f version in the OpenMP/Prime folder and then add the parallel directives as per the previous lecture slides. See how much it speeds up on various thread counts. Then...

2) Try various scheduling options to see if anything is effective at optimizing further. This “empirical” approach is a perfectly reasonable, and safe, way to find some low-hanging fruit.
Dynamic scheduling with a default chunksize (of 1).
We get a pretty big win for little work and even less danger. The Fortran and C times are almost exactly the same for this code.

<table>
<thead>
<tr>
<th>Threads</th>
<th>Default (s)</th>
<th>dynamic</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>32</td>
<td>32</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>23</td>
<td>16</td>
<td>1.4</td>
</tr>
<tr>
<td>4</td>
<td>14</td>
<td>8.1</td>
<td>1.7</td>
</tr>
<tr>
<td>8</td>
<td>7.7</td>
<td>4.2</td>
<td>1.8</td>
</tr>
<tr>
<td>16</td>
<td>4.2</td>
<td>2.1</td>
<td>2</td>
</tr>
<tr>
<td>28</td>
<td>2.4</td>
<td>1.2</td>
<td>2</td>
</tr>
</tbody>
</table>

500,000 iterations.
C++

- private /shared, etc. work with objects
  constructors/destructor are called for private
  things can get complicated with firstprivate, threadprivate, etc.

- Probably biggest question is std::vector
  Safe if no reallocation: No push_back(), pop_back(), insert()
  Iterators are even allowed in for loop here

- Other containers less likely to just work
  For example, std::list (a doubly linked list) updated by multiple threads would be a nightmare

- Note: MPI 3 and newer have dropped C++, so be aware if aiming for larger scalability
We have now covered everything up to (but not completely including) OpenMP 4.0. I hope you still recall how much we accomplished with just a parallel for/do. Let’s recap:

- Look at your large, time-consuming for/do loops first
  - Deal with dependencies and reductions
  - Using private and reductions
  - Consider scheduling

- If you find a lot of barrier time (via inspection or profiler) then:
  - Sections
  - Tasks
  - Run-time library
  - Locks
  - Barriers/nowaits