Shared Memory Programming with OpenMP

ISC5316: Applied Computational Science II

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SERIAL: von Neumann Architecture

For fifty years, we have used a simple model of the computer called the von Neumann computer, consisting of memory (input data and intermediate results), a processor (carrying out arithmetic and logical operations), an input/output device, and a clock.
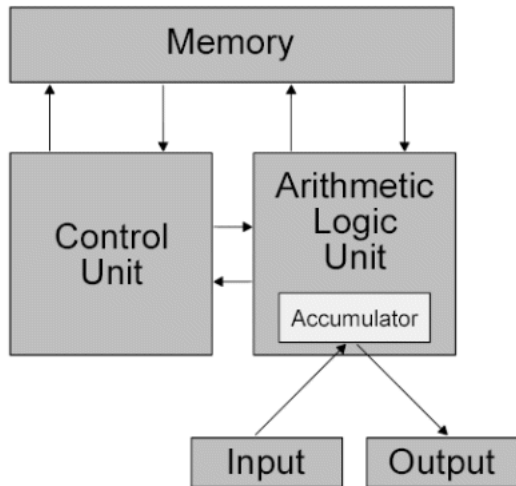
The von Neumann computer runs a program, also stored in memory.

The clock is surprisingly important, providing synchronization. Roughly speaking, nothing happens faster than a single clock tick.

In particular, no matter how many instructions there are in the program, just one instruction is carried out each tick. The von Neumann computer thus carries out sequential or serial execution of the program.

Logically, this is a beautiful and simple model. And we have kept if for so long, and designed computers and algorithms and programming languages around it, because over the years, computers have been fast enough to solve the problems we are interested in.

The problems we are interested in have grown enormously over the years, and the only reason computers were able to keep up was because it was possible to relentlessly increase the clock speed (of course, we had to make faster processors and memory access as well.)

The clock speed increased because of the increasing sophistication and miniaturization of computer chips.

Sometime around 2005, the clock speed curve hit an immovable ceiling.
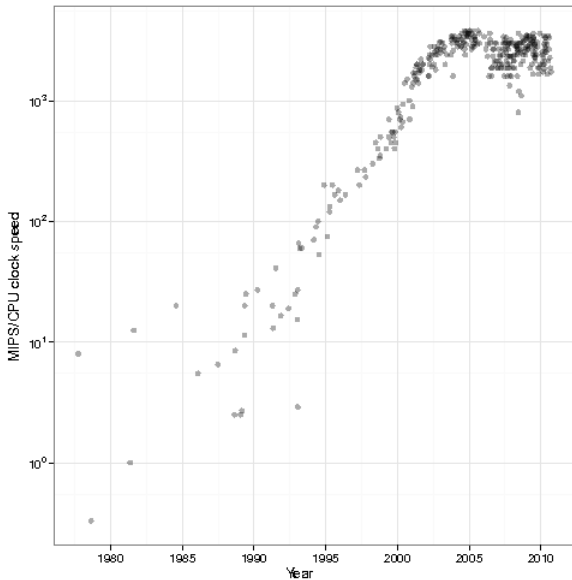
The are simple alternatives to the von Neumann model of computation.

Most of these involve the idea of parallel computing, that is, of carrying out more than one instruction or operation at a time.

if the clock can't tick faster, then somehow we have to carry out more work per clock cycle if we want to get done faster, or solve bigger problems.

One hardware advance involved communication: it was possible for two different computers to share information during a computation. This fact led to the development of MPI (next week's topic!).

Another advance was the development of multicore processors.
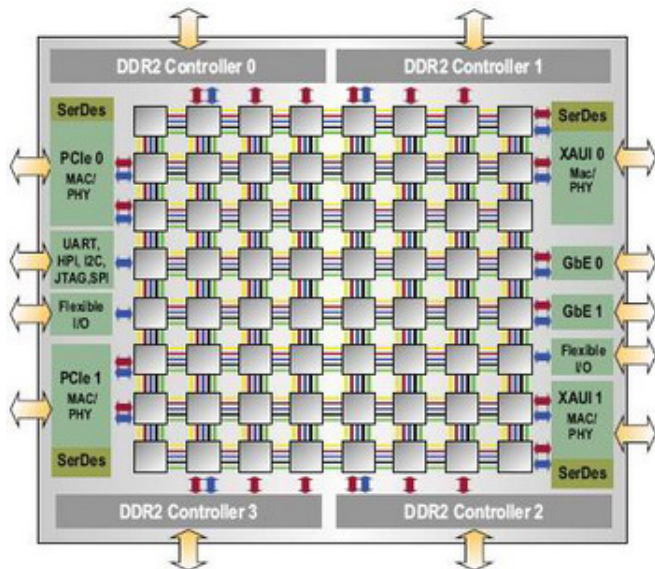
   With a multicore processor, we can make a simple modification to the von Neumann model of the computer. We have the same memory, I/O, and clock, but now we have many processors.
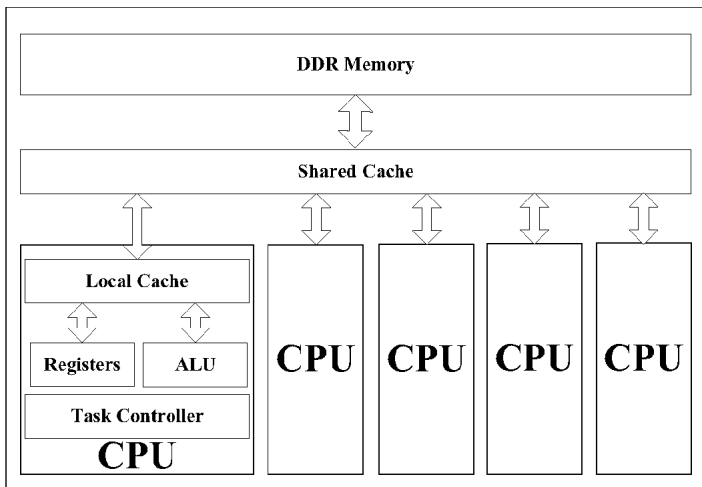
If these processors can cooperate, then even though the clock ticks at the same rate as before, we can get done faster.

The problem now: can we write a new kind of computer program that can correctly control multiple, cooperating processors?

We'll assume that the processors live in a shared memory space, so that any processor can read or write any piece of data.

I'd like you to think about this problem in a simple form. Suppose our program simply needs to square every number in memory.

Even if we have 64 processors available, each processor will need to get a copy of the instructions "square the number in the given location" and a (unique) subset of the memory locations.

So at least in this case, it's clear that more processors can be helpful; but it might not be clear how we, at the user level, can tell the processors how to divide up the work without interfering with each other.

OpenMP is a system that exactly allows us to write programs that will be correctly executed on multiple processors; if done correctly, such a parallel program can run a hundred times faster if we have 100 cores available.

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ALG: An Algorithm Need Not be "Step by Step"

We are use to definitions of algorithms as a step-by-step procedure, in which step 1 must be completed before step 2 can be started, but this is **not** an essential feature of an algorithm!

The step-by-step approach is called *serial* or *sequential* programming.

We may be so used to this idea that we look at a problem like

$$S = X1 + X2 + X3 + X4 + X5 + X6 + X7 + X8$$

and can only see a serial approach:

$$(\text{clock} = 1) \ S = X1$$
$$(\text{clock} = 2) \ S = S + X2$$
$$(\text{clock} = 3) \ S = S + X3$$
$$...$$
$$(\text{clock} = 8) \ S = S + X8$$

But for many algorithms, a few steps, maybe even many steps, can be going on at the same time. The point of parallel programming is to identify those opportunities.

ALG: Adding N Numbers Doesn't Need N Steps

If we have four processors, and room to store 4 temporary sums, and if all the processors can work at the same time, we can do the addition in 4 clock cycles (we are really working on a binary tree here):

(clock = 1) $S1 = X1, S2 = X3, S3 = X5, S4 = X7$
(clock = 2) $S1 = S1 + X2, S2 = S2 + X4, S3 = S3 + X6, S4 = S4 + X8$
(clock = 3) $S1 = S1 + S2, S3 = S3 + S4$
(clock = 4) $S1 = S1 + S3$

Assuming "unlimited resources" ($n/2$ processors!), we can add n numbers in $1 + log_2(n)$ rather than n cycles, so 1,000 numbers could be added in about 10 steps rather than 1,000, and 1,000,000 numbers could be added in about 20 steps rather than 1,000,000!

Of course, typically we don't have thousands of processors available, but it is still true that we really can solve problems faster if we can find, describe, and implement an appropriate parallel algorithm.

Are there classes of problems we can solve in parallel?

Search: if you need to:

- find the joker in a deck of cards;
- find the triangle in a mesh that contains a given point;
- find proteins in a database that are similar to a sample protein.

then you can divide up the deck, or the mesh, or the database, among the available processors, and run until one of the processors finds a match.

Sort: each processor can take a portion of the items and sort them, returning the sorted set to the "master" processor. The master then simply has to merge the sorted items.

Image Processing: An image is simply an array of pixels. We could be searching for patterns (a tumor, a star, a camouflaged missile battery).

We could be trying to "render" an image, that is, to simulate the look of a model with a given light source. A standard technique called **ray tracing** is to send out thousands of light rays from the source, letting them hit objects in the model, reflect and bounce off other objects, before exiting the model. We can do this in parallel by giving each processor its own set of random light rays to track.
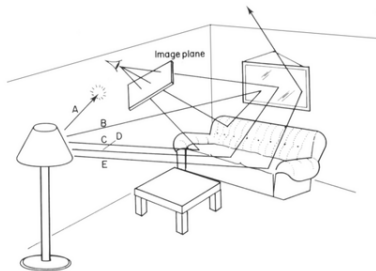
ALG: Gauss Elimination

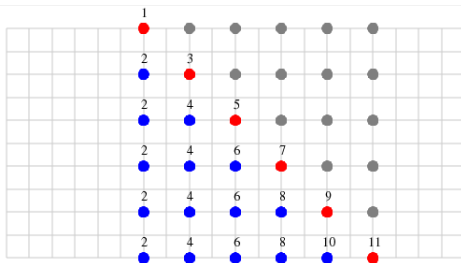**Gauss Elimination**: Suppose we have a linear system of the form:

$$A * x = b$$

Gauss elimination can produce the answer. The k-th step seeks a pivot row, which is used to eliminate elements in the matrix:

- Find $A_{p,k}$, the largest entry on or below the diagonal $A_{k,k}$;
- Swap rows p and k;
- Add a multiple of row k to rows $k+1$ through n to eliminate the entry in column k;

ALG: Jacobi Iteration

Jacobi Iteration: Suppose we have a linear system of the form:

$$A * x = b$$

where A is a symmetric positive definite matrix. Then Jacobi iteration can be used to estimate the solution. On the k-th step of Jacobi iteration, we compute the solution estimate x^k by

$$A_{i,i}\, x_i^k = b_i - \sum_{j=1; j\neq i}^{n} A_{i,j}\, x_j^{k-1}$$

or, in other words:

$$x_i^k = (b_i - \sum_{j=1; j\neq i}^{n} A_{i,j}\, x_j^{k-1})/A_{i,i}$$

so we can update all the entries in x^k at the same time.

ALG: An Ordinary Differential Equation (OOPS!)

An ordinary differential equation in time: Suppose we have a differential equation of the form:

$$u'(t) = f(u, t)$$
$$u(t = 0) = u_0$$

We can define a discretized problem, in which we seek approximate values of $u()$ at the sequence of points $t_1, t_2, ...$ equally spaced by dt. We might do this with a simple Euler method:

$$u_i = u_{i-1} + dt * f(u_{i-1}, t_{i-1})$$

But such an approach <u>cannot</u> be parallelized! Here, the problem is easy to see. The calculation of u_i cannot begin until the calculation of u_{i-1} is complete. But that can't begin until u_{i-2} is computed, and so on.
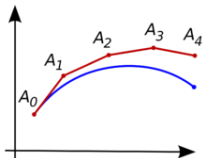
A partial differential equation in time and space: Suppose we have a differential equation of the form:

$$\frac{\partial u}{\partial t} + \nu\left(\frac{\partial^2 u}{\partial^2 x} + \frac{\partial^2 u}{\partial^2 y}\right) = f(u, t, x, y)$$

with corresponding initial and boundary conditions. If we discretize space and time, our solution is an array $u(t_i, x_j, y_k)$. If we use a forward difference for the time derivative, we relate each value $u(t_i, x_j, y_k)$ to known values at the previous time t_{i-1}. Given data at one time step, we can compute all the data at the next time step in parallel.

We have an estimate for the solution in this region.
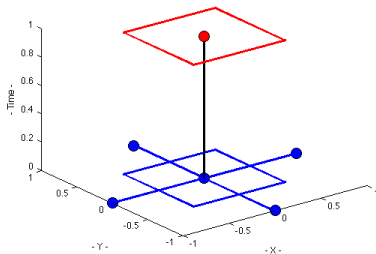
Solving F(X)=0 Using Newton's Method: Suppose we have a scalar equation $f(x) = 0$ to be solved for x. Newton's method produces a sequence of presumably improved estimates:

$$x^{i+1} = x^i - f(x^i)/f'(x^i)$$

However, we can't do this problem in parallel, since we can't start working on x^{17} until x^{16} has been computed.

We might be able to give each processor a different starting point. Or, if x is actually an m-dimensional vector, we might be able to solve the related linear systems in parallel.

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There are several ways that OpenMP allows you to create parallel programs. However, the simplest and most useful one concentrates entirely on operations that are carried out in loops - these are **for** loops in C/C++ and **do** loops in Fortran.

The idea is that a loop contains a lot of work (the number of loop iterations) and that each step is the same (we just repeat the loop logic, with a different loop index.) That makes it easy to break up the work into sections, and to tell each processor in advance what to do.

For example, we might imagine that the sequential loop:

```
for ( i = 0; i < 1000; i++ )
{
  x[i] = x[i] + s * y[i];
}
```

could be parallelized for two processors as:

```
Processor #1                      Processor #2

for ( i = 0; i < 500; i++ )  for ( i = 501; i < 1000; i++ )
{                            {
  x[i] = x[i] + s * y[i];      x[i] = x[i] + s * y[i];
}                            }
```

and it's easy to see how this could be extended to any number of
processors.

We can use more complicated formulas and indices. It's just important that distinct iterations in a loop don't try to set the same variable.

```
for ( j = 1; j <= n; j++ )
{
  x[j]   = sqrt ( y[j-1] );
}

for ( i = 0; i <= 1000; i = i + 2 )
{
  z[i]   = sin ( i * pi );
  z[i+1] = cos ( i * pi );
}
```

Things that only appear on the right hand side can have any form or index. They are simply variables that are "read", not modified:

```
for ( i = 0; i <= 1000; i = i + 2 )
{
  y[i] = y[i] + x[i-1] - 2.0 * x[i] + x[i+1] + z[99] + w;
}
```

LOOP: "Left Hand Side" Variables Can Conflict

Problems occur if more than one loop iteration tries to write or modify the same variable, which occurs on the left hand side of a statement. Here, we have a **y** vector; we'd want to add half of each entry to the corresponding "left" entry in **x** and half to the right.

```
for ( i = 0; i < n; i++ )
{
  if ( 0 < i )
  {
    x[i-1] = x[i-1] + 0.5 * y[i];
  }
  if ( i < n - 1 )
  {
    x[i+1] = x[i+1] + 0.5 * y[i];
  }
}
```

Even in our simple two-processor model, this code will have the potential of conflicts. Suppose that **n**=1000. Processor #1 might try to execute the second addition for $i = 499$ while processor #2 is executing the first addition for $i = 501$.

Sometimes a variable occurs on both the left and right hand side. Since this means that the variable's value changes during the loop execution, it means we can't safely run it in parallel.

```
for ( i = 1; i < n; i++ )
{
  x[i] = x[i] + x[i-1];
}
```

Note that if we try to compute
$x[2] = x[2] + x[1]$,
the value will depend on whether we have already executed the statement
$x[1] = x[1] + x[0]$.

LOOP: Another Example of Side Effects

   This simple model will work, as long as the loop is "appropriate" for parallel processing - in other words, it can go wrong. It will go wrong precisely if the loop has side effects, that is, information computed during one iteration of the loop is used or needed by a later iteration.

Here's a simple example:

```
x = 0.0;
for ( i = 0; i <= 1000; i++ )
{
  y[i] = x * x;
  x = x + 0.001;
}
```

This loop can't execute in parallel with the simple loop model.

Well, maybe it can, but it won't get the right answers! How could we easily fix this?

LOOP: Another Example of Left/Right Variables

Problems can occur if data appears on both the left and right hand side, and so is changed during the calculation.

Here is a sort of Gauss-Seidel iteration for solving a linear system. Why does the loop model fail here?

```
for ( i = 1; i < n - 1; i++ )
{
  x[i] = ( b[i] + x[i-1] + x[i+1] ) / 2.0;
}
```

LOOP: A Summation

Here's another example, (approximating an integral) which is actually important enough that we will see how to fix it later:

```
n = 1000;
q = 0.0;
for ( i = 0; i < n; i++ )
{
  x = i / ( double ) n;
  q = q + x * x;
}
q = q / n;
```

In this loop, **x** is not the problem, it's **q**, which is being modified on every iteration. In our two processor parallel version, would we have two separate variables called **q**? If so, what do we do with them at the end? If there's just one variable, and the processors have to share it, then how do we avoid conflicts?

In summary,

- If we want to run a loop in parallel, it should be written in such a way that the loop iterations would get the same results, even if they were executed in the reverse order, or any order;
- Moreover, we need to avoid cases in which the same variable is modified by two different iterations of the loop;
- Some loops, like the integral approximation, use a single variable to collect results from all the iterations. If we want to use such methods, we need to come up with a special approach.

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SAXPY: A Basic Linear Algebra Operation

Our simple example starts with an **n**-vector called **x** and adds to it the vector **y**, multiplied by the scalar **s**:

$$\vec{x} \leftarrow \vec{x} + s \cdot \vec{y};$$

We assume that the values of **x** and **y** are set by some formula, about which we don't really care that much.

If we have multiple processors, then, all we are asking is that the processors divide up the range of vector indices, and then carry out the arithmetic for their part of the work.

```
int main ( )
{
  int i, n = 1000;
  double s = 1.23, x[1000], y[1000];

  for ( i = 0; i < n; i++ )
  {
    x[i] = ( double ) ( ( i + 1 ) % 17 );
    y[i] = ( double ) ( ( i + 1 ) % 31 );
  }



  for ( i = 0; i < n; i++ )
  {
    x[i] = x[i] + s * y[i];
  }
  return 0;
}
```

SAXPY: C Example (After)

```c
# include <omp.h>

int main ( )
{
  int i, n = 1000;
  double s = 1.23, x[1000], y[1000];

  for ( i = 0; i < n; i++ )
  {
    x[i] = ( double ) ( ( i + 1 ) % 17 );
    y[i] = ( double ) ( ( i + 1 ) % 31 );
  }

# pragma omp parallel

# pragma omp for
  for ( i = 0; i < n; i++ )
  {
    x[i] = x[i] + s * y[i];
  }
  return 0;
}
```

```
program main


  integer, parameter :: n = 1000

  integer i
  double precision :: s = 1.23
  double precision x(n), y(n)

  do i = 1, n
    x(i) = mod ( i, 17 )
    y(i) = mod ( i, 31 )
  end do



  do i = 1, n
    x(i) = x(i) + s * y(i)
  end do



  stop
end
```

SAXPY: F90 Example (After)

```
program main

  use omp_lib

  integer, parameter :: n = 1000

  integer i
  double precision :: s = 1.23
  double precision x(n), y(n)

  do i = 1, n
    x(i) = mod ( i, 17 )
    y(i) = mod ( i, 31 )
  end do

!$omp parallel

!$omp do
  do i = 1, n
    x(i) = x(i) + s * y(i)
  end do
!$omp end do

!$omp end parallel

  stop
end
```

SAXPY: The Changes

Notice that our OpenMP program looks exactly the same as our original program, except for the OpenMP directives.

These directives, in fact, look like comments to the compiler. In other words, if you simply compile the OpenMP program in the usual way, it will compile and run just as it did before.

You might think this is not a big accomplishment, but what it means is that, as you modify your program to create an OpenMP version, you can always run the program in sequential mode as a check.

Moreover, we can work on our program one section at a time. There may be many loops in our program, but OpenMP will only parallelize the loops we select. So it's easy to experiment and to work in steps.

Now let's try to find out a little bit more about the directives that we added to the program.

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OpenMP includes a small number of functions and symbolic constants, which must be declared.

Therefore, a C or C++ program that uses OpenMP should usually have the following include statement at the beginning of the file:

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

Every Fortran77 subroutine or function that uses OpenMP should have the following include statement:

```
      include 'omp_lib.h'
```

A FORTRAN90 subroutine or function using OpenMP can use the Fortran77 include statement, or reference the OpenMP module:

```
  use omp_lib
```

The C/C++ **parallel** directive begins a *parallel region*.

```
# pragma omp parallel
{
    do things in parallel here, if directed!
}
```

If curly brackets aren't used to form a block, then the parallel region is taken to be just the next block of code.

Typically, this parallel region will contain one or more **for** loops; these loops may be selected for parallel execution if the user indicates so.

The FORTRAN **parallel** directive begins a *parallel region*.

```
!$omp parallel
  do things in parallel here, if directed!
!$omp end parallel
```

The parallel region must be closed with an **end parallel** directive.

Typically, this parallel region will contain one or more **do** loops; these loops may be selected for parallel execution if the user indicates so.

DIRECT: Variables in the Parallel Region

All variables inside the parallel region will be classified as:

- **shared**, leave this in shared memory;
- **private**, each processor needs a private copy;
- **reduction**, special treatment.

Except for loop indices, all variables are assumed to be shared.

It's important that no variable be misclassified. To override the defaults, or to declare some variables explicitly, add the **private()** or **shared()** clause to your **parallel** directive.

Our example doesn't need to specify this information, so we'll come back to discuss this in a later example!

The **private()** and **shared()** clauses modify the **parallel** directive.

In C, this might appear like this:

```
# pragma omp parallel \
    private ( i ) \
    shared ( n, s, x, y )
```
or:
```
# pragma omp parallel private ( i ) shared ( n, s, x, y )
```

while in FORTRAN, the same information would look like this:

```
!$omp parallel &
!$omp    private ( i ) &
!$omp    shared ( n, s, x, y )
```
or:
```
!$omp parallel private ( i ) shared ( n, s, x, y )
```

DIRECT: Parallel Loops are Marked by Directives

Inside the parallel region there should be one or more loops.

By default, a loop in the parallel region will **not** be executed in parallel. You explicitly indicate which loops are parallel by providing the appropriate directive.

In C/C++, this is the **for** directive, and in FORTRAN, the **do** directive.

If a parallel region has five loops, you can mark any or all of them to run in parallel.

```
# pragma omp for
for ( i = 0; i < m; i++ )
{
    ...xxx...
 }
# pragma omp for
for ( i = 0; i < 1000; i++ )
{
    ...xxx...
 }
```

DIRECT: Nested Loops

However, a nested loop should only be marked **once.**

```
# pragma omp for
for ( i = 0; i < m; i++ )
{
    for ( j = 0; j < n; j++ )
    {
      ...xxx...
    }
 }


!$ omp do
do i = 1, m
  do j = 1, n
     ...xxx...
  end do
 end do
!$ omp end do
```

```
# pragma omp for
  for ( i = 0; i < n; i++ )
  {
    x[i] = x[i] + s * y[i];
  }

!$omp do
  do i = 1, n
    x(i) = x(i) + s * y(i)
  end do
!$omp end do
```

DIRECT: SAXPY Example in C

```
# include <omp.h>          <-- OpenMP Definitions

int main ( )
{
  int i, n = 1000;
  double s = 1.23, x[1000], y[1000];

  for ( i = 0; i < n; i++ )
  {
    x[i] = ( double ) ( ( i + 1 ) % 17 );
    y[i] = ( double ) ( ( i + 1 ) % 31 );
  }

# pragma omp parallel   <-- Begin parallel region
{
# pragma omp for             <-- Next loop is parallel
  for ( i = 0; i < n; i++ )
  {
    x[i] = x[i] + s * y[i];
  }
}
  return 0;
}
```

DIRECT: SAXPY Example in F90

```
program main

  use omp_lib                  <-- OpenMP Definitions

  integer, parameter :: n = 1000

  integer i
  double precision :: s = 1.23
  double precision x(n), y(n)

  do i = 1, n
    x(i) = mod ( i, 17 )
    y(i) = mod ( i, 31 )
  end do

!$omp parallel                 <-- Begin parallel region

!$omp do                       <-- Next loop is parallel
  do i = 1, n
    x(i) = x(i) + s * y(i)
  end do
!$omp end do                   <-- End of that loop

!$omp end parallel             <-- End of parallel region

  stop
end
```

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Because the OpenMP directives look like comments, your program will run sequentially if you compile it the usual way:

- **gcc myprog.c**
- **g++ myprog.cpp**
- **gfortran myprog.f**
- **gfortran myprog.f90**

The compile statement results in the creation of what is called the *executable* program - that is, it's ready to run.

By default, the executable is stored in a file with the peculiar name of *a.out*. To avoid confusion, this should be renamed to something sensible:

```
mv a.out myprog
```

The executable program can be run by typing its name, preceding by ./, which is actually shorthand for the current directory:

```
./myprog
```

RUN: OpenMP Directives Can Be Activated

You build a parallel version of your program by telling the compiler to activate the OpenMP directives.

GNU compilers need the **fopenmp** switch:

- **gcc -fopenmp myprog.c**
- **g++ -fopenmp myprog.cpp**
- **gfortran -fopenmp myprog.f**
- **gfortran -fopenmp myprog.f90**

Again, we will want to rename the executable, but this time, perhaps we should choose a different name:

```
mv a.out myprog_omp
```

RUN: Intel Compiler Switches

Intel C compilers need the **openmp** and **parallel** switches:

- **icc myprog.c -openmp -parallel**
- **icpc myprog.cpp -openmp -parallel**

Intel Fortran compilers also require the **fpp** switch:

- **ifort myprog.f -openmp -parallel -fpp**
- **ifort myprog.f90 -openmp -parallel -fpp**

When we run a program whose OpenMP directives have been activated, then OpenMP looks for the value of an environment variable called **OMP_NUM_THREADS** to determine the default number of threads.

You can query this value by typing:

```
echo $OMP_NUM_THREADS
```

A blank value is the same as 1. Usually, however, it's set to a sensible value, such as the number of cores available.

You can reset this environment variable using a command like:

```
export OMP_NUM_THREADS=4   <-- (No spaces around equal sign!)
```

and this new value will hold for any programs you run interactively.

RUN: Trying Different Numbers of THreads

Changing the number of threads is easy, and can be done at run time.
Suppose our executable program is called **myprog_omp**.

We could experiment with 1, 2, 4 and 8 threads by:

```
export OMP_NUM_THREADS=1
./myprog_omp
export OMP_NUM_THREADS=2
./myprog_omp
export OMP_NUM_THREADS=4
./myprog_omp
export OMP_NUM_THREADS=8
./myprog_omp
```

We know a little bit about how to convert a sequential program into an OpenMP parallel program (include file, parallel and do/for directives).

We know how to compile;

We know how to run;

We know how to set the number of threads, which make the program "more parallel".

But the point of parallel programming is to run faster. Is there a good way to do timings?

Shared Memory Programming with OpenMP

1. Serial Programs Can't Accelerate
2. Parallel Algorithms Are Available
3. The Parallel Loop
4. SAXPY Example: Vector Addition
5. Basic OpenMP Directives
6. Compiling, Linking, Running
7. **Timing and Other Functions**
8. Private and Shared Variables
9. Reduction Operations
10. Using Random Numbers
11. The HPC Cluster

Parallel programming does the same amount of work as sequential programming, and in fact, it might even do more. So it's not a good idea, when making comparisons, to measure the amount of work. Nor is it a good idea to measure the total CPU time (how much time was used by all the processors), because this misses the point.

There are two important quantities in parallel programming:

- the **elapsed wall clock time** - how long did you wait for a result?
- the **relative speedup**, that is the wall clock time using 1 processor divided by the wall clock time using p processors.

TIME: Measuring Wall Clock Time

There are also several important things to keep in mind when measuring performance:

- parallelizing one big thing is much better than parallelizing many small things;
- some programs run too quickly, or work on too little data, to be worth parallelizing;
- if you let your problem get big enough, it will suddenly slow down drastically when it reaches the memory limit.

OpenMP includes the following functions:

- **omp_set_num_threads (t)** : set the number of threads;
- **t = omp_get_num_threads ( )** : get the number of threads;
- **p = omp_get_num_procs ( )** : how many processors are there?
- **id = omp_get_thread_num ( )** : which thread is executing?
- **wtime = omp_get_wtime()** : how much time has elapsed?

We may come back to review some of the other functions, but for now, I hope you can see which one we want to use!

TIME: How Much Time Has Passed?

The function **omp_get_wtime()** returns, as a double precision real number, the current reading of the wall clock.

You read the wall clock time before and after a parallel computation. The difference gives you the measured time.

```
wtime = omp_get_wtime ( );
# pragma omp parallel
# pragma omp for
for ( i = 0; i < n; i++ )
{
  Do a lot of work in parallel;
}
wtime = omp_get_wtime ( ) - wtime;
cout << "Work took " << wtime << " seconds.\n";
```

```c
# include <omp.h>

int main ( )
{
  int i, n = 1000;
  double wtime, s = 1.23, x[1000], y[1000];

  wtime = omp_get_wtime ( );   <-- Start the clock

# pragma omp parallel
  {   <-- parallel region begins with this bracket...
# pragma omp for
    for ( i = 0; i < n; i++ )
    {
      x[i] = ( double ) ( ( i + 1 ) % 17 );
      y[i] = ( double ) ( ( i + 1 ) % 31 );
    }

# pragma omp for
    for ( i = 0; i < n; i++ )
    {
      x[i] = x[i] + s * y[i];
    }
  }   <-- and parallel region ends with this bracket.
  wtime = omp_get_wtime ( ) - wtime;   <-- Stop the clock
  printf ( "%g seconds.\n", wtime );
  return 0;
}
```

```fortran
program main

  use omp_lib

  integer, parameter :: n = 1000

  integer i
  double precision :: s = 1.23
  double precision wtime, x(n), y(n)

  wtime = omp_get_wtime ( );   <-- Start the clock.

!$omp parallel

!$omp do
  do i = 1, n
    x(i) = mod ( i, 17 )
    y(i) = mod ( i, 31 )
  end do
!$omp end do

!$omp do
  do i = 1, n
    x(i) = x(i) + s * y(i)
  end do
!$omp end do

!$omp end parallel
  wtime = omp_get_wtime ( ) - wtime   <-- Stop the clock.
  write ( *, * ) wtime, ' seconds.'
  stop
end
```

TIME: Run SAXPY with Timings

Now our example program is tiny (as far as the number of instructions) and also as far as the amount of work.

So to start with, let's increase the value of **n** to 100,000.

Secondly, we are going to insert the timing calls (this should involve four new lines of code.)

I will recompile the program with OpenMP enabled, and run with 1, 2, 4, 8 and 16 threads.

If I plot the **time**, I am likely to get a hyperbola. If I plot the speedup, that is, **p**-processor time divided by the 1-processor time, I should get a diagonal line (if things are going well.). Lines that are diagonal (or not) are much easier to understand and judge than hyperbolas!
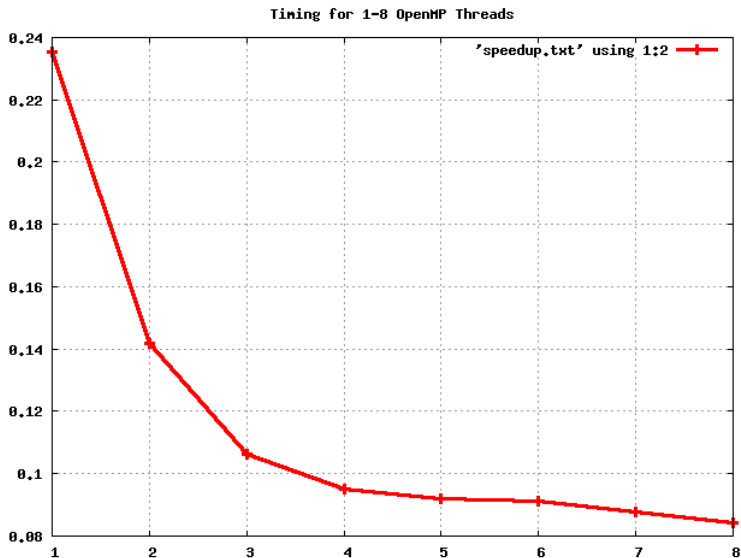
```
gnuplot
  set term png

  set output 'timing1.png'
  set style data linespoints
  set title "Timing for 1-8 OpenMP Threads"
  set grid
  plot 'speedup.txt' using 1:2 lw 3

  set output 'timing2.png'
  set style data linespoints
  set title "Timing for 1-8 OpenMP Threads"
  set grid
  set yrange [0:*]                          <-- Important!
  plot 'speedup.txt' using 1:2 lw 3

  quit
```
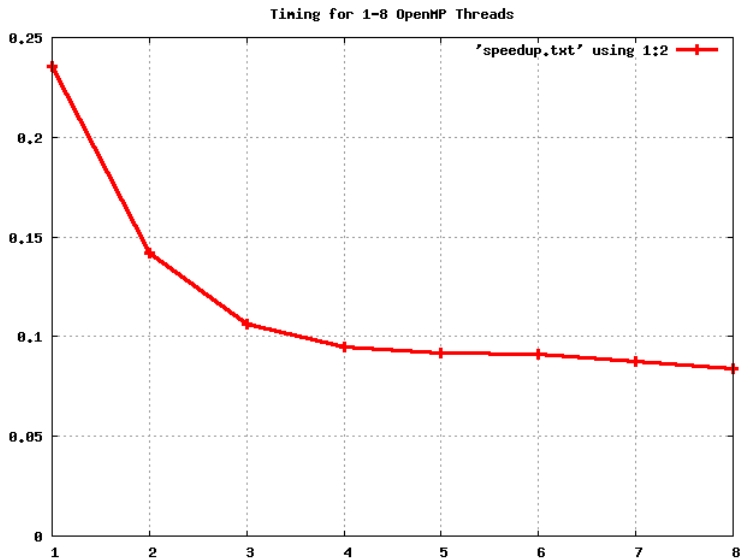
TIME: Time Plot (Deceptive)

Timing for 1-8 OpenMP Threads
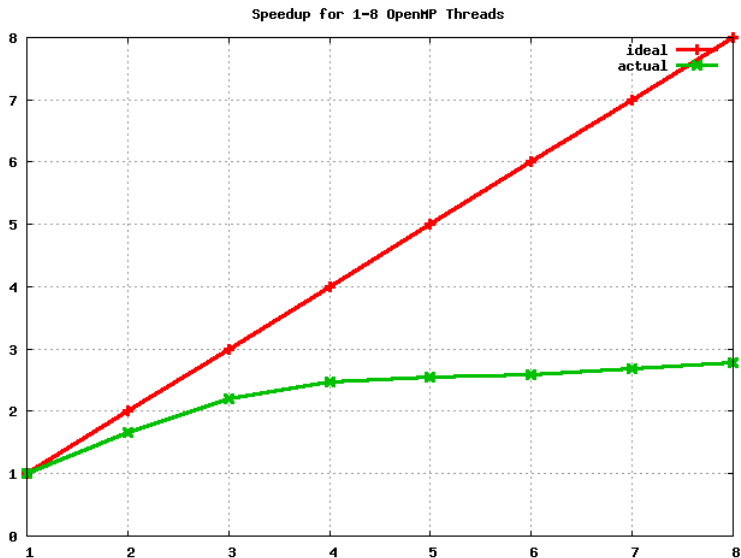
```
gnuplot
  set term png

  set output 'speedup.png'
  set style data linespoints
  set title "Speedup for 1-8 OpenMP Threads"
  set grid
  plot 'speedup.txt' using 1:1 title 'ideal' lw 3, \
       'speedup.txt' using 1:3 title 'actual' lw 3
  quit
```

Speedup for 1-8 OpenMP Threads

# Shared Memory Programming with OpenMP

PRIV: Lambert's W Function

Lambert's W function is the solution of the equation

$$w(x)e^{w(x)} = x$$

It's might not be obvious why this function needed to be invented, but there was a reason. It's really not obvious how to evaluate the function, but there is an algorithm. As you might expect, $w(x)$ is more difficult to compute than a polynomial or the sine function, but these complications are typical of what you will encounter in scientific computing. And they point out some problems that OpenMP will have to work around!
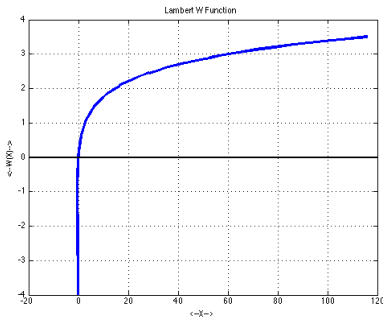
PRIV: Code to Compute W

```
for ( i = 0; i < 8; i++ )
{
  x = x_vec[i];           <-- x_vec contains test values.
  w = x + log ( x );      <-- Initial guess for w(x).

  it = 0;

  while ( 1 )
  {
    if ( 100 < it )
    {
      break;
    }

    if ( fabs ( ( x - w * exp ( w ) ) ) <
      tol * fabs ( ( w + 1.0 ) * exp ( w ) ) )
    {
      break;
    }
    a = w * exp ( w ) - x;
    b = ( w + 1.0 ) * exp ( w )
      - ( w + 2.0 ) * ( w * exp ( w ) - x ) / ( 2.0 * w + 2.0 );
    w = w - a / b;
    it = it + 1;
  }
  printf ( " %8.4f  %3d  %14g  %14g  %8.2e\n",
    x, it, w, w_vec[i], fabs ( w - w_vec[i] ) );   <-- Compare with exact.
}
```

PRIV: Lambert's W Function

We want to compute a table of 100,000 values for $w(x)$ over the range $1 \leq x \leq 100$. We'd like to use OpenMP to do so.

Do you see some real problems here? This computation is much messier than the "saxpy" example. In that example, the only variables that appeared on the left hand side were vector entries, indexed by the loop index. So there was no possibility of a conflict. Each loop iteration was working with completely distinct data.

Here, however, notice the variables **x, w, it, a, b** which all appear on the left hand side of equations inside the loop. These are all potential conflicts.

We presumably will fix the problem with **x** and **w** by storing them in arrays for our table. But how do we deal with **it, a, b**? Remember, if these variables each represent a single shared location in memory, then all the processors can be putting and reading stuff from the same location, which will cause total confusion!

PRIV: Code to Compute W

We are used to the loop index **i** being "private"; each process has its own copy. But now the variables **a, b, it** must also be stored this way.

```
# pragma omp parallel shared ( n, tol, w, x ) private ( a, b, i, it )
{
# pragma omp for
  for ( i = 0; i < n; i++ )
  {
    x[i] = ( ( n - i ) * 1.0 + i * 100.0 ) / n;
    w[i] = x[i] + log ( x[i] );

    it = 0;

    while ( 1 )
    {
      if ( 100 < it )
      {
        break;
      }

      if ( fabs ( ( x[i] - w[i] * exp ( w[i] ) ) ) <
        tol * fabs ( ( w[i] + 1.0 ) * exp ( w[i] ) ) )
      {
        break;
      }
      a = w[i] * exp ( w[i] ) - x[i];
      b = ( w[i] + 1.0 ) * exp ( w[i] )
        - ( w[i] + 2.0 ) * ( w[i] * exp ( w[i] ) - x[i] ) / ( 2.0 * w[i] + 2.0 );
      w[i] = w[i] - a / b;
      it = it + 1;
    }
  }
}
```

The very name "shared memory" suggests that the threads share one set of data that they can all "touch".

By default, OpenMP assumes that all variables are to be shared – with the exception of the loop index in the **do** or **for** statement.

It's obvious why each thread will need its own copy of the loop index. Even a compiler can see that!

However, some other variables may need to be treated specially when running in parallel. In that case, you must explicitly tell the compiler to set these aside as **private** variables.

Usually, such variables are temporary or convenience variables, whose values are not needed before or after the loop is executed.

PRIV: Private/Shared

What variables here are private?

Note that **pfun** is the name of a user function.

```
do i = 1, n
  do j = 1, n
    d = 0.0
    do k = 1, 3
      dif(k) = coord(k,i) - coord(k,j)
      d = d + dif(k) * dif(k)
    end do
    do k = 1, 3
      f(k,i) = f(k,i) - dif(k) * pfun ( d ) / d
    end do
  end do
end do
```

I've had to cut this example down a bit. So let me point out that **coord** and **f** are big arrays of spatial coordinates and forces, and that **f** has been initialized already.

The variable **n** is counting particles, and where you see a 3, that's because we're in 3-dimensional space.

The mysterious **pfun** is a function that evaluates a factor that will modify the force.

List all the variables in this loop, and try to determine if they are **shared** or **private**.

Which variables are already shared or private **by default**?

```
do i = 1, n              <-- I?   N?
  do j = 1, n            <-- J?
    d = 0.0              <-- D?
    do k = 1, 3          <-- K
      dif(k) = coord(k,i) - coord(k,j)  <-- DIF?
      d = d + dif(k) * dif(k)              -- COORD?
    end do
    do k = 1, 3
      f(k,i) = f(k,i) - dif(k) * pfun ( d ) / d
    end do               <-- F?, PFUN?
  end do
end do
```

PRIV: Private/Shared

```
!$omp parallel private ( i, j, k, d, dif ) &
!$omp shared ( n, coord, f )

  !$ omp do
  do i = 1, n
    do j = 1, n
      d = 0.0
      do k = 1, 3
        dif(k) = coord(k,i) - coord(k,j)
        d = d + dif(k) * dif(k)
      end do
      do k = 1, 3
        f(k,i) = f(k,i) - dif(k) * pfun ( d ) / d
      end do
    end do
  end do
  !$ omp end do

!$omp end parallel
```

PRIV: The SAXPY Example

Remember the SAXPY example?

We didn't specify any **shared()** or **private()** information there, but the programs compiled, ran correctly, and ran faster, under OpenMP. Are there rules for when we have to specify this information?

Indeed. By default, OpenMP will assume that the index of any loop marked with a **for** or **do** directive is **private** (which it must be). In FORTRAN, it will also assume that the indices of any loops nested inside such a loop are also private - but in C/C++, it does not make this assumption.

By default, all other variables are assume to be **shared**. Therefore, although it can be useful to indicate the status of all variables, you really only have to indicate any non-loop index variables that are private, and any reduction variables.

Just for review, here is the SAXPY example, with the extra clauses that it turned out we didn't actually need.

PRIV: The SAXPY Example

```
# include <omp.h>

int main ( )
{
  int i, n = 1000;
  double s = 1.23, x[1000], y[1000];

  for ( i = 0; i < n; i++ )
  {
    x[i] = ( double ) ( ( i + 1 ) % 17 );
    y[i] = ( double ) ( ( i + 1 ) % 31 );
  }

# pragma omp parallel \
    private ( i ) \
    shared ( n, s, x, y )

# pragma omp for
  for ( i = 0; i < n; i++ )
  {
    x[i] = x[i] + s * y[i];
  }
  return 0;
}
```

```
program main

  use omp_lib

  integer, parameter :: n = 1000

  integer i
  double precision :: s = 1.23
  double precision x(n), y(n)

  do i = 1, n
    x(i) = mod ( i, 17 )
    y(i) = mod ( i, 31 )
  end do

!$omp parallel &
!$omp   private ( i ) &
!$omp   shared ( n, s, x, y )

!$omp do
  do i = 1, n
    x(i) = x(i) + s * y(i)
  end do
!$omp end do

!$omp end parallel

  stop
end
```

Shared Memory Programming with OpenMP

Recall the Lambert function $w(x)$ and suppose that we wish to estimate the integral of this function over the range $1 \leq x \leq 100$.

For simplicity, let's also assume that we have rewritten the computation so that there is now a C or FORTRAN function called **w(x)** which carries out the evaluation of the Lambert function for any value of x.

We'll use a simple approximation that divides $[1, 100]$ into n subintervals $[a, b]$, and sums the products of $w(x)$ at the midpoints multiplied by the length of the subintervals.

$$\int_1^{100} w(x)dx \approx \sum_{i=1}^n w\left(\frac{a_i + b_i}{2}\right)(b_i - a_i)$$

REDUCTION: Is Q Private? Shared?

What kind of variable is Q? It can't be shared, because every process is trying to update it. It can't be private, because it has a value before the loop, and after the loop.

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

int main ( );
double w ( double x );

int main ( )
{
  double a;
  double b;
  int i;
  int n = 1000;
  double q;
  double x;

  q = 0.0;
  for ( i = 0; i < n; i++ )
  {
    a = ( ( n - i     ) * 1.0 + ( i     ) * 100.0 ) / n;
    b = ( ( n - i - 1 ) * 1.0 + ( i + 1 ) * 100.0 ) / n;
    x = 0.5 * ( a + b );
    q = q + ( b - a ) * w ( x );
  }

  printf ( "Q = %g\n", q );

  return 0;
}
```

REDUCTION: Q is a Reduction Variable

Q has an intermediate status between private and shared, called a **reduction variable**, because a single result is formed from contributions of all the processes. To indicate such a variable, a reduction clause must be added to the **for** or **do** loop where the variable is computed.

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

int main ( );
double w ( double x );

int main ( )
{
  double a;
  double b;
  int i;
  int n = 1000;
  double q;
  double x;

  q = 0.0;
# pragma omp parallel shared ( n ) private ( a, b, i, x )

# pragma for reduction ( + : q )
  for ( i = 0; i < n; i++ )
  {
    a = 1.0 + ( 100.0 - 1.0 ) * ( double ) ( i     ) / n;
    b = 1.0 + ( 100.0 - 1.0 ) * ( double ) ( i + 1 ) / n;
    x = 0.5 * ( a + b );
    q = q + ( b - a ) * w ( x );
  }

  printf ( "Q = %g\n", q );

  return 0;
}
```

A reduction operation occurs when you

- sum a set of numbers;
- compute the dot product of two vectors;
- compute the product of a set of numbers;
- find the maximum of a set of numbers.

The OpenMP **reduction** clause is used to indicate variables that are used to store such computations.

REDUCTION: The Reduction clause

The **reduction** clause modifies a **for** or **do** directive.

Reduction clause examples include:

- **# omp for reduction (+ : xdoty)** ;
- **# omp for reduction (+ : sum1, sum2, sum3)** :
  several sums in one loop;
- **# omp for reduction (* : factorial)**: a product;
- **!$omp do reduction (max : pivot)** :
  maximum or minimum value (Fortran only);)

If a variable occurs in a reduction clause, it cannot also occur in a private or shared clause for that parallel region!

Within a parallel region, a variable is private, shared or reduction.

REDUCTION: Norm Example

A dot product is another example of reduction:

```
# pragma omp parallel private ( i ) shared ( n, x, y )
  dot = 0.0;
  # pragma for reduction ( + : dot )
  for ( i = 0; i < n; i++ )
  {
    dot = dot + x[i] * y[i];
  }
```

Shared Memory Programming with OpenMP

Now suppose that we wish to approximate the integral of the Lambert W function from 1 to 100, but instead of using a quadrature rule, we want to use a Monte Carlo approach.

For this simple problem, the advantages of a Monte Carlo approach aren't obvious, but for problems with complicated geometries, or probabilistic components, or simulations, sometimes this is the only way to do computations.

Our approximation selects n sample points x_i from $[1, 100]$ at random, and computes the estimate as

$$\int_1^{100} w(x)dx \approx \frac{100 - 1}{n} \sum_{i=1}^{n} w(x_i)$$

REDUCTION: The Sequential Code

Each time we call **drand()**, we get a new sample point. We also get a new value of **seed**, which is actually what controls the computation.

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

int main ( );
double w ( double x );
double drand ( int *seed );

int main ( )
{
  double a;
  double b;
  int i;
  int n = 1000;
  double q;
  int seed = 123456789;
  double u;
  double x;

  q = 0.0;
  for ( i = 0; i < n; i++ )
  {
    u = drand ( seed );            <-- some random number generator.
    x = 1.0 + ( 100.0 - 1.0 ) * u;
    q = q + w ( x );
  }
  q = q * ( 100.0 - 1.0 ) / n;
  printf ( "Q = %g\n", q );

  return 0;
}
```

If we want this calculation to run in parallel, then we want each process to be able to call **drand()** and get a distinct set of random numbers. That means each process needs a separate, distinct, private value of **seed**. Let's call this quantity **my_seed**.

A simple idea would be to set

```
my_seed = seed + id
```

where **seed** is our original seed value and **id** is the identifier or index of the process. This will give us distinct seeds.

This idea will work, but look carefully at the details in the revised code:

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

int main ( );
double w ( double x );
double drand ( int *seed );

int main ( )
{
  double a;
  double b;
  int i;
  int my_seed;
  int n = 1000;
  double q;
  int seed = 123456789;
  double u;
  double x;

  q = 0.0;
# pragma omp parallel shared ( n, seed ) private ( i, my_seed, u, x )

  my_seed = seed + omp_thread_num ( );   <-- omp_thread_num() gets the id.

# pragma omp for reduction ( q : + )
  for ( i = 0; i < n; i++ )
  {
    u = drand ( my_seed );
    x = 1.0 + ( 100.0 - 1.0 ) * u;
    q = q + w ( x );
  }
  q = q * ( 100.0 - 1.0 ) / n;
  printf ( "Q = %g\n", q );

  return 0;
}
```

Shared Memory Programming with OpenMP

If you have a really big job, or lots of them, or you need a lot of parallel threads, you are not going to want to mess around on our lab system. Instead, you want to try to run your program on a cluster, such as the FSU HPC system.

The system we have access to for this class is a cluster, but since we are using OpenMP, we will only be using one "node" of that cluster. Each node has 32 cores, so that's the most parallelism we can get.

This is one important difference between OpenMP and MPI. For OpenMP to work, all the processors must share memory, which generally means they are on the same physical processor or chip. That means we are typically talking about cores on a multicore chip, and right now, 32, 48 and 64 core chips are available, but not much more. MPI, on the other hand, can run hundreds or thousands of parallel processes.

HPC: File Transfer with SFTP

If you plan to use the cluster, your program file, perhaps called *md.c*, is probably sitting on the lab machine, or your laptop. A copy of this file must be sent to the login node of the cluster. You do this using the **sftp** program.

```
sftp sc.hpc.fsu.edu
put md.c

quit        <-- (You can keep the connection and transfer other files.)
```

The command for bringing something from the HPC back to your local system is **get** instead of **put**.

You may find other file transfer programs that you prefer.

You need to log into the HPC. The standard way to do this is with the **ssh** command.

```
ssh sc.hpc.fsu.edu
Carry out your login session on the HPC
quit
```

One of the things you will definitely need to do is to recompile your program on the cluster. You can use the same Gnu compilers that are available on the lab machines:

- **gcc -fopenmp md.c**
- **g++ -fopenmp md.cpp**
- **gfortran -fopenmp md.f**
- **gfortran -fopenmp md.f90**

Now rename your executable program to something more memorable than "a.out".

```
mv a.out md
```

At this point, on the lab machines, we could run the program (and we might want to set the number of threads as well).

On the HPC, we are not supposed to run interactively. Instead, we prepare a script file for the run...which might be called *md_batch.sh*.

HPC: An HPC Batch Script

```bash
#!/bin/bash                    << Job uses BASH shell

#MOAB -N md                    << Job name is "MD"
#MOAB -q classroom             << Run job in this queue
#MOAB -l nodes=1:ppn=8         << Want 1 node, 8 processors.
#MOAB -l walltime=00:02:00     << Request 2 minutes of time.
#MOAB -j oe                    << Join output and error files.

cd $PBS_O_WORKDIR              << Move to directory

export OMP_NUM_THREADS=8       << Number of threads <= PPN
./md > output.txt              << Finally!
```

HPC: Running Your Job

Briefly, once you have a compiled version of **md** on the HPC, and your batch script file *md_batch.sh*, you "submit" the job with the command

```
msub md_batch.sh
```

and then you wait for the job to complete. You can check the job's program using the command

```
showq
```

and, the way this script was written, the interesting results will show up in the file *output.txt*.

We will go over the details of HPC job execution during the lab.