An Introduction to HPC and Scientific Computing

Lecture six: How to multi-task on CPUs using OpenMP.

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Overview

In this lecture we will learn about:

- The Basic Idea Behind Parallelism
- What OpenMP is
- How to divide work amongst threads
- How to synchronise threads
- How to go about parallelising a simple program with OpenMP

Parallelism – How to do we split up the work?

Scenario: The application takes too long to run!

Parallel processing can shorten the run-time:

- Parallelism in the workload (in algorithms and data) and
- Assign portions of the workload to different workers (processors)

Parallelism – How to do we split up the work?

Analogy:

Shorten the time it takes to build an entire row of houses by:

- dividing the work into parts that can be carried out in parallel and
- scheduling different (teams of) workers to work on these parts concurrently.

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Parallelism – How to do we split up the work?

Perfect (linear) scaling is the holy grail:

- execution time is inversely proportional with the number of processors
- by analogy: halve the time by using twice the workers
- in practice, scaling is not linear but can be close enough

Many ways to parallelise

- Consider the row of houses analogy
  - One could hire one man for each house
  - Or you could hire a brickie, a roofer, a plumber, an electrician, etc.
- The second obviously requires more communication between the workers
  - They have to coordinate their activities
  - Can’t put a roof on the house before you have built the walls
- But the second also doesn’t require every person to know everything about how to build a house
  - The required knowledge is split across many people
- Another possibility is a hybrid approach
  - Hire N brickies, N roofers, N plumbers, N electricians
  - And form N teams each of which works on 1/Nth of the houses

Parallelism – A maths example

- Consider adding two vectors:

$$a_i = b_i + c_i$$

- The operations required for each value of i are independent from any other value
- Thus for parallelism we require *independent operations*
- We can perform the operations *in any order*
- We also require *independent data*
  - Consider the apparently very similar $a_i = b_i + a_{i-1}$
  - Can't calculate a_i until has been a_{i-1} calculated

Parallelism – Communication and Synchronisation

- Now consider a dot product

$$a=\sum b_i \times c_i$$

- Could give a subset of the indices to each process and form the local contribution to a
- Sum together all the local contributions for final answer
- This last phase requires the processes or threads to work together
  - i.e. they are no longer totally independent
  - They need to communicate with each other
  - If one finishes before the others it will have to wait for them
- Very typical way parallelism work inside real codes
  - Independent iterations
  - Coordinate local results into global one

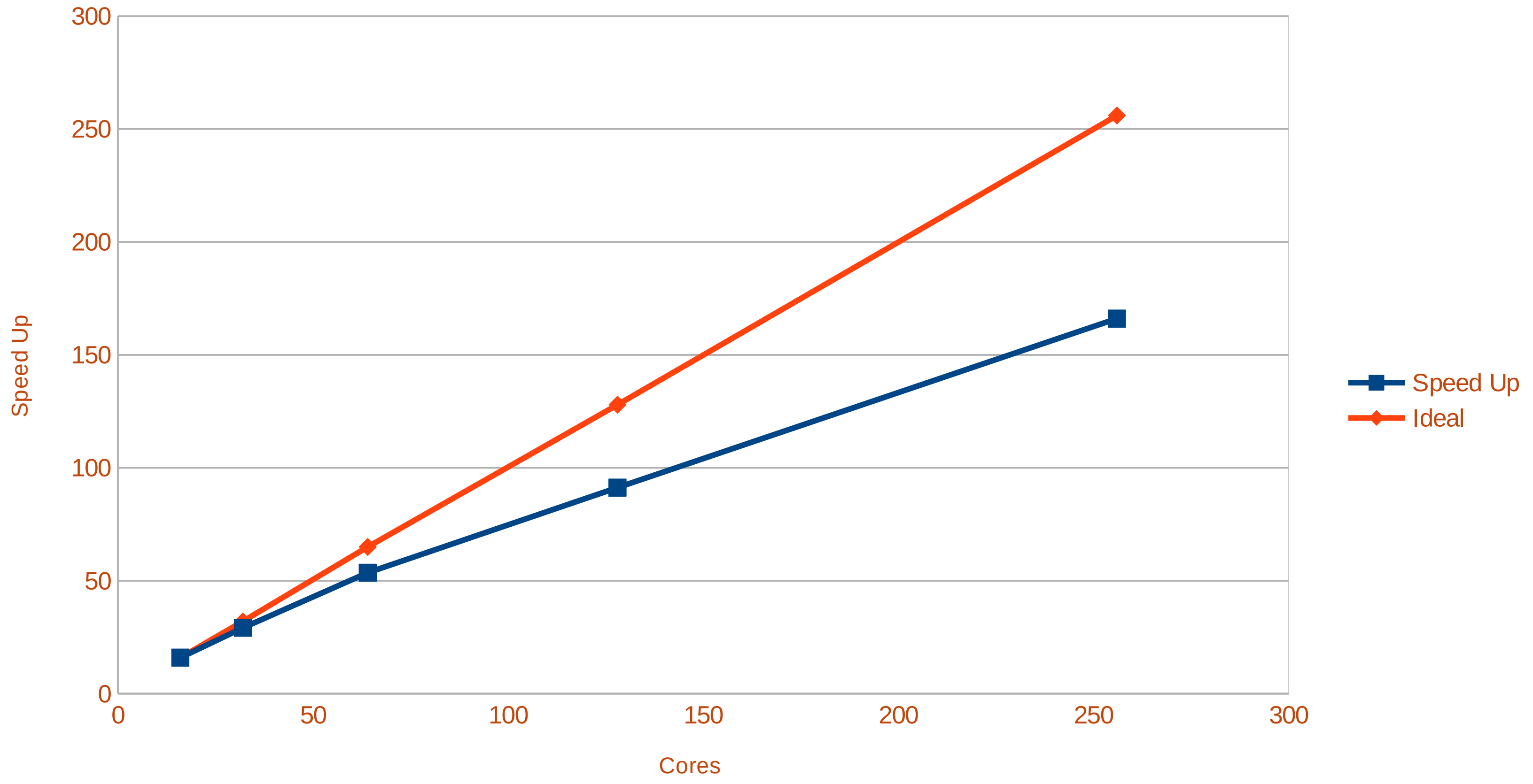
Parallel Scaling

- Consider the time to solution for our dot product.
- Vectors of order N
- P threads or processes
- The time to compute the local sum will be proportional to N/P
  - A **decreasing** function of the number of threads
- The time to synchronise and is more complicated
  - But it will be an **increasing** function of the number of threads
  - and independent of N
  - A deeper analysis shows a suitable model is log(P)
- Thus our model is:
- $t(P) = \alpha N/P + \beta \log(P)$

- Thus parallelism is most efficient
  - For large N
  - For small P
  - Too many threads may cause your program to slow down!

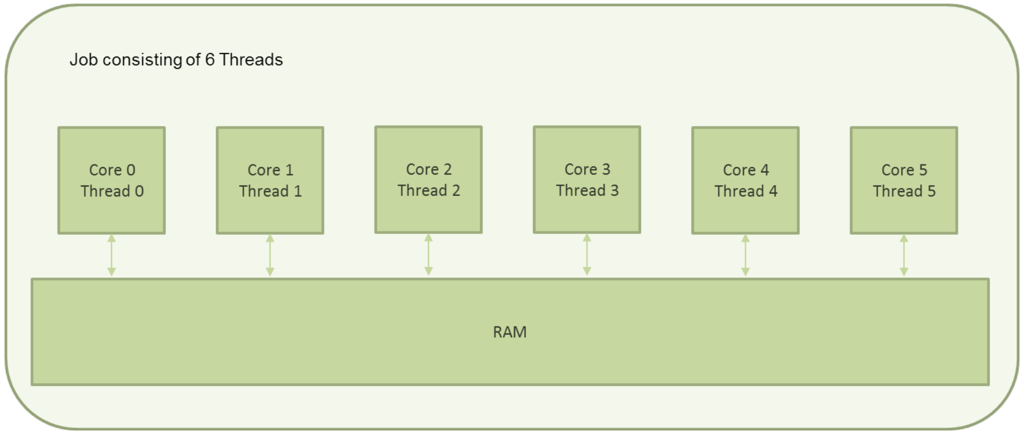
Measuring Scalability – Speed Up

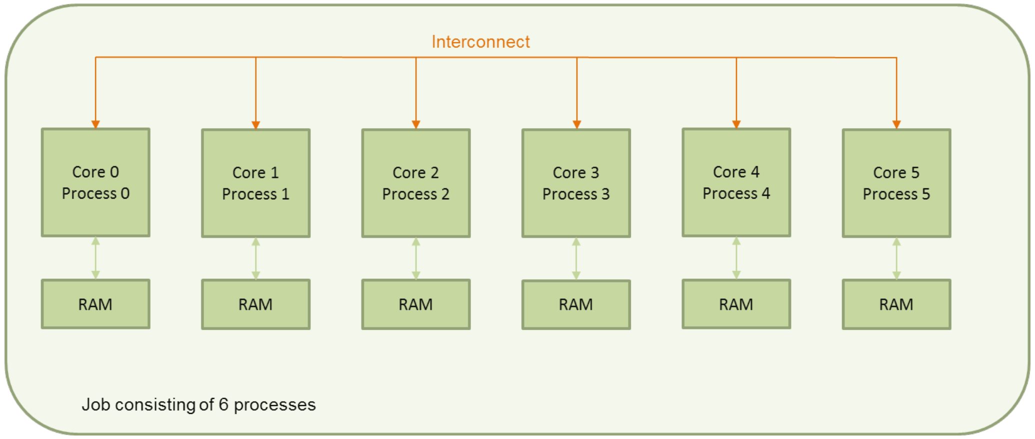
S = t(1)/t(P)



Parallelising Scientific Programs

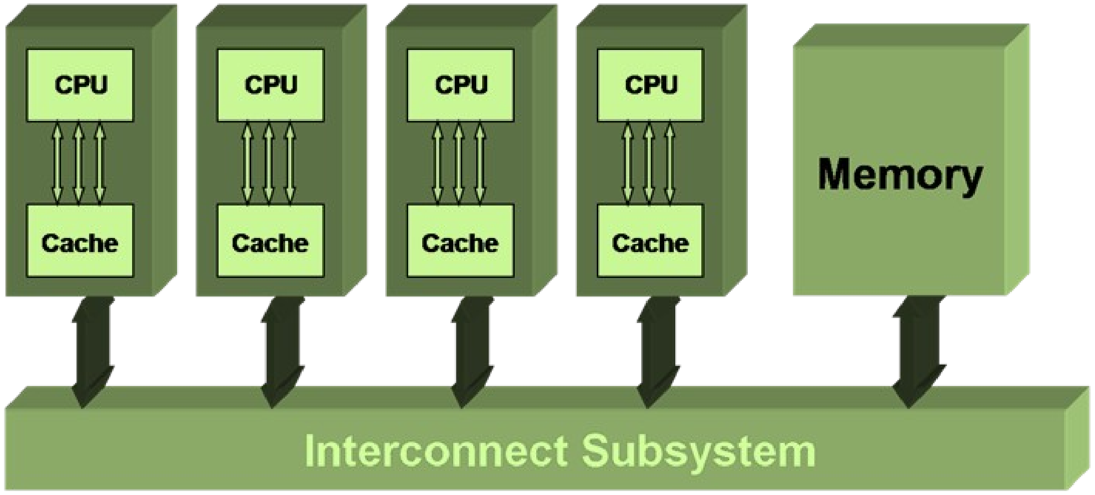
- **Shared memory programming**
  - Each core can see all of the memory
  - This is generally done via *OpenMP*
  - Generally limited to a single node
- **Distributed memory programming**
  - Each core can only see its memory
  - Have to use the interconnect
  - Can use an unlimited number of cores
  - Generally done via *MPI*
  - We don't cover it here but there are free ARC and ARCHER courses
- Hybrids of the two are possible and are used





Shared memory model

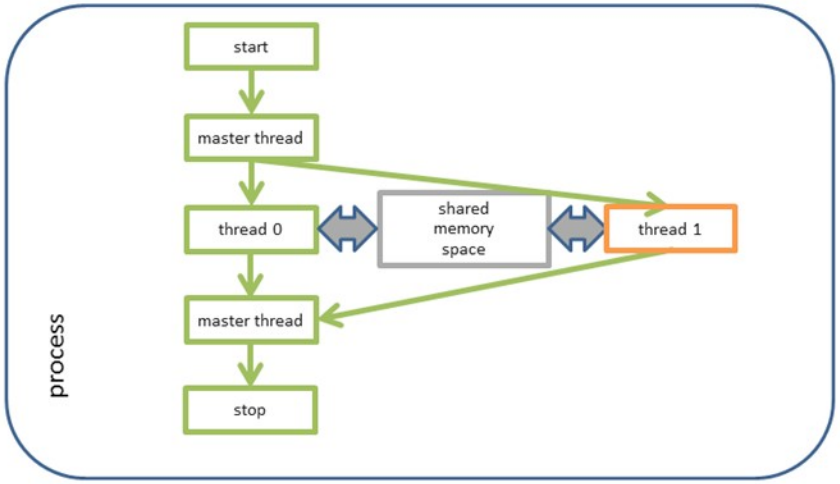
- Represents computing on a multi-processor architecture which links multiple (identical) CPUs to a single unified main memory;
- Uses a shared-memory programming model, with data that can be shared between processors
- Also called SMP, Symmetric Multi-Processor systems (for historical reasons)

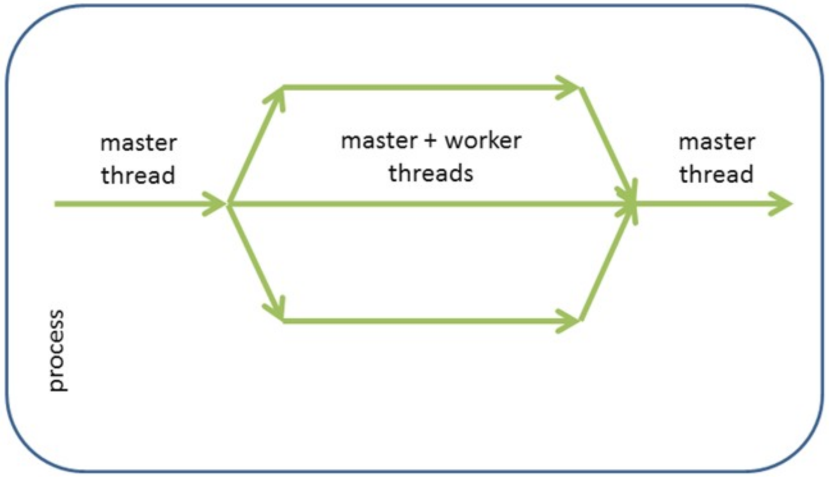


Processes and Threads

In shared-memory computing:

- An "application" is a single process – May be many threads
- The "process" is the "master thread"
- Master thread can spawn/destroy other threads (fork/join strategy)





Thread programming

- Explicit, low-level thread programming:
  - start several threads and explicitly tell each what to do
  - tedious, difficult to write and difficult to maintain
  - standards not universal (POSIX pthreads, Windows threads)
  - may be suited to task parallelism
- High-level programming using the OpenMP API:
  - instruct the compiler what can be done in parallel
  - let the compiler do the tedious stuff
  - threads are generated at runtime and scheduled by the OS
  - “standard” supported by a large number of compilers and operating systems
  - by design, suited to data parallelism

OpenMP Status

- OpenMP specification is not a formal standard.
- Agreement between industrial vendors and users

an agreement between industrial vendors and users and

- Version 2.5 (May 2005)
- Version 3.0 (May 2008)
- Version 3.1 (July 2011)
- Version 4.0 (July 2013)
  - Currently this is probably the most common implementation you will meet
- Vesion 5.0 (November 2018)

The OpenMP API

- OpenMP is
  - An API for portable and scalable shared memory programming
  - Defined and supported by a group of major vendors
  - Supported by most compilers for Fortran, C, C++
- OpenMP programming is
  - Standardised parallelism (fine-grained – loops, coarse-grain – regions)
  - If we’re careful, usable serial code
- OpenMP API components:
  - Compiler directives
  - Runtime library routines
  - Environment variables

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OpenMP “Hello World” in C

```
#include <stdio.h>
#include <stdlib.h>
#include "omp.h"
int main( void ) {
  int my_thread;
  /* Scope the variables and create the threads */
#pragma omp parallel default( none ) private( my_thread )
  {
    my_thread = omp_get_thread_num();
    printf( "Hello from thread %d\n", my_thread );
  }
  return EXIT_SUCCESS;
}
$ gcc -fopenmp -O -std=c89 -Wall -Wextra -pedantic hello.c -o hello
$ export OMP_NUM_THREADS=5
$ ./hello
Hello from thread 2
Hello from thread 4
Hello from thread 3
Hello from thread 0
Hello from thread 1
$ export OMP_NUM_THREADS=3
$ ./hello
Hello from thread 0
Hello from thread 2
Hello from thread 1
```

Running In Batch

```
#!/bin/bash

# set the number of nodes, which is always 1 for OpenMP codes
#SBATCH --nodes=1

# set number of cores per node -- grab the whole node (why?)
#SBATCH --ntasks-per-node=16

# set max wallclock time
#SBATCH --time=00:10:00

# set name of job
#SBATCH --job-name hello

# Set up the software environment
module purge
module load intel-compilers

# set the number of threads we will use
export OMP_NUM_THREADS=5

# run the OpenMP program
./my_prog
```

A More Complex Example

```
#include <stdlib.h>
#define N 50
int main( void ) {
  double a[ N ], b[ N ], c[ N ];
  int i;
  for( i = 0; i < N; i++ ) {
    b[ i ] = ( (double) rand() ) / RAND_MAX;
    c[ i ] = ( (double) rand() ) / RAND_MAX;
  }
/* Scope the variables for the parallel region and create the threads */
#pragma omp parallel default( none ) shared( a, b, c ) private( i )
  {
  /* A work sharing directive */
#pragma omp for
    for( i = 0; i < N; i++ ) {
      a[ i ] = b[ i ] + c [ i ];
    }
  }
  return EXIT_SUCCESS;
}
```

Scoping and Work Sharing

- So there are two main steps

1. Create the threads with a parallel directive and at that point “scope” the variables.
   - **`default none`** forces you to scope all the variables – USE THIS.
   - Variables can be one of
     - **`Shared`** – each thread can access the variable
     - **`Private`** – each thread has its own, unique copy
   - Note thread creation is *expensive.*
2. Once the threads are created you split the work up between them with a “work sharing” directive
   - Without a work sharing directive all threads will do exactly the same thing on the same data!
   - You can have as many work sharing constructs as you want within a parallel region
   - As thread creation is expensive exploit this – don’t create threads every time you need to share work, reuse the threads as many times as you can!

Problems Of Sharing Data

- Shared variables makes writing parallel code easy
- But what happens if multiple threads are trying to update (the same part of) a shared variable at the same time?
  - The result is not well defined!
  - And will probably vary from run to run!
- This is called a “race condition” and OpenMP does NOTHING by default to protect you from them
- So if multiple threads need to access a shared variable you will need to synchronize the threads somehow
- Rule of thumb: **If a shared variable is on the left hand side of an = sign it is time to stop and think about thread synchronisation**
- Race conditions are very easy to write and very hard to debug! Be careful!
  - To fully cover this subject we need to have discussed the OpenMP memory model, which is well beyond what we have time to cover here.

Synchronising Threads

- So how can we synchronise threads?
- OpenMP provides a number of mechanisms. Here we will cover
  - Barrier: a given thread can only proceed once all threads have reached the barrier
    - **Important**: By default there is an implicit barrier at the end of each worksharing construct
  - Critical region: Only 1 thread can be executing codes within a critical region. All other threads must wait at the start until the thread executing the region has exited it
  - Reduction: Combining multiple private values into a single shared value

Summary: OpenMP Directives So Far

parallel region constructs	blocks of code executed by all threads
	(most data shared by default)
		`#pragma omp parallel (C,C++)`
		`!$omp parallel (Fortran)`
		• shared data are visible to all threads
		• private data is local to thread and invisible outside, created on entry to scope, destroyed on exit

work-sharing constructs
(within a parallel region)
	parallel DO loops
	(distribute iterations over active threads)
		`#pragma omp for`
		`!$omp do`

critical section	protects action on the shared variables (only one thread at a time allowed)	`#pragma omp critical`
		`!$omp critical`

synchronisation	barriers	`#pragma omp barrier`
		`!$omp barrier`
		Threads can proceed only after all execute the barrier; implied at end of parallel region and loop (unless overridden by nowait)

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Bringing It Together – A More Complex Example

Task:
Orthogonalise 2 NORMALIZED vectors **x** and **y** on 2 threads.

There are several problems to watch out for.

Thread 1

```
z = 0
for i = 1 to n/2
   z = z + $x_i$ * $y_i$
end for
[ w = w + z ]
< barrier >
for i = 1 to n/2
 $y_i$ = $y_i$ - w * $x_i$
end for
```

de

```
1 to
z + x

1 to
- z
```

Thread 2

```
z = 0
for i = n/2+1 to n
   z = z + $x_i$ * $y_i$
end for
[ w = w + z ]
< barrier >
for i = n/2+1 to n
 $y_i$ = $y_i$ - w * $x_i$
end for
```

Problem
A thread may finish bef
other has updated **w**

This now works!

d **z** private

( )

OpenMP program example

Wait for all Threads (Barrier)

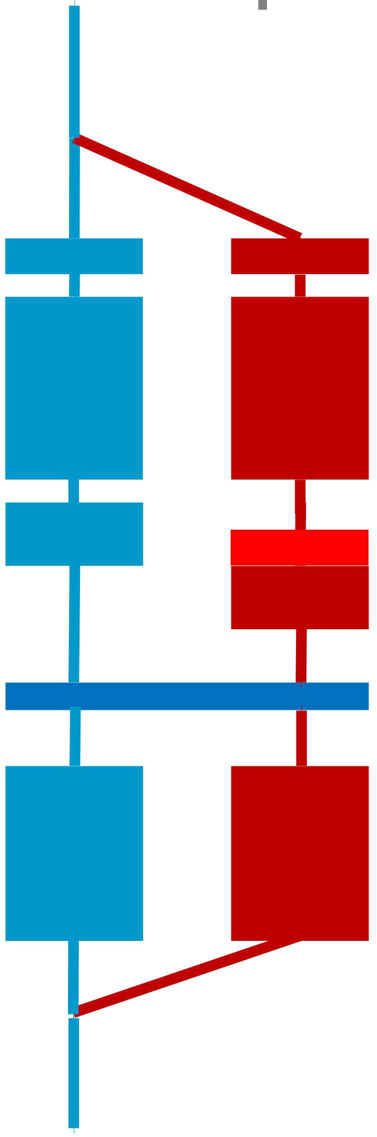
Fortran

```
w = 0.0

!OMP PARALLEL SHARED(n,w,x,y), &
!OMP          PRIVATE (i,z)
   z = 0.0
!OMP DO
   DO  i = 1, n
      z = z + x(i)*y(i)
   END DO
!OMP END DO
!OMP CRITICAL
   w = w + z
!OMP END CRITICAL
!OMP BARRIER
!OMP DO
DO  i = 1, n
   y(i) = y(i) – w*x(i)
END DO
!OMP END DO
!END PARALLEL
```

```
w = 0.0;

#pragma omp parallel shared (n,w,x,y) \
                 private(i,z)
{
   z = 0.0;
   #pragma omp for
   for (i=0; i<n; i++) {
      z = z + x[i]*y[i];
   }
   #pragma omp critical
   {
      w = w + z;
   }
   #pragma omp barrier
   #pragma omp for
   for (i=0; i<n; i++) {
      y(i) = y(i) – w*x(i);
   }
}
```

OpenMP program example

```
w = 0.0;

#pragma omp parallel shared (n,w,x,y) \
                     private(i,z)
{
   z = 0.0;

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

   #pragma omp critical
   {
      w = w + z;
   }

   #pragma omp barrier


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



Serial code

Spawn threads

Same code

Do loop
Each thread execute a different set of loop iterations

Only one thread at a time can execute this

Barrier
All threads synchronise

Do loop
Each thread execute a different set of loop iterations

Destroy threads

Serial code

Reductions

- In the above example we are adding up the value of the private z's across all threads to produce a shared value in w
  - So we are reducing many values to a single one via the + operator
- This is so common that reduction operations are supplied directly by OpenMP
- And if it is applicable reductions should be used rather than critical as it will be faster
  - Critical is all purpose, reduction is the precision tool
- Reductions can be applied to whole parallel regions or parallel do/for work share constructs
  - In the latter the reduction variable should be shared

```
w = 0.0;

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

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

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

Reduction Operators

- C/C++ Syntax:
  reduction (operator : list)
- Where
  - operator is one of: `+ * - & ^ | && || min max`

More OpenMP

- There is much more in OpenMP
  - More run time library routines
    - Inquiry, timers, locks …
  - More work share directives
    - Sections, work share, task …
  - More synchronisation directives
    - atomic, flush …
  - More environment variables than you can imagine
- We have only scratched the surface here
  - ARC courses
  - ARCHER Courses

OpenMP: best practices

- thread creation / destruction can be expensive, so threads should be re-used
  - maximise parallel loops (large loops has more opportunities for reuse of cached data)
  - avoid parallel regions in inner loops (aim for the coarsest data parallelism)
  - minimise the number of times parallel regions are entered/exited
  - example: parallel inner loop moved to parallel outer region

```
# initial
for (n=0;n<NN;n++)
  #pragma omp parallel private(m)
  #pragma omp for
  for (m=0;m<MM;m++)
```

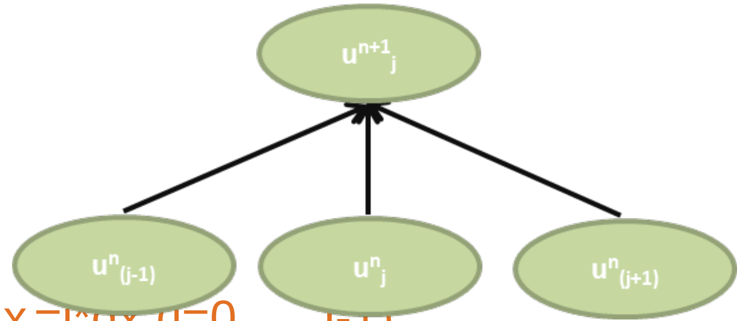
```
# improved
#pragma omp parallel private (n,m)
for (n=0;n<NN;n++)
  # pragma omp for
  for (m=0;m<MM;m++)
```

OpenMP: best practices

- Do not overuse synchronisation and explicit barriers
  - Remember every workshare construct by default has an implicit barrier on exit – this is normally enough
- Scope all your variables and use default(none)
- Think carefully about potential race conditions
  - Remember – a shared variable on the left hand side of an = should start alarm bells ringing

Example – The 1D Heat Equation

- The **physics**: find the time-varying distribution of temperature along a rod, starting from an initial distribution, given the fixed temperature at the ends
- The **maths** (an initial value problem): find u(x,t) on the interval [0, 1] given
  - u(0, t) = u(1, t) = 0 and u(0, x) = u_0(x).



- The **numerics** (a finite difference scheme):
  - sample the interval [0, 1] at equidistant points x_j=j*dx (j=0,…,J-1) and fixed time intervals t_n=n*dt, n>0 and find the values of all temperature samples u^n_j at the sample points
  - discretised equations give:

$$u^{(n+1)}_j = u^n_j + nu*(u^n_{(j+1)} - 2*u^n_j + u^n_{(j-1)})$$

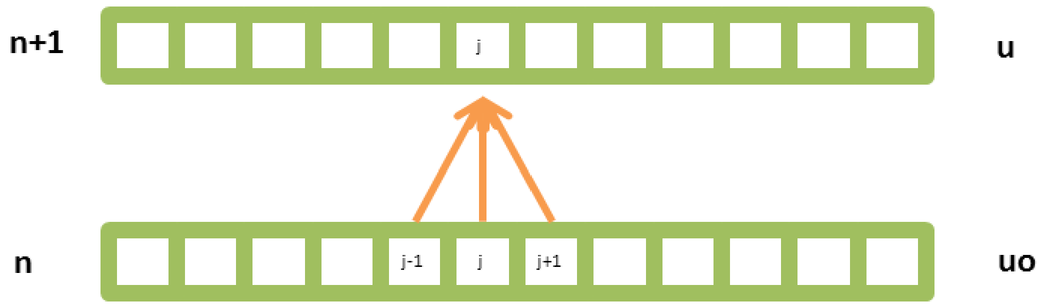
  - 4 point stencil

Example: 1D Heat Equation

- The core of the program is to use two vectors u and uo (u “old”).

At every time step,

- copy u into uo (not efficient but simple to understand)
- apply the finite difference scheme (the 4 point stencil)



- apply boundary conditions: $u_1=u_J=0$

Example – 1D Heat Equation

```
// boundary conditions
   u[0]   = 0.0; uo[0]   = 0.0;
   u[J-1] = 0.0; uo[J–1] = 0.0;

// time loop
  for (n=0; n<n_time_steps; n++) {

    // store solution
    for (j=1; j<J-1; j++) {
      uo[j] = u[j];
    }

    // finite difference scheme
    for (j=1; j<J-1; j++) {
      u[j] = uo[j] + nu*(uo[j-1]-2.0*uo[j]+uo[j+1]);
    }

}
```

Problem: 1D heat equation in Parallel – The Easy Way

```
// time loop
for (t=0; t<n_time_steps; t++) {
   // store solution



   for (j=1; j<n-1; j++) {
      uo[j] = u[j];
   }

   // finite difference scheme



   for (j=1; j<n-1; j++) {
      u[j] = uo[j] +
      nu*(uo[j-1]-2.0*uo[j]+uo[j+1]);
   }

}
```

```
// time loop
for (t=0; t<n_time_steps; t++) {
  // store solution
  #pragma omp parallel shared(n,u,uo,J) private(j)
  {
    #pragma omp for
    for (j=1; j<n-1; j++) {
      uo[j] = u[j];
    }
  }
  // finite difference scheme
  #pragma omp parallel shared(n,u,uo,nu,J) private(j)
  {
    #pragma omp for
    for (j=1; j<n-1; j++) {
      u[j] = uo[j] +
      nu*(uo[j-1]-2.0*uo[j]+uo[j+1]);
    }
  }
}
```

Problem: 1D Heat Equation in Parallel – The Better Way

```
// time loop
for (t=0; t<n_time_steps; t++) {
  // store solution
  #pragma omp parallel shared(n,u,uo,J) private(j)
  {
    #pragma omp for
    for (j=1; j<n-1; j++) {
      uo[j] = u[j];
    }
  }
  // finite difference scheme
  #pragma omp parallel shared(n,u,uo,nu,J) private(j)
  {
    #pragma omp for
    for (j=1; j<n-1; j++) {
      u[j] = uo[j] +
      nu*(uo[j-1]-2.0*uo[j]+uo[j+1]);
    }
  }
}
```

```
// time loop
  # pragma omp parallel default( none ) \
         shared(n,n_time_steps,u,uo,nu,) \
         private(t,j)
  {
    for (t=0; t<n_time_steps; t++) {
      // store solution
      # pragma omp for
      for (j=1; j<n-1; j++) {
     uo[j] = u[j];
      }

      // finite difference scheme
      # pragma omp for
      for (j=1; j<n-1; j++) {
        u[j] = uo[j] +
        nu*(uo[j-1]-2.0*uo[j]+uo[j+1]);
      }
    }
  }
```

What have we learnt?

We have learnt

- The basic ideas behind parallelism
- How OpenMP implements the shared memory programming model
- How to create threads with #pragma omp parallel
- How to scope variables
- How to share the work between the threads with #pragma omp for
- How to synchronise the threads with barriers, critical regions and reductions
- How to parallelise a small but realistic program

Further learning

- The best way to learn OpenMP is to go on a longer course. Two free possibilities are
  - The courses run here in Oxford by the Advanced Research Computing Service
    - http://www.arc.ox.ac.uk/content/training
    - https://oxford.imparando.com/accessplan/LMSPortal/UI/Page/Courses/book.aspx?courseid=HP014 is the direct link to the OpenMP course
  - Courses run by the national supercomputing service, ARCHER and it's soon to come replacement, ARCHER2
    - http://www.archer.ac.uk/training/
    - https://www.archer2.ac.uk/training/

- Unfortunately there are no books I know of that I can totally recommend
  - Probably the best is **Parallel Programming in OpenMP** by Chandra *et al.*
  - But it is a bit old now