

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 by:

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

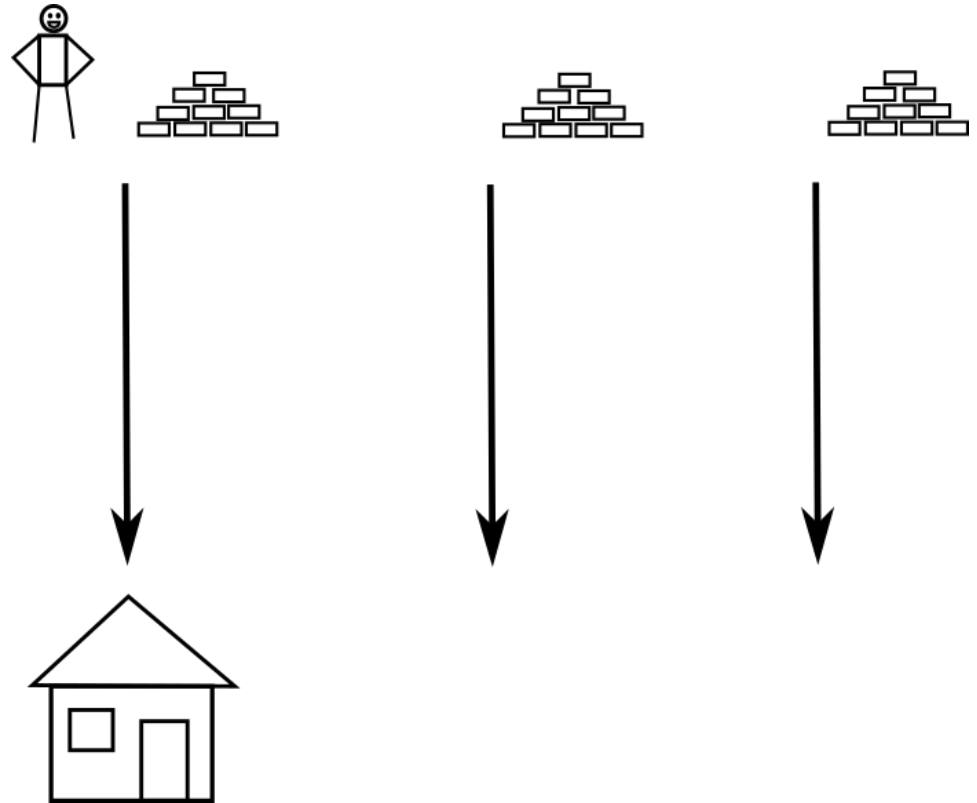
Parallelism – How to do we split up the work?

Analogy:

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

-

-

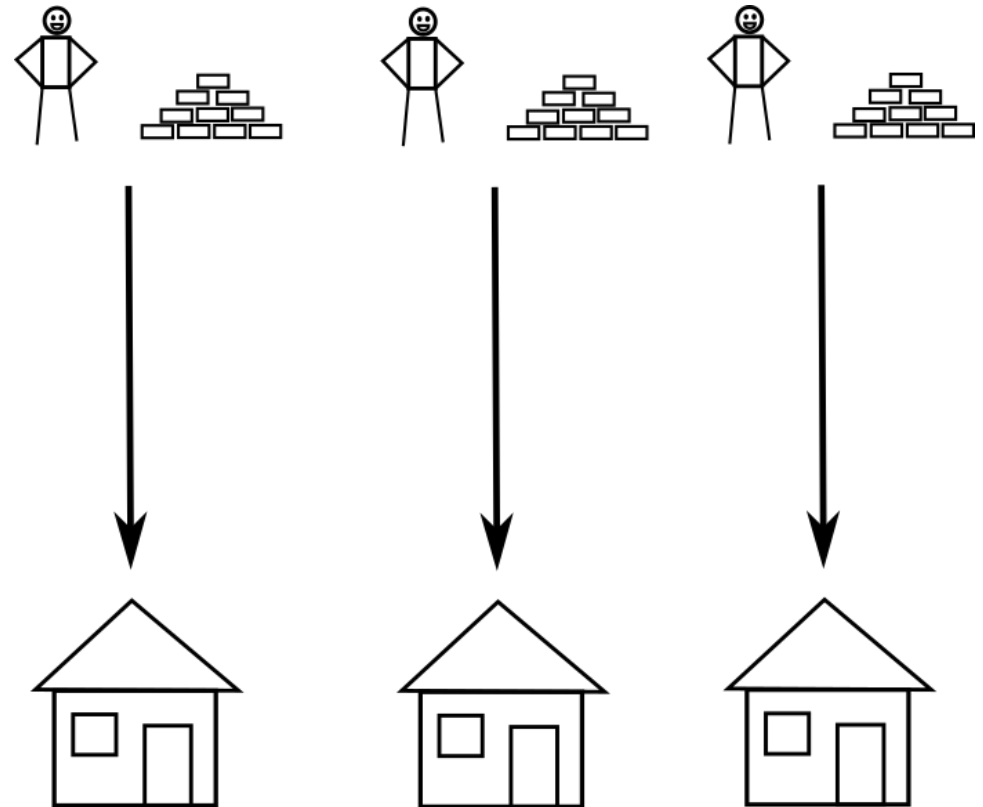


Parallelism – How to do we split up the work?

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 building multiple houses at the same time as one

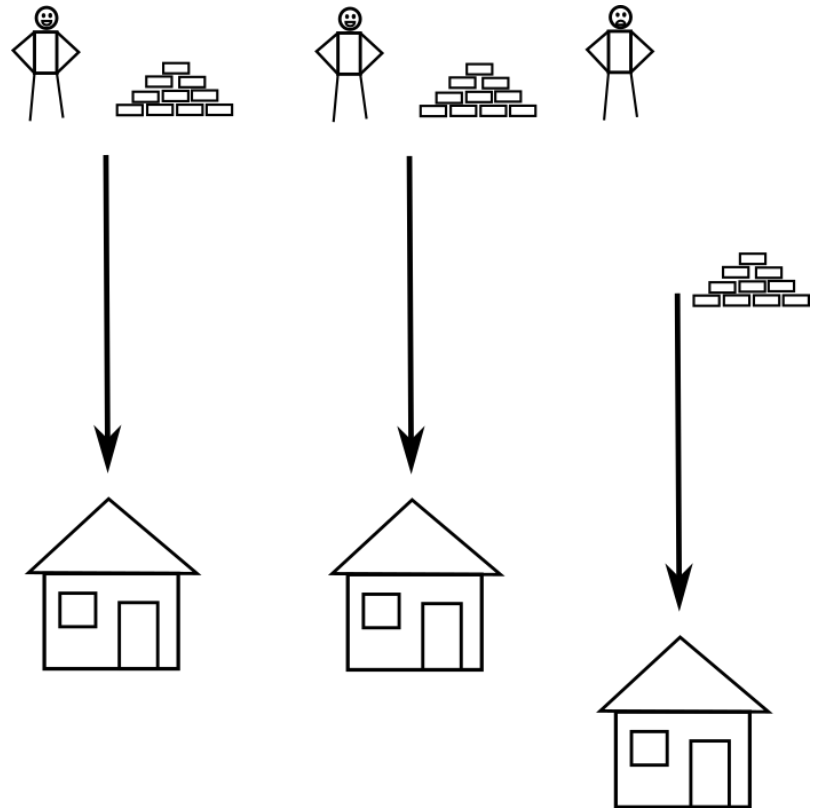


Parallelism – How to do we split up the work?

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 building multiple houses at the same time as one
- Oh no! Supply issues!

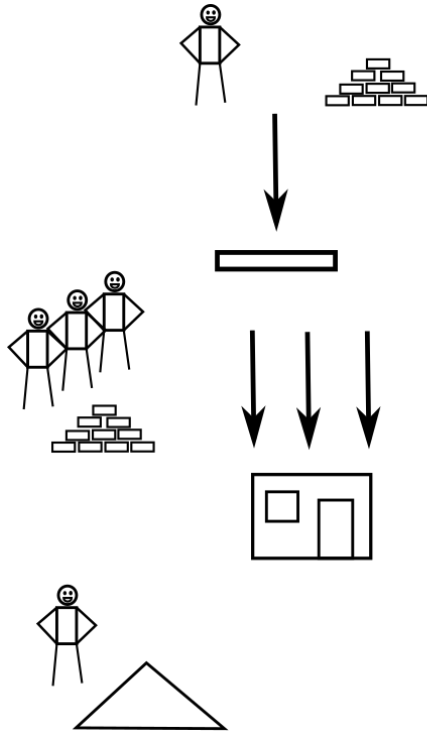


Parallelism – How to do we split up the work?

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

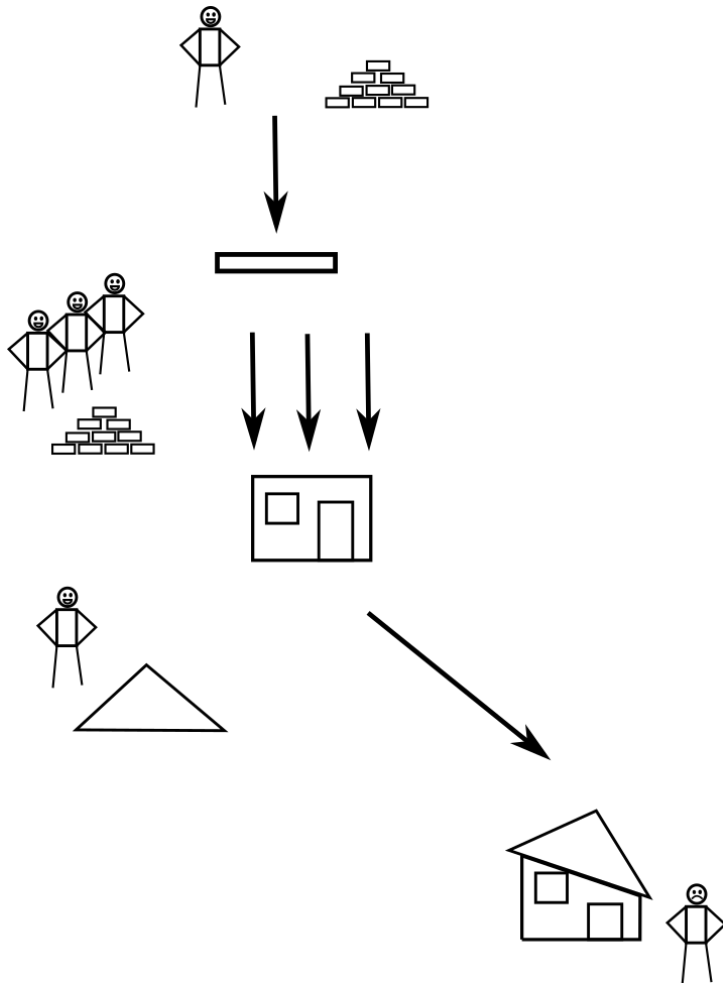
Parallelism – How to do we split up the work?



Division of work for one house:

- We can divide the work on a single house between teams
- Lay the foundations (one worker)
- Build walls (three workers)
- When to build a roof?

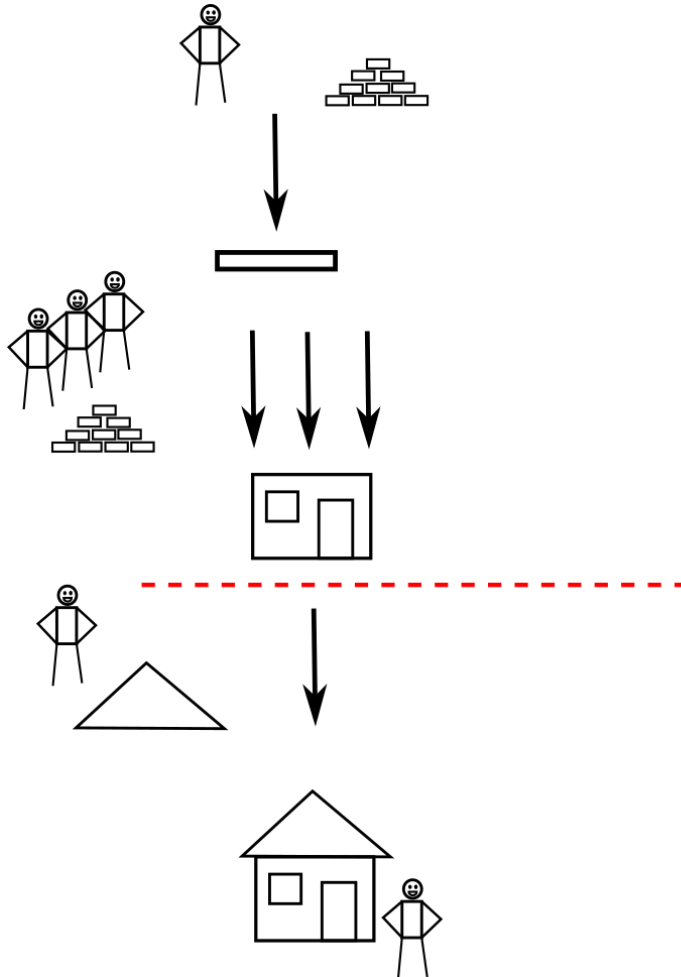
Parallelism – How to do we split up the work?



Division of work for one house:

- We can divide the work on a single house between teams
- Lay the foundations (one worker)
- Build walls (three workers)
- When to build a roof? Whenever we want?

Parallelism – How to do we split up the work?



Division of work for one house:

- We can divide the work on a single house between teams
- Lay the foundations (one worker)
- Build walls (three workers)
- When to build a roof? Whenever we want? NO!
- After walls are build!

Parallelism – A maths example

- Consider adding two vectors:

$$a_i = b_i + c_i$$

- The operations required for each value of i are independent of 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

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

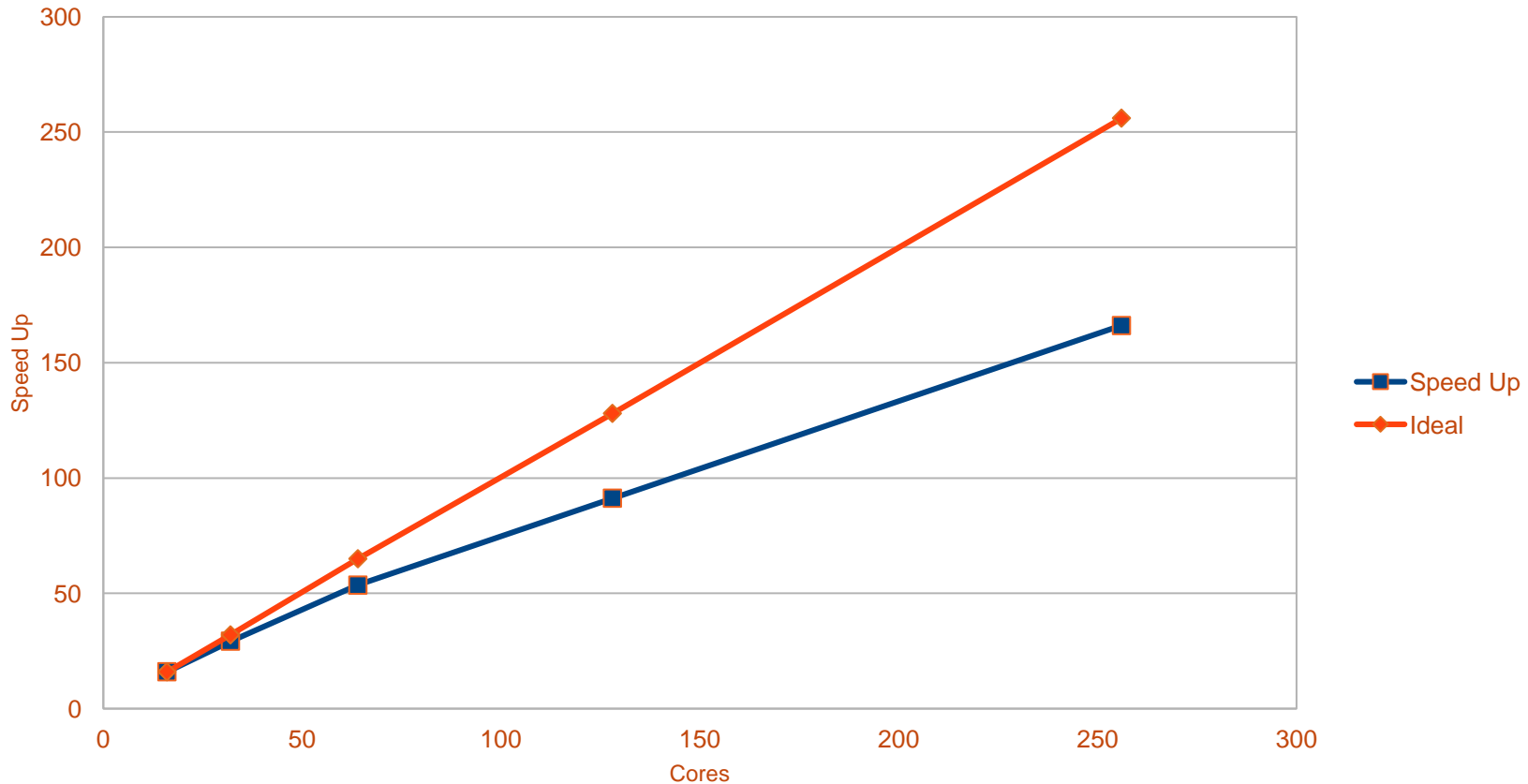
- Could give a subset of the indices to each process and form the local contribution to a
- Sum together all the local contributions for final answer
- This last phase requires the processes or threads to work together
 - i.e. they are no longer totally independent
 - They need to communicate with each 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 a 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 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 the most efficient
 - For large N
 - For small P
 - Too many threads may cause your program to slow down!

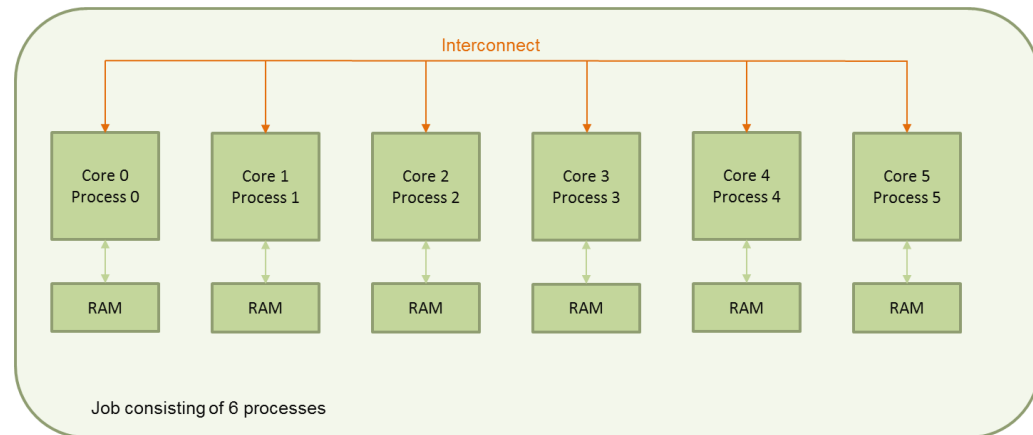
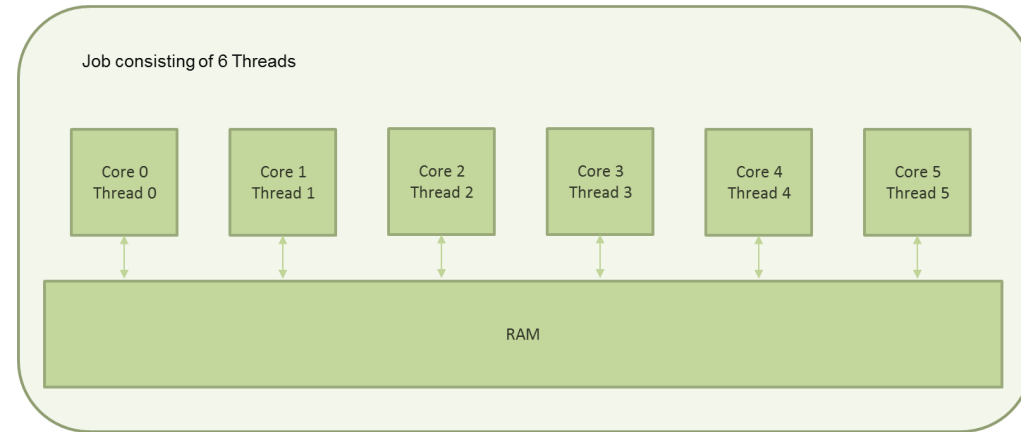
Measuring Scalability – Speed Up

$$S = t(1)/t(P)$$



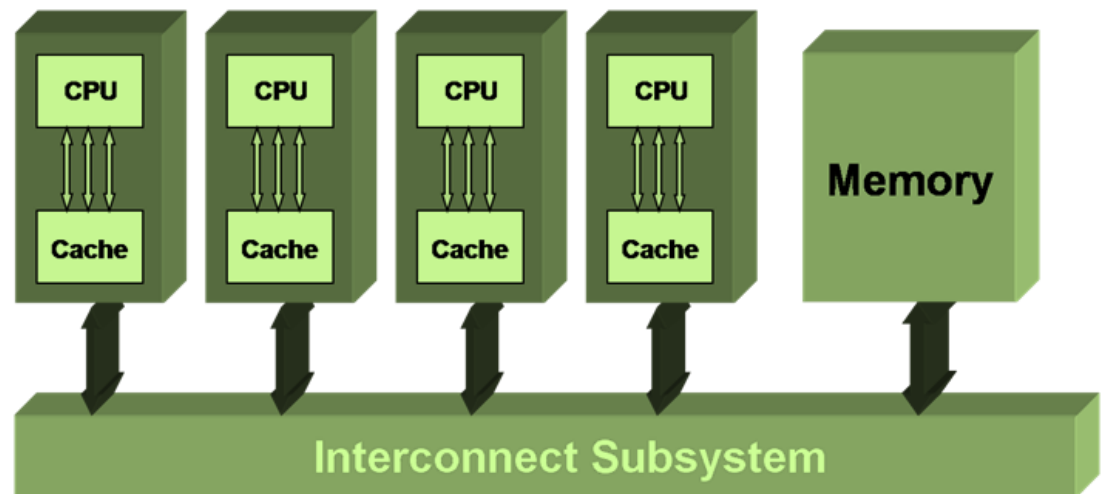
Parallelising Scientific Programs

- **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

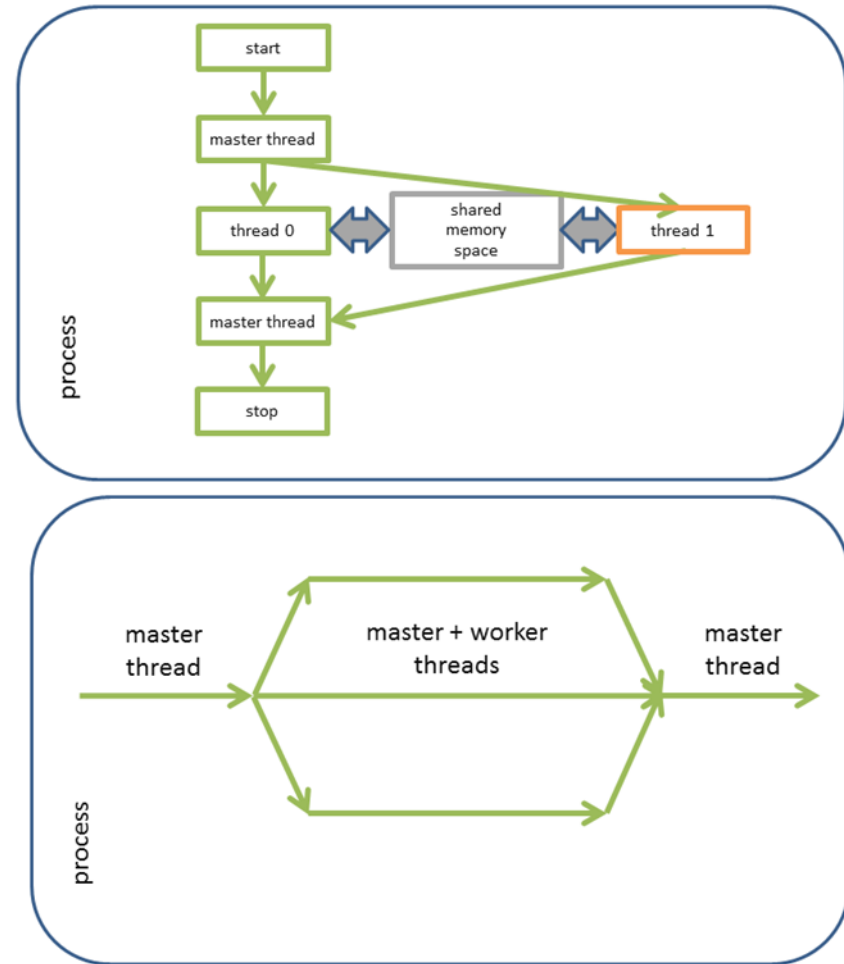
- Represents computing on a multi-processor architecture which links multiple (identical) CPUs to a single unified main memory;
- Uses a shared-memory programming model, with data that can be shared between processors
- Also called SMP, Symmetric Multi-Processor systems (for historical reasons)



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.
- Version 1.0 (1997)
- Version 2.0 (2002)
- Version 2.5 (2005)
- Version 3.0 (2008)
- Version 3.1 (2011)
- Version 4.0 (2013)
- Version 5.0 (2018)
- Version 5.1 (2020)
- Version 5.2 (2021)

It is live and well

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

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;
}
```

OpenMP “Hello World” in C

```
$ 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)	<pre>#pragma omp parallel (C,C++) !\$omp parallel (Fortran)</pre> <ul style="list-style-type: none">• 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)	<pre>#pragma omp for !\$omp do</pre>
critical section	protects action on the shared variables (only one thread at a time allowed)	<pre>#pragma omp critical !\$omp critical</pre>
synchronisation	barriers	<pre>#pragma omp barrier !\$omp barrier</pre> <p>Threads can proceed only after all execute the barrier; implied at end of parallel region and loop (unless overridden by nowait)</p>

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 + xi * yi
end for
[ w = w + z ]
< barrier >
for i = 1 to n/2
    yi = yi - w * xi
end for
```

Thread 2

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

Problem

A thread may finish before
other has updated **w**

This now works!

z private

OpenMP program example

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
```

C

```
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;

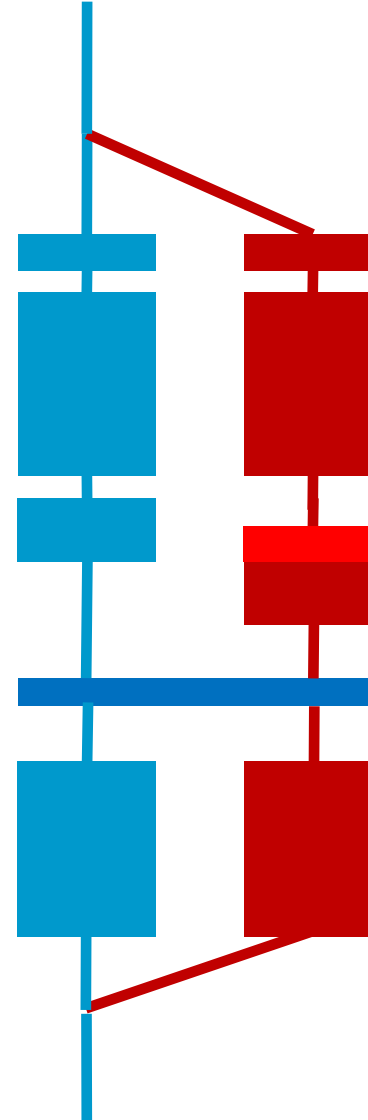
#pragma omp parallel shared (n,w,x,y) \
    private(i,z)
{
    z = 0.0;

    #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

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++)
```

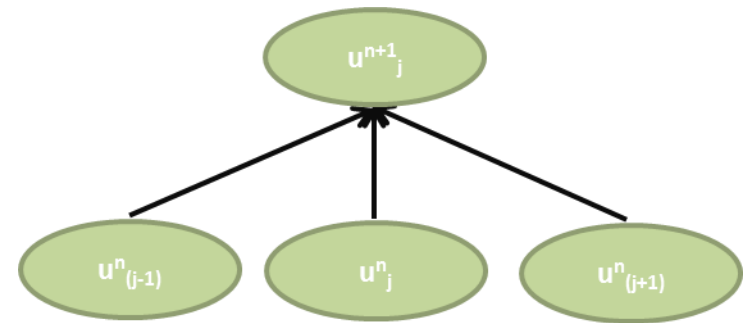
```
// improved
#pragma omp parallel private (n,m)
for (n=0;n<NN;n++)
  # pragma omp for
  for (m=0;m<MM;m++)
```

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
 - $\frac{\partial u}{\partial t} = k \frac{\partial^2 u}{\partial x^2}$
 - Boundary conditions $u(0, t) = u(1, t) = 0$
 - Initial conditions $u(x, 0) = u_0(x)$.



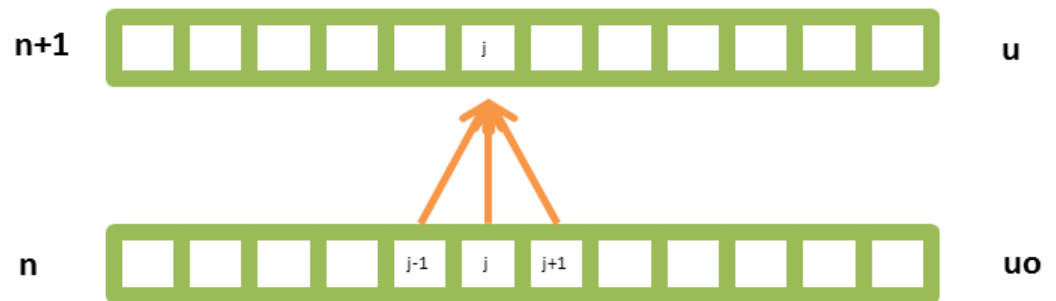
- The **numerics** (a finite difference scheme):
 - sample the interval $[0, 1]$ at equidistant points $x_j = j \cdot dx$ ($j=0, \dots, J-1$) and fixed time intervals $t_n = n \cdot dt$, $n > 0$ and find the values of all temperature samples u^n_j at the sample points
 - discretised equations give:
$$u^{(n+1)}_j = u^n_j + nu \cdot (u^n_{j+1} - 2 \cdot u^n_j + u^n_{j-1})$$
 - 4 point stencil

Example: 1D Heat Equation

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

At every time step,

- copy u into u_o (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

- There is more to OpenMP
 - More run-time library routines (times, locks, execution)
 - More work-sharing directives (sections, work share, task, ...)
 - More synchronization directives (atomic, flush, ...)
 - More environmental variables
- The best way to learn OpenMP is to go on a longer course run by the national supercomputing service, ARCHER2
 - <https://www.archer2.ac.uk/training/>
 - <https://www.archer2.ac.uk/training/courses/211005-advanced-openmp/>

In the next lecture...

Introduction to GPUs

- Hardware architecture
- Software tools
- NVIDIA libraries