CFD exercise

Regular domain decomposition

Reusing this material

Aims

- An introduction to geometric decomposition
  - Partitioning into sub-grids and assigning these to difference processes
  - Halo swapping for communications
- Gain hands on experience with performance metrics
- Understand in more detail how specific configuration choices can impact our performance
  - The choice of compiler
  - Level of optimisation

Computational Fluid Dynamics

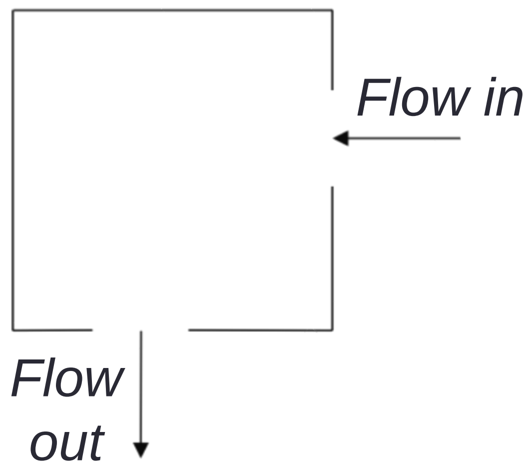
Algorithm, implementation and the problem

Fluid Dynamics

- The study of the mechanics of fluid flow, liquids and gases in motion.
- Commonly requires HPC.
- Continuous systems typically described by partial differential equations.
- For a computer to simulate these systems, these equations must be *discretised* onto a grid.
- One such discretisation approach is the *finite difference method*.
- This method states that the value at any point in the grid is some combination of the neighbouring points

The Problem

- Determining the flow pattern of a fluid in a cavity
  - a square box
  - inlet on one side
  - outlet on the other



- For simplicity, we are assuming zero viscosity for this exercise

The Maths

- In two dimensions, easiest to work with the stream function Ψ
- At zero viscosity, Ψ satisfies:

$$\nabla^2\Psi = \frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} = 0$$

- With finite difference form:

$$\Psi_{i-1,j} + \Psi_{i+1,j} + \Psi_{i,j-1} + \Psi_{i,j+1} - 4\Psi_{i,j} = 0$$

- Jacobi iterative method can be used to find solutions:
  - With boundary values fixed, stream function can be calculated for each point in the grid by averaging the value at that point with its four nearest neighbours.
  - Process continues until the algorithm converges on a solution which stays unchanged by the averaging.
  - Iterative methods are a very common computational approach used for solving systems of equations

Jacobi iterative method

- To solve $$\Psi_{i-1,j} + \Psi_{i+1,j} + \Psi_{i,j-1} + \Psi_{i,j+1} - 4\Psi_{i,j} = 0$$

Repeat for many iterations:

loop over all points *i* and *j:*

```
psinew(i,j) = 0.25*(psi(i+1,j) + psi(i-1,j) + psi(i,j+1) + psi(i,j-1))
```

copy psinew back to psi for next iteration

- In the Fortran version of the code, array notation (arrays of size m x n) removes explicit loops:

```
psinew(1:m,1:n) = 0.25*(psi(2:m+1, 1:n) + psi(0:m-1, 1:n) +
                        psi(1:m, 2:n+1) + psi(1:m, 0:n-1)   )
```

Notes

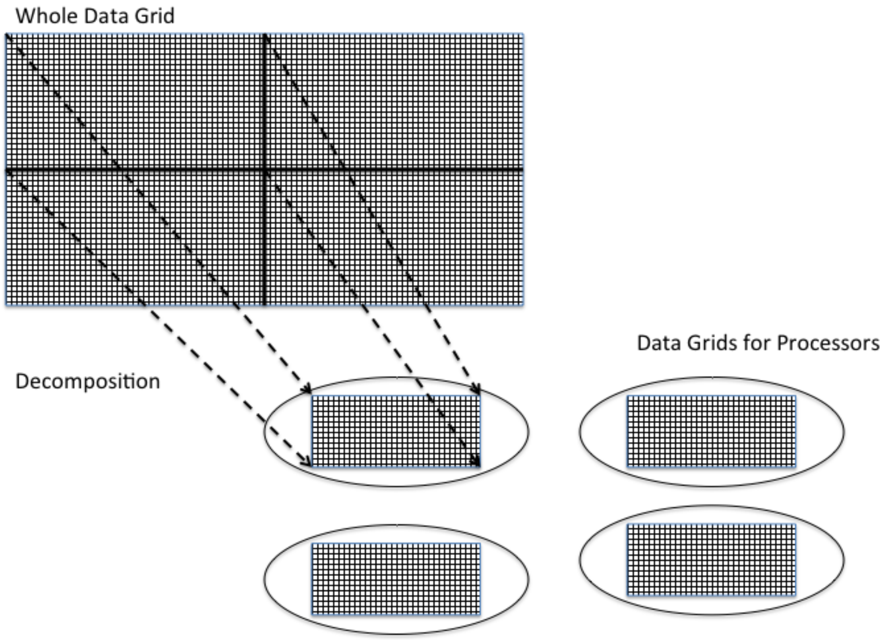
- Finite viscosity gives more realistic flows
  - introduces a new field zeta related to the vorticity
  - equations a bit more complicated but same basic approach
- Terminating the process
  - larger problems require more iterations
  - fixed number of iterations OK for performance measurement but not if we want an accurate answer
  - compute the RMS change in psi and stop when it is small enough
- There are many more efficient iterative methods than Jacobi
  - But Jacobi is the simplest and easy to parallelise

Parallelisations

How does our code take advantage of multiple processes?

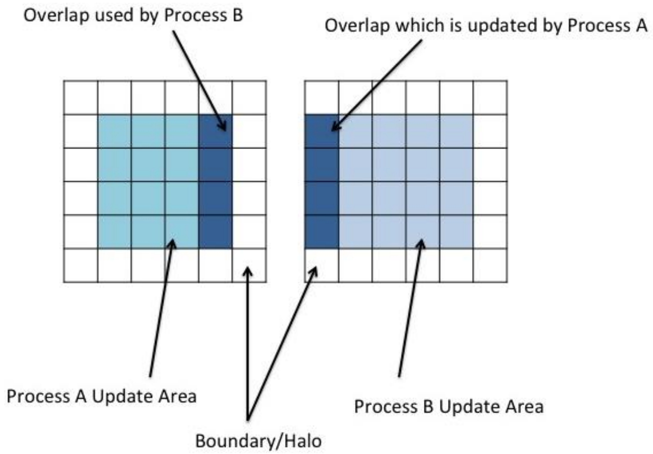
Parallel Programming – Grids

- The algorithm involves calculating the value at each grid point by combining it with the value of its neighbours.
- Same amount of work needed to calculate each grid point – ideal for the geometric decomposition approach.
- Grid is broken up into smaller grids and one is allocated to each process.



Parallel Programming – Halo Swapping

- Points on the edge of a grid present a challenge. Required data is shipped to a remote processor. Processes must therefore communicate.
- Solution is for processor grid to have a boundary layer on adjoining sides.
- Layer is not writable by the local process.
- Updated by another process which in turn will have a boundary updated by the local process.
- Layer is generally known as a *halo* and the inter-process communication which ensures their data is correct and up to date is a *halo swap*.



Characterising Performance

- Speed up (*S*) is how much faster the parallel version runs compared to a non-parallel version.
- Efficiency (*E*) is how effectively the available processing power is being used.

$$S = \frac{T_1}{T_N} \qquad E = \frac{S}{N} = \frac{T_1}{N T_N}$$

- Where:
  - N number of processors
  - T_1 time taken on 1 processor
  - T_N time taken on *N* processors

Over to you

Details of the exercise

Practical

- Compile and run the code on ARCHER
  - on different numbers of cores
  - for different problem sizes

- Will return to this later to study compiler optimisation
  - following slides are for interest only

Exercise outcomes

What do the timings tell us about HPC machines?

Parallel Scaling – Number of Processors

- Addition of parallel resources subject to diminishing returns.
- Depends on scalability of underlying algorithms.
- Any sources of inefficiency are compounded at higher numbers of processes.
- In the CFD example, run time can become dominated by MPI communications rather than actual processing work.

CFD Code	Iterations: 10,000	Scale Factor: 40	Reynolds number: 2
MPI procs	Time	Speedup	Efficiency
1	100.5	1.00	1.00
2	53.61	1.87	0.94
4	35.07	2.87	0.72
8	31.34	3.21	0.40
16	17.81	5.64	0.35

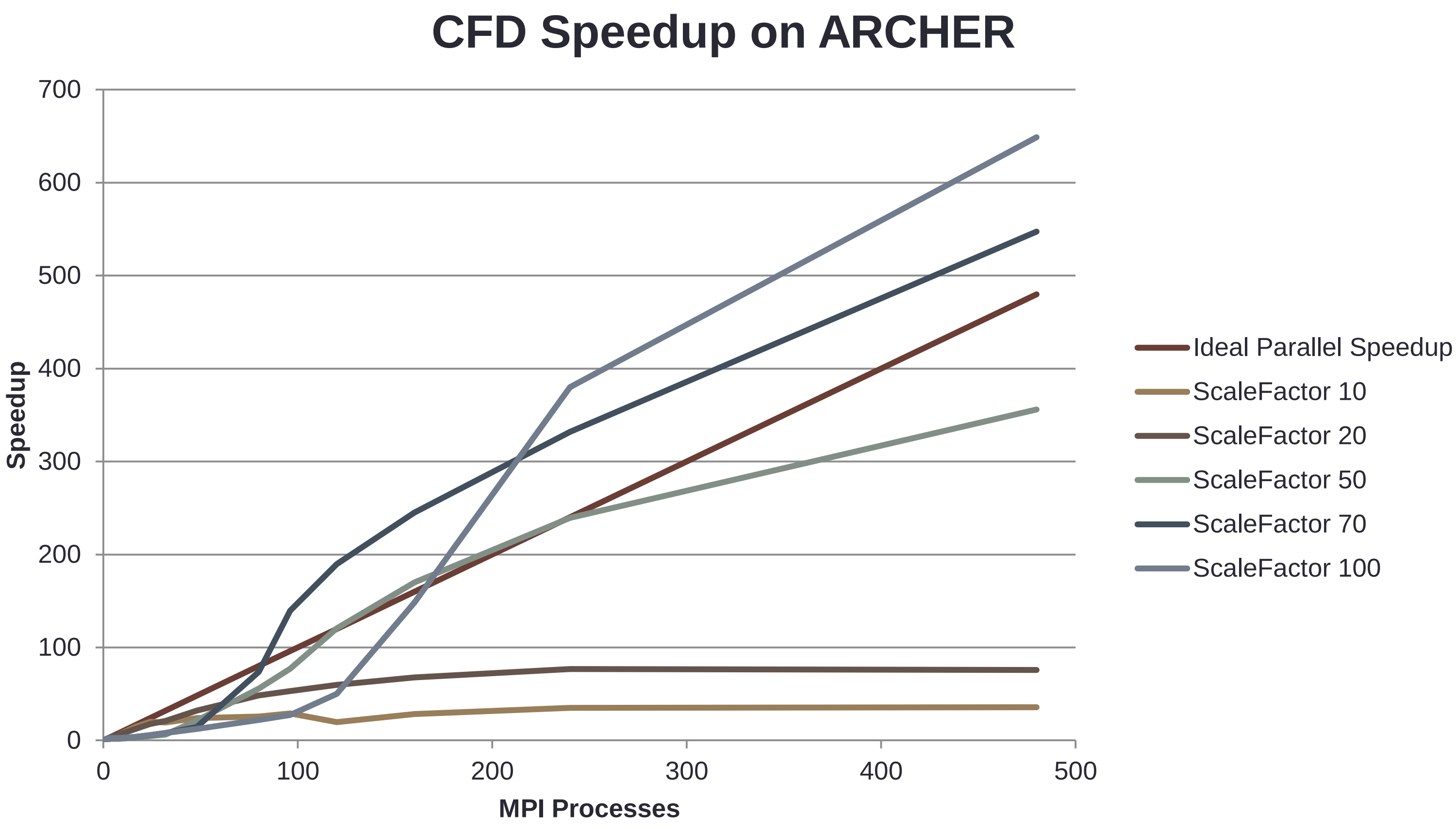
Parallel Scaling – Problem Size

- Problem scale affects memory interactions – notably cache accesses.
- Additional processors provide additional cache space.
- Can lead to more, or even all, of a program's working set being available at the cache level.
- Configurations that achieve this will show a sudden efficiency "spike".

CFD Code Iterations: 10000 Scale Factor: 70

MPI procs	Time	Speedup	Efficiency
1	331.34	1.00	1.00
48	23.27	14.24	0.30
96	2.37	139.61	1.45

- 2x the number of MPI processes gives ~9.8x the speed up.



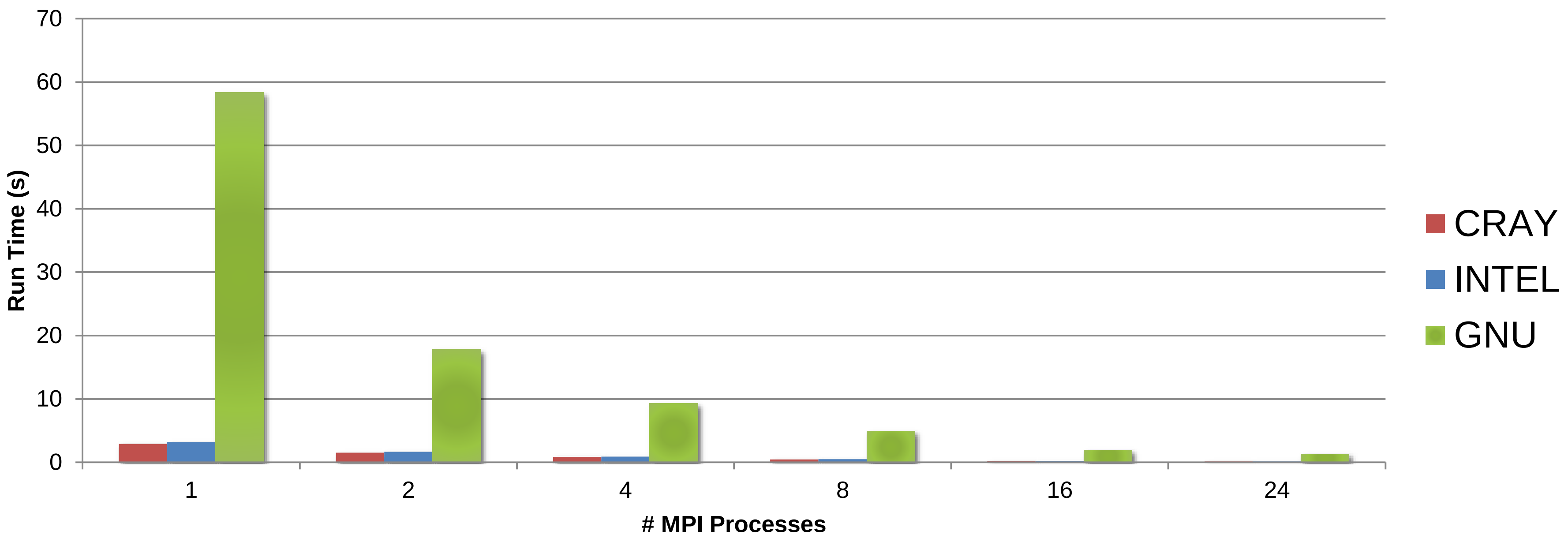
CFD Speedup on ARCHER
Speedup
MPI Processes
0
100
200
300
400
500
600
700
0
100
200
300
400
500
Ideal Parallel Speedup
ScaleFactor 10
ScaleFactor 20
ScaleFactor 50
ScaleFactor 70
ScaleFactor 100

The impact of configuration choices

Different compilers, optimisations and hyper-threading

Compiler Implementation and Platform

- Use ARCHER as an example, where we have the Cray, Intel and GNU compilers.
- Cray and Intel: more optimisations on by default, likely to give more performance out-of-the-box.
- ARCHER is a Cray system using Intel processors. Cray compiler tuned for the platform, Intel compiler tuned for the hardware.



- GNU compiler likely to require additional compiler options...

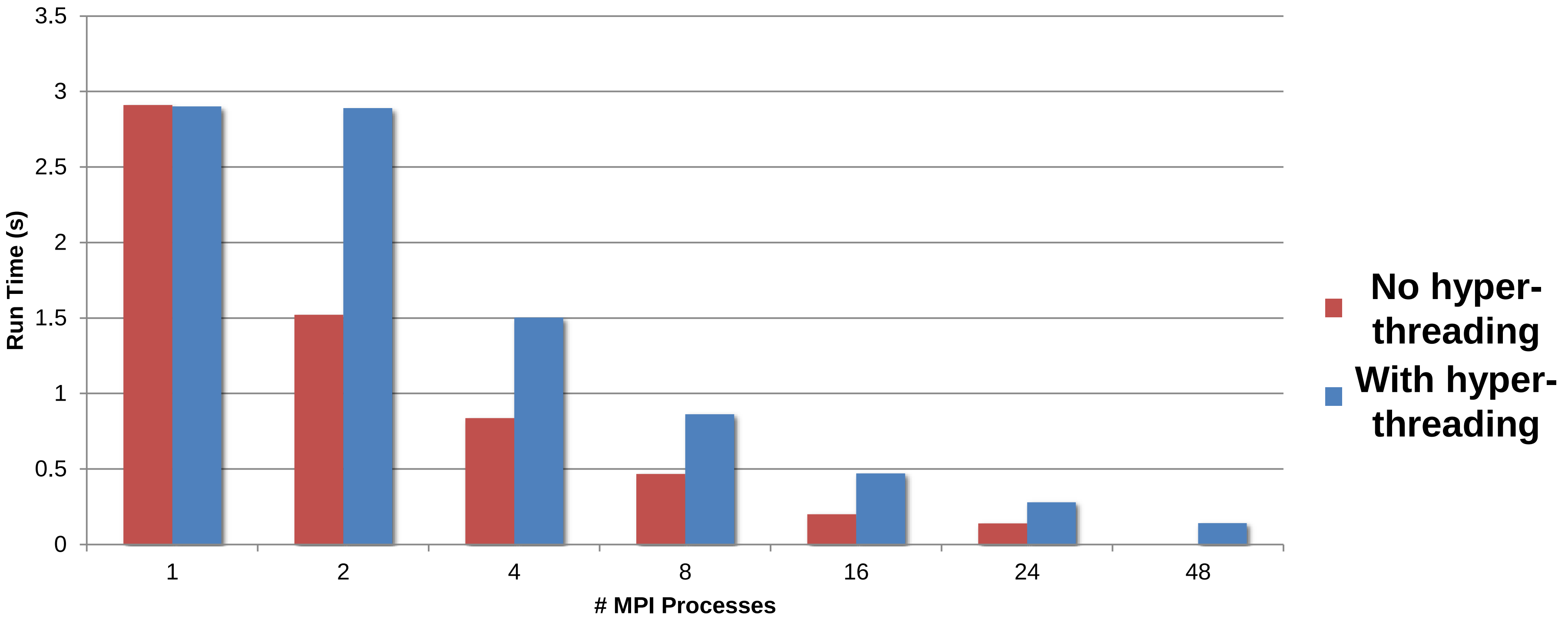
Hyper-Threading

- Intel technology – designed to increase performance using simultaneous multi-threading (SMT) techniques.
- Presented as one additional *logical core* per physical one on the system.
- Each node therefore reports double available processors (48 on ARCHER, 72 on Cirrus).
- Must be explicitly requested with the "-j 2" option:

```
#PBS -l select=1
aprun -n 48 -j 2 ./myMPIProgram
```

- Hyper-Threading doubles the number of available parallel units per node at no additional resource cost.
- However, performance effects are highly dependent on the application

Hyper-Threading Performance



- Can have a positive or negative effect on run times.
- Hyper-Threading is a bad idea for the CFD problem.
- Experimentation is key to determining if this technique would be suitable for your code.