

# CFD exercise

---

Regular domain decomposition



# Reusing this material



This work is licensed under a Creative Commons Attribution-NonCommercial-ShareAlike 4.0 International License.

[http://creativecommons.org/licenses/by-nc-sa/4.0/deed.en\\_US](http://creativecommons.org/licenses/by-nc-sa/4.0/deed.en_US)

This means you are free to copy and redistribute the material and adapt and build on the material under the following terms: You must give appropriate credit, provide a link to the license and indicate if changes were made. If you adapt or build on the material you must distribute your work under the same license as the original.

Acknowledge EPCC as follows: “© EPCC, The University of Edinburgh, [www.epcc.ed.ac.uk](http://www.epcc.ed.ac.uk)”

Note that this presentation contains images owned by others. Please seek their permission before reusing these images.

# 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

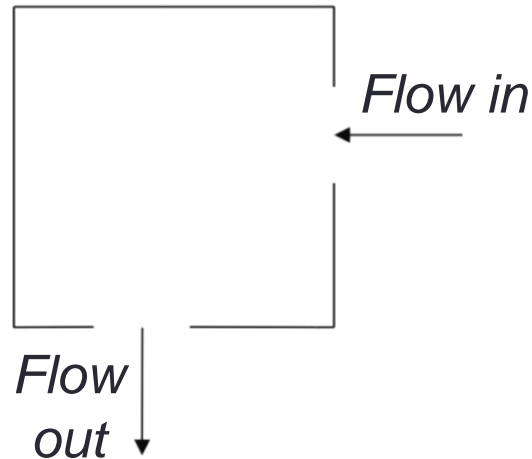
Algorithm, implementation and the problem

# Fluid Dynamics

- 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 assume zero viscosity for this exercise

# The Maths

- In two dimensions, easiest to work with the stream function  $\Psi$
- At zero viscosity,  $\Psi$  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 by averaging 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  $m \times n$ ) 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

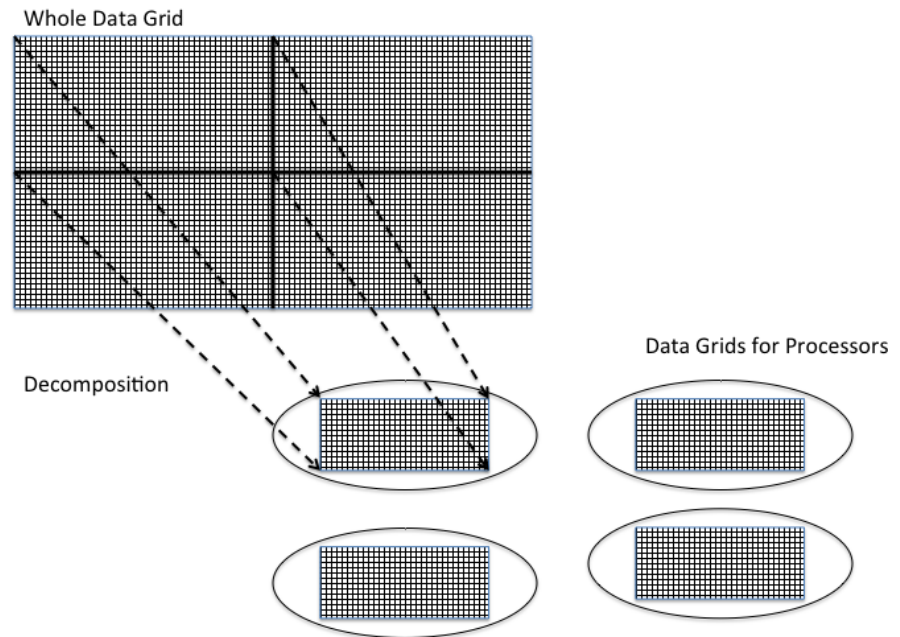
- Finite viscosity gives more realistic flows
  - introduces a new field zeta related to the vorticity
  - equations a bit more complicated but same basic approach
- Terminating the process
  - larger problems require more iterations
  - fixed number of iterations OK for performance measurement but not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

# Parallelisations

How does our code take advantage of multiple processes?

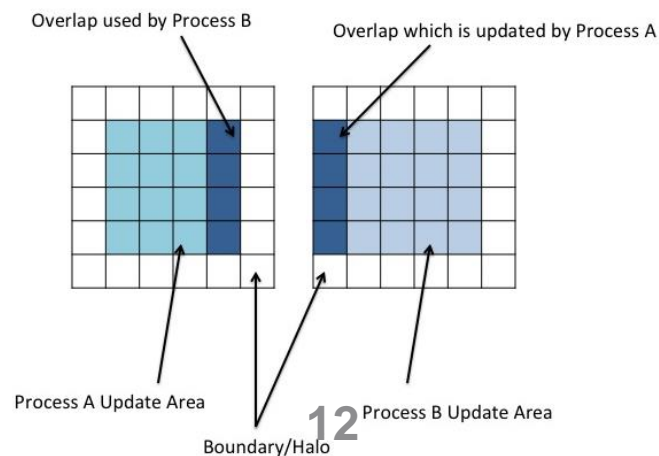
# Parallel Programming – Grids

- 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

- Speedup ( $S$ ) 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.

$$S(N, P) = \frac{T(N, 1)}{T(N, P)} \qquad E(N, P) = \frac{S(N, P)}{P} = \frac{T(N, 1)}{P T(N, P)}$$

- Where:
  - $P$  = number of processors
  - $N$  = problem size (number of grid points)
  - $T(N, 1)$  time taken on 1 processor
  - $T(N, P)$  time taken on  $P$  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”.

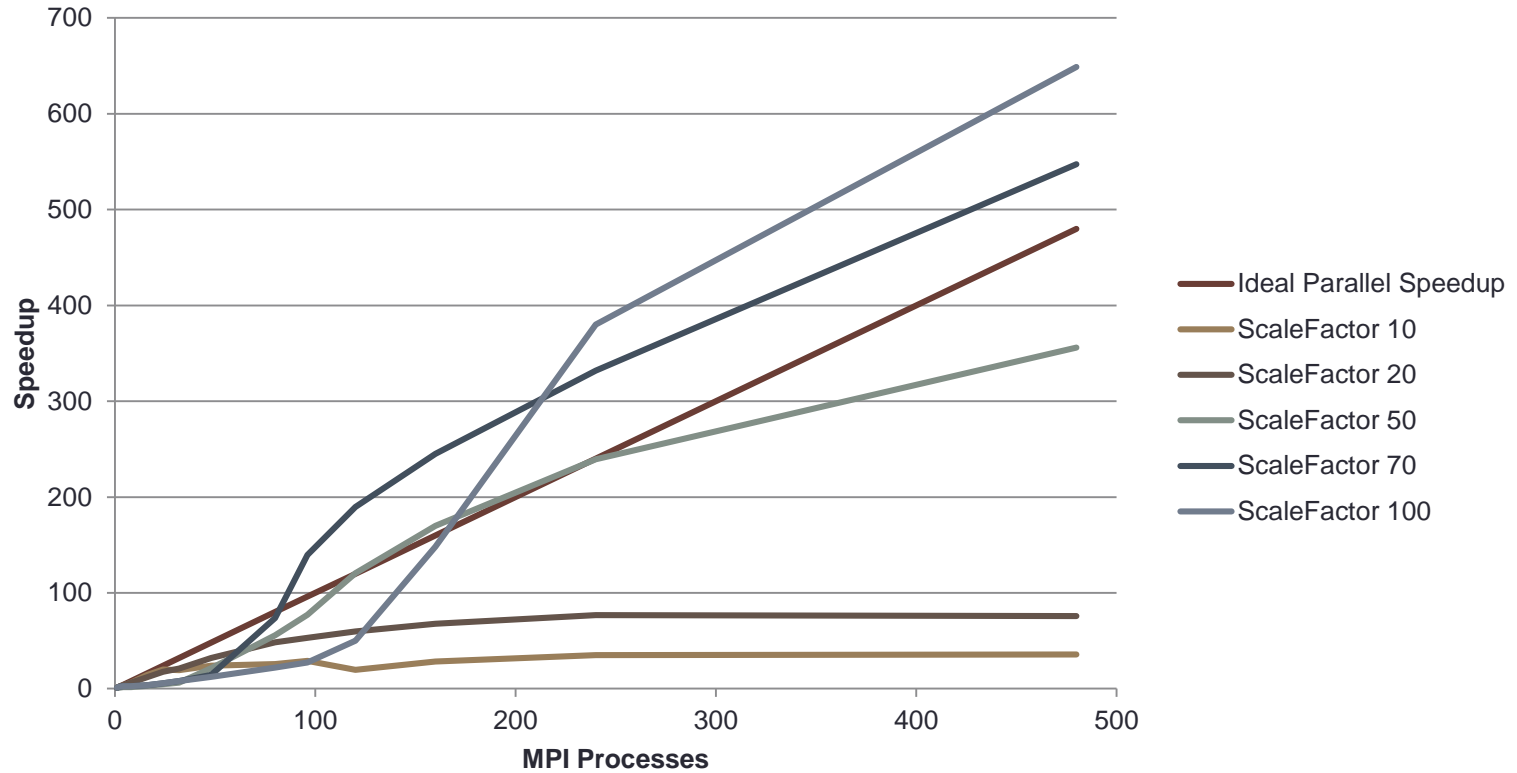
---

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

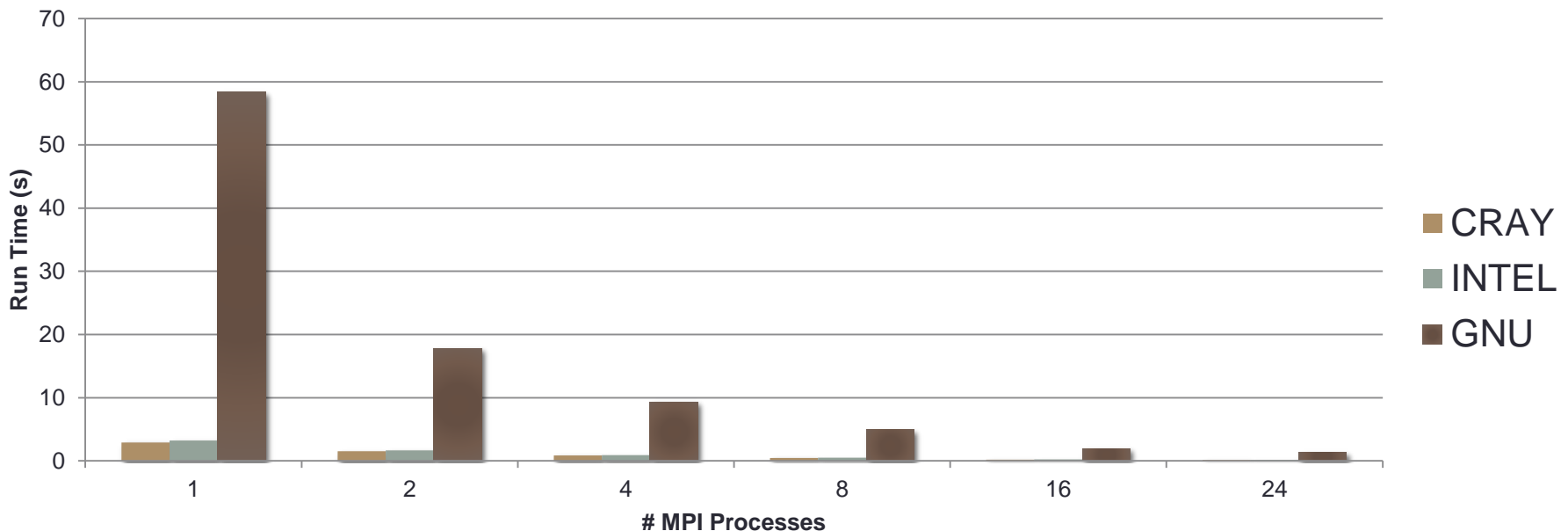


# The impact of configuration choices

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...

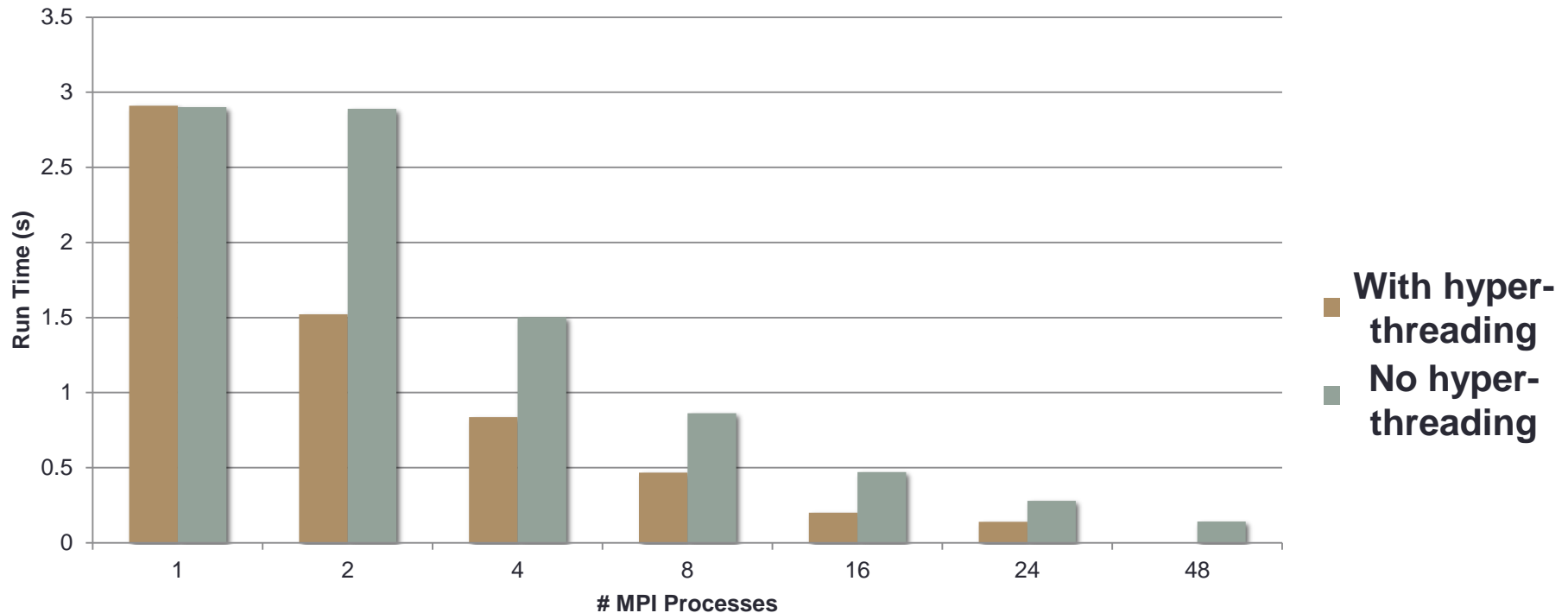
# Hyper-Threading

- 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.

# Process Placement

- Many HPC machines are NUMA systems – processors access different regions of memory at different speeds.
- In ARCHER compute nodes have two NUMA regions – one for each CPU. Hence 12 cores per region.
- It may be desirable to control which NUMA regions processes are assigned to.
- For example, with hybrid MPI and OpenMP jobs, it is suggested that processes are placed such that shared-memory threads in the same team access the same local memory.
- Can be controlled with *aprun* flags such as:
  - -N [parallel processes per node]
  - -S [parallel processes per NUMA region]
  - -d [threads per parallel process]