CFD example

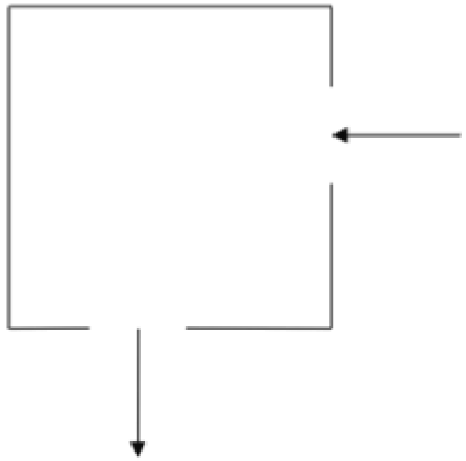
Regular domain decomposition

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



The Cavity

- For simplicity, assuming zero viscosity.

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 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.

The Maths

- In order to obtain the flow pattern of the fluid in the cavity we want to compute the velocity field: u
- The x and y components are related to the stream function by:

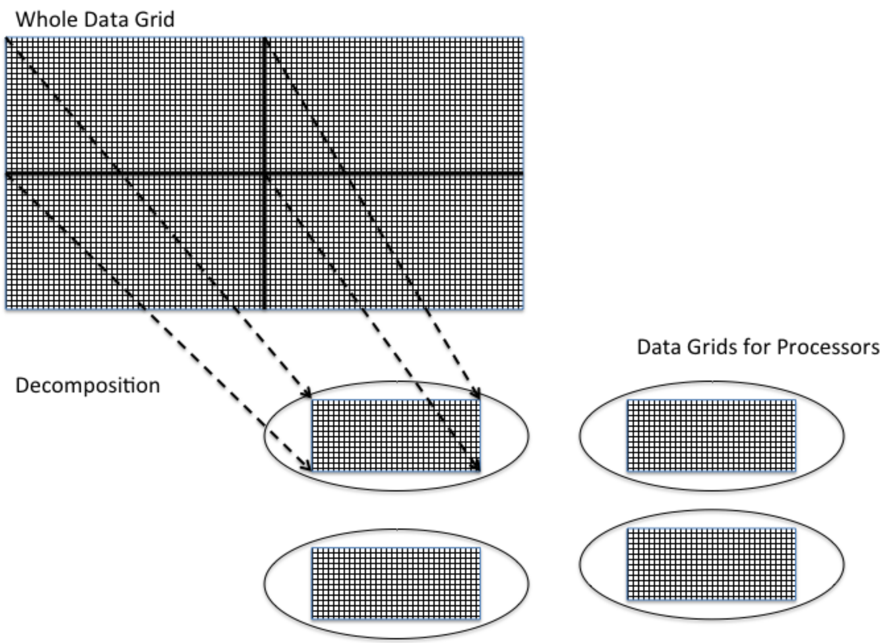
$$u_x = \frac{\partial \Psi}{\partial y} = \frac{1}{2}(\Psi_{i,j+1} - \Psi_{i,j-1})$$

$$u_y = -\frac{\partial \Psi}{\partial x} = \frac{1}{2}(\Psi_{i-1,j} - \Psi_{i+1,j})$$

- General approach is therefore:
  - Calculate the stream function.
  - Use this to calculate the two dimensions of the velocity.

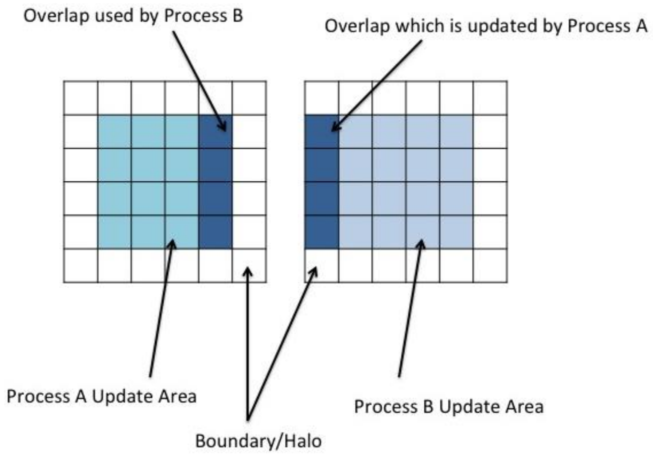
Parallel Programming – Grids

- Both stages involve 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 regular domain decomposition approach.
- Grid is broken up into smaller grids for each processor.



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

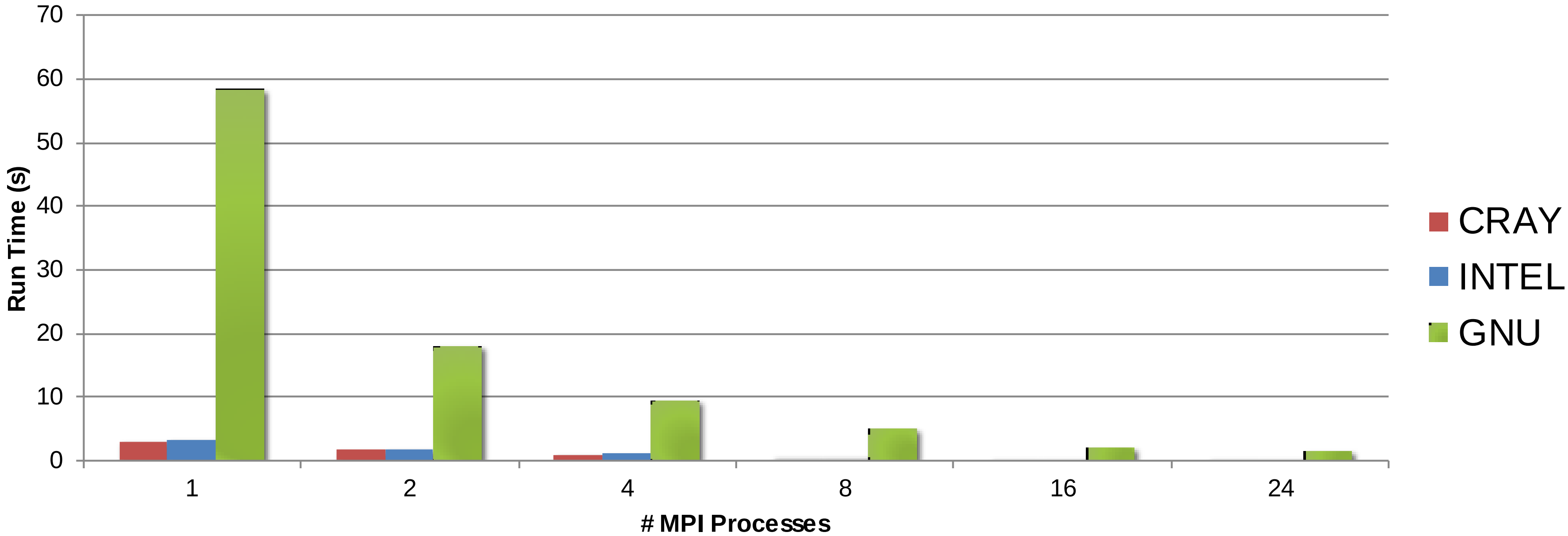
- Speed up (*S*) is how much faster the parallel version runs compared to a non-parallel version.
- Efficiency (*E*) is how effectively the available processing power is being used.

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

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

Compiler Implementation and Platform

- Three compilers on ARCHER: Cray, Intel and GNU.
- 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...

Compiler Optimisation Options

- Flags for the compiler. Can be set on the command line or in the Makefile.
- Standard levels:
  - O3 Aggressive
  - O2 Suggested
  - O Conservative
  - O0 Off (for debugging)
- Finer tuning available. Details in compiler man pages.
- Higher levels aren't always better. Increased code size from some optimisations may negatively impact cache interactions.
- Can increase compilation time.

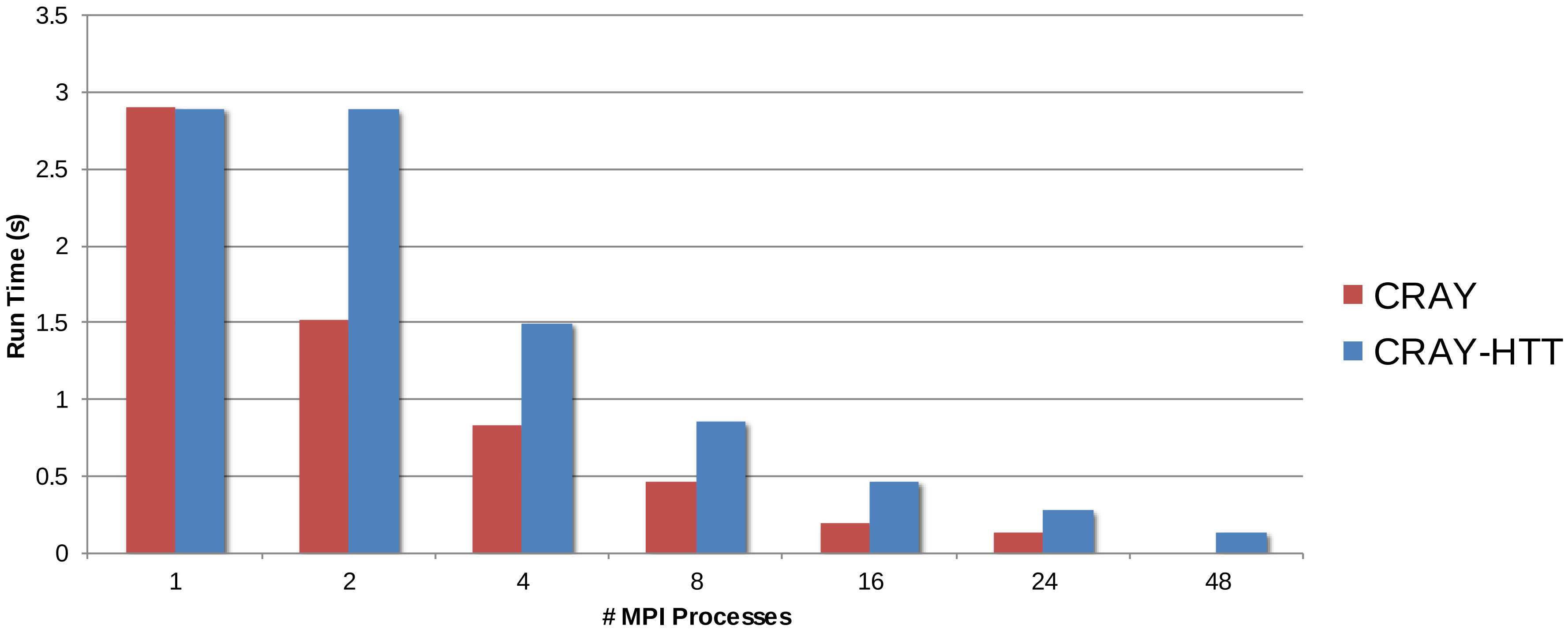
Hyper-Threading

- 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 ARCHER node therefore reports a total of 48 available processors (can be confirmed by checking /proc/cpuinfo).
- 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

- ARCHER is a NUMA system – processors access different regions of memory at different speeds.
- 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 hyrbid 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]

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.

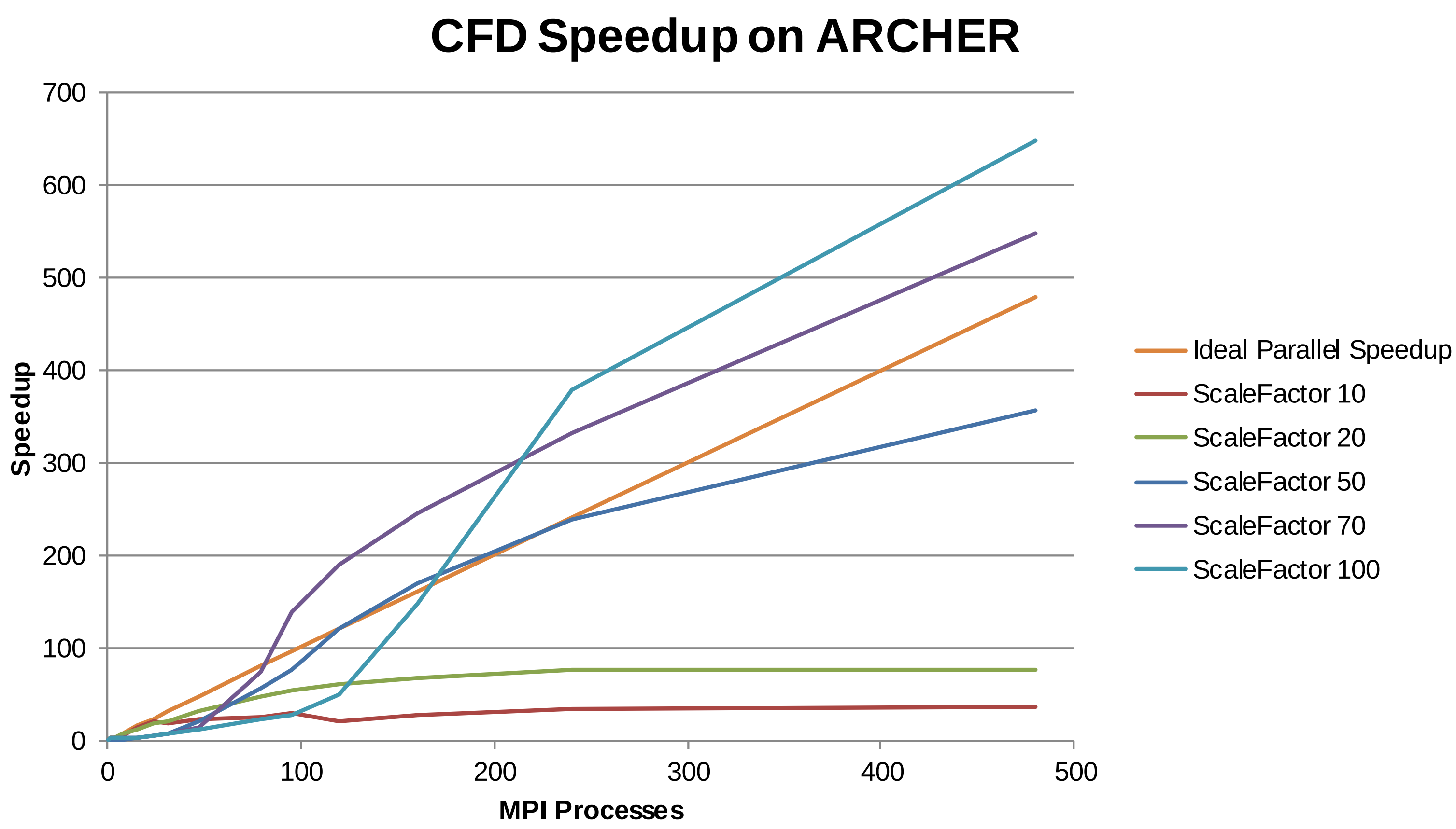
CFD Code	Iterations: 10,000	Scale Factor: 70	
MPI procs	Time	Speedup	Efficiency
1	331.34	1.00	1.00
2	180.30	1.84	0.92
4	132.16	2.51	0.63
8	121.23	2.73	0.34
16	89.02	3.72	0.23
24	58.70	5.64	0.24

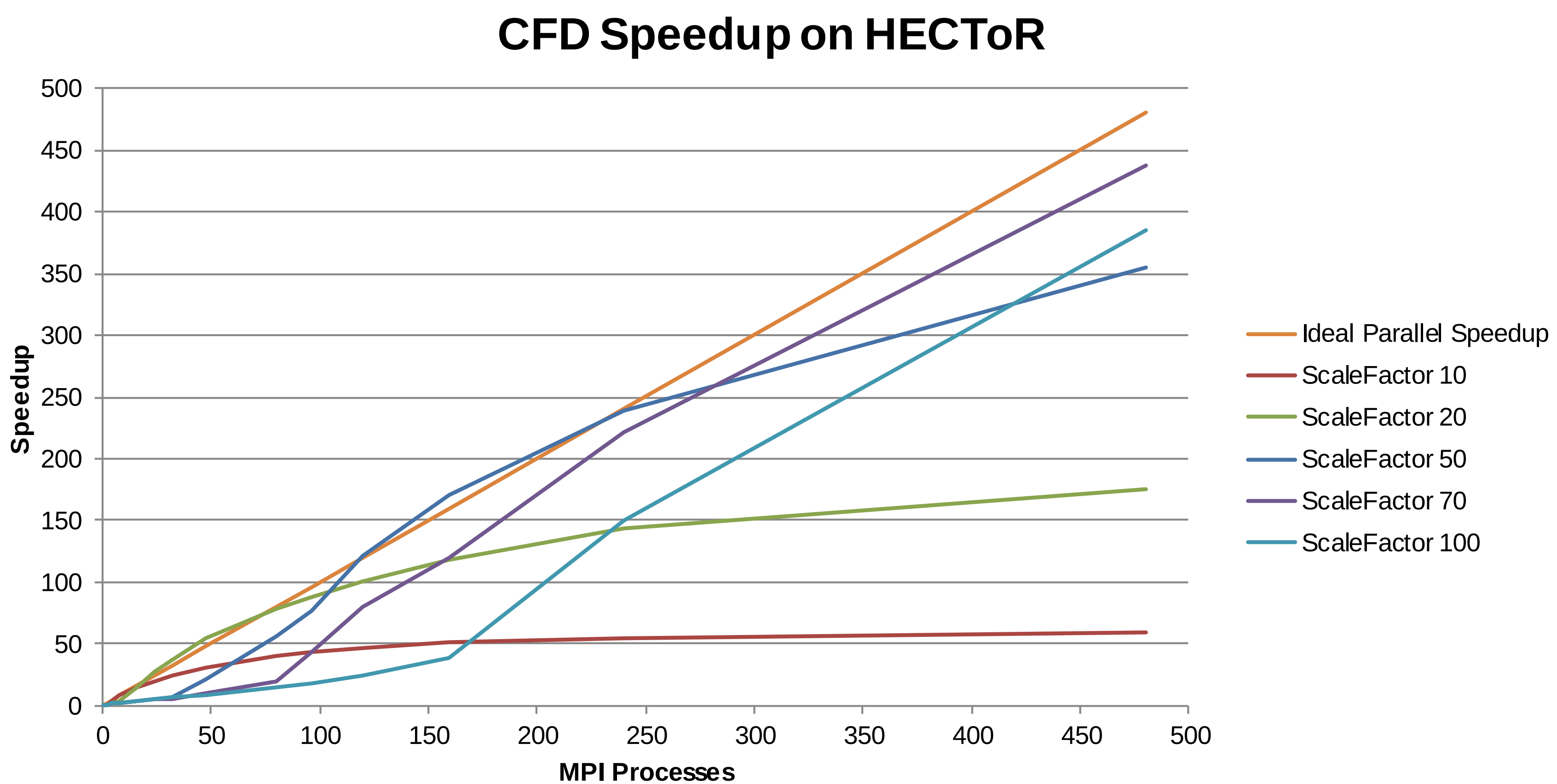
Parallel Scaling – Problem Size

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



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ARCHER-ScaleFactor 10

MPI procs	Time	Speedup	Efficiency
1	2.91	1.00	1.00
2	1.52	1.91	0.96
4	0.84	3.47	0.87
8	0.47	6.22	0.78
16	0.20	14.46	0.90
24	0.15	19.92	0.83
32	0.15	19.45	0.61
48	0.12	23.90	0.50
80	0.11	25.63	0.32
96	0.10	28.95	0.30
120	0.15	19.78	0.16
160	0.10	28.36	0.18
240	0.08	35.14	0.15
480	0.08	35.87	0.07

ARCHER-ScaleFactor 20

MPI procs	Time	Speedup	Efficiency
1	11.92	1.00	1.00
2	6.21	1.92	0.96
4	3.38	3.52	0.88
8	1.86	6.41	0.80
16	1.00	11.91	0.74
24	0.68	17.52	0.73
32	0.57	21.03	0.66
48	0.37	31.95	0.67
80	0.25	48.43	0.61
96	0.22	53.17	0.55
120	0.20	59.86	0.50
160	0.18	67.90	0.42
240	0.16	76.77	0.32
480	0.16	75.94	0.16

HECToR-ScaleFactor 10

MPI procs	Time	Speedup	Efficiency
1	8.91	1.00	1.00
2	8.01	1.11	0.56
4	2.77	3.21	0.80
8	1.12	7.99	1.00
16	0.61	14.56	0.91
24	0.46	19.16	0.80
32	0.37	24.28	0.76
48	0.29	31.00	0.65
80	0.22	39.80	0.50
96	0.21	43.06	0.45
120	0.19	46.47	0.39
160	0.17	51.25	0.32
240	0.16	54.58	0.23
480	0.15	59.81	0.12

HECToR-ScaleFactor 20

MPI procs	Time	Speedup	Efficiency
1	48.42	1.00	1.00
2	44.30	1.09	0.55
4	30.68	1.58	0.39
8	11.97	4.04	0.51
16	3.34	14.49	0.91
24	1.71	28.27	1.18
32	1.29	37.59	1.17
48	0.89	54.28	1.13
80	0.62	78.63	0.98
96	0.55	88.33	0.92
120	0.48	100.57	0.84
160	0.41	118.94	0.74
240	0.34	143.04	0.60
480	0.28	175.50	0.37

ARCHER-ScaleFactor 100			
MPI procs	Time	Speedup	Efficiency
1	694.66	1.00	1.00
2	378.47	1.84	0.92
4	272.62	2.55	0.64
8	250.92	2.77	0.35
16	184.39	3.77	0.24
24	121.45	5.72	0.24
32	88.64	7.84	0.24
48	56.98	12.19	0.25
80	31.66	21.94	0.27
96	25.26	27.50	0.29
120	13.89	50.02	0.42
160	4.68	148.34	0.93
240	1.83	379.89	1.58
480	1.07	648.81	1.35

ARCHER-ScaleFactor 150			
MPI procs	Time	Speedup	Efficiency
1	1577.00	1.00	1.00
2	856.87	1.84	0.92
4	617.34	2.55	0.64
8	569.49	2.77	0.35
16	423.34	3.73	0.23
24	280.15	5.63	0.23
32	207.53	7.60	0.24
48	134.89	11.69	0.24
80	77.95	20.23	0.25
96	69.59	22.66	0.24
120	53.61	29.42	0.25
160	37.43	42.14	0.26
240	19.89	79.30	0.33
480	4.96	317.79	0.66

HECToR-ScaleFactor 100			
MPI procs	Time	Speedup	Efficiency
1	1229.85	1.00	1.00
2	1135.95	1.08	0.54
4	810.08	1.52	0.38
8	803.56	1.53	0.19
16	404.02	3.04	0.19
24	270.39	4.55	0.19
32	203.32	6.05	0.19
48	135.61	9.07	0.19
80	80.72	15.24	0.19
96	66.10	18.61	0.19
120	50.12	24.54	0.20
160	31.63	38.88	0.24
240	8.23	149.44	0.62
480	3.19	385.72	0.80

HECToR-ScaleFactor 150			
MPI procs	Time	Speedup	Efficiency
1	2794.46	1.00	1.00
2	2545.46	1.10	0.55
4	1823.64	1.53	0.38
8	1803.73	1.55	0.19
16	903.92	3.09	0.19
24	604.05	4.63	0.19
32	454.35	6.15	0.19
48	304.80	9.17	0.19
80	183.54	15.23	0.19
96	152.96	18.27	0.19
120	122.20	22.87	0.19
160	91.26	30.62	0.19
240	58.37	47.87	0.20
480	11.20	249.48	0.52