An Introduction to Parallel Programming

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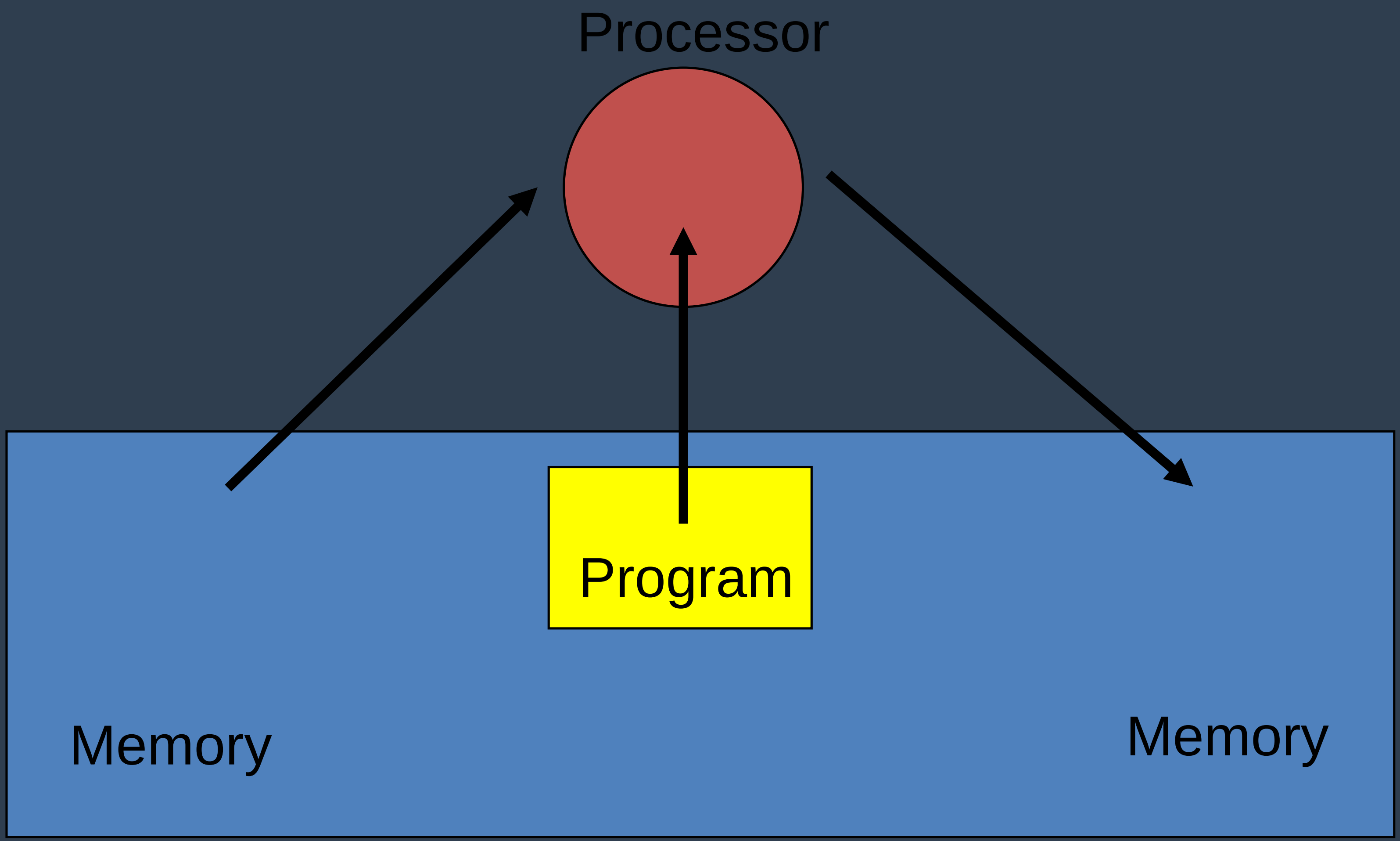
Introduction

- Syntax is easy
  - And can always be found in books/web pages if you can’t remember!
- How to think about parallel programming is more difficult
  - But it’s essential!
  - A good mental model enables you to use the OpenMP and MPI we will teach you
  - It can be a struggle to start with
  - Persevere!
- What this module will cover
  - Revision : What does a parallel computer look like
  - Different programming models and how to think about them
  - What is needed for best performance

More than one way of looking at things!

- What can you see?

What does a computer do?



How do we make a computer go faster? [1]

- Make the processor go faster
  - Give it a faster clock (more operations per second)
- Give the processor more ability
  - For example – allow it to calculate a square root
- But…
  - It gets very expensive to keep doing this
  - Need to keep packing more onto a single silicon chip
    - Need to make everything smaller
  - Chips get increasingly complex
    - Take longer to design and debug
  - Difficult and very expensive for memory speed to keep up
  - Produce more and more heat

How do we make a computer go faster? [1]

- Introduce multiple processors
- Advantages:
  - “Many hands make light work”
  - Each individual processor can be less powerful
    - Which means it’s cheaper to buy and run (less power)
- Disadvantages
  - “Too many cooks spoil the broth”
  - One task – many processors
    - We need to think about how to share the task amongst them
    - We need to co-ordinate carefully
  - We need a new way of writing our programs

What limits parallel performance?

- Parallelisation is not a limitless way to infinite performance!
- Algorithms and computer hardware give limits on performance
- Amdahl's Law
  - Consider an algorithm (program!)
  - Some parts of it (fraction "p") can be run in parallel
  - Some parts of it (fraction "s") cannot be run in parallel
    - Nature of the algorithm
    - Hardware constraints (writing to a disk for example)
  - Takes time "t" to run on a single processor
  - On "n" processors it takes : $T = s \times t + (p \times t)/n$

Consequences of Amdahl's Law [1]

- T = s x t + (p x t)/n
  - Looks simple, but "s" has devastating consquences!

- Consider the case as the number of processors "n" grows large, then we get:
  - T = s x t + [something small]

- So our performance is limited by the non-parallel part of our algorithm

Consequences of Amdahl's Law [2]

- For example, assume we can parallelise 99% of our algorithm, which takes 100 seconds on 1 processor.

- On 10 processors we get : T[10]= 0.01*100 + (0.99*100)/10
  - T[10]=1 + 9.9 = 10.9 seconds
  - 9.2 times speedup : not too bad - we're "wasting" 8%

- But on 100 processors we get :
  - T[100] = 1 + 0.99 = 1.99 seconds
  - 50 times speedup : not so good – we're "wasting" 50%

- And on 1000 processors we get :
  - T[1000] = 1 + 0.099 = 1.099 seconds = 90 times speedup : terrible!
    - We're "wasting" 91%!

How do we program a parallel computer? [1]

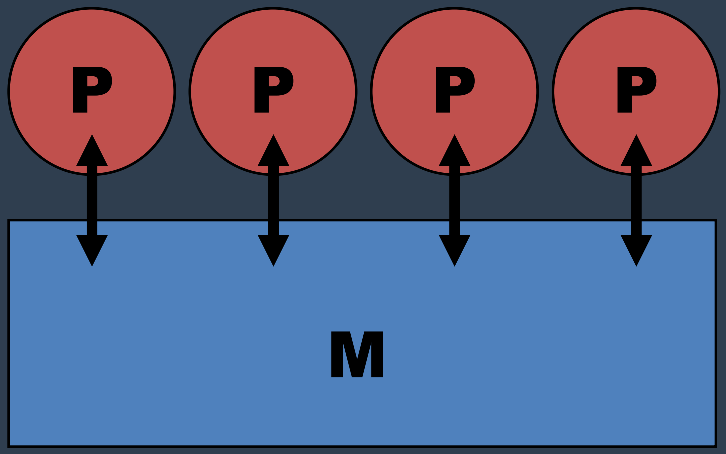
- Decompose (split) into parts
- We can think both about the data and the algorithm…
  - Apply the same operation to many different pieces of data simultaneously
    - SIMD : SINGLE Instruction MULTIPLE Data
    - Requires us to decompose (split) the data, but the algorithm can stay put
    - eg. Factory making widgets – 1000 employees each producing 10 widgets per hour
  - Apply different operations to many different pieces of data simultaneously
    - MIMD : MULTIPLE Instruction MULTIPLE Date
    - Now we need to decompose (split) the algorithm too
    - eg. Factory assembly line making cars – split into stages with a few staff at each stage doing a specific operation (Instruction)
- To maximise parallelism, typically we want to take a MIMD approach

How do we program a parallel computer? [2]

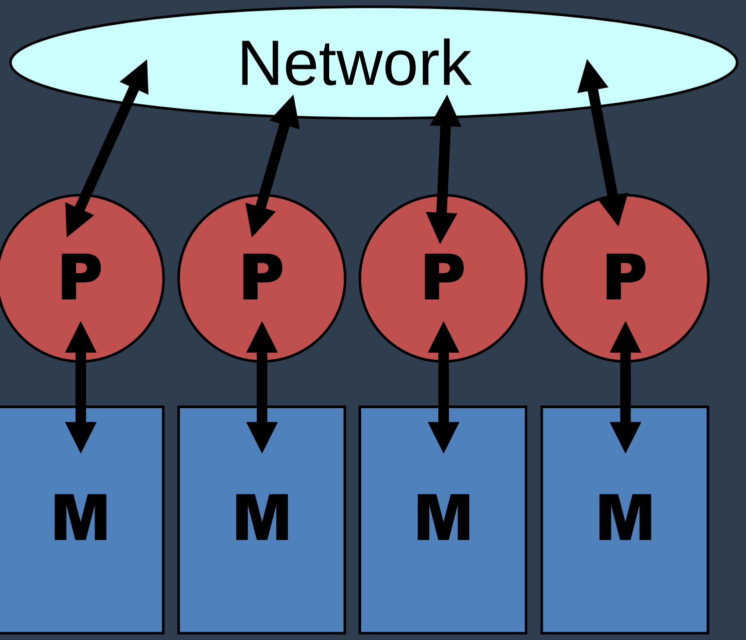
- We need to work out how to distribute the data
  - Need to enable multiple processors work simultaneously
- Algorithmic Considerations
  - Does the algorithm create a data dependency?
    - This may be a function of how to decompose the data
    - What is the most efficient decomposition to achieve this?
  - Need to ensure the work is properly synchronised
    - When there is a data dependency, we need to wait for dependencies to be satisifed
  - Possibly need to communicate between processors
    - As little as possible!
  - Can we split the work equally between all processors?
- Hardware Considerations
  - What parallel architecture (hardware) are we using?
  - Does our decomposition map neatly onto our hardware (or future hardware?)

Parallel programming techniques will reflect the architecture

Shared Memory Architecture

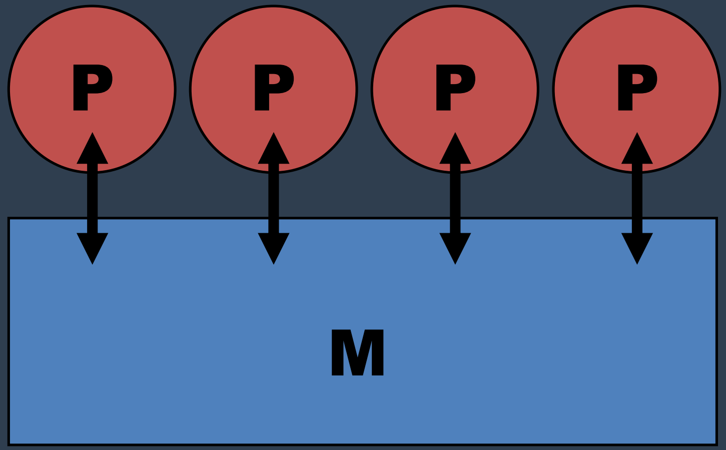


Distributed Memory Architecture



Shared memory programming

Each processor runs a single independent “**thread**”



- Split (decompose) the computation
  - “Functional parallelism”
- Each thread works on a subset of the computation
- No explicit communication required
  - Implicit through common memory
- Advantages
  - Easier to program
    - no communications
    - no need to decompose data
- Disadvantages
  - Memory contention?
  - How do we split an algorithm?

A simple program

```
INTEGER, PARAMETER       :: SIZE=100
REAL, DIMENSION (SIZE) :: A,B,C,D,E,F
INTEGER                  :: i

! Read arrays A,B,C,D from a disk
CALL READ_DATA ( A , B , C , D , 100 )

! Calculate E=A+B
DO i = 1 , SIZE
  E(i) = A(i) + B(i)
ENDDO


! Calculate F=C*D
DO i = 1 , SIZE
  F(i) = C(i) * D(i)
ENDDO

! Write results
CALL WRITE_DATA( E , F , 100 )
```

We'll ignore these bits for now…

A shared memory approach

- Split the function across the threads
  - In the example we have two functions:
    `E=A+B` and `F=C*D`
  - But we have 4 processors (threads) – two would be idle ☹
- So what we do is split the computation of each loop between the threads
  - Each thread will be responsible for executing a subset of the iterations
  - Each iteration *****MUST***** be independent of the others for this to work
- We need some new syntax to tell the computer what we want it to do
  - OpenMP – compiler directive
  - For now we'll just use some descriptive text
- We don't really care which processor/thread does which computations
  - The shared memory means that each processor/thread can read/write to any array element

Shared memory program

```
INTEGER, PARAMETER      :: SIZE=100
REAL, DIMENSION (SIZE) :: A,B,C,D,E,F
INTEGER                 :: i

! Read arrays A,B,C,D from a disk
CALL READ_DATA ( A , B , C , D , 100 )


! Calculate E=A+B and F=C*D
! (Merged loops to fit onto slide!)
! OpenMP : Distribute loop over NPROC threads
! OpenMP : Private variables : i
DO i = 1 , SIZE
  E(i) = A(i) + B(i)
  F(i) = C(i) * D(i)

ENDDO

! Write results
CALL WRITE_DATA( E , F , 100 )
```

This is easy with shared memory as all threads can read/write to the whole of each array

Directives

- Usually before a loop

- Tells the computer
  - How many threads to split the iterations of the loop between
  - Any variables which are “private” (default is that variables are “shared”)
    - “private” – each thread has an independent version of the variable
    - “shared” – all threads can read/write the same variable
    - The loop index must be private - each thread must have its own independent loop index so that it can keep track of what it’s doing
  - Optionally some tips on how to split the iterations of the loop between threads

How you might want to try and think about it…

- The program runs on a single processor P1 – as a single thread.

- Until…
  - It meets an OpenMP directive (typically before a loop)
  - This starts up the other processors (P2,P3,P4) – each running a single “thread”
    - Each thread takes a “chunk” of computations
    - This is repeated until all the computations are done
  - When the loop is finished (`ENDDO`) all the other processors (P2,P3,P4) go back to sleep, and execution continues on a single thread running on processor P1

How to do it

- Identify parts of the algorithm (typically loops) which can be split (parallelised) between processors

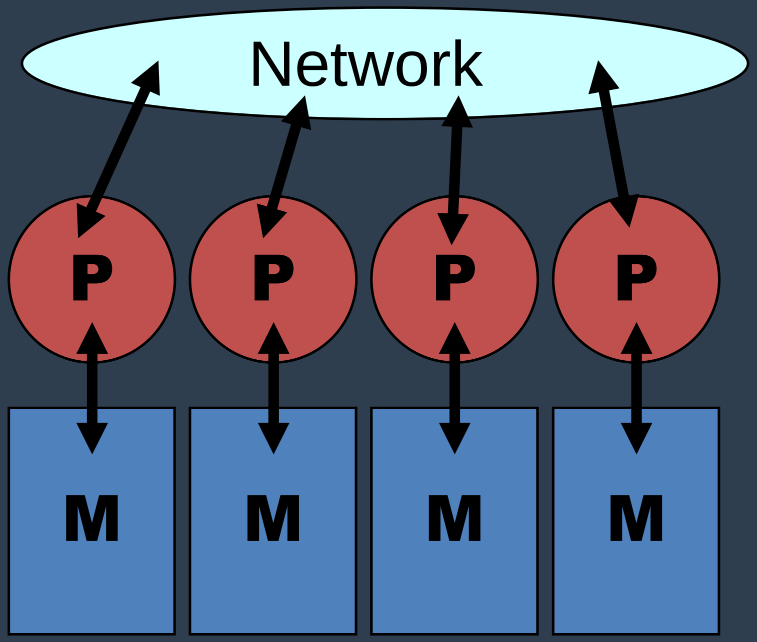
- Possibly rewrite algorithm to allow it to be (more efficiently) parallelised
  - In our example we merged two loops – this can be more efficient than starting up all the parallel threads multiple times

- For a given loop, identify any “private” variables
  - eg. Loop index, partial sum etc.

- Insert a directive telling the computer how to split the loop between processors

Distributed memory programming

Each processor runs a single independent "**task**"



- Split (decompose) the data
  - "Data Parallelism"
- Each processor/task works on a subset of the data
- Processors communicate over the network
- Advantages
  - Easily scalable (assuming a good network)
- Disadvantages
  - Need to think about how to split our data
  - Need to think about dependencies and communications

A distributed memory approach [1]

- Split (decompose) the data between the tasks

- We'll need to do something clever for input/output of the data
  - Each task will only read/write it's particularly subset of the data
  - We'll ignore this for now

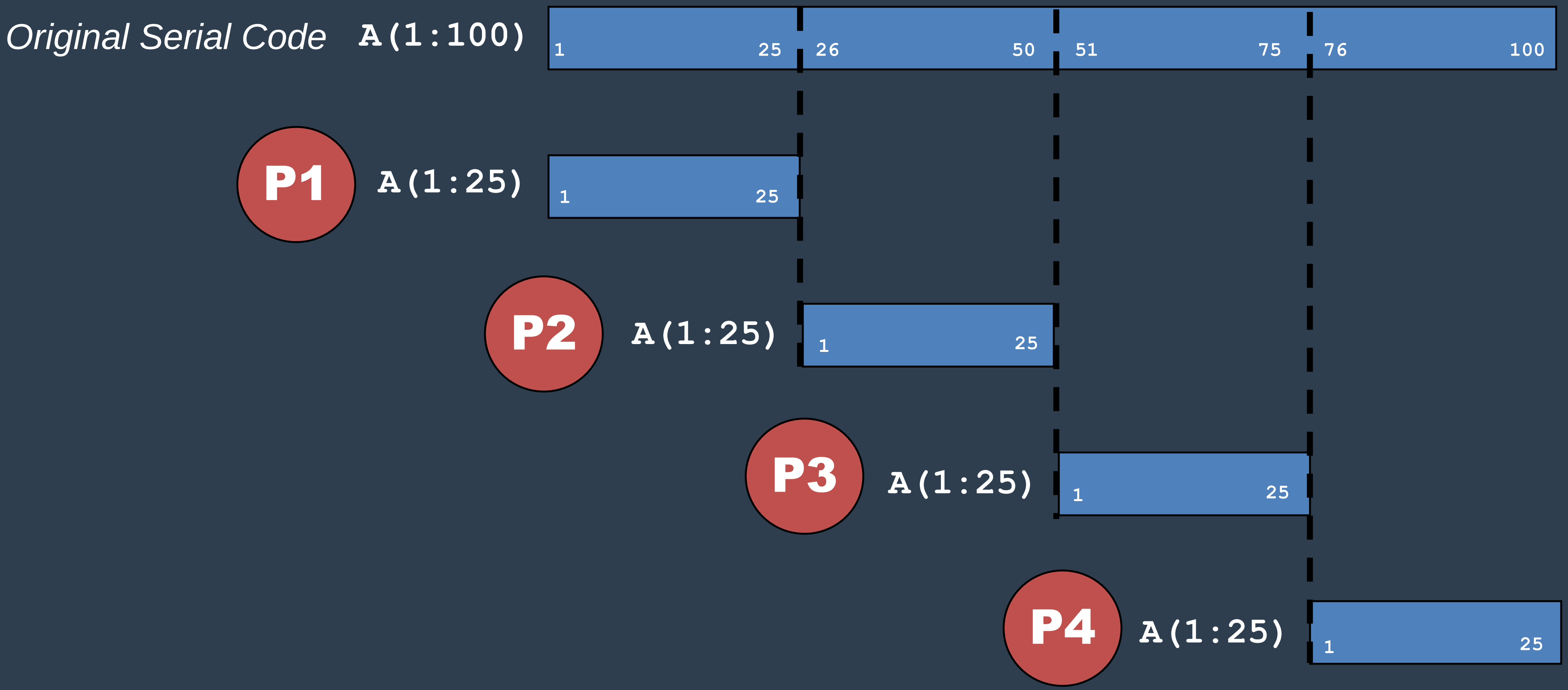
- Each task will compute its subset of the full data set
  - Shouldn't be any problem with load balance (if we decompose the data well!)

- Computation is easy in this example
  - No dependencies between different elements of the arrays
  - If we had expressions like `A(i)=B(i-1)+B(i+1)`
    we would need to be a bit more clever…

A distributed memory approach [2]

- Split the data between processors
  - Each processor will now have 25 (100 / 4) elements per array
  - `REAL, DIMENSION (SIZE/4) :: A,B,C,D,E,F`
- Processor 1
  - `A(1) .. A(25)` which corresponds to
    `A(1) .. A(25)` in the original (single processor code)
- Processor 2
  - `A(1)  .. A(25)` which corresponds to
    `A(26) .. A(50)` in the original (single processor code)
- Processor 3
  - `A(1)  .. A(25)` which corresponds to
    `A(51) .. A(75)` in the original (single processor code)
- Processor 4
  - `A(1)  .. A(25)` which corresponds to
    `A(76) .. A(100)` in the original (single processor code)

Distributed memory data mapping (array “A”)



Distributed memory program

```
INTEGER, PARAMETER      :: NPROC=4
INTEGER, PARAMETER      :: SIZE=100/NPROC
REAL, DIMENSION (SIZE)  :: A,B,C,D,E,F
INTEGER                 :: i

! Read arrays A,B,C,D from a disk
CALL READ_DATA ( A , B , C , D , 100 )

! Calculate E=A+B
DO i = 1 , SIZE
  E(i) = A(i) + B(i)
ENDDO


! Calculate F=C*D
DO i = 1 , SIZE
  F(i) = C(i) * D(i)
ENDDO

! Write results
CALL WRITE_DATA( E , F , 100 )
```

We'll ignore these bits for now… But it is very important and will need attention

How you might want to try and think about it…

- Each task runs its own copy of the program

- Each task's data is private to it

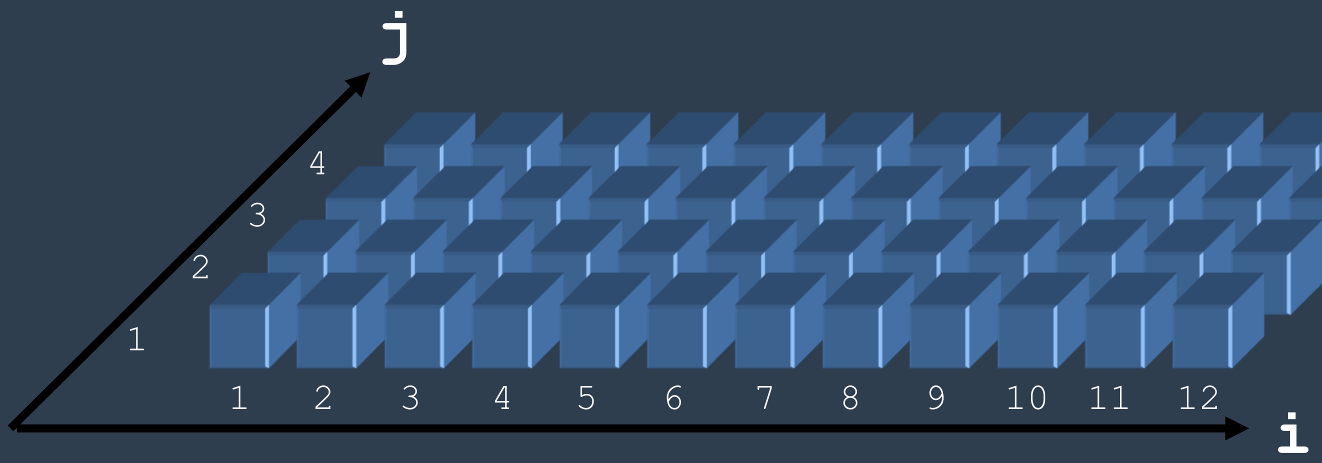
- Each task operates on a subset of the data

- Sometimes there may be dependencies between data on different tasks
  - Tasks must explicitly communicate with one another
  - Message Passing key concepts
    - One task sends a message to one or more other tasks
    - These tasks receive the message
    - Synchronisation : All (or subset of) tasks wait until they have all reached a certain point

How to do it

- Think about how to split (decompose) the data
  - Minimize dependencies (which array dimension should we decompose?)
  - Equal load balance (size of data and/or computation time required)
  - May need different decompositions in different parts of the code
- Add code to distribute input data across tasks
  - And to collect when writing out
- Watch out for end cases / edge conditions
  - For example code which implements a wrap-around at the boundaries
  - First/Last item in a loop isn't necessarily the real "edge" of the data on every task
  - Maybe some extra logic required to check
- Identify data dependencies
  - Communicate data accordingly
  - Add code to transpose data if changing decomposition

Decomposing Data [1]

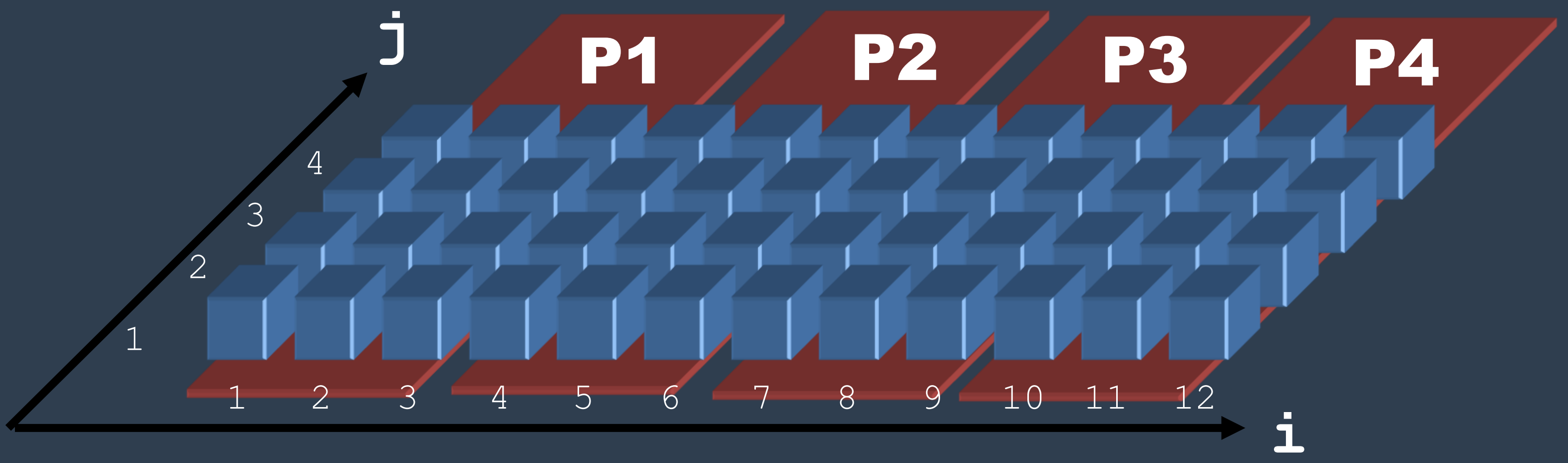



```
REAL, DIMENSION (12,4) :: OLD,NEW

DO j=1,4
  DO i=2,11
    NEW(i,j)=0.5*(OLD(i-1,j)+OLD(i+1,j))
  ENDDO
ENDDO
```

Decomposing Data [2]

- Let's consider decomposing in the "i" dimension…

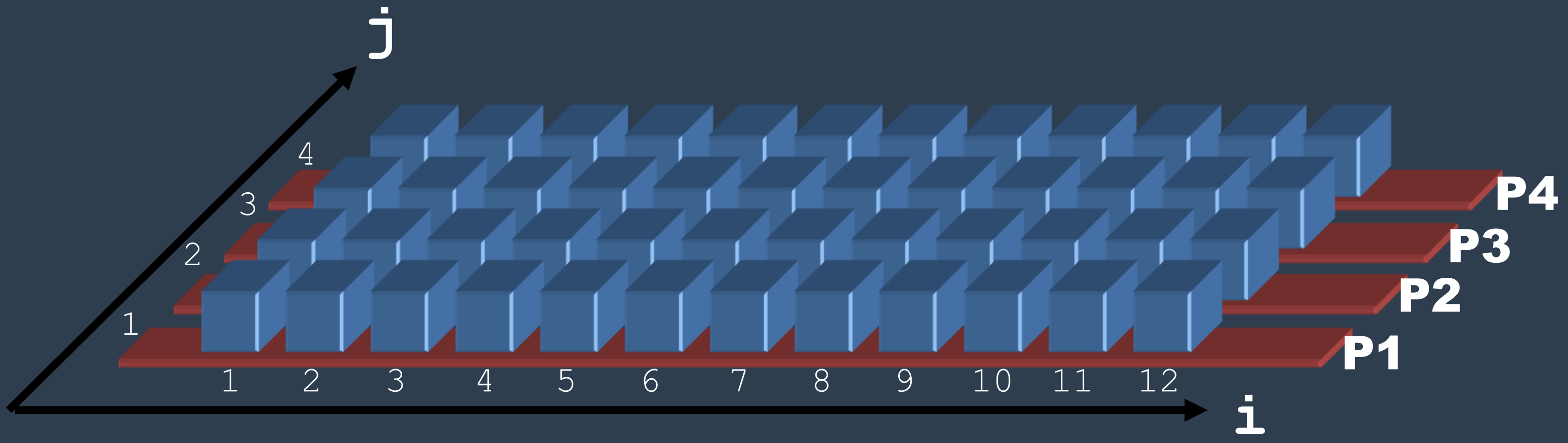



```
NEW(i,j)=0.5*(OLD(i-1,j)+OLD(i+1,j))
```

- How do we calculate element (3,1) – on P1?
  - We need element (2,1) which is on P1 – OK
  - And element (4,1) which is on P2 – how do we get that?
- Message passing will be required

Decomposing Data [3]

- Instead, let’s consider decomposing in the “j” dimension…

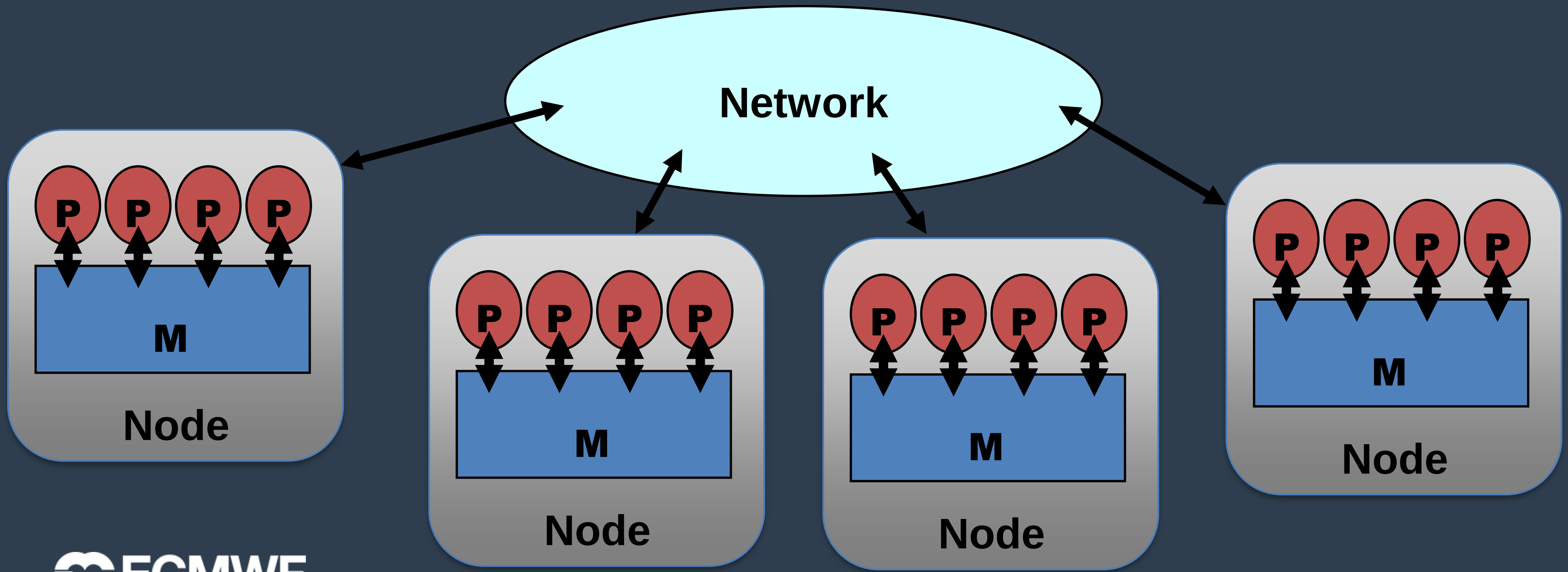



```
NEW(i,j)=0.5*(OLD(i-1,j)+OLD(i+1,j))
```

- Now no communication is required
  - So this is a much better decomposition for this problem
- Real life is rarely this simple unfortunately!
  - Real codes often have data dependencies across all dimensions
  - So we attempt to identify the decomposition which will minimise the overall communication traffic or transpose the data

Hybrid architecture : Shared & Distributed Memory

- Nearly all HPC systems combine architectures
  - Many shared memory “nodes”
    - Each node has processors accessing a single shared memory
    - Each node behaves as a single (compound) processor with distributed memory
- Shared memory programming on a node (OpenMP)
- Distributed memory programming between nodes (Messaging Passing, MPI)



Load Balancing

- Aim to have an equal computational load on each processor
  - Maximum efficiency is gained when all processors are working
- Consequences of poor load balance:
  - Some processors sit idle waiting for others to complete some work – inefficient
  - Run time is determined by the slowest processor

Causes of Load Imbalance

- Different sized data on different processors
  - Array dimensions and NPROC mean it's impossible to decompose data equally between processors
    - Change dimensions, or collapse loop:
      `A(13,7)` -> `A(13*7)`
  - Regular geographical decomposition may not have equal work points (eg. land/sea not uniformly distributed around globe)
    - Different decompositions required

- Different computational load for different data points
  - Physical parameterisations such as convection, short wave radiation
  - Sometimes this load can be predetermined, sometimes it is effectively random or unknowable

Improving Load Balance : Distributed Memory

- Transpose data
  - Change decomposition so as to minimize load imbalance
  - Good solution if we can predict load per point (eg. land/sea)
- Implement a master/slave solution & distribute work dynamically
  - If we don't know the load per point

```
IF (L_MASTER) THEN
  DO chunk=1,nchunks
    Wait for "I'm ready for work" message from a slave
    Send DATA(offset(chunk)) to that slave
  ENDDO
  Send "Finished" message to all slaves
ELSEIF (L_SLAVE) THEN
  WHILE ("Finished" message not received) DO
    Send "I'm ready for work" message to MASTER
    Receive DATA(chunk_size) from MASTER processor
    Compute DATA
    Send DATA back to MASTER
  ENDWHILE
ENDIF
```

Improving Load Balance : Shared memory

- Generally much easier
- In IFS we add an extra “artificial” dimension to arrays
  - Distribute chunks of this dimension to threads
  - Allows arrays to be easily handled using OpenMP
- It allows us write loops like this:

```
REAL, DIMENSION (SIZE/NPROMA,NCHUNKS) :: A,B
! OpenMP : Distribute loop over NPROC (NPROC<=NCHUNKS) processors
! OpenMP : Private variables : chunk,i
DO chunk=1,NCHUNKS
  DO i=1,SIZE/NCHUNKS
    B(i,chunk)=Some_Complicated_Function(A(I,chunk))
  ENDDO
ENDDO
```

- Make NCHUNKS >> NPROC
  - Load balancing will happen automatically
- Other performance benefits by tuning inner loop size

Steps to parallelisation (1)

- Identify parts of the program that can be executed in parallel

- Requires a thorough understanding of the algorithm

- Exploit any inherent parallelism which may exist

- Expose parallelism by
  - Re-ordering the algorithm
  - Tweaking to remove dependencies
  - Complete reformulation to a new more parallel algorithm
  - Google is your friend!
    - You’re unlikely to be the first person to try and parallelise a given algorithm!

Steps to parallelisation (2)

- Decompose the program

- Probably a combination of
  - Data parallelism (hard!) for distributed memory
  - Functional parallelism (easier, hopefully!) for shared memory

- If you're likely to need more than a few 10's of processors to run your problem then a distributed memory solution will be required
  - Shared memory parallelism can be added as a second step, and can be added to individual parts of the algorithm in stages

- Identify the key data structures and data dependencies and how best to decompose them

Steps to parallelisation (3)

- Code development
  - Parallelisation may be influenced by your machine's architecture
    - But try to have a flexible design – you won't use this machine for ever!
  - Decompose key data structures
  - Add new data structures to describe and control the decomposition (eg. offsets, mapping to/from global data, neighbour identification)
  - Identify data dependencies and add the necessary communications

- And finally, the fun bit : CAT & DOG
  - Compile And Test
  - Debug, Optimise and Google!

Some questions to think about

- Which do you think is easier to understand?
  - Distributed memory parallelism (message passing) or Shared memory parallelism
- Which do you think is easier is implement?
- Which do you think might be easier to debug?
  - Can you imagine the kind of errors that you might make and how you might be able to find them?
- Do you think one may be more scalable than the other? Why?
- Why should we have to do all this work anyway. Why can't the compiler do it all for us?

Parallel Computing Game

- A chance to put your understanding of parallel computers to the test!
- Your chance to be part of a “human computer”!
- Two equal sized teams
  - Team A : Distributed Memory Computer
  - Team B : Shared Memory Computer
- Plus a “team” of 1 person representing a non-parallel single-processor computer

- Your task : Add together 36 single-digit integers as fast (& accurately!) as possible

- You will have some time within your teams before we start the game to formulate your “algorithm” or strategy – a set of instructions on how you are going to complete the problem
  - These must be agreed and briefly written down before the game starts

Game : General Rules

- The data will be supplied from a disk
  - Each team has its own disk
  - Each disk is an envelope containing 12 pieces of paper, each piece has 3 integers on it
  - Only one player can come to the disk at a time to get some numbers
  - Each player can take as many pieces of paper as they wish on any visit to the disk
  - A player can come to the disk more than once if they wish to
- The game is played in silence
  - Once the game starts, no talking or hand-gestures are allowed
  - The only communication allowed is via writing as described in your team's rules
  - So all team members must understand and agree on the algorithm before the game starts!
- The final answer (sum of integers) must be supplied written on a sheet of paper to the disk
- Each team will be timed. A penalty of 5 seconds is added for any errors (SUM-TRUTH)*5

Game : Team Rules

- TEAM A : DISTRIBUTED MEMORY
  - Each player must sit at least one empty seat away from their neighbour(s)
  - Each player is supplied with many pieces of blank paper (their distributed “memory”)
  - The only permitted communication is by writing information onto a piece of paper and giving it to any other team member
- TEAM B : SHARED MEMORY
  - All players to sit closely around a shared desk
  - Each player has pieces of blank paper to use if necessary (private variables)
  - There is a single, shared sheet of paper on the desk (shared variable) and a single special pen. The only permitted communication is by writing information onto this piece of paper with the special pen
- TEAM C : SINGLE PROCESSOR
  - Good luck!