# MPI / OpenMP Track IHPCSS 2016, Ljubljana

## Overview

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# Who am I?

- David Henty
  - EPCC (Edinburgh Parallel Computing Centre)
    - University of Edinburgh, Scotland, UK
  - background in theoretical particle physics
    - (computational)
  - at EPCC since 1995
  - in charge of training including our 1-year masters course in HPC, PRACE Advanced Training Centre, ARCHER training, ...
  - generally interested in parallel languages and models
- EPCC runs the UK national supercomputer ARCHER
  - Cray XC30 with 118,000 cores
  - around 70 full time staff
  - a range of work: national systems, research projects, European collaborations, MSc in HPC, commercial software development, ...

# Edinburgh

# ARCHER


archer
EPSRC
archer


EPSRC
Engineering and Physical Sciences Research Council
archer

# Overview

- An introduction to
  - message-passing programming with MPI
  - shared-memory programming with OpenMP
  - hybrid (both MPI and OpenMP at the same time)
- Assumptions
  - you have used MPI
  - you have some knowledge of OpenMP
  - you have looked at the background material:
  - www.xsede.org/web/international-hpc-summer-school/2016-wiki
  - see Hands-on Session Prerequisites -> MPI/OpenMP (Classic Track)
- All exercises are based around the parallel traffic model

# Materials

- Slides on XSEDE wikiw
  - www.xsede.org/web/international-hpc-summer-school/2016-wiki
- Also at: **`tinyurl.com/ihpcss-mpi-openmp`**
- Additional material other than slides:
  - intructions for running on Bridges: **`Bridges-cribsheet.pdf`**
  - MPI/OpenMP exercise sheet: **`traffic-ihpcss16.pdf`**
  - MPI/OpenMP codes: **`IHPCSS-pi.tar`** and **`IHPCSS-traffic.tar`**
  - challenge talk: **`IHPCSS2016_Hybrid_Computing_Challenge.pdf`**
  - challenge code: **`challenge.tar`**

# Timetable: Monday

- 13:30 Introduction and recap
- 14:00 Log on; walkthrough of pi example
- 14:30 Communicators, tags and modes
- 15:00 Break
- 15:30 Non-blocking communications
- 16:15 Practical session: traffic model
- 17:30 Close

# Timetable: Tuesday

- 11:45 OpenMP overview
- 12:15 Walkthrough of pi example
- 12:30 Lunch
- 13:30 Advanced worksharing and orphaning
- 14:15 Practical session: traffic model
- 15:00 Coffee
- 15:30 Hybrid MPI / OpenMP
- 16:15 Practical session
- 17:15 HPC Challenge example
- 17:30 Close

# Lecture / practical rationale

- A challenge to teach an audience with such a wide variety of previous experiences ...

- Practical
  - a range of options from basic to advanced
  - identical parallelisation to HPC challenge so a useful playground

- Lectures
  - I am happy to cover whatever you want to know
  - let me know!

# Message-Passing

Parallel Programming using Processes

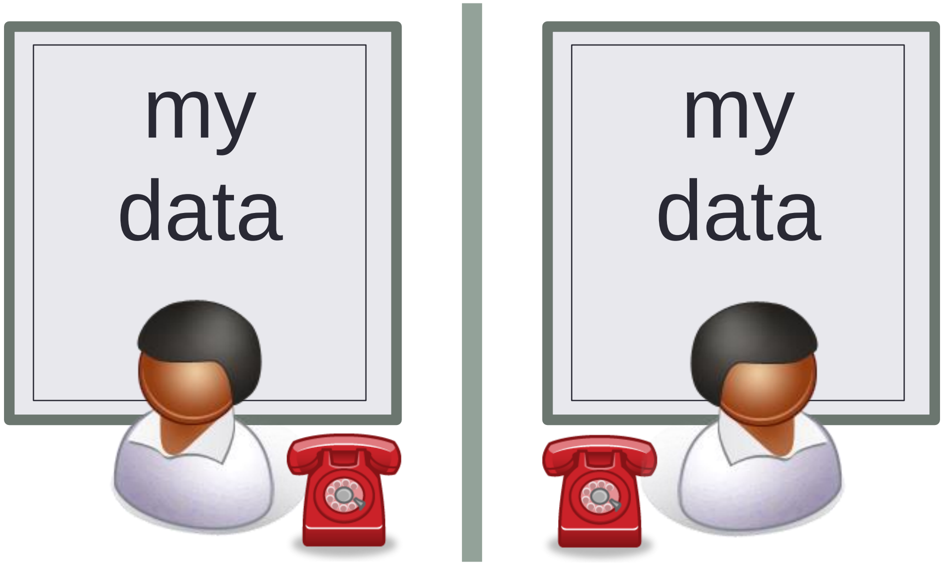
# Outline

- Message-Passing Parallelism
  - processes
  - messages
  - communications patterns

- Practicalities
  - usage on real HPC architectures

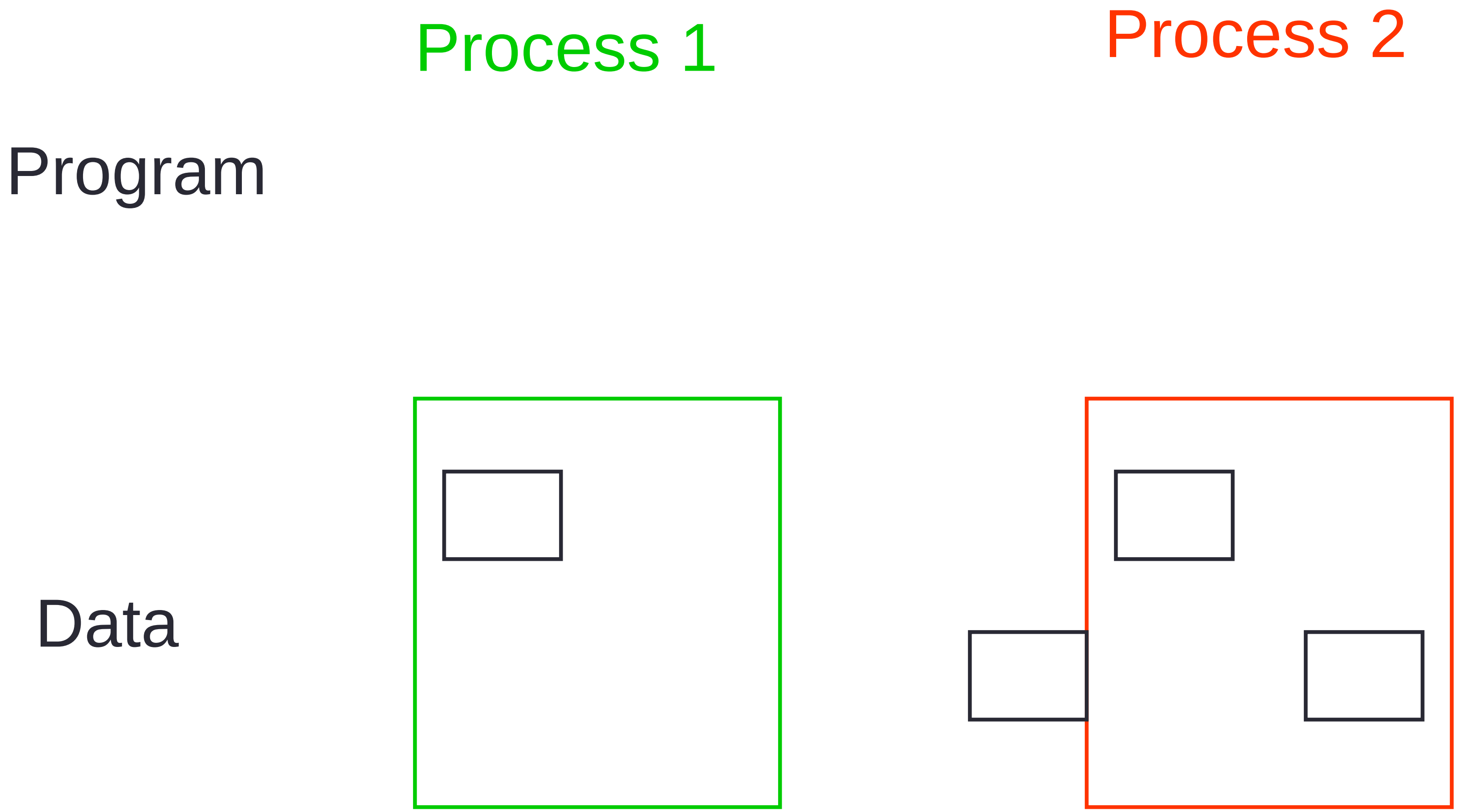
# Analogy

- Two whiteboards in different single-person offices
  - the distributed memory
- Two people working on the same problem
  - the processes on different nodes attached to the interconnect




- How do they collaborate?
  - to work on single problem
- Explicit communication
  - e.g. by telephone
  - no shared data

# Process communication



# Process communication

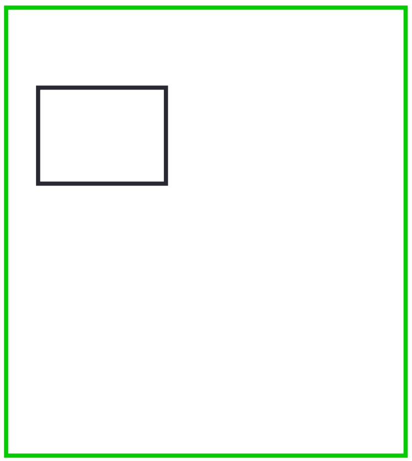
Process 1

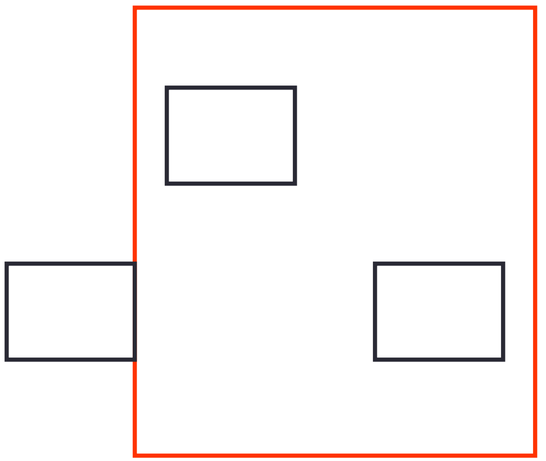
Process 2

Program

a=23

Data





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Program

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a=23
```

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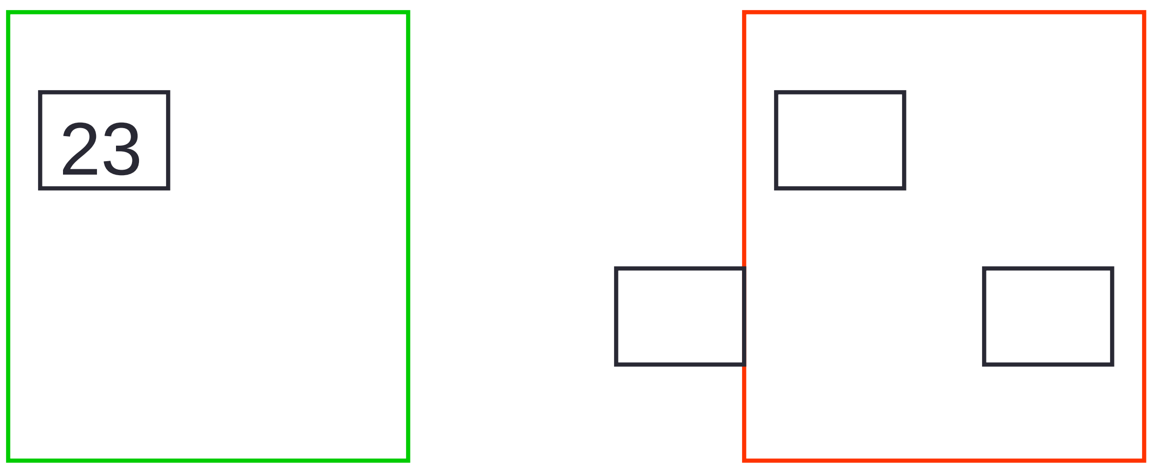


# Process communication

Process 1

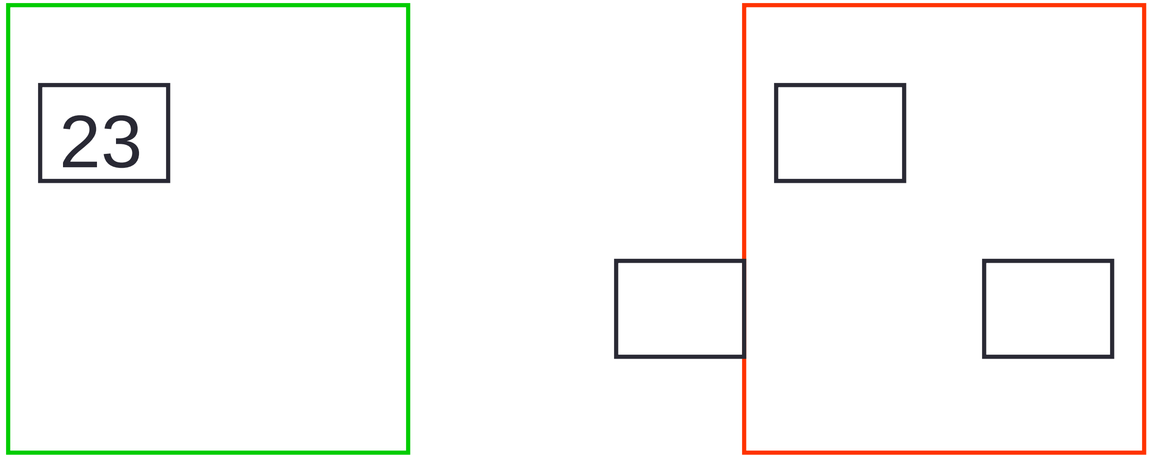
Process 2

Program

```
a=23

Send(2,a)
```

Data



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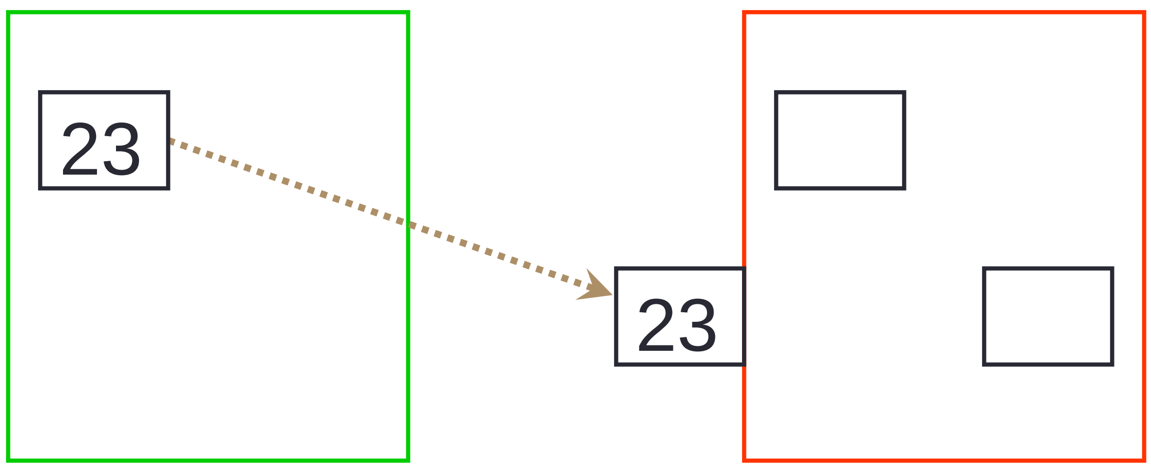
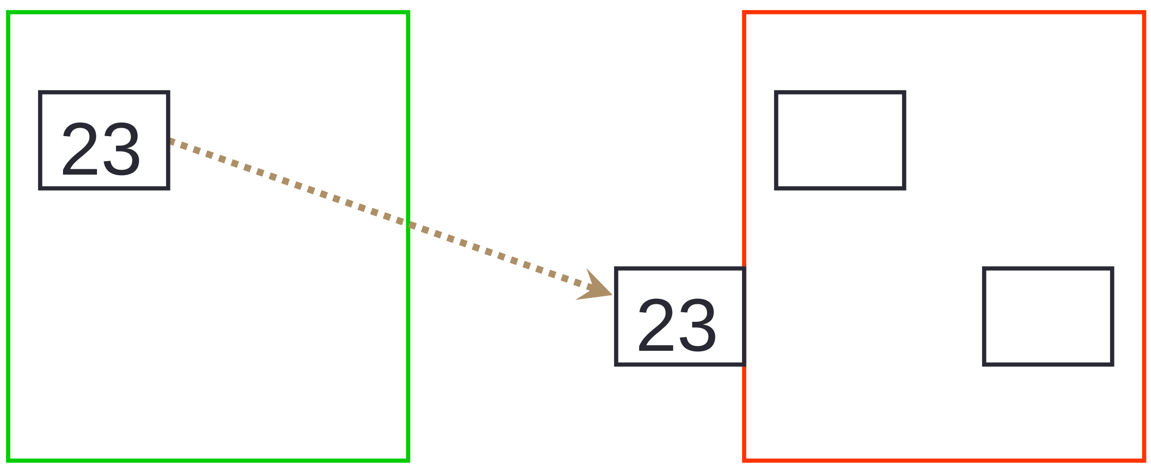


# Process communication

| | Process 1 | Process 2 |
|---|---|---|
| Program | `a=23`<br>`Send(2,a)` | `Recv(1,b)` |
| Data | | |



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Process 1 | Process 2

Program

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Send(2,a)
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Recv(1,b)
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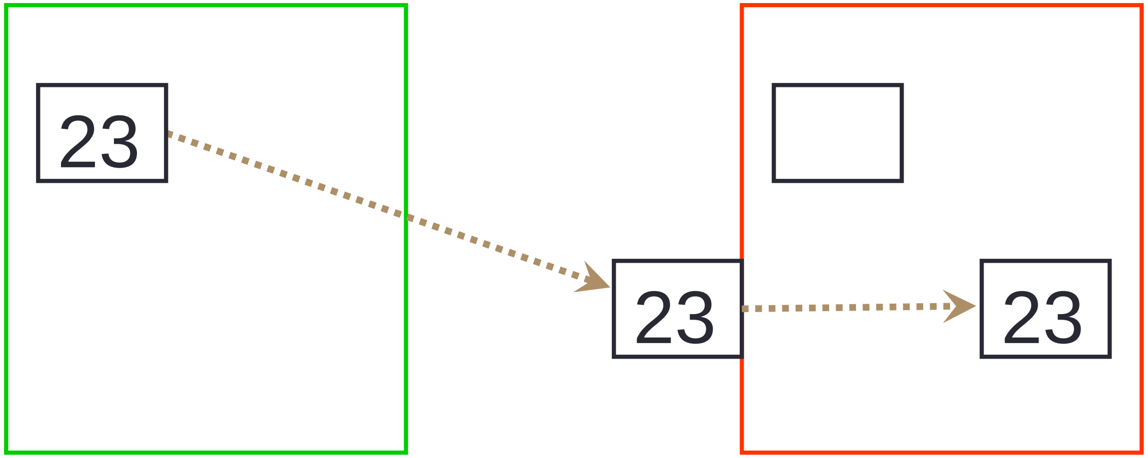

# Process communication

| | Process 1 | Process 2 |
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| Program | `a=23`<br>`Send(2,a)` | `Recv(1,b)`<br>`a=b+1` |

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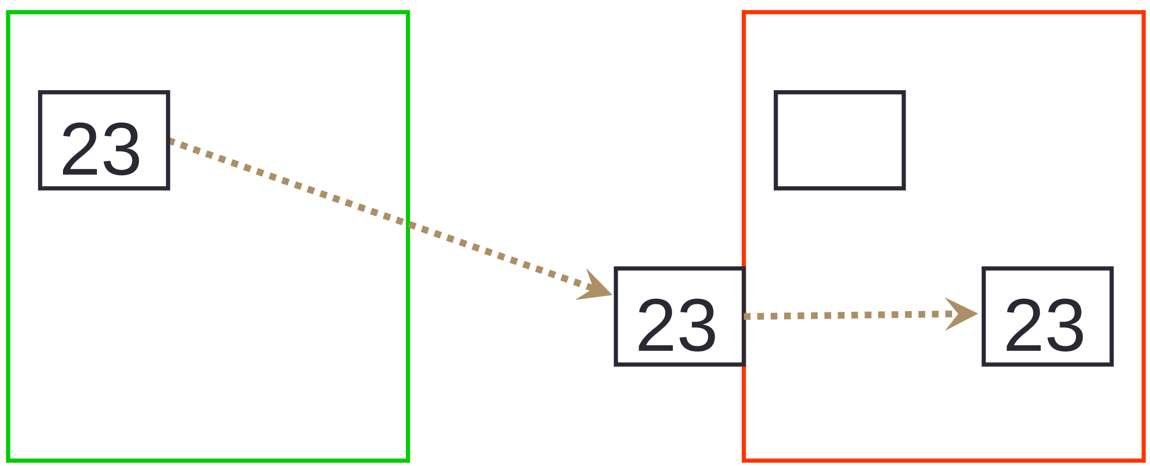

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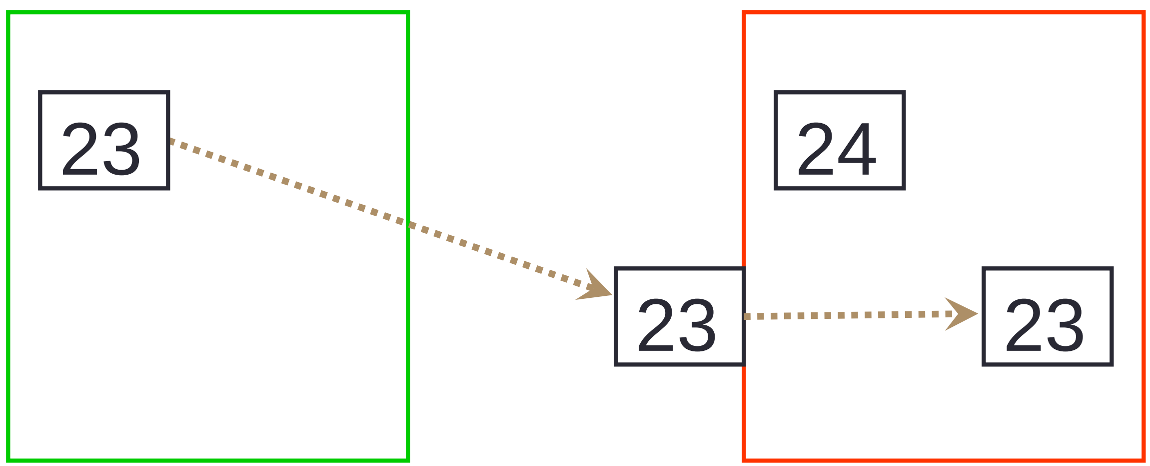


# Synchronisation

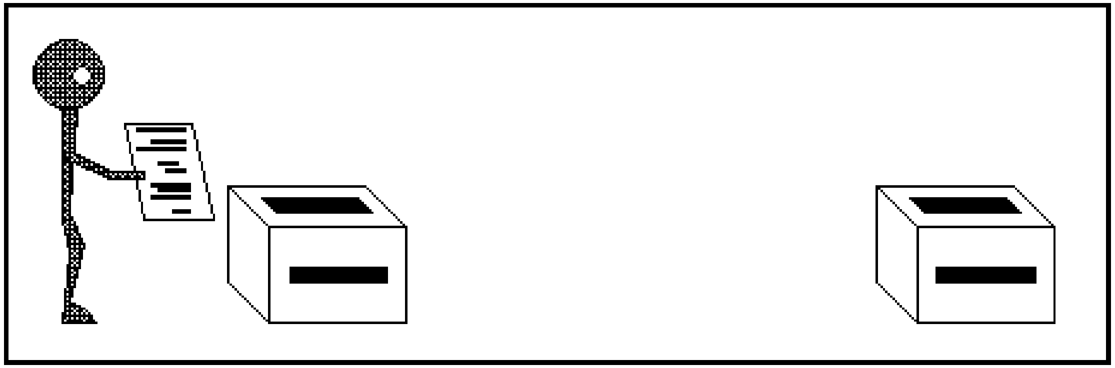
- Synchronisation is automatic in message-passing
  - the messages do it for you
- Make a phone call …
  - … wait until the receiver picks up
- Receive a phone call
  - … wait until the phone rings
- No danger of corrupting someone else's data
  - no shared blackboard

# Communication modes

- Sending a message can either be synchronous or asynchronous
- A synchronous send is not completed until the message has started to be received
- An asynchronous send completes as soon as the message has gone
- Receives are usually synchronous - the receiving process must wait until the message arrives

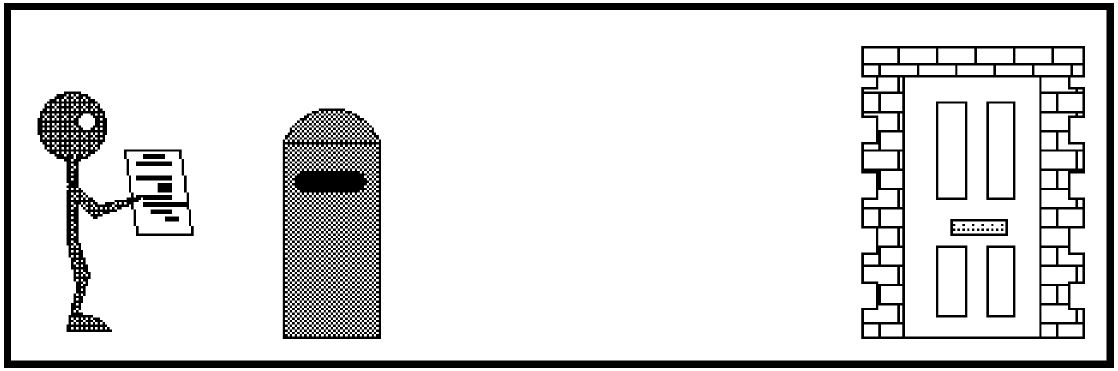
# Synchronous send

- Analogy with faxing a letter.
- Know when letter has started to be received.



# Asynchronous send

- Analogy with posting a letter.
- Only know when letter has been posted, not when it has been received.



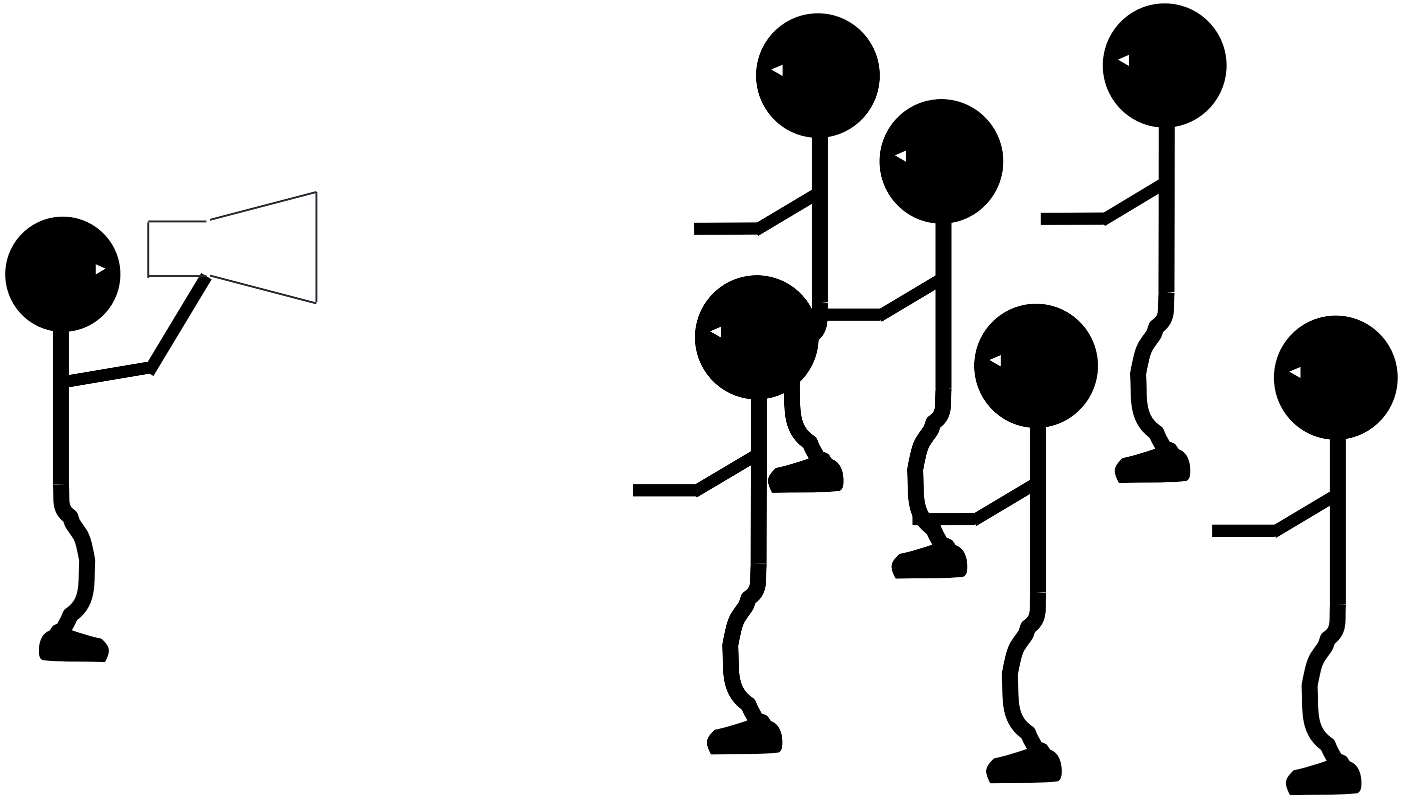
# Point-to-Point Communications

- We have considered two processes
  - one sender
  - one receiver
- This is called point-to-point communication
  - simplest form of message passing
  - relies on matching send and receive
- Close analogy to sending personal emails

# Collective Communications

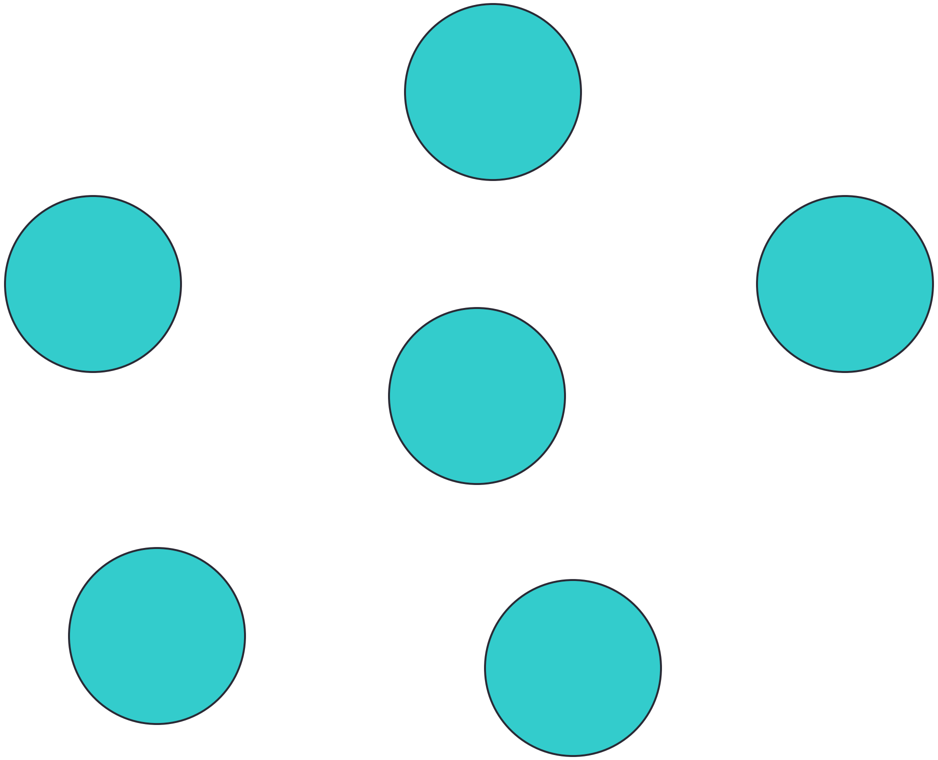
- A simple message communicates between two processes
- There are many instances where communication between groups of processes is required
- Can be built from simple messages, but often implemented separately, for efficiency

# Broadcast: one to all communication



# Broadcast

- From one process to all others



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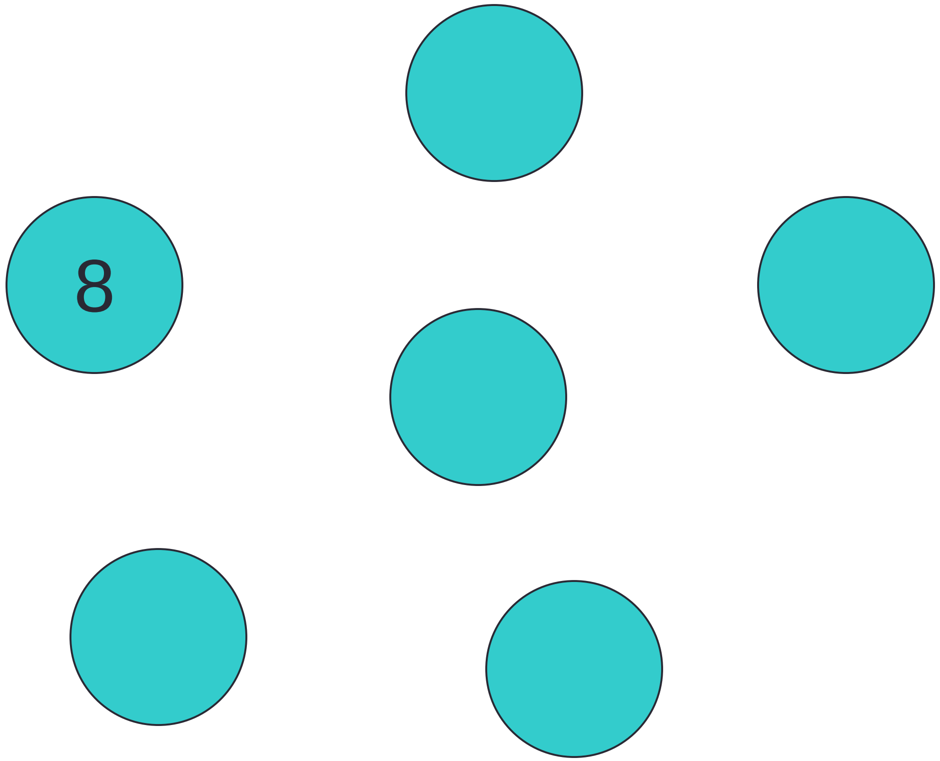

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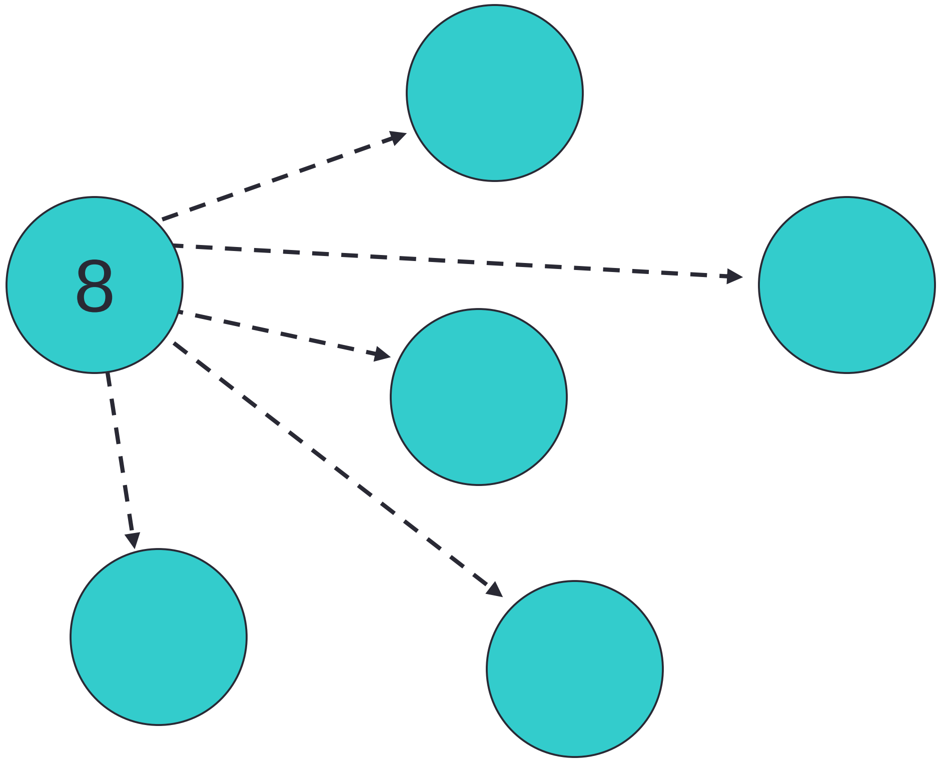

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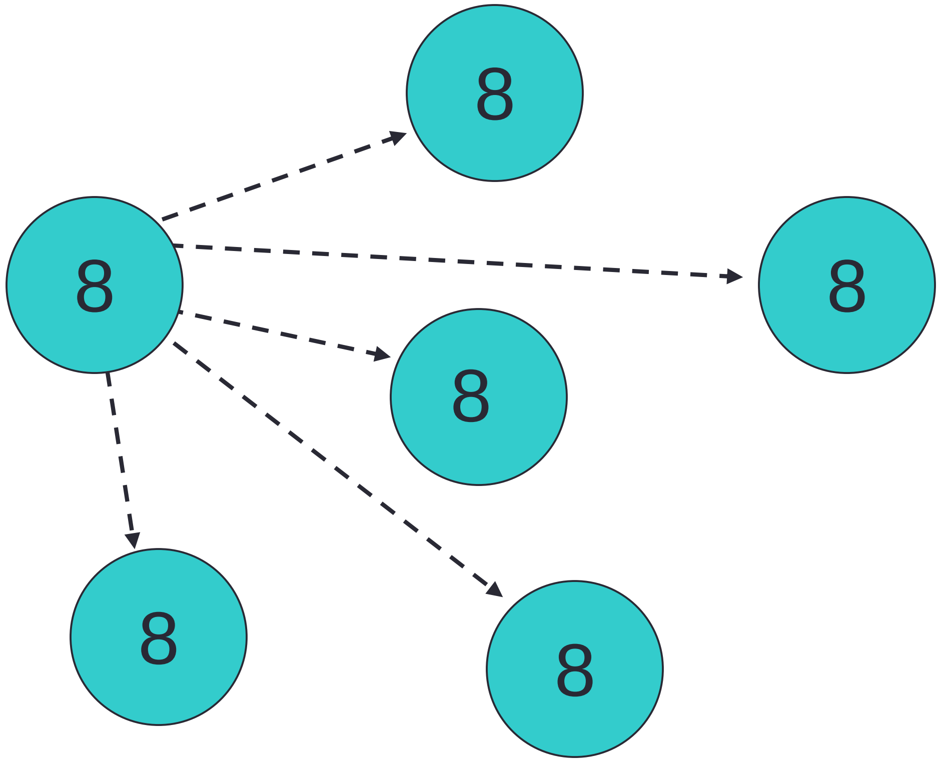
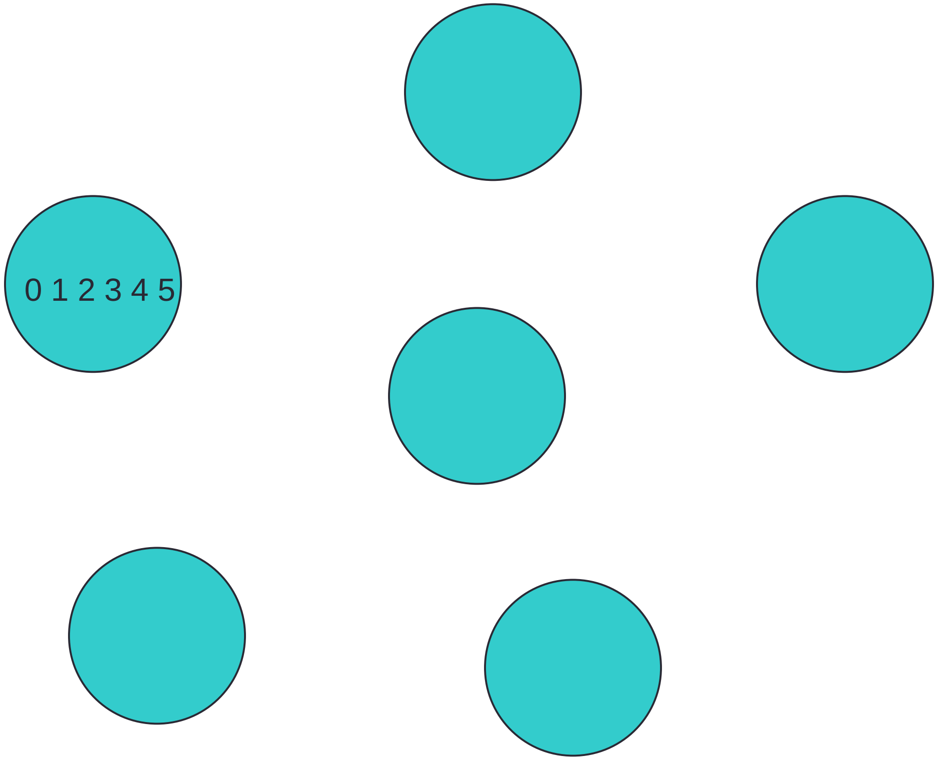


# Scatter

- Information scattered to many processes



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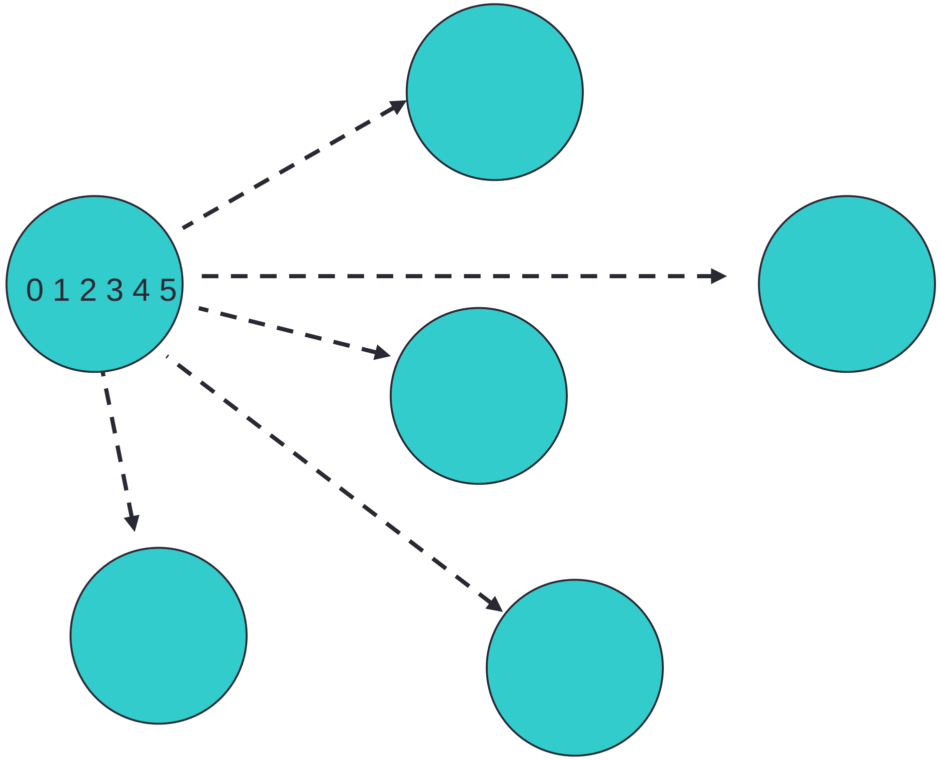

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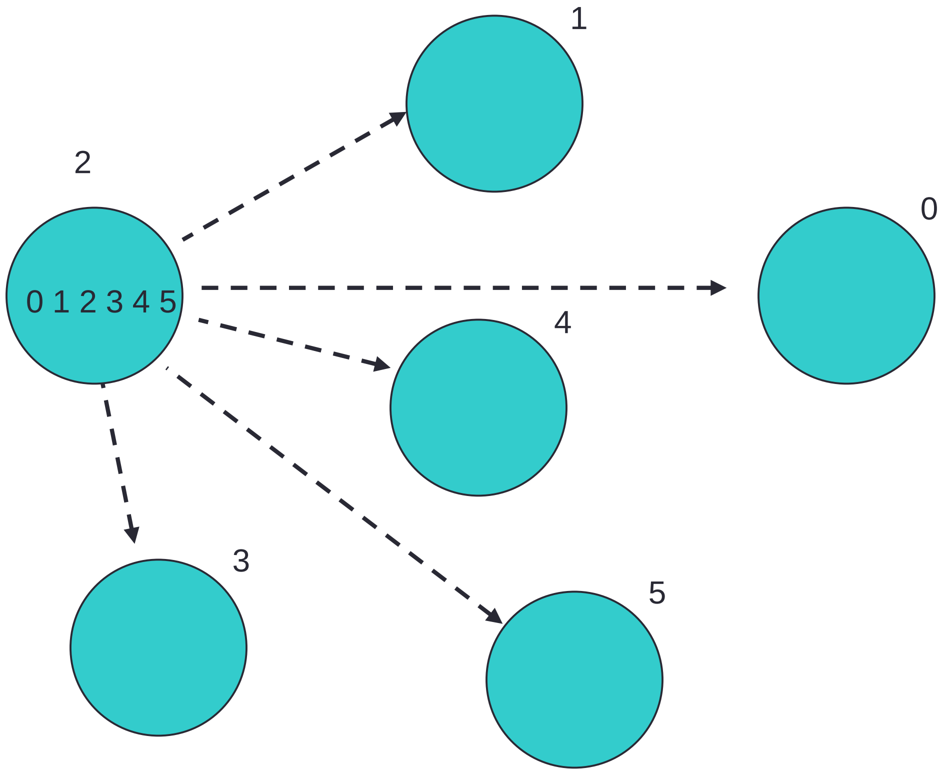
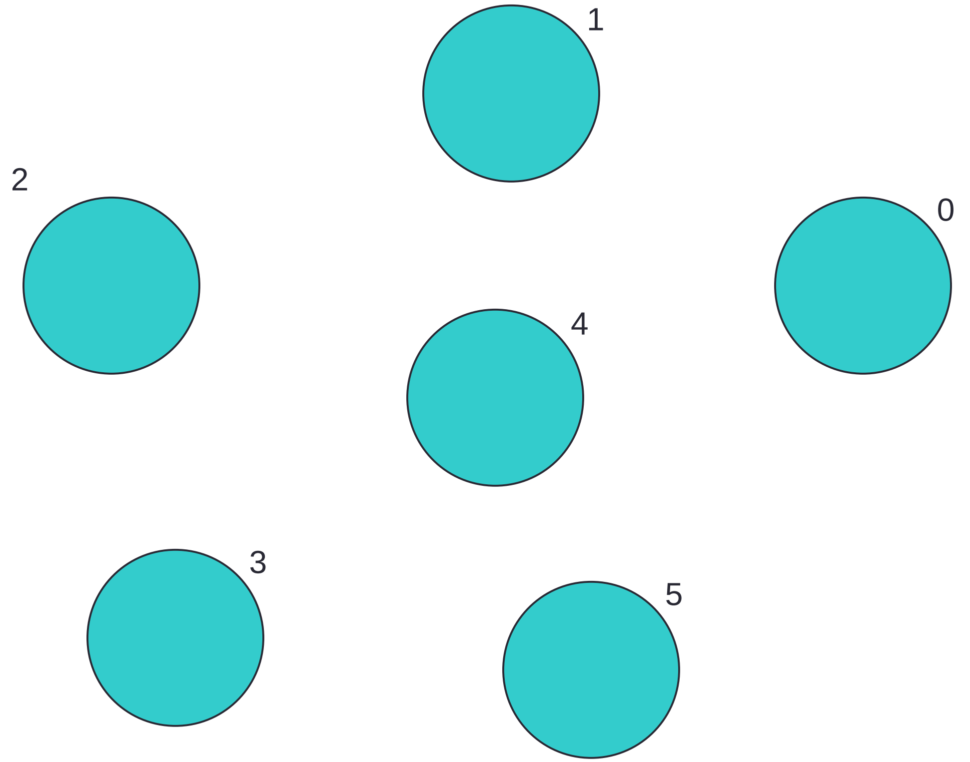


# Gather

- Information gathered onto one process



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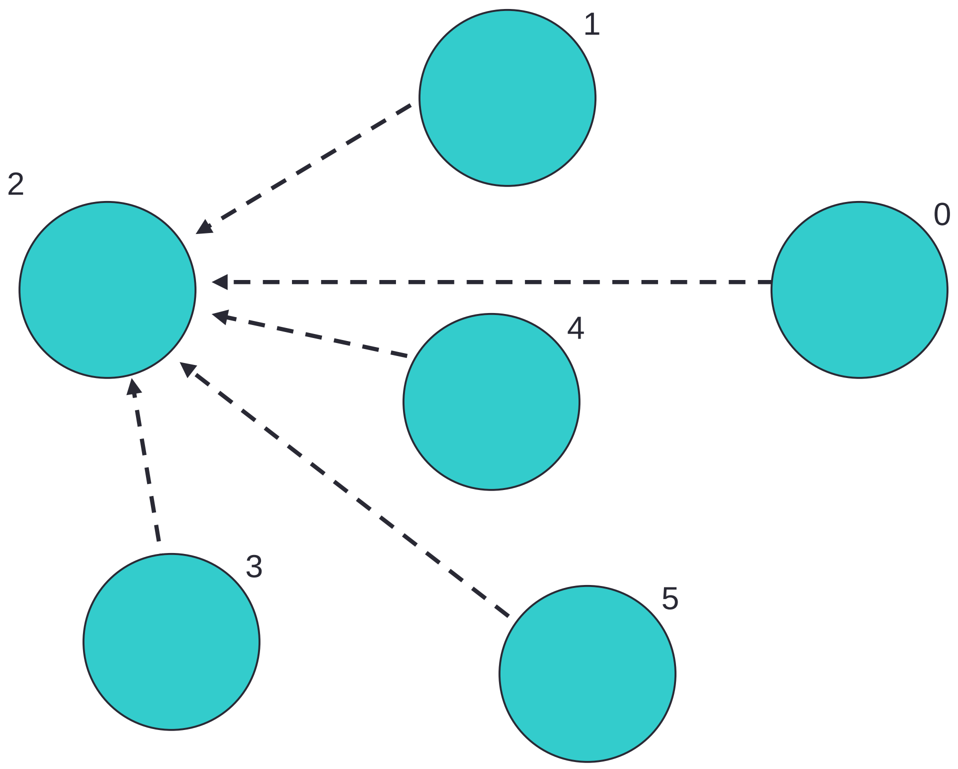

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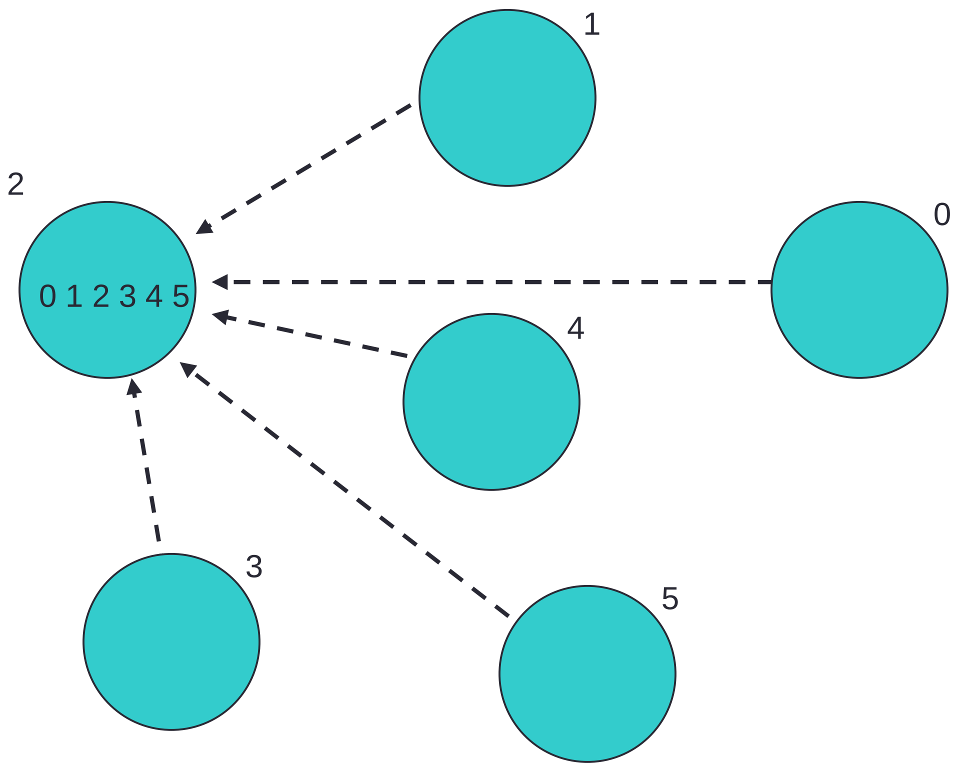
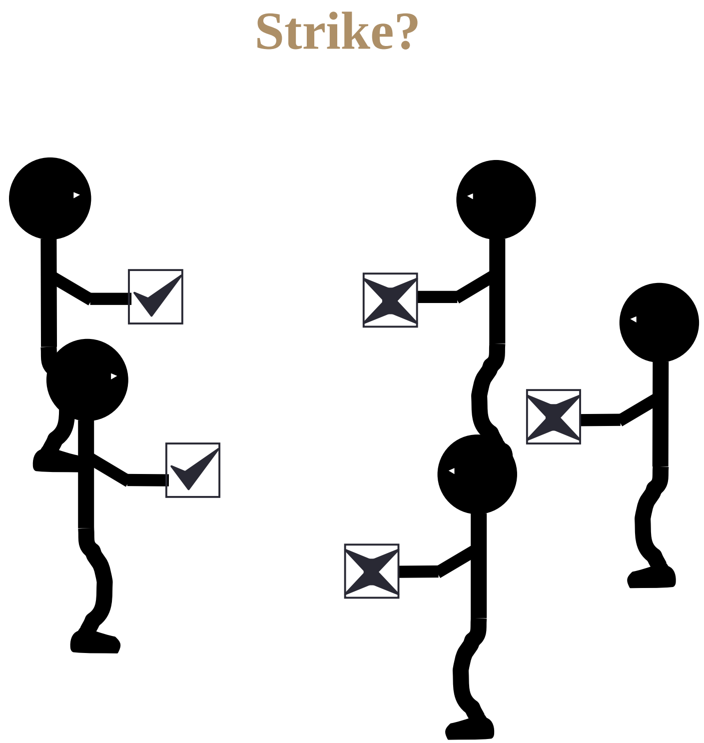


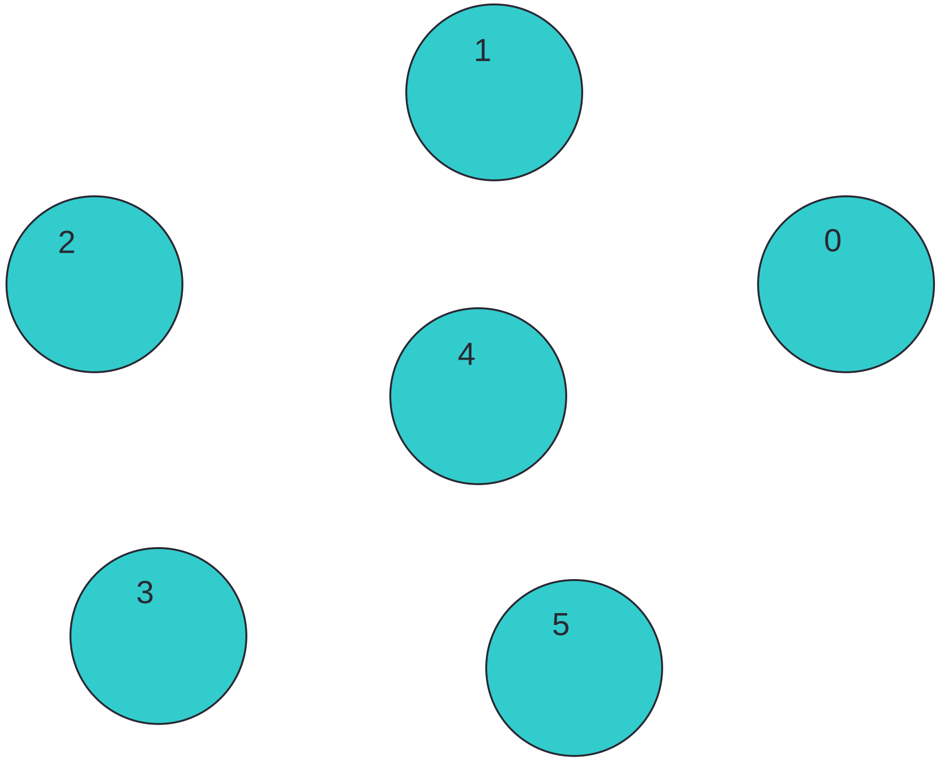
# Reduction Operations

- Combine data from several processes to form a single result



# Reduction

- Form a global sum, product, max, min, etc.



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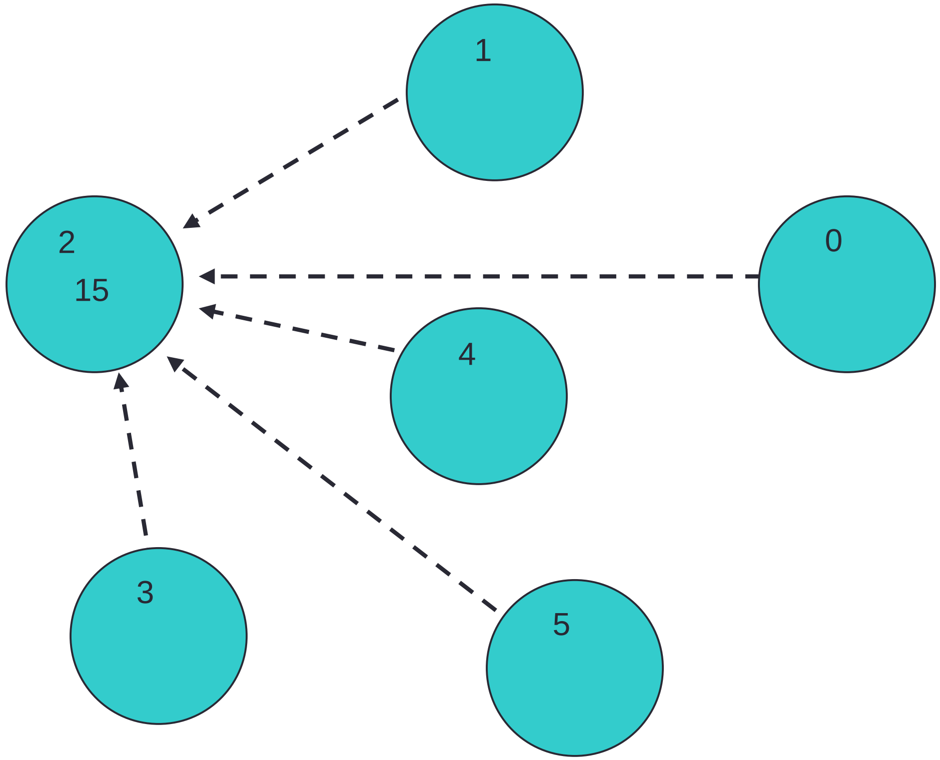
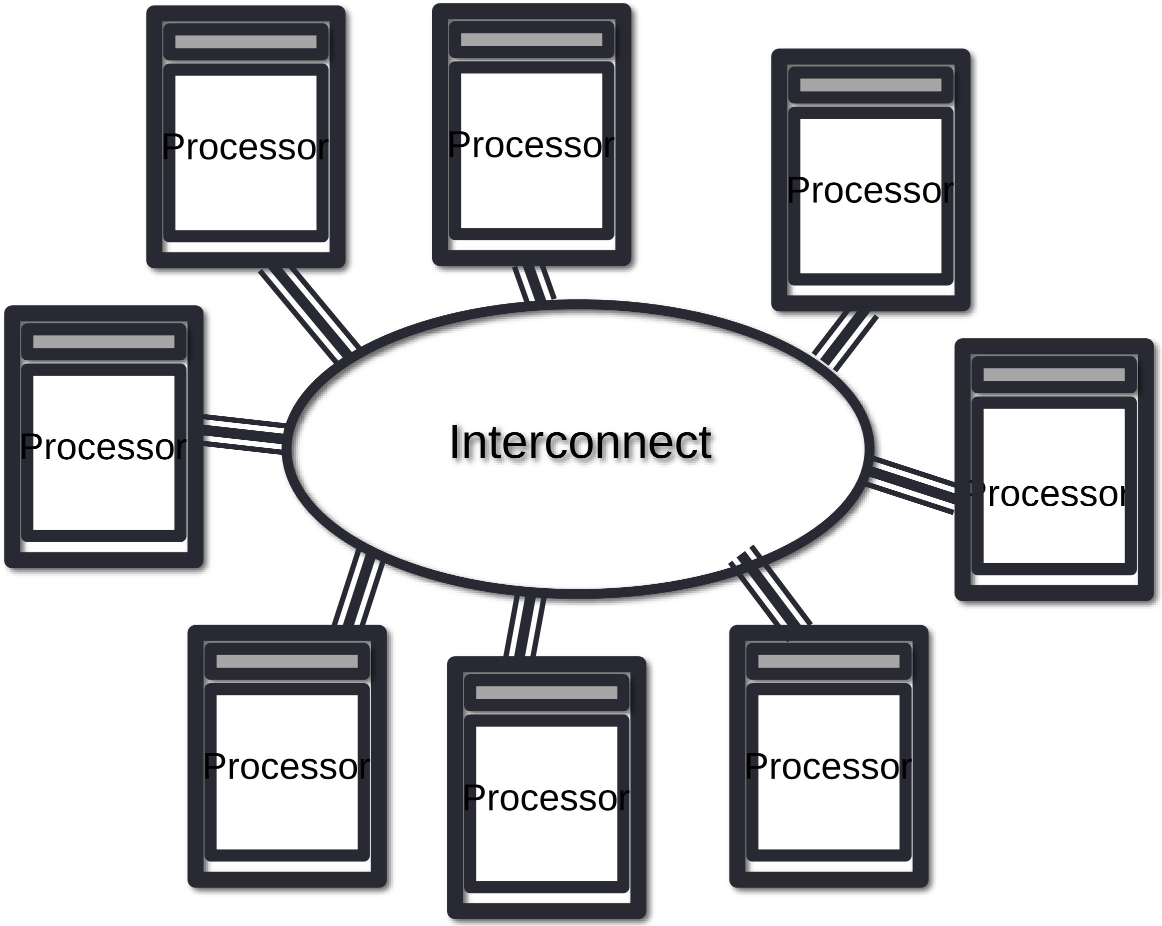
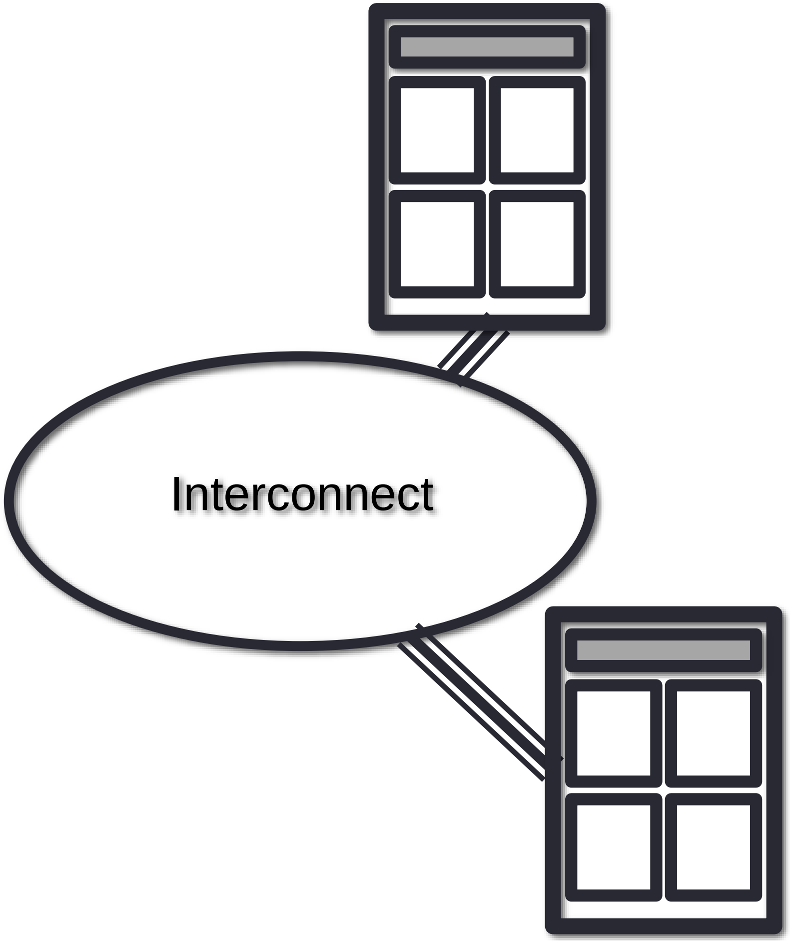


# Hardware




- Natural map to distributed-memory
  - one process per processor-core
  - messages go over the interconnect, between nodes/OS's

# Practicalities

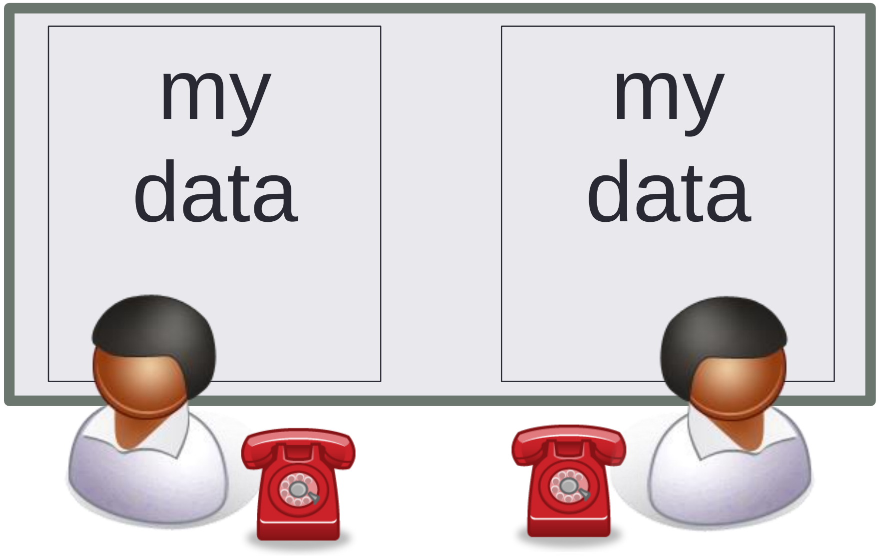



- 8-core machine might only have 2 nodes
  - how do we run MPI on a real HPC machine?
- Mostly ignore architecture
  - pretend we have single-core nodes
  - one MPI process per processor-core
  - e.g. run 8 processes on the 2 nodes
- Messages between processes on the same node are fast
  - but remember they also share access to the network

# Message Passing on Shared Memory

- Run one process per core
  - don't directly exploit shared memory
  - analogy is phoning your office mate
  - actually works well in practice!

- Message-passing programs run by a special job launcher
  - user specifies #copies
  - some control over allocation to nodes



# Issues

- Sends and receives must match
  - danger of deadlock
  - program will stall (forever!)
- Possible to write very complicated programs, but …
  - most scientific codes have a simple structure
  - often results in simple communications patterns
- Use collective communications where possible
  - may be implemented in efficient ways

# Summary (i)

- Messages are the *only* form of communication
  - all communication is therefore explicit
- Most systems use the SPMD model
  - Single Program Multiple Data
  - all processes run exactly the same code
  - each has a unique ID
  - processes can take different branches in the same codes
- Basic communications form is point-to-point
  - collective communications implement more complicated patterns that often occur in many codes

# Summary (ii)

- Message-Passing is a programming model
  - that is implemented by MPI
  - the Message-Passing Interface is a library of function/subroutine calls
- Essential to understand the basic concepts
  - private variables
  - explicit communications
  - SPMD
- Major difficulty is understanding the Message-Passing model
  - a very different model to sequential programming

```
if (x < 0)
   print("Error");
   exit;
```

# Exercise: computing pi

An approximation to the value $\pi$ can be obtained from the following expression

$$\frac{\pi}{4} = \int_0^1 \frac{dx}{1+x^2} \approx \frac{1}{N} \sum_{i=1}^{N} \frac{1}{1+\left(\frac{i-\frac{1}{2}}{N}\right)^2}$$

where the answer becomes more accurate with increasing $N$. Iterations over $i$ are independent so the calculation can be parallelised.

- Will use this as a simple example for MPI and OpenMP
- Traffic Model (see later) is a much better analogue of a real simulation code
  - but pi calculation illustrates basic concepts