Programming with MPI

Parallel programming

Jan Thorbecke

Acknowledgments

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  - Rolf Rabenseifner at the High-Performance Computing-Center Stuttgart (HLRS), University of Stuttgart in collaboration with the EPCC Training and Education Centre, Edinburgh Parallel Computing Centre, University of Edinburgh.
    http://www.hlrs.de/home/
    https://www.epcc.ed.ac.uk

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- http://mpitutorial.com

Contents

Amdahl's Law

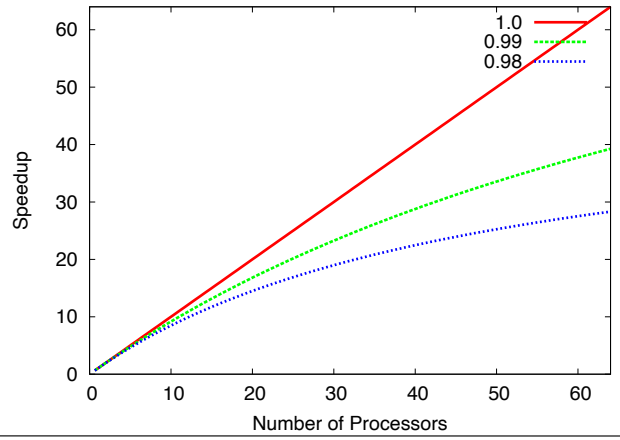
- Describes the relation between the parallel portion of your code and the expected speedup

$$speedup = \frac{1}{(1-P) + \frac{P}{N}}$$

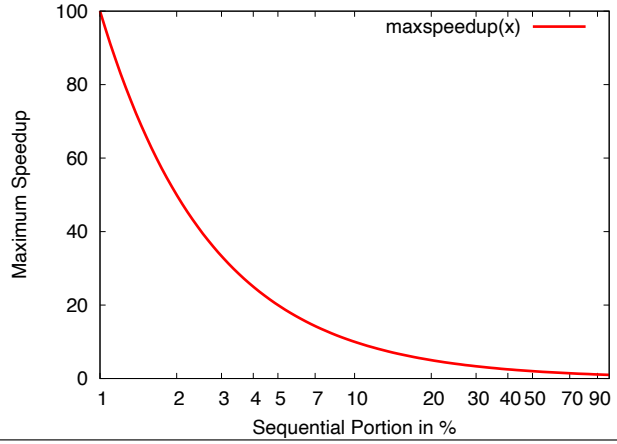
- P = parallel portion
- N = number of processors used in parallel part

- P/N is the ideal parallel speed-up, it will always be less

Amdahl's Law

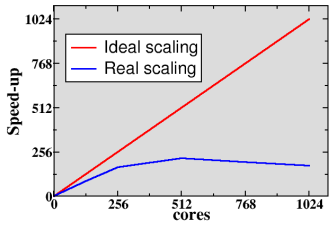


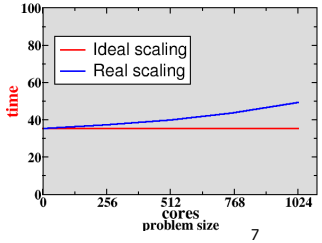
Amdahl's Law



Concepts

- Strong parallel scaling
  - constant problem size
  - execution time decreases in proportion to the increase in the number of cores
  - shortens the time to solve a problem
- Weak parallel scaling
  - increasing problem size
  - execution time remains constant when number of cores increases in proportion to the problem size
  - enables to solve larger problems

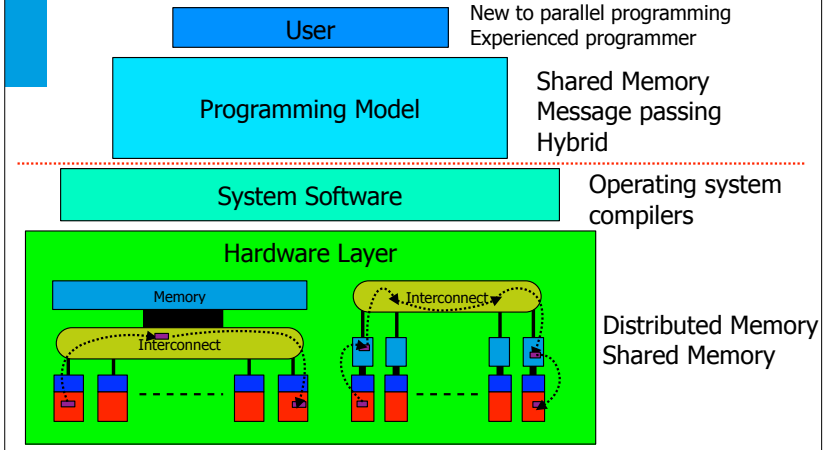




Parallel Programming Models

- Shared Memory
  - tasks share a common address space, which they read and write asynchronously.
- Threads
  - a single process can have multiple, concurrent execution paths. Example implementations: POSIX threads & **OpenMP**
- Message Passing
  - tasks exchange data through communications by sending and receiving messages. Example: MPI
- Data Parallel languages
  - tasks perform the same operation on their partition of work. Example: Co-array Fortran (CAF), Unified Parallel C (UPC), Chapel
- Hybrid
  - MPI + OpenMP

Programming Models



Parallel Programming Concepts

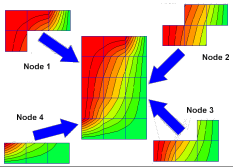
- Work distribution
  - Which parallel task is doing what?
  - Which data is used by which task?
- Synchronization
  - Do different parallel tasks meet?
- Communication
  - Is communication between parallel parts needed?
- Load Balance
  - Does every task has the same amount of work?
  - Are all processors of the same speed?

Distributing of Work and/or Data

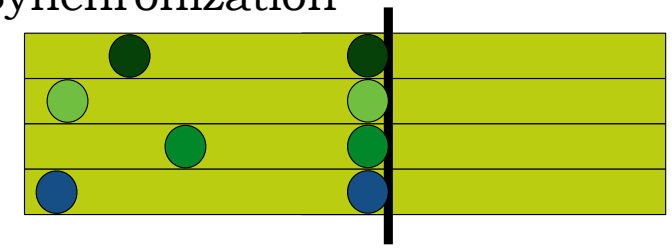
- Work decomposition
  - based on loop counter
- Data decomposition
  - all work for a local portion of the data is done by the local processor
- Domain decomposition
  - decomposition of work and data

```
do i=1,100
  1: i=1,25
  2: i=26,50
  3: i=51,75
  4: i=76,100

A(1:10,1:25)
A(1:10,26:50)
A(11:20,1:25)
A(11:20,25:50)
```



Synchronization



- Synchronization: all parallel processes must reach this point
  - causes overhead
  - idle time, when not all tasks are finished at the same time: load imbalance

Communication

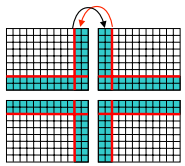
- communication is necessary on the boundaries

```
do i=2,99
   b(i) = b(i) + h*(a(i-1)-2*a(i)+a(i+1))
end do

e.g. b(26) = b(26) + h*(a(25)-2*a(26)+a(27))
```

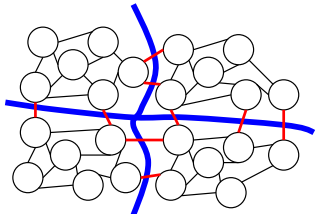
A(1:25)
A(26:50)
A(51:75)
A(76:100)

- domain decomposition



Load Imbalance

- Load imbalance is the time that some processors in the system are idle due to:
  - less parallelism than processors
  - unequal sized tasks together with too little parallelism
  - unequal processors

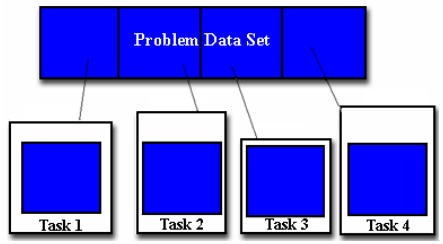


Examples of work distribution

- Domain Decomposition
- Master Worker
- Task Decomposition

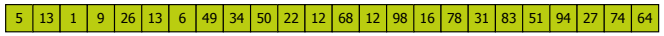
Domain Decomposition

- First, decide how data elements should be divided among processors
- Second, decide which tasks each processor should be doing



Domain Decomposition

Find the largest element of an array



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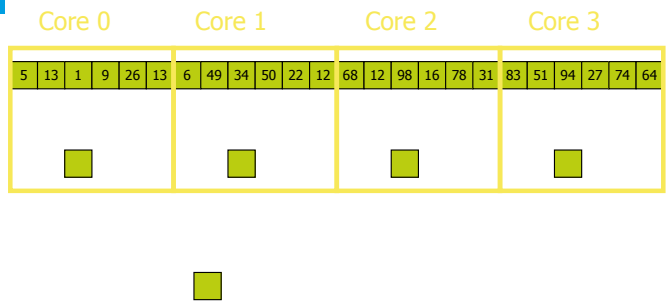

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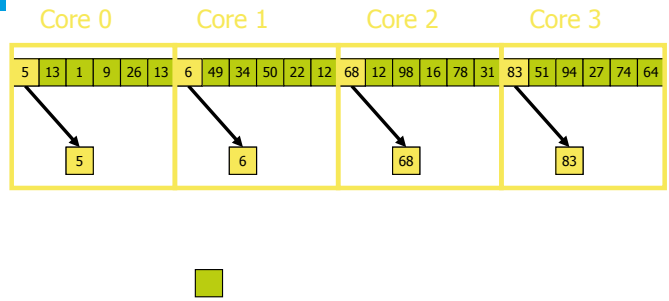

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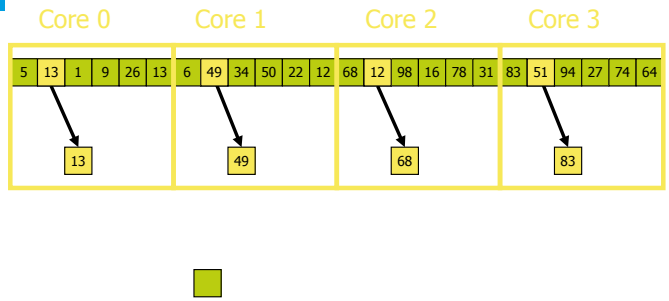

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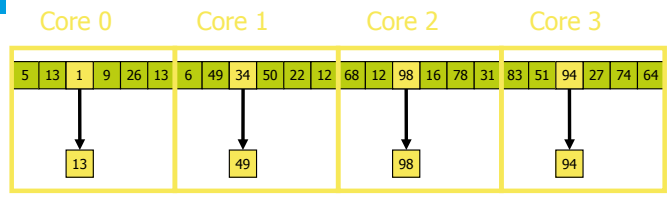

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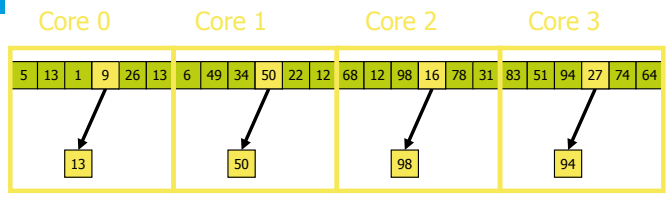

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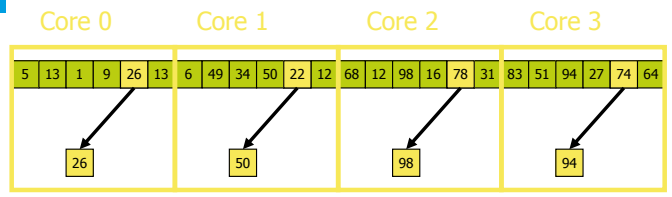

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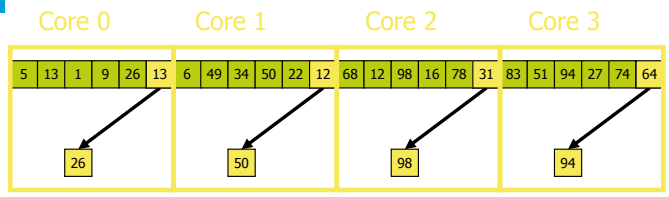

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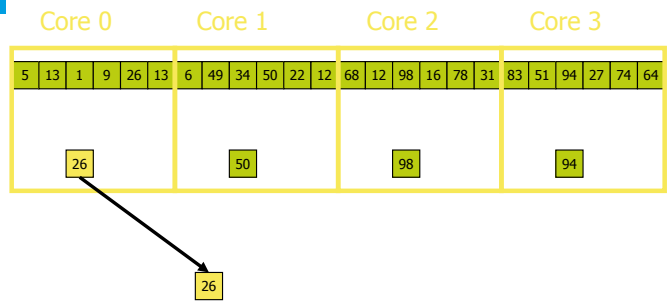

TU Delft

Domain Decomposition

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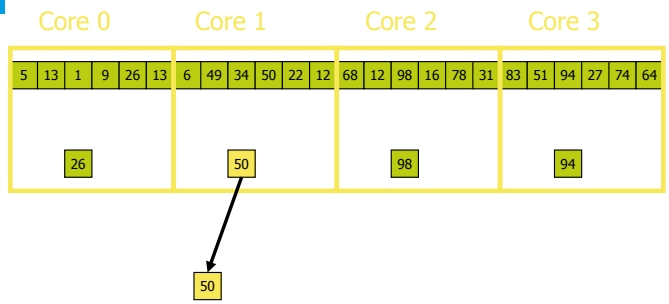

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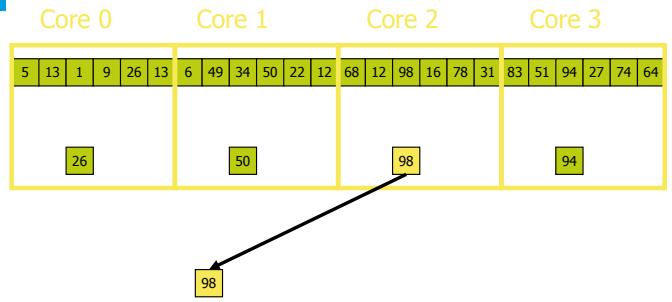

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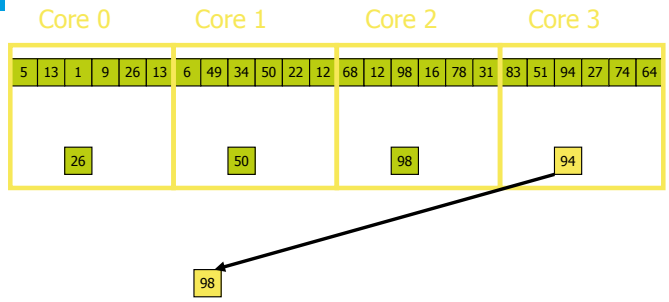

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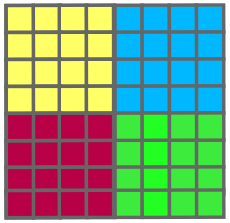
Domain decomposition of sum

- Data is distributed to processor cores
- Each core performs (nearly) identical tasks with different data
- Example: summing the elements of an 2 D array

core 1: ∑= core 2: ∑=

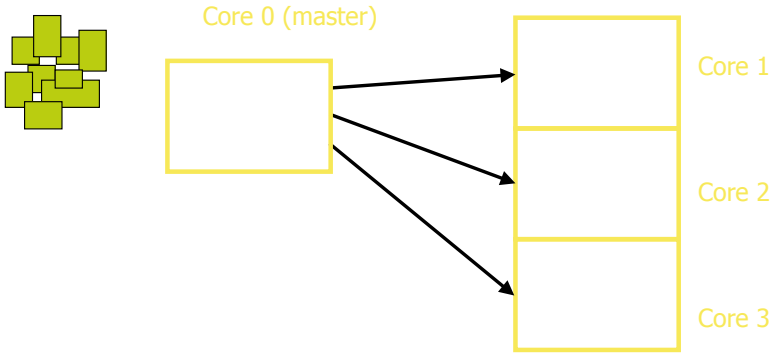


core 3: ∑= core 4: ∑=

- Each core sums it's part of the array
- The individual sums have to be combined in the end

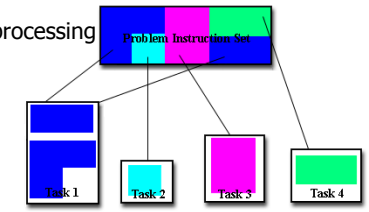
Master Worker

Get a pile of work done



Task/Functional Decomposition

- The problem is decomposed according to the work that must be done. Each task then performs a portion of the overall work.
- Divide computation based on natural set of independent tasks
  - Assign data for each task as needed
- Example: pipeline seismic data pre-processing
  - static-correction
  - deconvolution
  - nmo correction
  - stacking
  - ....



OpenMP™

What Is OpenMP?

- Compiler directives for multithreaded programming
- Easy to create threaded Fortran and C/C++ codes
- Supports data parallelism model
- Portable and Standard
- Incremental parallelism
  - Combines serial and parallel code in single source

Directive based

- Directives are special comments in the language

– Fortran fixed form: `!$OMP, C$OMP, *$OMP`

– Fortran free form: `!$OMP`

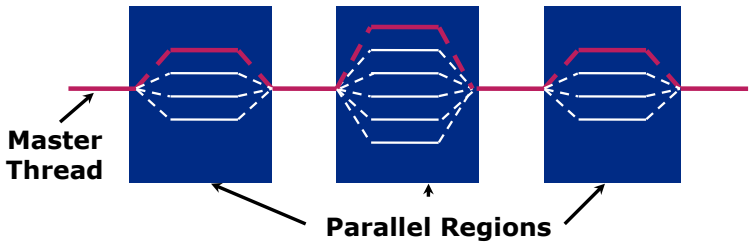
Special comments are interpreted by OpenMP compilers

```
      w = 1.0/n
      sum = 0.0
!$OMP PARALLEL DO PRIVATE(x) REDUCTION(+:sum)
      do I=1,n
        x = w*(I-0.5)
        sum = sum + f(x)
      end do
      pi = w*sum
      print *,pi
      end
```

Comment in Fortran but interpreted by OpenMP compilers

Programming Model

- Fork-join parallelism:
  - Master thread spawns a team of threads as needed
  - Parallelism is added incrementally: the sequential program evolves into a parallel program

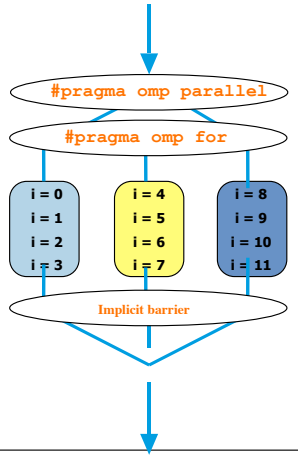


Work-sharing Construct

```
#pragma omp parallel
#pragma omp for
   for(i = 0; i < 12; i++)
      c[i] = a[i] + b[i]
```

Threads are assigned an independent set of iterations

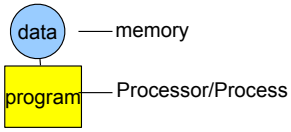
Threads must wait at the end of work-sharing construct



MPI

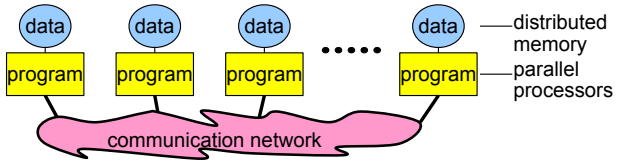
The Message-Passing Programming model

- Sequential Programming



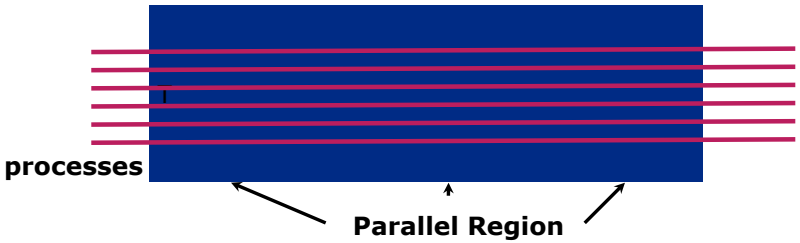
A processor may run many processes

- Message-Passing Programming



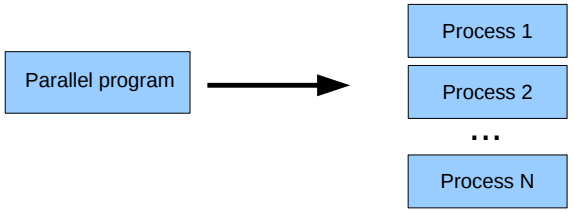
Programming Model

- Explicit parallelism:
  - All processes starts at the same time at the same point in the code
  - Full parallelism: there is no sequential part in the program



Execution model

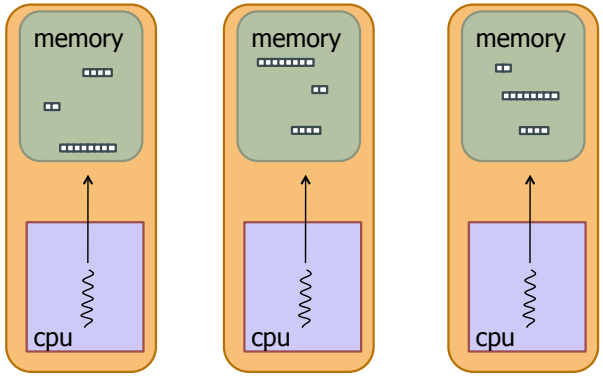
- Parallel program is launched as set of **independent, identical processes**



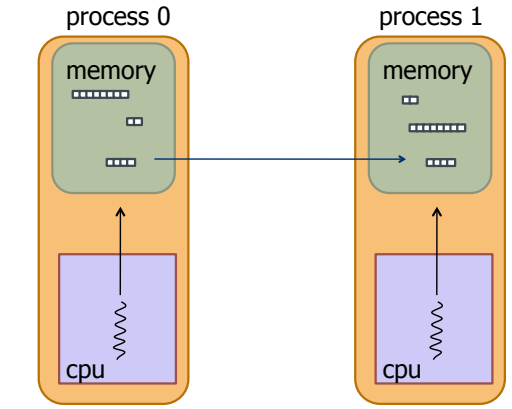
- All the processes contain the same program code and instructions
- Processes can reside in different nodes or even in different computers
- The way to launch parallel program is implementation dependent
  - mpirun, mpiexec, aprun, poe, ...

MPI

processes



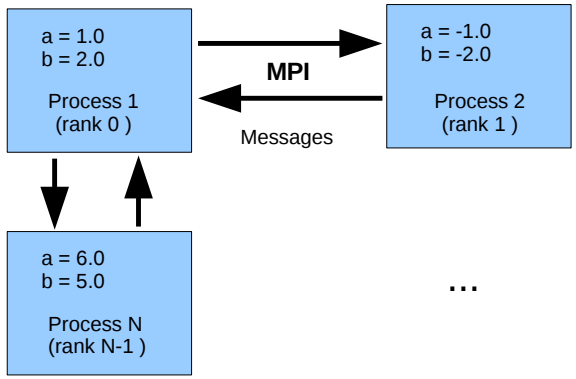
MPI




```
MPI_Send(a,...,1,…)  MPI_Recv(a,...,0,…)
```


Data Model

- All variables and data structures are local to the process
- Processes can exchange data by sending and receiving messages



MPI advantages

- Mature and well understood
  - Backed by widely-supported formal standard (1992)
  - Porting is "easy"
- Efficiently matches the hardware
  - Vendor and public implementations available
- User interface:
  - Efficient and simple
  - Buffer handling
  - Allow high-level abstractions
- Performance

MPI learning

- MPI 3.1 includes many features beyond message passing

- Execution control environment depends on implementation

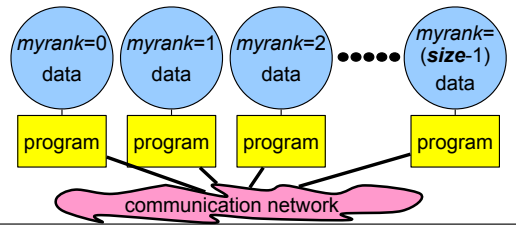
Basic Concepts

Work Distribution

- All processors run the same executable.
- Parallel work distribution must be explicitly programmed into the algorithm:
  - domain decomposition
  - master worker

Data and Work Distribution

- To communicate together mpi-processes need identifiers: rank = identifying number
- all distribution decisions are based on the rank
  - i.e., which process works on which data

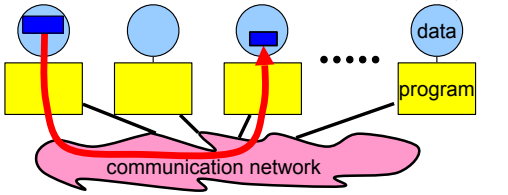


Message passing

- Point-to-Point
- Requires explicit commands in program
  - Send, Receive
- Must be synchronized among different processors
  - Sends and Receives must match
- Multi-processor communications
  - e.g. broadcast, reduce

Message passing

- Messages are packets of data moving between sub-programs
- Necessary information for the message passing system:
  - sending process – receiving process } i.e., the ranks
  - source location – destination location
  - source data type – destination data type
  - source data size – destination buffer size

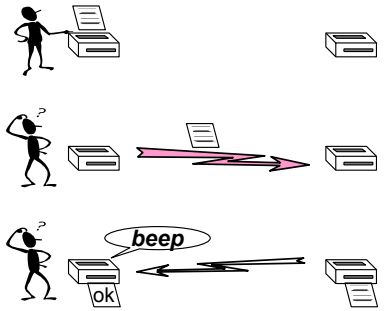


Point-to-Point Communication

- Simplest form of message passing.
- One process sends a message to another.
- Different types of point-to-point communications
  - **synchronous** send
  - buffered = **asynchronous** send

Synchronous Sends fax(?)

- The sender gets an information that the message is received.
- Analogue to the beep or okay-sheet of a fax.



Synchronous Sends in

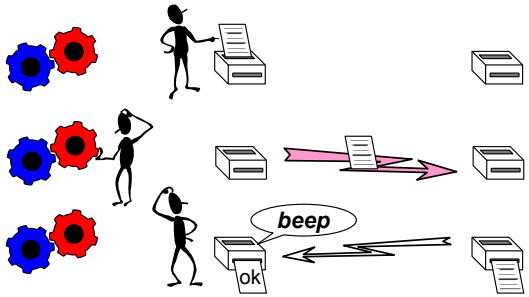
- Check marks will appear next to each message you send. Here's what each one indicates:
  - ✓ The message was successfully sent.
  - ✓✓ The message was successfully delivered to the recipient's phone or any of their linked devices.
  - ✓✓ The recipient has read your message.

Blocking Operations

- Some sends/receives may block until another process acts:
  - synchronous send operation blocks until receive is issued;
  - receive operation blocks until message is sent.
- Blocking subroutine returns only when the operation has completed.
- Don't confuse this with blocking messages in what's app !

Non-Blocking Operations

- Non-blocking operations return immediately and allow the sub-program to perform other work.

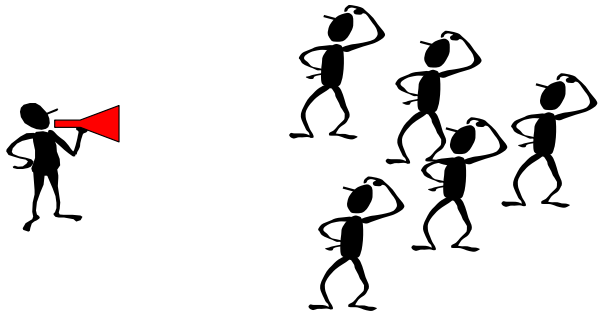


Collective Communications

- Collective communication routines are higher level routines.
- Several processes are involved at a time.
- May allow optimized internal implementations, e.g., tree based algorithms

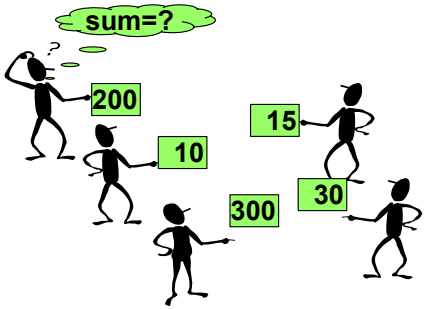
Broadcast

- A one-to-many communication.



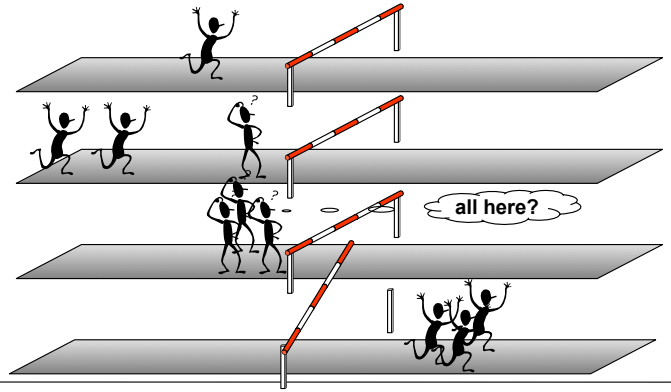
Reduction Operations

- Combine data from several processes to produce a single result.



Barriers

- Synchronize processes.



End of brief overview