HPC & BigData

High Performance computing Curriculum

UvA-SURFsara

http://www.hpc.uva.nl/

How to score 6 EC?

Core modules

- Lectures (6 hours)
  - Introduction to distributed systems
  - BigData
- Introduction to Linux (3.30 hours)

Workshops

- openMP / MPI (4 hours)
- Hadoop (8 hours)
- HPC CLoud (8 hours)
- Local and Remote visualization (4 hours)
- GPU

How to score 6 EC?

Grading

- Literature study: read 2 papers and summarize
- Following workshops you will have to do a assignment (none-supervised assignment)
  - Hadoop
  - HPCCloud
  - Local and Remote visualization
  - GPU programming
  - MPI/OpenMP

If you know these concepts you are attending the wrong class …

- **Supercomputing / High Performance Computing (HPC)**
- **Node**
- **CPU / Socket / Processor / Core**
- **Task**
- **Pipelining**
- **Shared Memory**
- **Symmetric Multi-Processor (SMP)**
- **Distributed Memory**
- **Communications**
- **Synchronization**
- **Granularity**
- **Observed Speedup**
- **Parallel Overhead**
- **Massively Parallel**
- **Embarrassingly Parallel**
- **Scalability**

Introduction to distributed systems

- Parallel programming MPI/openMP/RMI …
- Grid computing
- Cloud Computing
- SOA and Web Service
- Workflow
- Discussions

BigData

- General introduction to BigData
- MapReduce
- Analytics of BigData
- Technology for Big Data

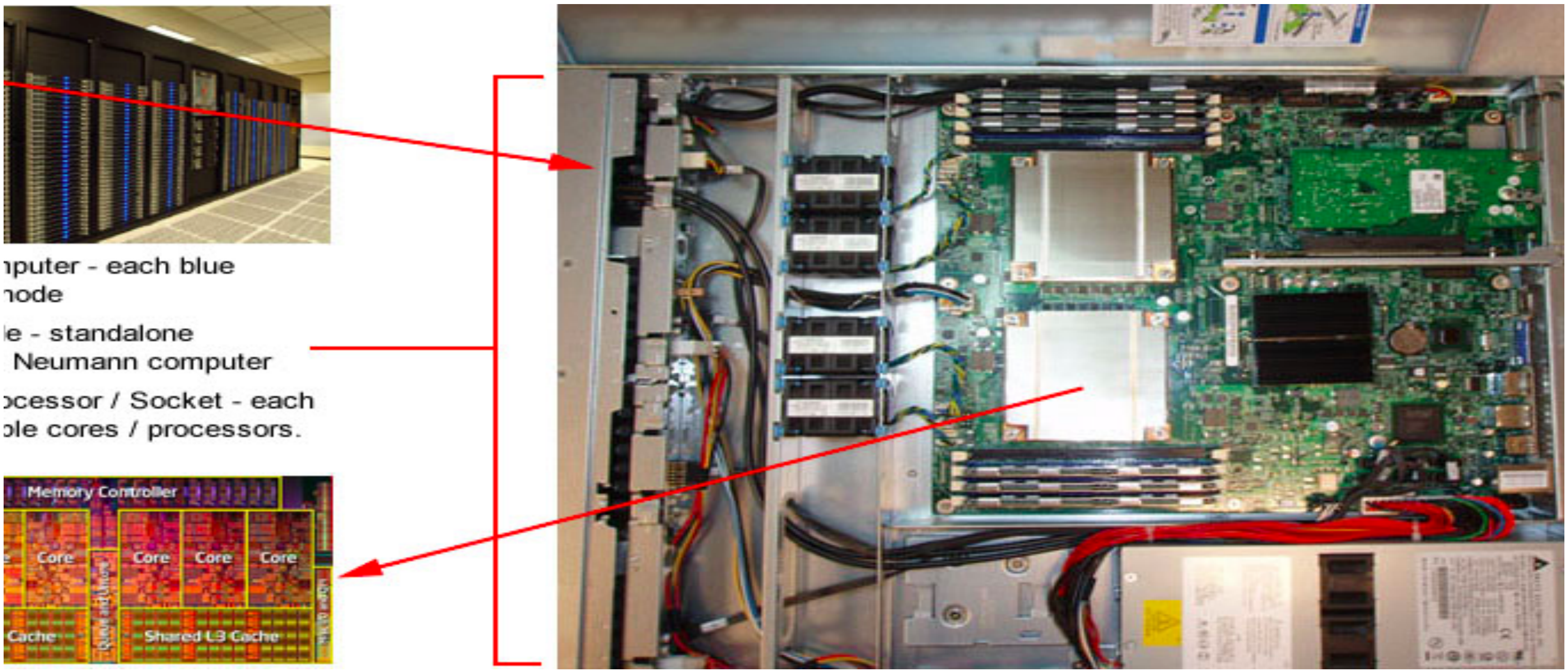
Content

- Computer Architectures
- High Performance Computing (HPC)
- Speed up
- Parallel programming models

Computer Architecture

- supercomputers **use many CPUs** to do the work
- All supercomputing architectures have
  - **processors** and some **combination cache**
  - some form of **memory** and **IO**
  - the processors are separated from every other processors by some distance
- there are **major differences** in the way that the parts are connected

some problems fit into different architectures better than others



- How CPU works http://www.youtube.com/watch?v=cNN_tTXABUA
- How Computers Add Numbers In One Lesson: http://www.youtube.com/watch?v=VBDoT8o4q00&feature=fvwp
- Computer Architecture Lesson 1: Bits and Bytes http://www.youtube.com/watch?v=UmSelKbP4sc
- Computer Architecture Lesson 2: Memory addresses http://www.youtube.com/watch?v=yF_txERujps&NR=1&feature=episodic
- Richard Feynman Computer Heuristics Lecture http://www.youtube.com/watch?v=EKWGGDXe5MA

Architectures: Michael J. Flynn (1972)

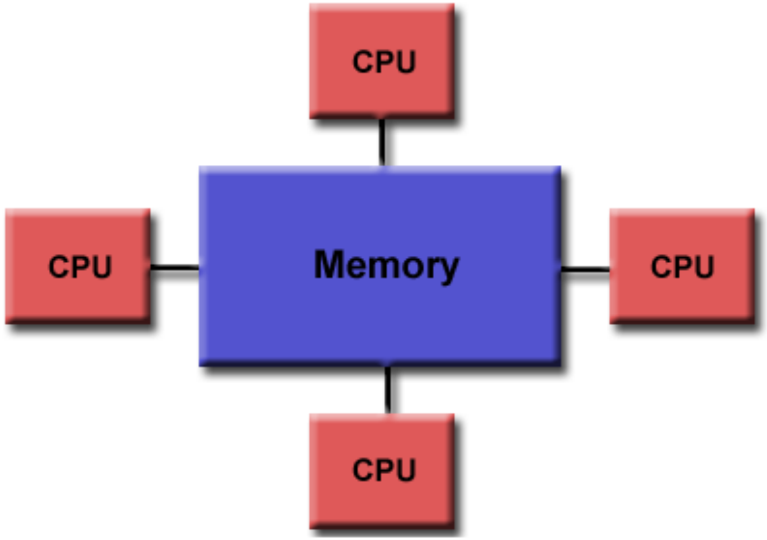
- Flynn's taxonomy distinguish multi-processor computer according to independent dimensions
  - **Instruction**
  - **Data**

- Each dimension
  - **Single**
  - **Multiple**

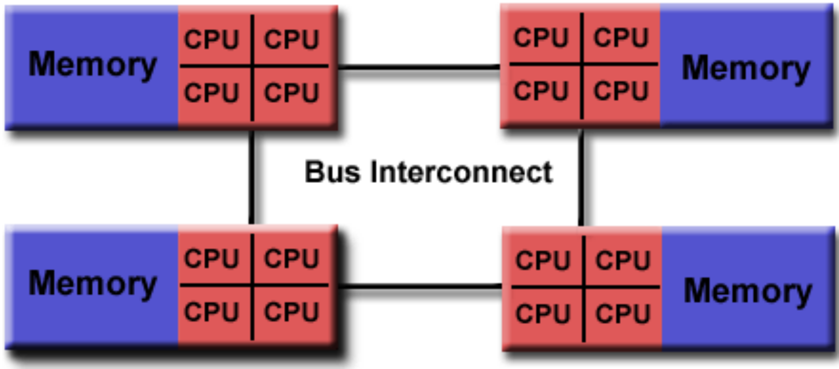
SISD Single Instruction, Single Data	SIMD Single Instruction, Multiple Data
MISD Multiple Instruction, Single Data	MIMD Multiple Instruction, Multiple Data

Parallel Computer Memory Architectures

- we can also **classify** supercomputers according to how the **processors** and **memory** are connected
  - **couple of processors** to a single large memory address space



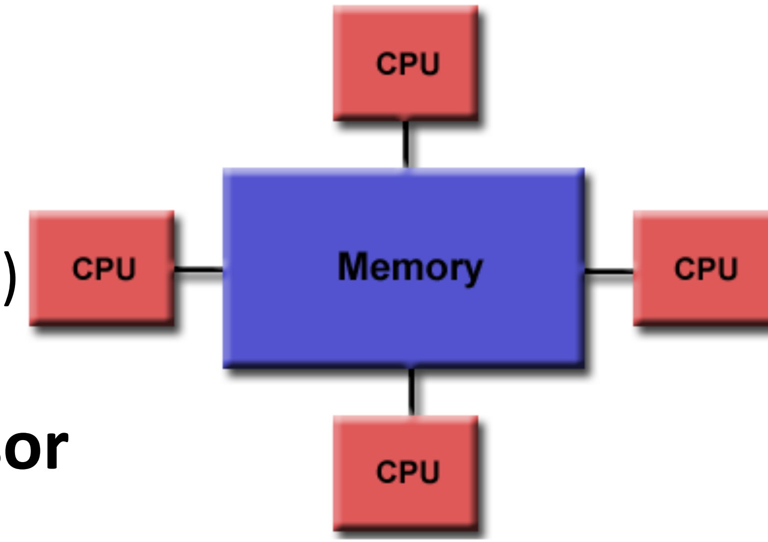
  - **couple of computers**, each with its own memory address space



Parallel Computer Memory Architectures

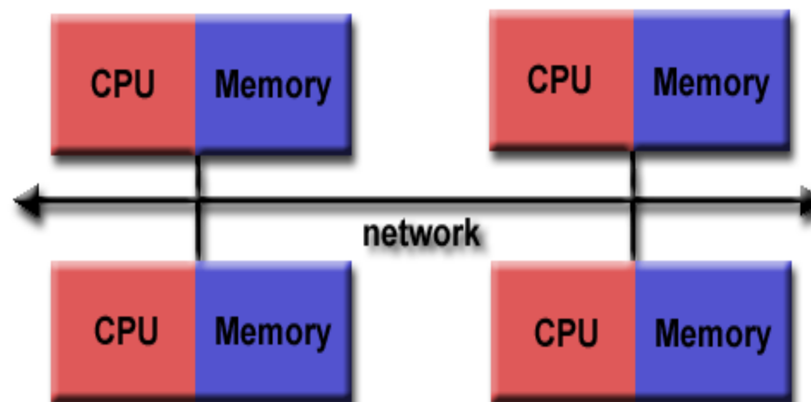
Shared Memory

- Uniform Memory Access (UMA)
- Non-Uniform Memory Access (NUMA)



Distributed Memory Multiprocessor

- Processors have their own local memory
- Changes it makes to its local memory have no effect on the memory of other processors.



High Performance Computing

- increasing **computing power** available allows
  - increasing the **problem dimensions**
  - adding more **particles** to a system
  - increasing the **accuracy** of the result
  - improve experiment turnaround time
  - …

Why Use Parallel Computing?

- Save time and/or money
- Solve larger problems
- Provide concurrency
- Use of non-local resources
- Limits to serial computing

DreamWorks Presents the Power of Supercomputing
http://www.youtube.com/watch?v=TGSRvV9u32M&feature=fvwp

https://computing.llnl.gov/tutorials/parallel_comp/

High Performance Computing

- **What does *High-Performance Computing (HPC)* mean?**
  - High-performance computing (HPC) is **the use of super computers** and **parallel processing techniques** for solving complex computational problems.
  - *HPC technology* focuses on **developing** parallel processing systems by incorporating both **administration** and **parallel computational** techniques.

    The terms high-performance computing and supercomputing are sometimes used interchangeably.

http://www.techopedia.com/definition/4595/high-performance-computing-hpc

Content

- High Performance Computing
- Computer Architectures
- Speed up
- Parallel programming models
- Example of Parallel programs

Speedup

- how can we measure how much faster our program runs when using more than one processor?
- define **Speedup** S as:
  - the ratio of 2 program execution times
  - constant problem size

$$S = \frac{T_1}{T_P}$$

- **T1** is the execution time for the problem on a single processor (use the “best” serial time)
- **TP** is the execution time for the problem on P processors

Speedup: Limit of Parallel programming

- A program **always** has a **sequential** part and a parallel part

```
(1) A = B+C;
(2) D = A + 1;
(3) E = D + A;
(4) For (I=0; I<E; I++)
(5)     M(I) = 0;
```

- the best you can do is to sequentially execute 4 instructions no mater how many processors you get

http://www.docstoc.com/docs/2698537/Introduction-to-Parallel-Programming

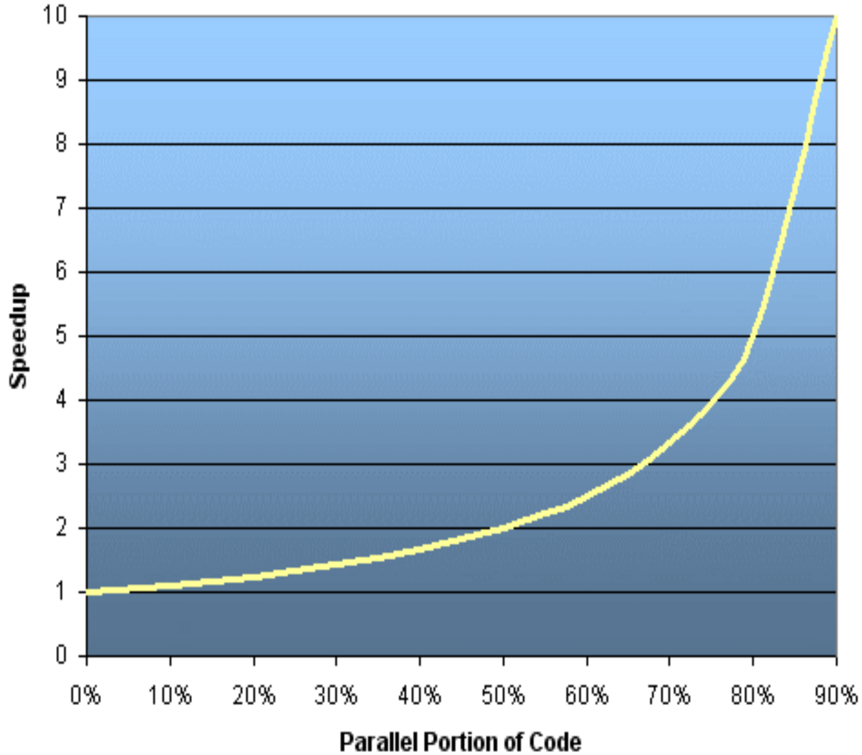
Speedup: Implication

- Parallel programming is **great** for programs with a lot of parallelism
  - Jacobi, scientific applications (weather prediction, DNA sequencing, etc)
- Parallel programming **may not be that great** some traditional applications:
    - Computing Fibonacci series F(K+2)=F(k+1) + F(k)

http://www.docstoc.com/docs/2698537/Introduction-to-Parallel-Programming

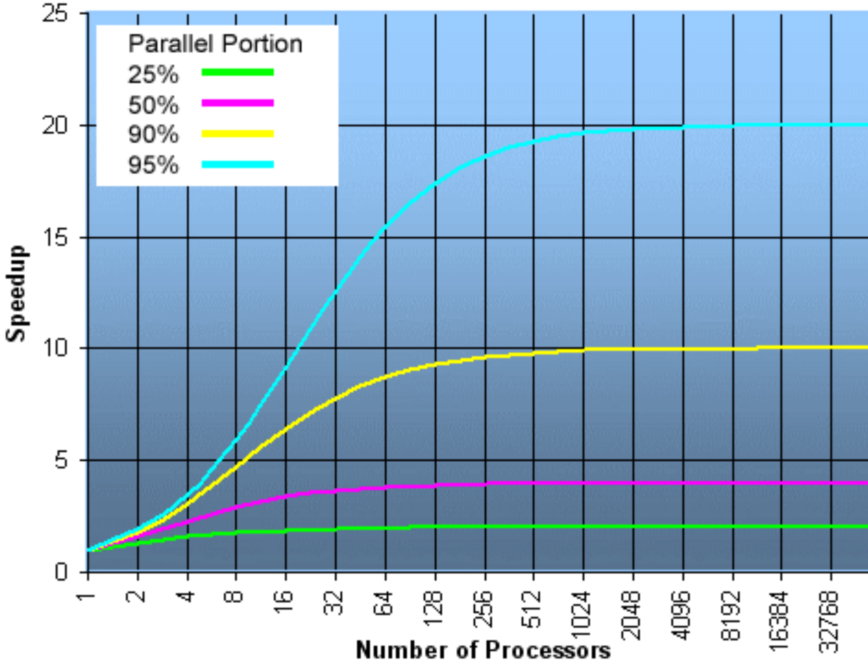
Speedup: Amdahl's Law (1967)

- **Amdahl's Law** states that potential program **speedup** is defined by the **fraction of code** (P) that can **be parallelized**:
  - speedup = $\dfrac{1}{1 - P}$



Speedup: Amdahl's Law (1967)

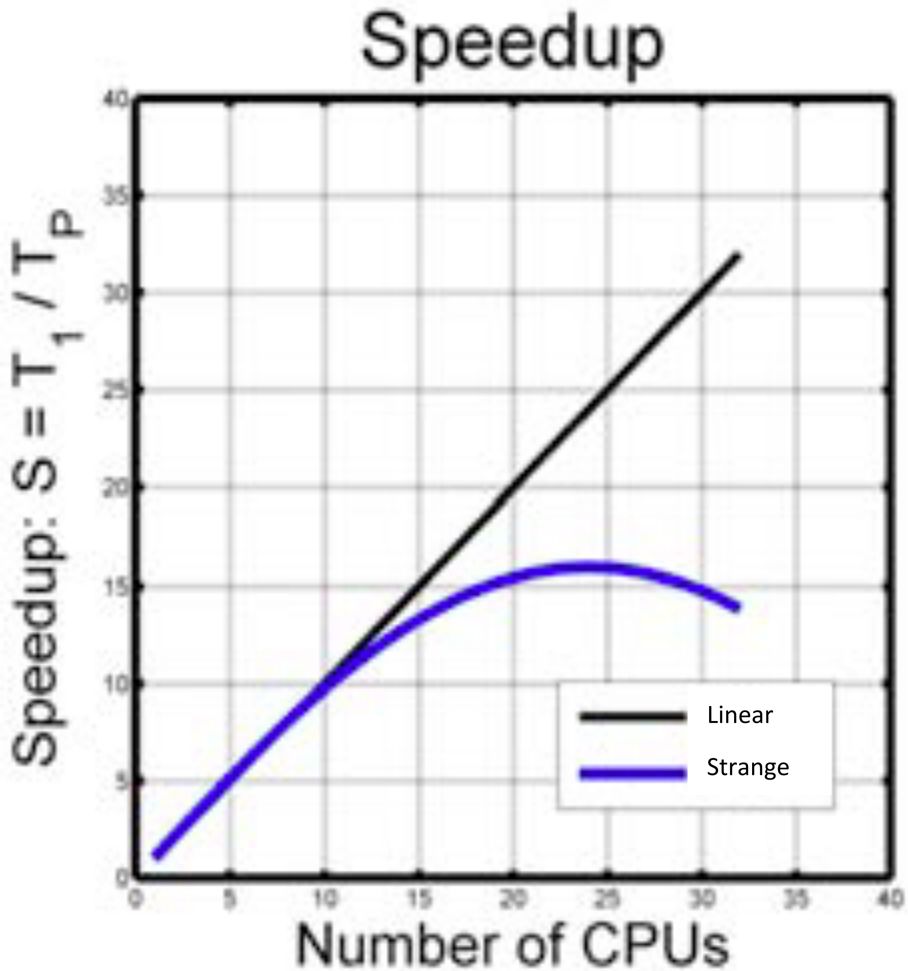
- Introducing the **number of processors** performing the parallel fraction of work, the relationship can be modeled by:
  - $$\text{speedup} = \frac{1}{\frac{P}{N} + S}$$



Speedup

- Linear speedup
- Sublinear speedup
- Superlinear speedup

- why do a speedup test?



Content

- High Performance Computing
- Computer Architectures
- Speed up
- How to design Parallel programs
- Parallel programming models
- Example of Parallel programs

Design Parallel programs

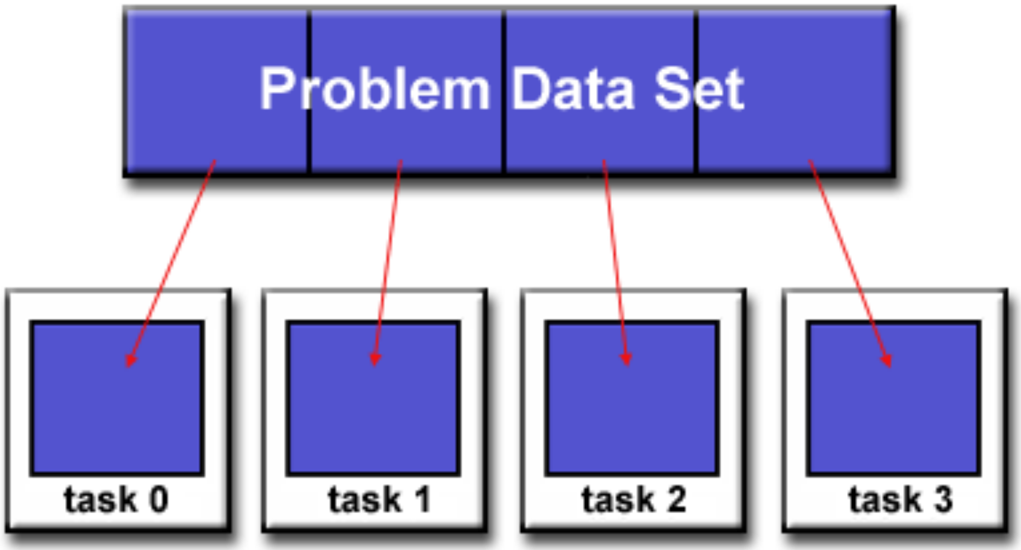
- Domain decomposition and functional decomposition
  - **Domain decomposition**: DATA associate with a problem is decomposed.
    - Each parallel **task** then **works** on **a portion of data**
  - **Functional deposition**: focus on the computation that is be performed. The problem is decomposed according to the work that must be done.
    - Each **task** then **performs** **a portion of the overall work**

http://www.docstoc.com/docs/2698537/Introduction-to-Parallel-Programming

Design Parallel programs

Domain decomposition:

- Also Called data parallelism
- DATA associate with a problem is decomposed.
- Each parallel task then works on **a portion of data**
- **Example: MapReduce**



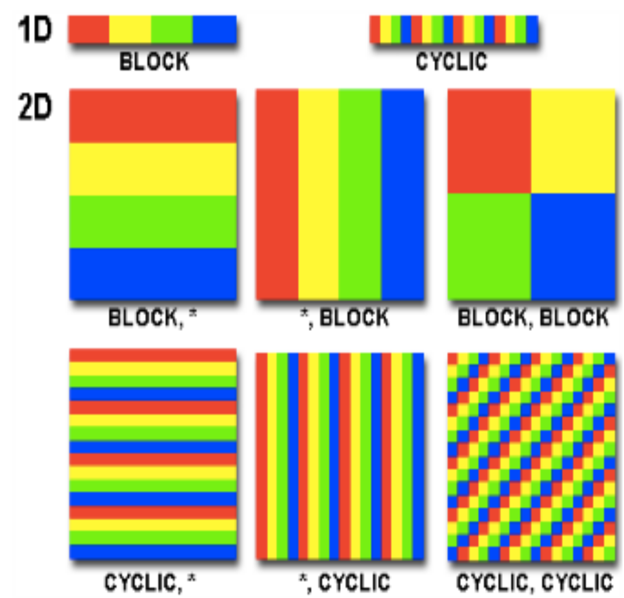
http://www.docstoc.com/docs/2698537/Introduction-to-Parallel-Programming

Design Parallel programs

Domain decomposition methods:

- Same datum may be needed by **multiple tasks**
- Decompose the data in such a manner that the **required communication is minimized**
- Ensure that the computational loads on processes are **balanced**

Domain deposition methods



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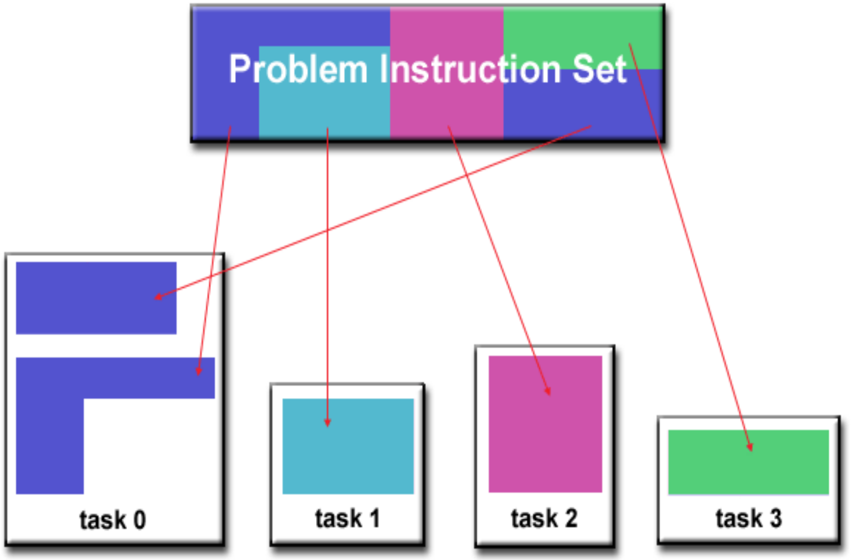
Functional deposition

- the focus is on the **computation** that is to be performed rather than on the data manipulated by the computation.
- The problem is decomposed according to the **work that must be done**.
- **Each task** then **performs** a **portion** of the overall work.



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Data Dependence

- A **dependence** exists between programs when the **order** of statement execution **affects** the results of the program.

- A data dependence results from multiple use of the same location(s) in storage by different tasks.

  (task 1) – (task2)

  - True dependence: Write X – Read X
  - Output dependence: Write X – Write X
  - Anti dependence: Read X – Write X

Dependencies: are important to parallel programming because the are one of the inhibitors to parallelism.

http://www.docstoc.com/docs/2698537/Introduction-to-Parallel-Programming

Data Dependence

- The value of a(I-1) must be computed before the value of a(I)

- A(I) exhibits **a data dependenc**y on a(I-1).

- Parallelism is inhibited.

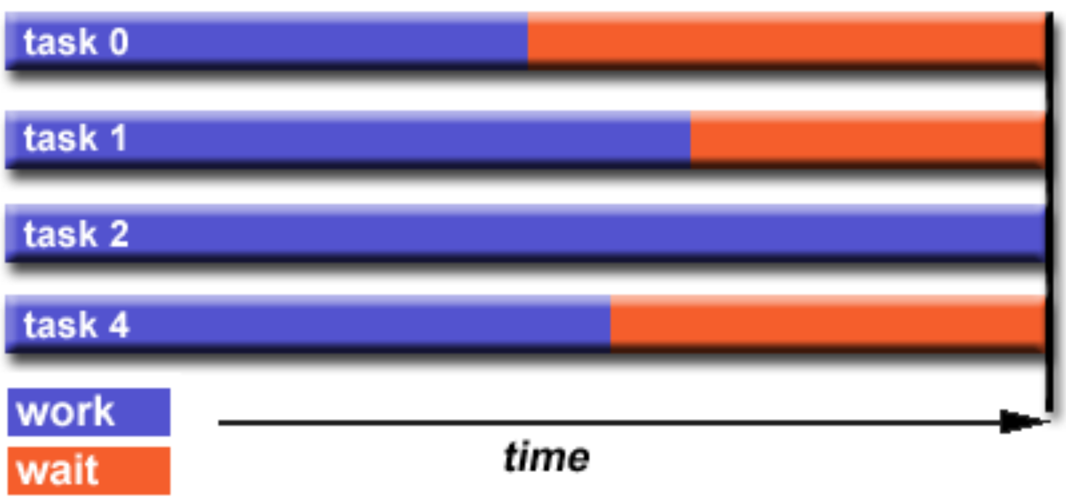
Data dependency examples

```
For (I=0; I<500; i++)
    a(I) = 0;
```

```
For (I=0; I<500; i++)
    a(I) = a(I-1) + 1;
```

Load balancing

- Distribute the **computation/communication** such that all the processor are busy all the time.
- At a synchronization point, the worst case performance is the real performance



Communications

- Parallel applications that do not need communications are called **embarrassingly parallel programs**
  - Monte carlo method, Seti at home
  - Most programs (e.g. Jacobi) are not like that
  - Communication is inherent to exploit parallelism in a program

Communications

- Factors to consider:
  - Cost of the communication
  - Latency and bandwidth
  - Synchronous and asynchronous
  - Point to point or collective

Overlapping communication and computation

- Make processors busy when **waiting** for **communication** results
  - Usually achieved by using **non-blocking** communicating primitives

Loading balancing, **minimizing communication** and **overlapping communication** with computation are keys to develop efficient parallel applications

Some basic load balancing techniques

- **Equally partition the work each task receives**
  - For array/matrix operations where each task performs similar work, evenly **distribute the data** set among the tasks.
  - For loop iterations where the work done in each iteration is similar, evenly **distribute the iterations** across the tasks.
- **Use dynamic work assignment**
  - Sparse arrays
  - Adaptive grid method
  - If a **heterogeneous mix of machines** with **varying performance**

    → ***scheduler* - *task pool*** approach

Granularity

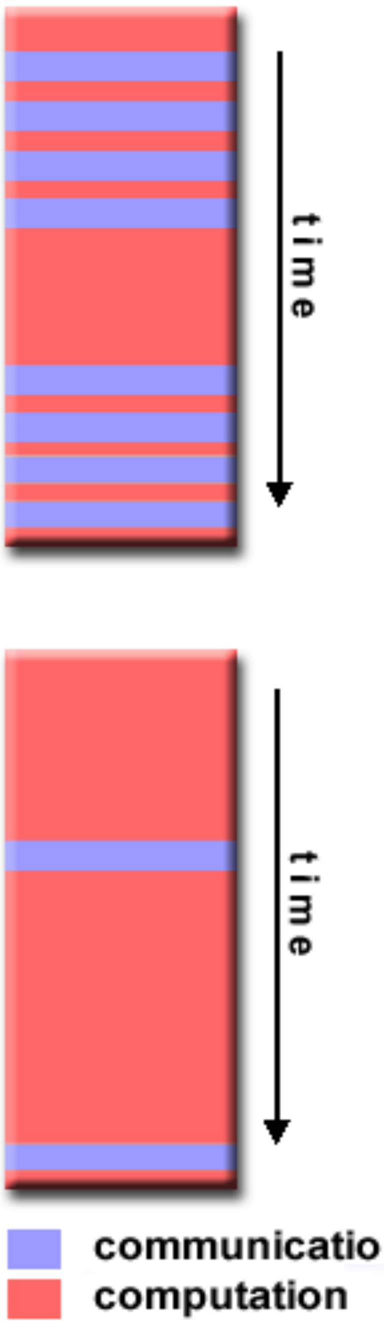
- Computation/ Communication
  - In parallel programming, granularity is a **qualitative** measure of the **ratio** of the **computation** to **communication**.

  - **Periods of computation** are typically **separated** form **periods of communication** by synchronization events
    - Computation phase and communication phase

Granularity

- Fine-grain parallelism
  - Relatively **small amount of computational** work are done between communication events
  - Low computation to communication ratio
  - Implies **high commutation over head** and less opportunity for performance enhancement

- Coarse-grain parallelism
  - Relatively **large amounts of computation** work are done between communication/synchronization events
  - High computation to communication ratio
  - Implies **more opportunity for performance** increase
  - Harder to load balance efficiently



Deadlock/Livelock

- Deadlock appears when two or more programs are waiting and none can make progress
- Livelock results from indefinite loop.

content

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- Shared Memory (without threads)
- Threads
- Distributed Memory / Message Passing
- Data Parallel
- Hybrid
- Single Program Multiple Data (SPMD)
- Multiple Program Multiple Data (MPMD)

Parallel programming

- need to do something to your program to use **multiple processors**
- need to **incorporate commands** into your program which allow **multiple threads** to run
  - one thread per processor
  - each thread gets a piece of the work

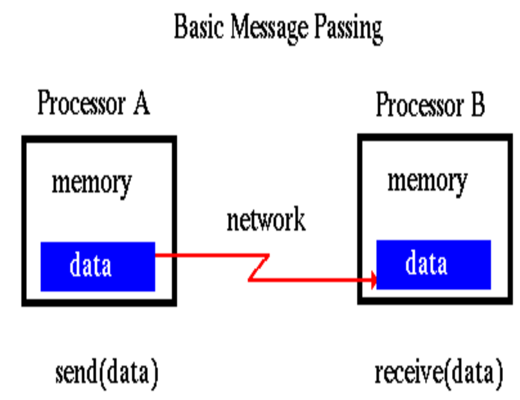
- several ways (APIs) to do this …

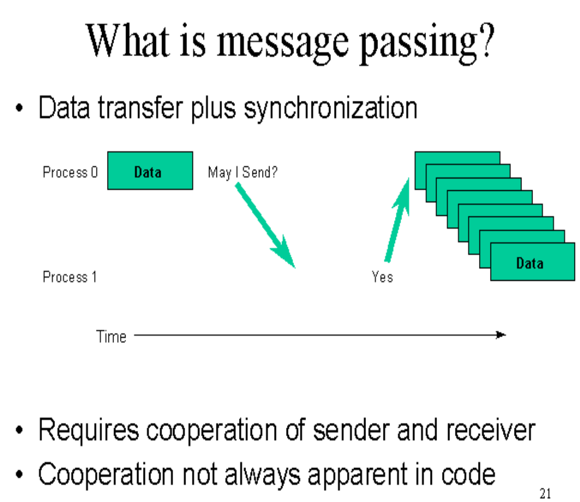
Parallel programming

Message Passing Interface (MPI)

- **Interprocess** communication which have separate address spaces

- Data is **explicitly** sent by one process and received by another
  - Data transfer usually requires cooperative operations to be performed by each process.
  - For example, a send operation must have a matching receive operation



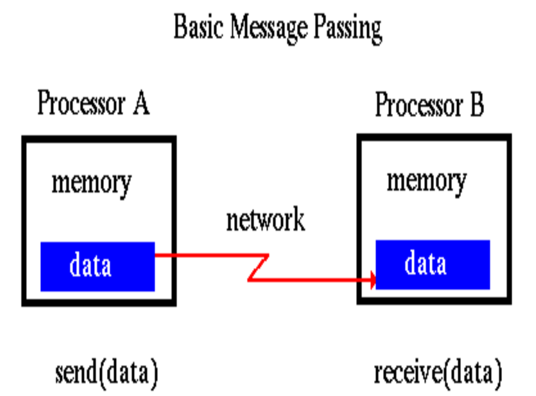


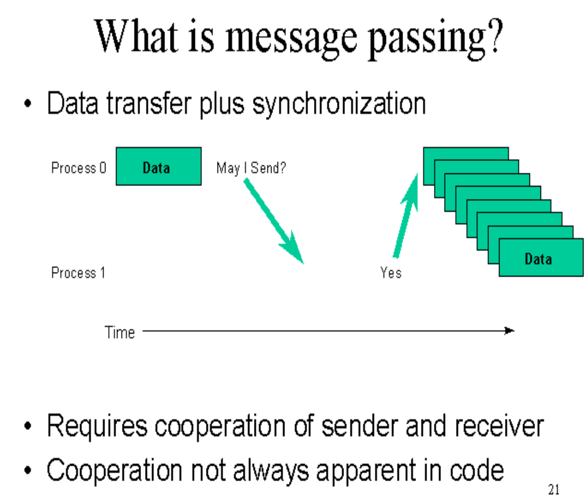
Parallel programming

Message Passing Interface (MPI)

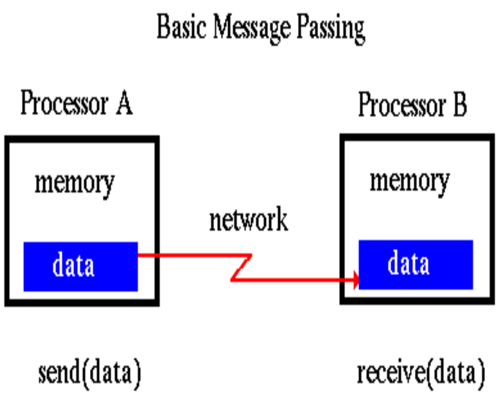
- What is MPI?
  - A message-Passing **Library** specification
  - Not a language or compiler specification
  - Not a specific implementation or product

- For parallel computers, clusters, and heterogeneous networks.
  - Designed to provide access to advanced parallel hardware for:
    - End users, library writers, tools developers



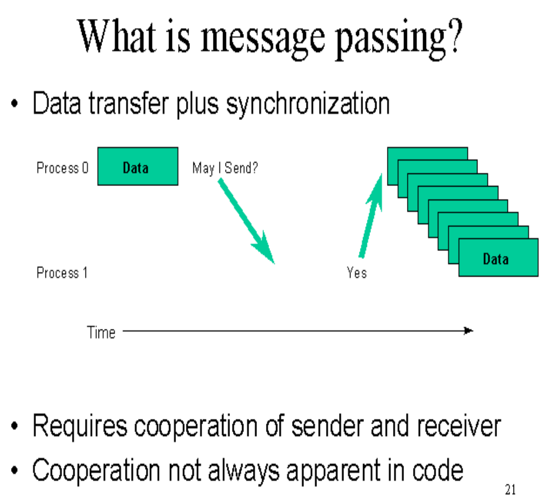


Parallel programming



Message Passing Interface (MPI)

- Why use MPI?
  - Optimized for performance
  - Will take advantage of fastest transport found
    - Shared memory (within a computer)
    - Fast cluster interconnects (Infiniband, Myrinet..) between computers (nodes)
    - TCP/IP if all else fails



Parallel programming

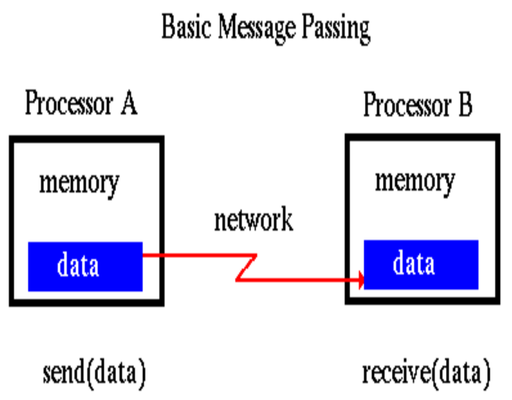
Message Passing Interface (MPI)

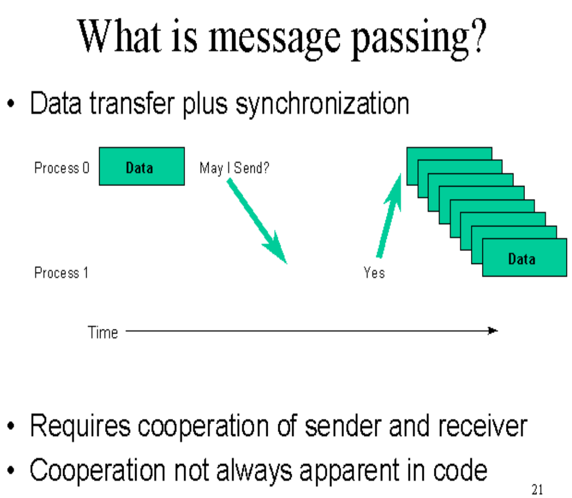
Deadlocks?

- Send a large message from proc A to proc B
  - If there is insufficient storage at the destination, the send must wait for the user to provide the memory space (through a receive)

- What will happen? (unsafe)
  - Process 0 Process 1

Process 0	Process 1
Send(1)	**Send(0)**
Recv(1)	**Recv(0)**

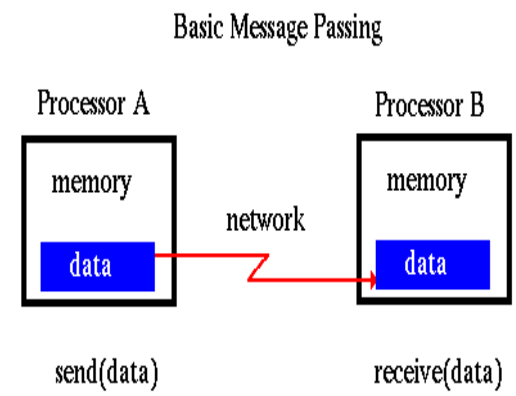


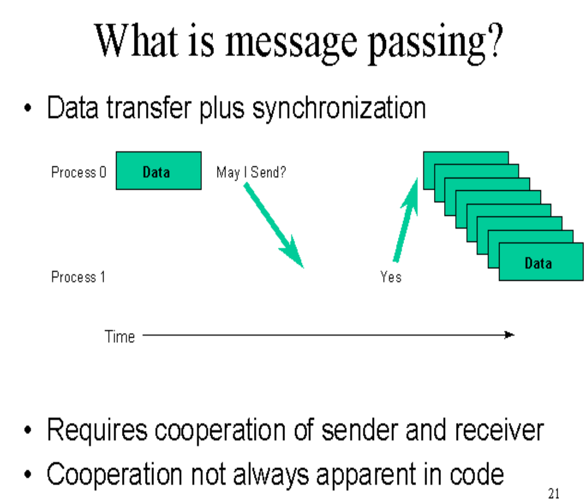


Parallel programming

Message Passing Interface (MPI)

- Very good for distributing large computations across reliable network
- Would be terrible for a distributed internet chat client or BitTorrent server





Example MPI Hello World

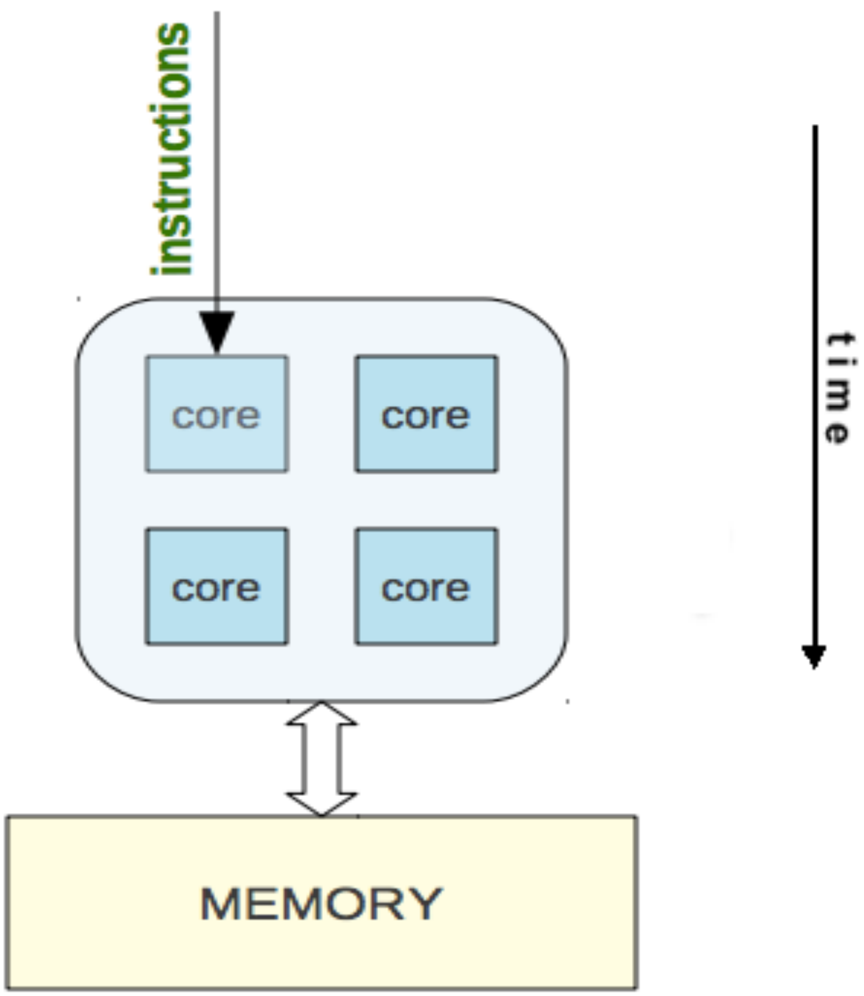
```c
#include <mpi.h>;

int main(int argc, char** argv) {
  // Initialize the MPI environment
  MPI_Init(NULL, NULL);

  // Get the number of processes
  int world_size;
  MPI_Comm_size(MPI_COMM_WORLD, &world_size);

  // Get the rank of the process
  int world_rank;
  MPI_Comm_rank(MPI_COMM_WORLD, &world_rank);

  // Get the name of the processor
  char processor_name[MPI_MAX_PROCESSOR_NAME];
  int name_len;
  MPI_Get_processor_name(processor_name, &name_len);

  // Print off a hello world message
  printf("Hello world from processor %s, rank %d"
         " out of %d processors\n",
         processor_name, world_rank, world_size);

  // Finalize the MPI environment.
  MPI_Finalize();
}
```

```
>>> export MPIRUN=/home/kendall/bin/mpirun
>>> export MPI_HOSTS=host_file
>>> ./run.perl mpi_hello_world
/home/kendall/bin/mpirun -n 4 -f host_file ./mpi_hello_world
Hello world from processor cetus2, rank 1 out of 4 processors
Hello world from processor cetus1, rank 0 out of 4 processors
Hello world from processor cetus4, rank 3 out of 4 processors
Hello world from processor cetus3, rank 2 out of 4 processors
```

Threads

- threads model of parallel programming, a **single** process can have **multiple**, **concurrent execution paths**
- Each thread has local data, but also, shares the entire resources of executable a.out.

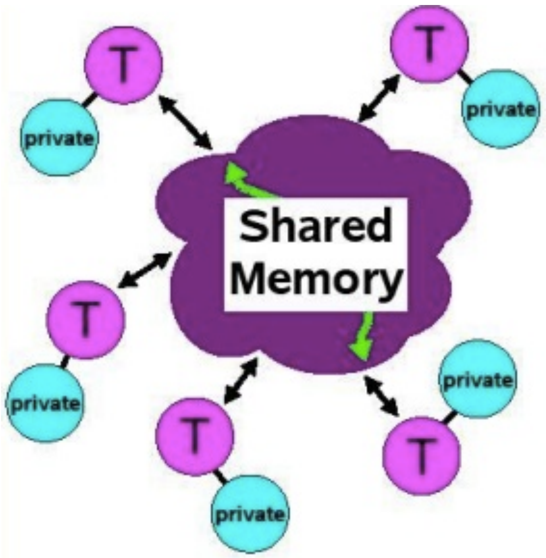
- Threads **communicate** with each other through **global memory**

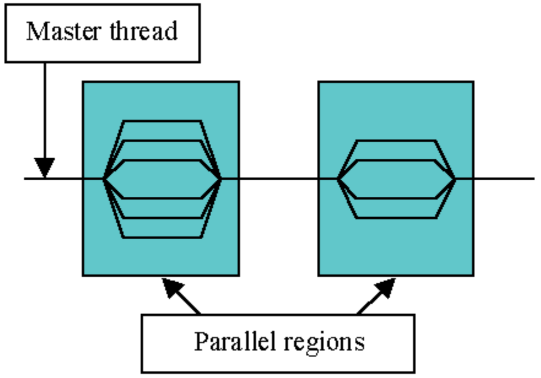


Parallel programming

Open MultiProcessing (OpenMP)

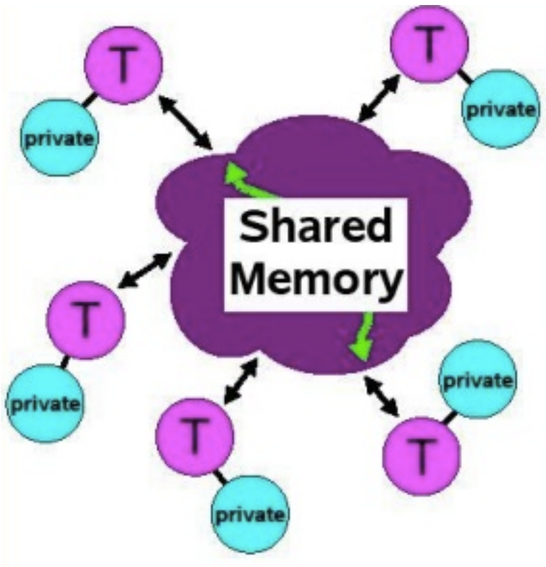
- What is OpenMP?
  - is a library that supports parallel programming in **shared-memory** parallel machines.
  - allows for the parallel execution of code (*parallel DO loop*), the definition of shared data (*SHARED*), and synchronization of processes





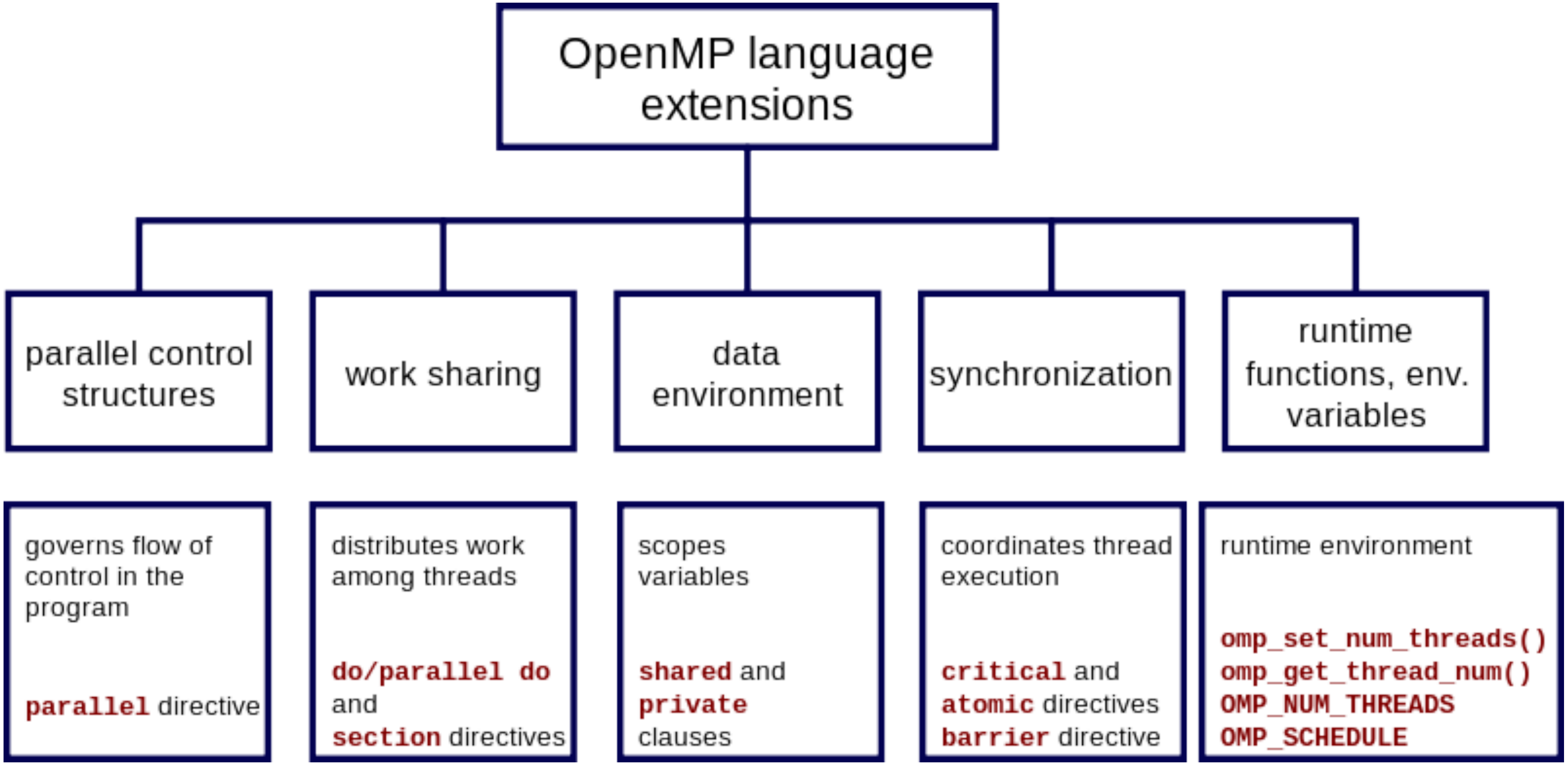
Parallel programming

- Open MultiProcessing (OpenMP)
  - What is the programming model?
    - All threads have access to the **same**, globally **shared**, memory
    - Data can be **shared** or **private**
      - Shared data is accessible by all threads
      - Private data can be accessed only by the threads that owns it
    - Data transfer is **transparent** to the **programmer**
    - **Synchronization** takes place, but it is mostly **implicit**



Parallel programming

Open MultiProcessing (OpenMP)



Example OpenMP Hello World

```c
#include <omp.h>
#include <stdio.h>
#include <stdlib.h>
int main (int argc, char *argv[]) {

int nthreads, tid;

/* Fork a team of threads giving them their own copies of variables */
#pragma omp parallel private(nthreads, tid)
 {

 /* Obtain thread number */
 tid = omp_get_thread_num();
 printf("Hello World from thread = %d\n", tid);

 /* Only master thread does this */
 if (tid == 0)
 {
  nthreads = omp_get_num_threads();
 printf("Number of threads = %d\n", nthreads);
 }

 } /* All threads join master thread and disband */

}
```

```
$ icc -o omp_helloc -openmp omp_hello.c
omp_hello.c(22): (col. 1) remark: OpenMP DEFINED REGION WAS PARALLELIZED.
$ export OMP_NUM_THREADS=3
$ ./omp_helloc
Hello World from thread = 0
Hello World from thread = 2
Hello World from thread = 1
Number of threads = 3
```

Parallel programming

Pros/Cons of OpenMP

- ✓ easier to program and debug than MPI
- ✓ directives can be added incrementally - gradual parallelization
- ✓ can still run the program **as a serial code**
- ✓ serial code statements usually don't need modification
- ✓ code is easier to **understand** and maybe more easily maintained

- ➢ can only be run in **shared memory computers**
- ➢ requires a **compiler** that supports OpenMP
- ➢ mostly used **for loop parallelization**

Pros/Cons of MPI

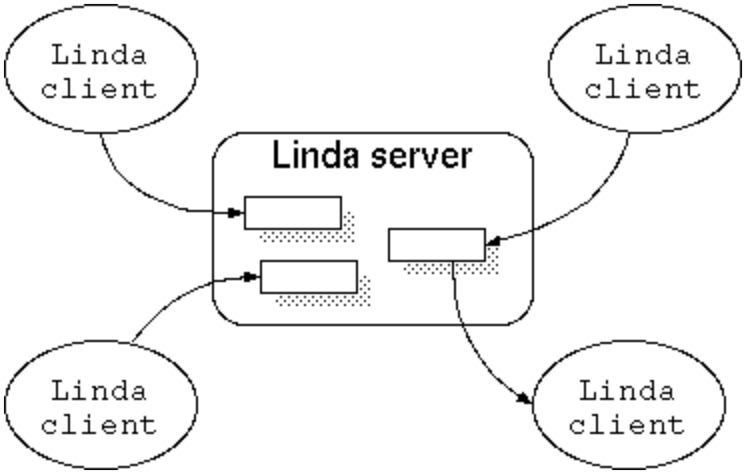
- ✓ runs on either **shared** or **distributed** memory architectures
- ✓ can be used on **a wider range of problems** than OpenMP
- ✓ each process has its **own local variables**
- ✓ distributed memory computers are less expensive than large shared memory computers

- ➢ requires more **programming changes** to go from serial to parallel version
- ➢ can be harder to debug
- ➢ **performance is limited** by the communication network between the nodes

Parallel programming

Shared State Models

- Views an application as a collection of processes communicating by putting/getting objects into one or more *spaces*
- A *space* is a shared and persistent object repository that is accessible via network
- The processes use the repository as an exchange mechanism to get coordinated, instead of communicating directly with each other



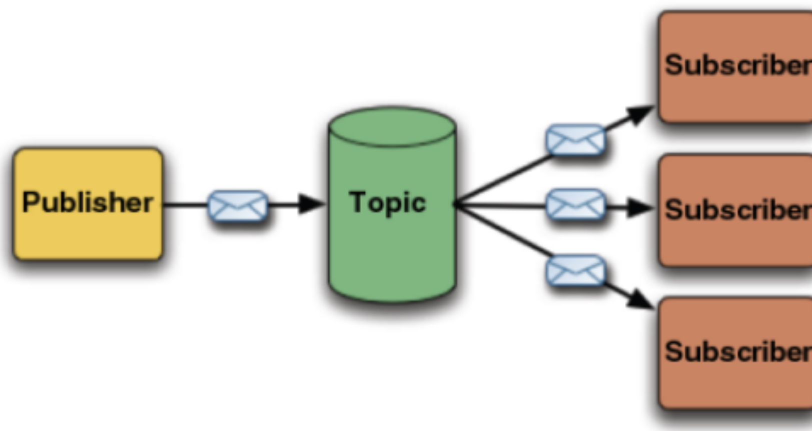
implementation: Java (JavaSpaces), Lisp, Prolog, Python, Ruby, and the .NET framework

Parallel programming

Shared State Models: Publish/
Subscribe

- Publish/subscribe systems are programming capability provided by associative matching

- Allows the producers and consumers of data to coordinate in a way where they can be decoupled and may not even know each other's identity
  - SOA, Web service etc.

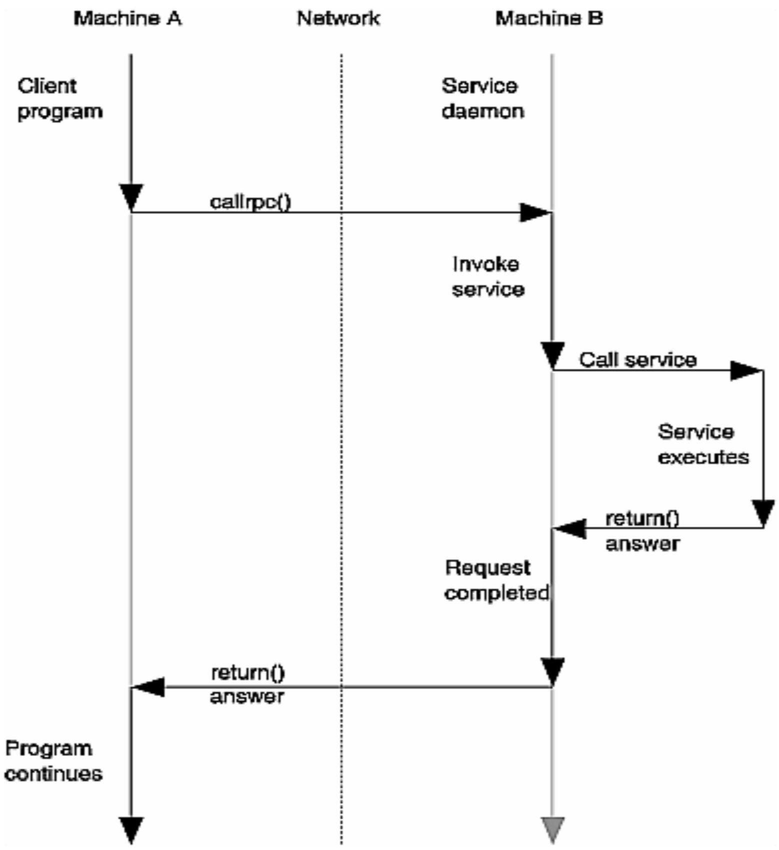


Parallel programming

RPC and RMI Models

- Structure the interaction between sender and receiver as:
  - a language construct, rather than a library function call that simply transfers an un-interpreted data.

- provide a simple and well understood mechanism for managing remote computationss



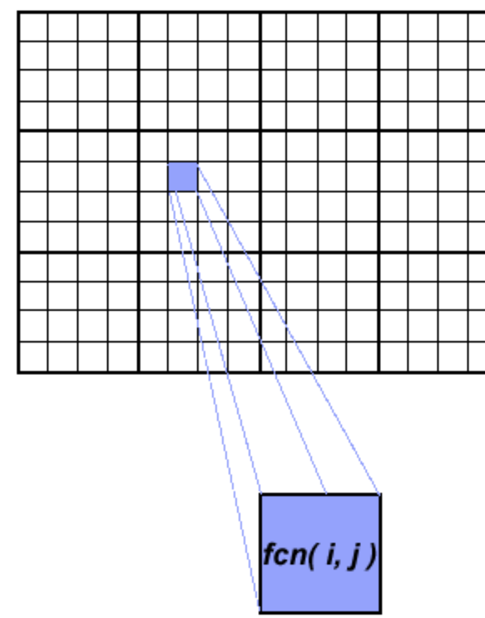
content

- High Performance Computing
- Computer Architectures
- Speed up
- How to design parallel applications
- Parallel programming models
- Example of Parallel programs

calculations on 2-dimensional array elements

- The serial program calculates one element at a time in sequential order.
- Serial code could be of the form:

```
do j = 1,n
do i = 1,n
  a(i,j) = fcn(i,j)
end do
end do
```

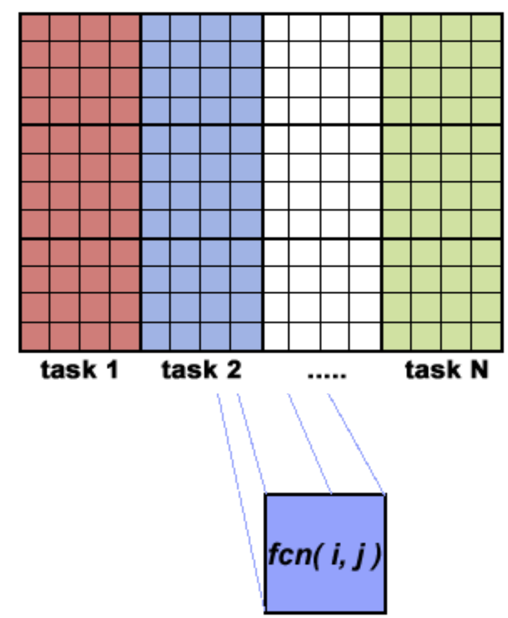


https://computing.llnl.gov/tutorials/parallel_comp/#MemoryArch

calculations on 2-dimensional array elements: solution 1

- Implement as a Single Program Multiple Data (SPMD) model.
- each task executes the portion of the loop corresponding to the data it owns.

```
do j = mystart, myend
do i = 1,n
  a(i,j) = fcn(i,j)
end do
end do
```



https://computing.llnl.gov/tutorials/parallel_comp/#MemoryArch

calculations on 2-dimensional array elements: implementation

- Implement as a Single Program Multiple Data (SPMD) model.
- **Master process** initializes array, sends info to worker processes and receives results.
- **Worker process** receives info, performs its share of computation and sends results to master.

https://computing.llnl.gov/tutorials/parallel_comp/#MemoryArch

calculations on 2-dimensional array elements: implementation

```
find out if I am MASTER or WORKER

if I am MASTER

  initialize the array
  send each WORKER info on part of array it owns
  send each WORKER its portion of initial array

  receive from each WORKER results

else if I am WORKER
  receive from MASTER info on part of array I own
  receive from MASTER my portion of initial array

  # calculate my portion of array
  do j = my first column,my last column
  do i = 1,n
    a(i,j) = fcn(i,j)
  end do
  end do

  send MASTER results

endif
```

https://computing.llnl.gov/tutorials/parallel_comp/#MemoryArch

calculations on 2-dimensional array elements: solution 2

- Solution1: demonstrated **static load** balancing:
  - Each task has a fixed amount of work to do
  - May be significant idle time for faster or more lightly loaded processors - **slowest tasks determines overall performance**.
- If you have a **load balance problem** (some tasks work faster than others),
  - you may benefit by using a "**pool of tasks**" scheme.

https://computing.llnl.gov/tutorials/parallel_comp/#MemoryArch

calculations on 2-dimensional array elements: solution 2

- Master Process:
  - Holds pool of tasks for worker processes to do
  - Sends worker a task when requested
  - Collects results from workers
- Worker Process: repeatedly does the following
  - Gets task from master process
  - Performs computation
  - Sends results to master

calculations on 2-dimensional array elements: solution 2

```
find out if I am MASTER or WORKER

if I am MASTER

  do until no more jobs
    if request send to WORKER next job
    else receive results from WORKER
  end do

else if I am WORKER

  do until no more jobs
    request job from MASTER
    receive from MASTER next job

    calculate array element: a(i,j) = fcn(i,j)

    send results to MASTER
  end do

endif
```

References

1. Introduction to Parallel Computing
   https://computing.llnl.gov/tutorials/parallel_comp/#MemoryArch
2. Intro to Parallel Programming . Lesson 2, pt. 1- Shared Memory and threads
   http://www.youtube.com/watch?v=6sL4C2SwszM
3. Intro to Parallel Programming . Lesson 2, pt. 2- Shared Memory and threads
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   http://www.youtube.com/watch?v=403LWbrA5oU