An introduction to High Performance Computing and its Applications

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Outline

- Introduction to HPC
- Architecting a HPC system
- Approach to Parallelization
- Parallelization Paradigm
- Applications in area of Science and Engineering

What is a HPC?

High Performance Computing

- Set of Computing technologies for very fast numeric simulation, modeling and data processing
- Employed for specialised applications that require lot of mathematical calculations
- Using computer power to execute a few applications extremely fast

What is HPC?(continued)

Definition 1

- High Performance Computing (HPC) is the use of parallel processing for running advanced application programs efficiently, reliably and quickly.
- A supercomputer is a system that performs at or near the currently highest operational rate for computers.

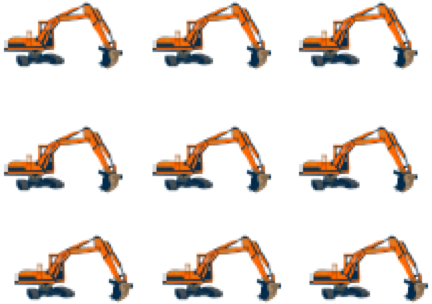
Definition 2 (Wikipedia)

- High Performance Computing (HPC) uses Supercomputers and Computer Clusters to solve advanced computation problems.

Evolution of Supercomputers

- Supercomputer in the 1980s and 90s
  - Custom-built computer systems
  - Very expensive

- Supercomputer after 1990s
  - Build using commodity off-the-shelf" components
  - Uses cluster computing techniques

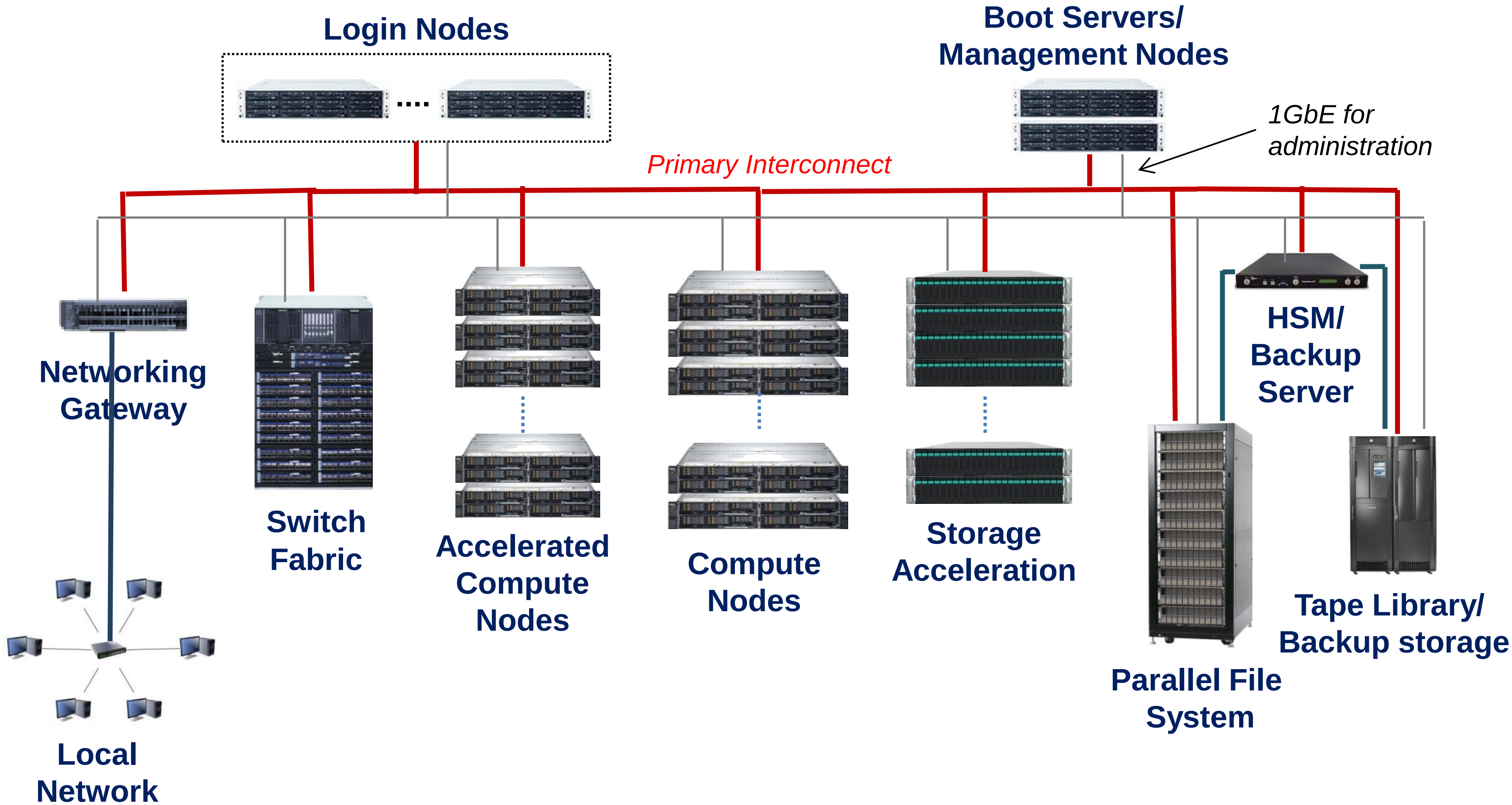


Supercomputers

Cray Supercomputer

PARAM Yuva II

Components of Cluster



HPC Software Stack

HPC Programming Tools	Performance Monitoring	HPCC, IOR, PAPI/IPM, NPB, Netperf
HPC Programming Tools	Development Tools	Alliena DDT/ TAU, Intel Cluster Studio/IBM XC, PGI (PGI SDK), GNU Compiler
HPC Programming Tools	Application Libraries	Ferret/GRADS/PARA view/VISIT, MVAPICH2/ OpenMPI, ACML/ESSL, MPSS/CUDA, BLAS, LAPACK
Middleware Applications and Management	Resource Management/ Job Scheduling	SLURM, Grid Engine, MOAB, Altair PBS Pro, IBM Platform LSF, Torque/ Maui
Middleware Applications and Management	File System	NFS, Local FS (ext3, ext4, XFS), GPFS, Lustre
Middleware Applications and Management	Provisioning	XCAT / ROCKS / C-DAC Developed tools
Middleware Applications and Management	Cluster Monitoring	XCAT / ROCKS / C-DAC Developed tools
Operating Systems	Operating System	Linux (Red Hat, CentOS, SUSE)

Single CPU Systems

- Can run a single stream of code
- Performance can be improvement through
    - Increasing ALU width
    - Increasing clock frequency
    - Making use of pipelining
    - Improved compilers
- But still, there is a limit to each of these techniques
  - Parallel computing, provides relief

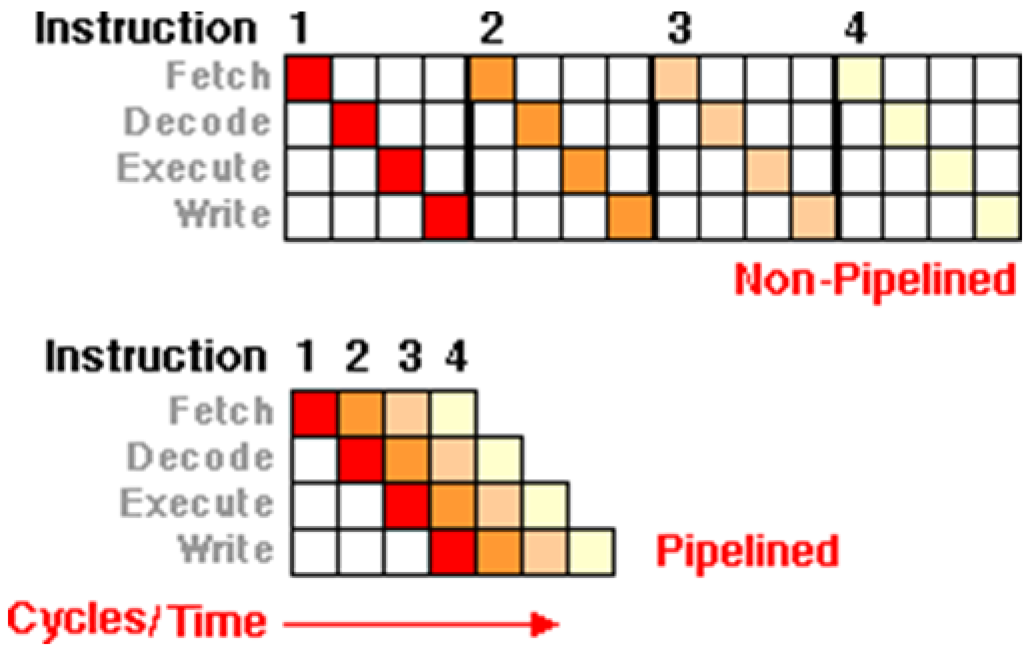
Why use Parallel Computing?

- Overcome limitations of single CPU systems
  - Sequential systems are slow
    - Calculations make take days, weeks, years
    - More CPUs can get job done faster
  - Sequential systems are small
    - Data set may not fit in memory
    - More CPUs can give access to more memory
- So, the advantages are
  - Save time
  - Solve bigger problems

Single Processor Parallelism

- Instruction level Parallelism is achieved through
  - Pipelining
  - Superscaler implementation
  - Multicore architecture
  - Using advanced extensions

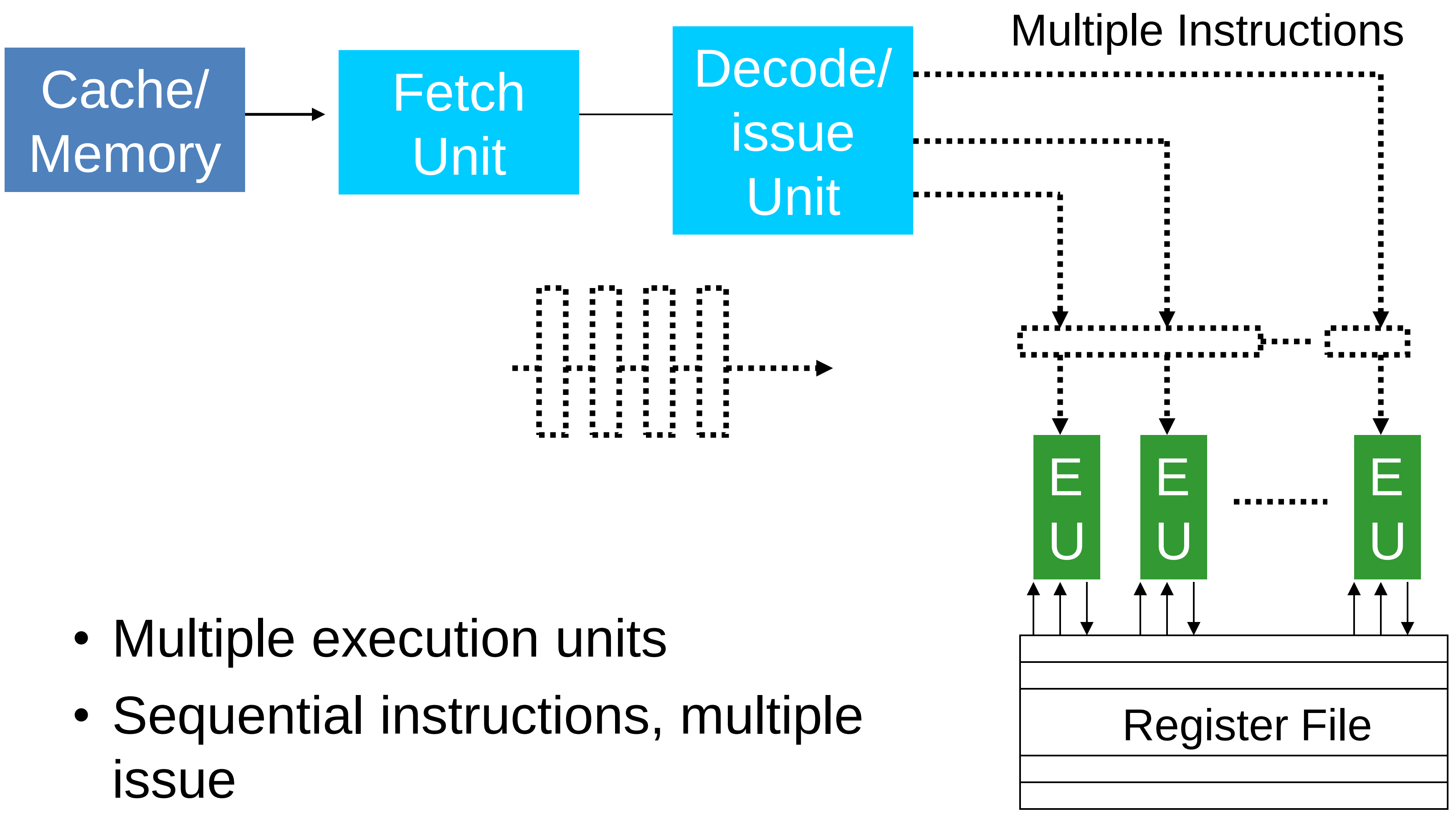
Pipelined Processors



- A new instruction enters every clock
- Instruction parallelism = No. of pipeline stages

Diagram Souce: Quora

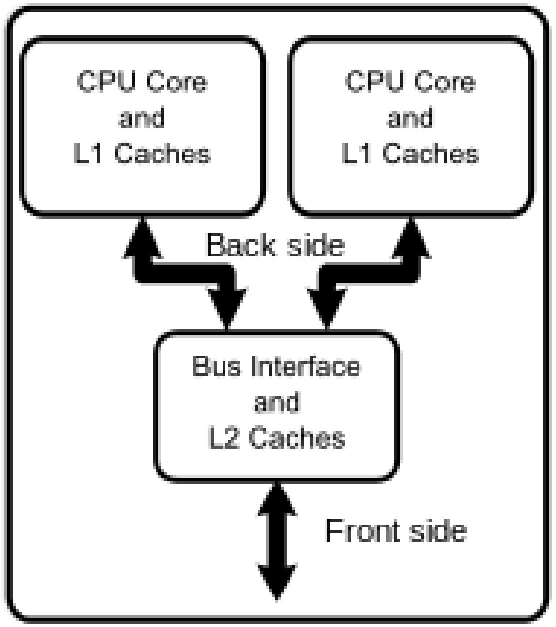
Superscaler



- Multiple execution units
- Sequential instructions, multiple issue

Multicore Processor

- Single computing component with two or more independent processing units
- Each unit is called cores, which read and execute program instructions



Source: Wikipedia.

Advanced Vector eXtensions

- Useful for algorithms that can take advantage of SIMD
- AVX were introduced by Intel and AMD in x86
- Using AVX-512, applications can pack
  - 32 double precision or 64 single precision floating point operations or
  - eight 64-bit and sixteen 32-bit integers
- Accelerates performance for workloads such as
  - Scientific simulations, artificial intelligence (AI)/deep learning, image and audio/video processing

Parallelization Approach

Means of achieving parallelism

- Implicit Parallelism
  - Done by the compiler and runtime system
- Explicit Parallelism
  - Done by the programmer

Implicit Parallelism

- Parallelism is exploited implicitly by the compiler and runtime system
  - Automatically detects potential parallelism in the program
  - Assigns the tasks for parallel execution
  - Controls and synchronizes execution

(+) Frees the programmer from the details of parallel execution

(+) it is a more general and flexible solution

(-) very hard to achieve an efficient solution for many applications

Explicit Parallelism

- It is the programmer who has to
  - Annotate the tasks for parallel execution
  - Assign tasks to processors
  - Control the execution and the synchronization points

(+) Experienced programmers achieve very efficient solutions for specific problems

(-) programmers are responsible for all details

(-) programmers must have deep knowledge of the computer architecture to achieve maximum performance.

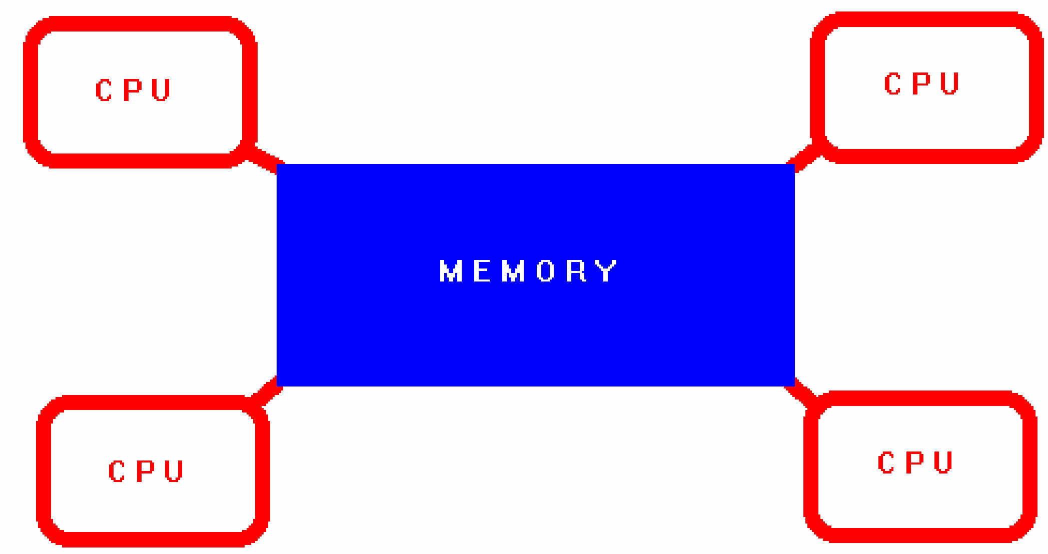
Explicit Parallel Programming Models

Two dominant parallel programming models

- Shared-variable model
- Message-passing model

Shared Memory Model

- Uses the concept of single address space
- Typically SMP architecture is used
  - Scalability is not good



Shared Memory Model

- Multiple threads operate independently but share same memory resources
- Data is not explicitly allocated
- Changes in a memory location effected by one process is visible to all other processes
- Communication is implicit
- Synchronization is explicit

Advantages & Disadvantages of Shared Memory Model

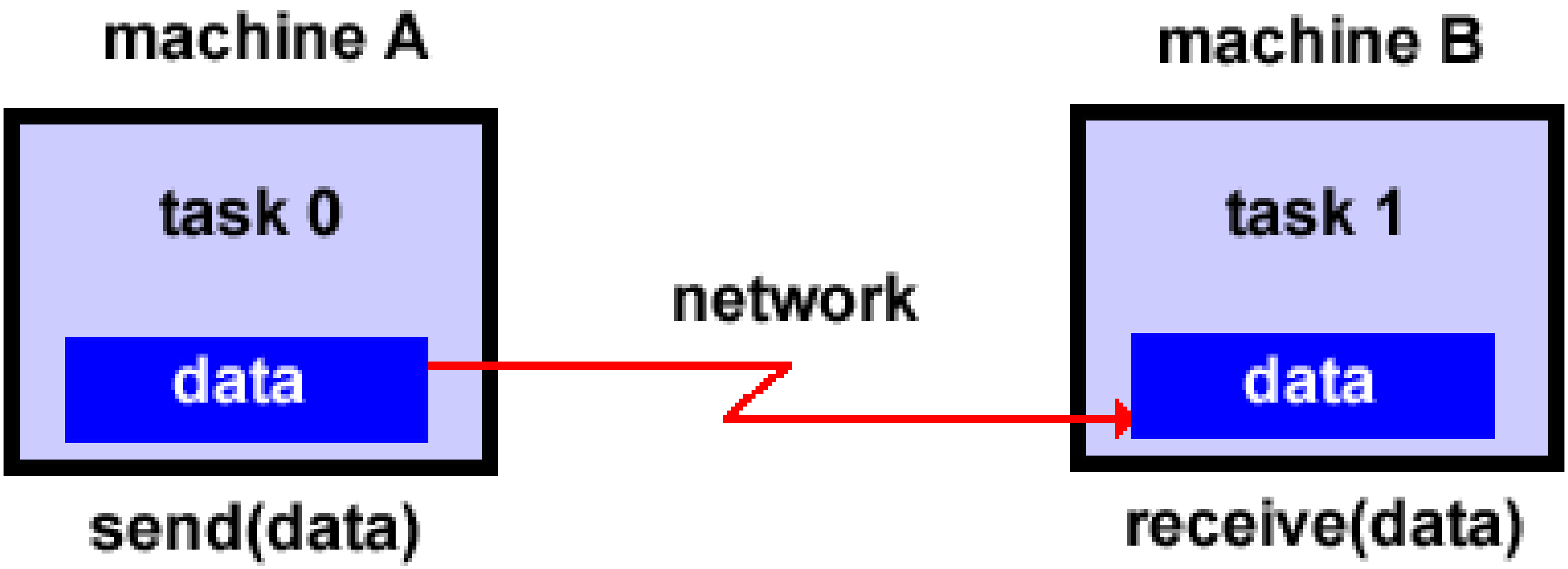
Advantages :

- Data sharing between threads is fast and uniform
- Global address space provides user friendly programming

Disadvantages :

- Lack of scalability between memory and CPUs
- Programmer is responsible for specifying synchronization, e.g. locks
- Expensive

Message Passing Model



Characteristics of Message Passing Model

- Asynchronous parallelism
- Separate address spaces
- Explicit interaction
- Explicit allocation by user

How Message Passing Model Works

- A parallel computation consists of a number of processes
- Each process has purely local variables
- No mechanism for any process to directly access memory of another
- Sharing of data among processes is done by explicitly message passing
- Data transfer requires cooperative operations by each process

Usefulness of Message Passing Model

- Extremely general model
- Essentially, any type of parallel computation can be cast in the message passing form
- Can be implemented on wide variety of platforms, from networks of workstations to even single processor machines
- Generally allows more control over data location and flow within a parallel application than in, for example the shared memory model
- Good scalability

Parallelization Paradigms

Ideal Situation !!!

- Each Processor has a Unique work to do
- Communication among processes is largely unnecessary
- All processes do equal work

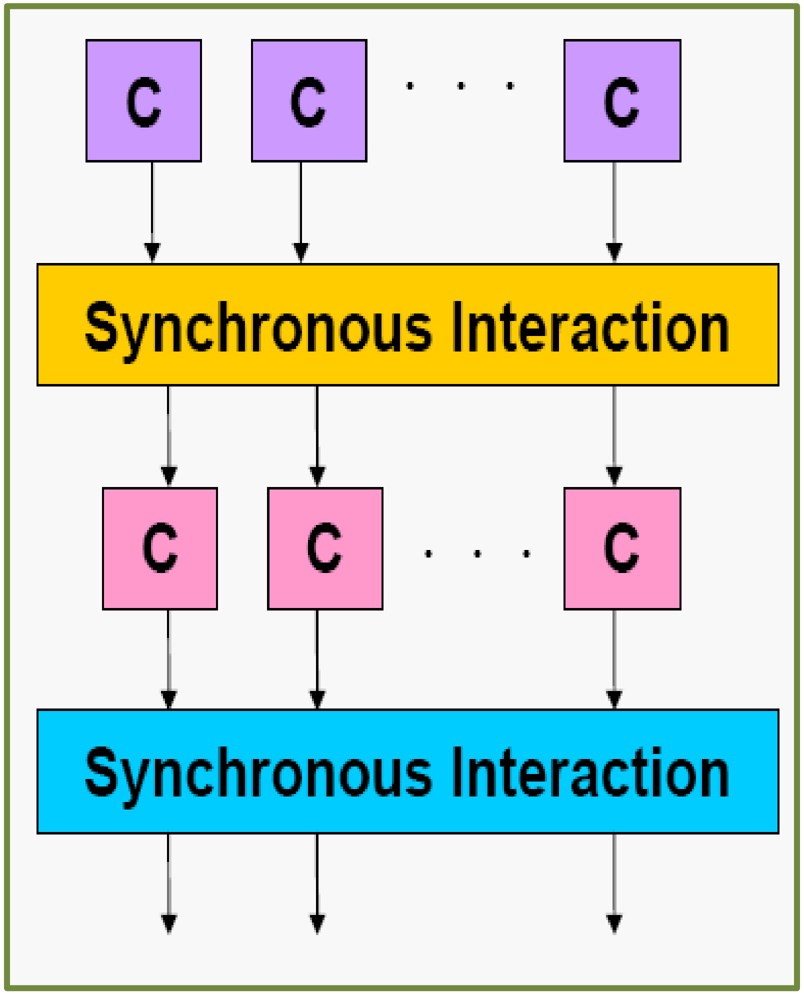
Writing parallel codes

- Distribute the data to memories
- Distribute the code to processors
- Organize and synchronize the workflow
- Optimize the resource requirements by means of efficient algorithms and coding techniques

Parallel Algorithm Paradigms

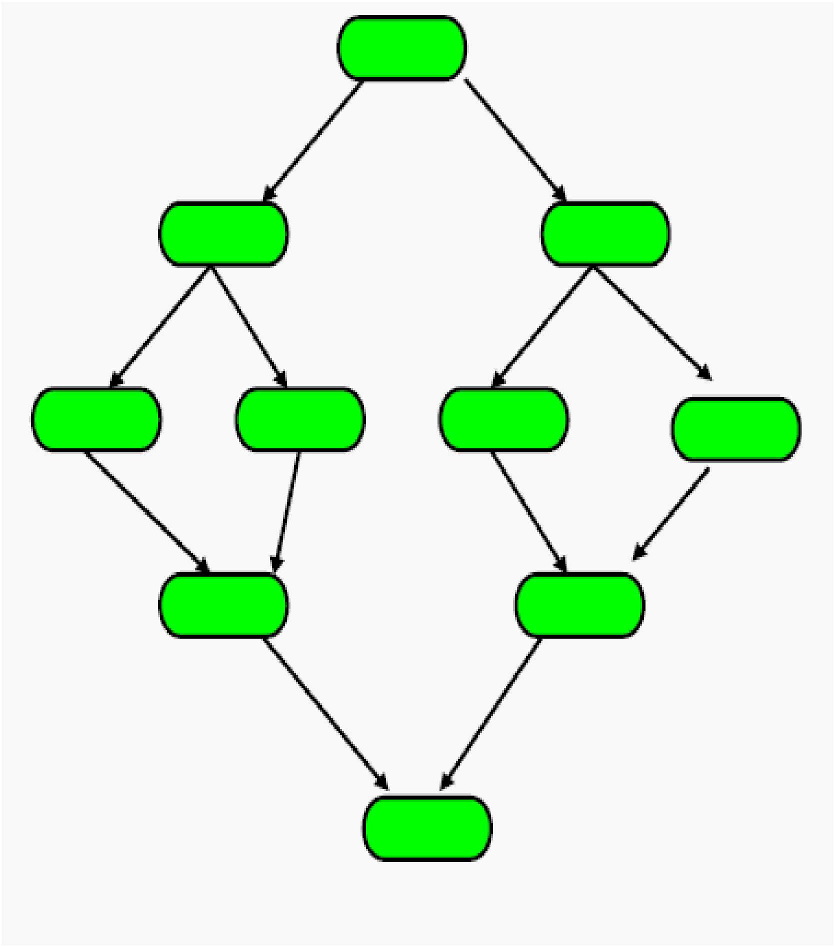
- Phase parallel
- Divide and conquer
- Pipeline
- Process farm
- Domain Decomposition

Phase Parallel Model



- The parallel program consists of a number of super steps, and each has two phases.
- In a computation phase, multiple processes each perform an independent computation.
- In interaction phase, the processes perform one or more synchronous interaction operations, such as a barrier or a blocking communication.

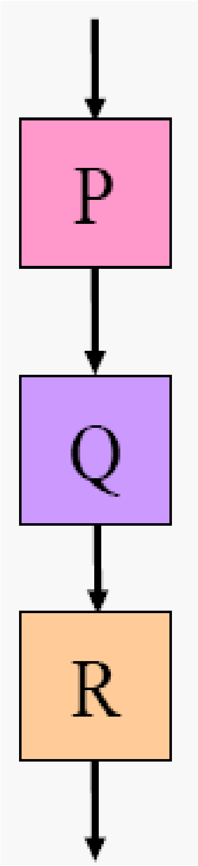
Divide and Conquer model



- A parent process divides its workload into several smaller pieces and assigns them to a number of child processes.
- The child processes then compute their workload in parallel and the results are merged by the parent.
- This paradigm is very natural for computations such as quick sort.

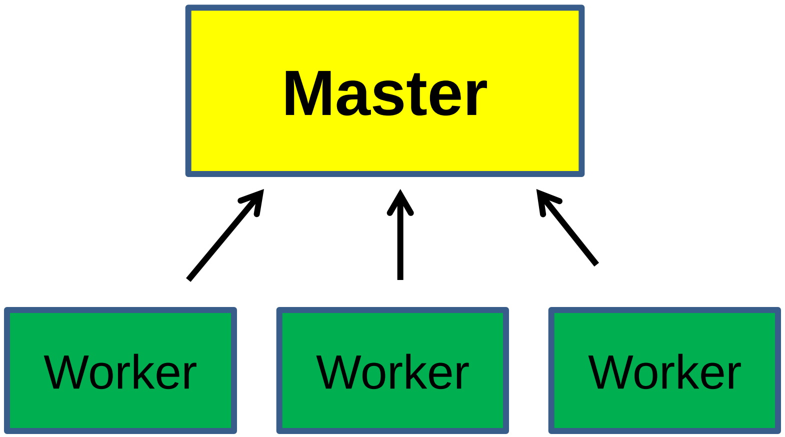
Pipeline Model

Data Stream



- In pipeline paradigm, a number of processes form a virtual pipeline.
- A continuous data stream is fed into the pipeline, and the processes execute at different pipeline stages simultaneously.

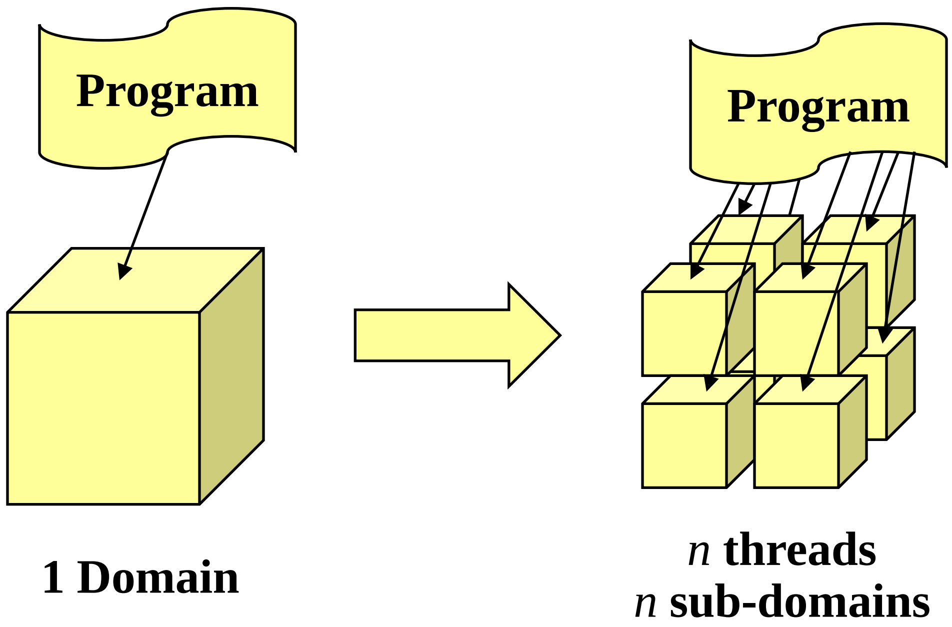
Process Farm Model



- Also known as the master-worker paradigm.
- A master process executes the essentially sequential part of the parallel program
- It spawns a number of worker processes to execute the parallel workload.
- When a worker finishes its workload, it informs the master which assigns a new workload to the slave.

- The coordination is done by the master.

Domain Decomposition



This methods solve a boundary value problem by splitting it into smaller boundary value problems on subdomains and iterating to coordinate the solution between adjacent subdomains.

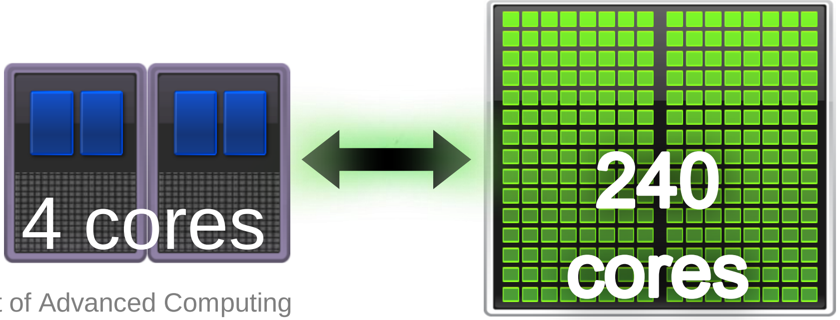
Desirable Attributes for Parallel Algorithms

- Concurrency
  - Ability to perform many actions simultaneously
- Scalability
  - Resilience to increasing processor counts
- Data Locality
  - High ratio of local memory accesses to remote memory accesses (through communication)
- Modularity:
  - Decomposition of complex entities into simpler components

Heterogeneous Computing: GPUs + CPUs

Massive processing power introduces I/O challenge

- Getting data to and from the processing units can take as long as the processing itself
- Requires careful software design and deep understanding of algorithms and architecture of
  - Processors (Cache effects, memory bandwidth)
  - GPU accelerators
  - Interconnects (Ethernet, IB, 10 Gigabit Ethernet),
  - Storage (local disks, NFS, parallel file systems)

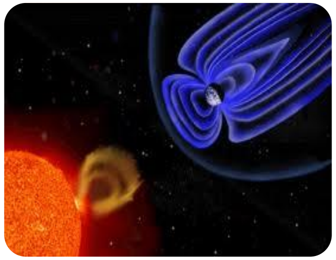


Application Areas of HPC in Science & Engineering

HPC in Science

Space Science

- Applications in Astrophysics and Astronomy



Earth Science

- Applications in understanding Physical Properties of Geological Structures, Water Resource Modelling, Seismic Exploration

Atmospheric Science

- Applications in Climate and Weather Forecasting, Air Quality

HPC in Science

Life Science

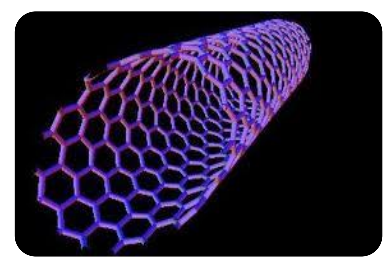
- Applications in Drug Designing, Genome Sequencing, Protein Folding

Nuclear Science

- Applications in Nuclear Power, Nuclear Medicine (cancer etc.), Defence

Nano Science

- Applications in Semiconductor Physics, Microfabrication, Molecular Biology, Exploration of New Materials



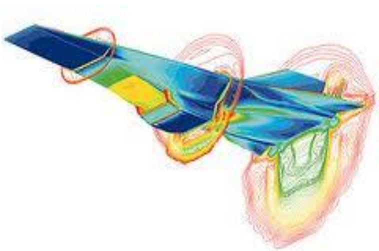
HPC in Engineering

Crash Simulation

- Applications in Automobile and Mechanical Engineering

Aerodynamics Simulation & Aircraft Designing

- Applications in Aeronautics and Mechanical Engineering



Structural Analysis

- Applications in Civil Engineering and Architecture

Multimedia and Animation

DreamWorks Animation SKG produces all its animated movies using HPC graphic technology

Graphical Animation Application in Multimedia and Animation

Thank You

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