Introduction to Parallel Computing

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

Converted into slides by Olivier Ricou <ricou@lrde.epita.fr>
Sources available on `http://www.lrde.epita.fr/~ricou`.

Warning: few modifications have been made during the convertion.

Abstract

This presentation covers the basics of parallel computing. Beginning with a brief overview and some concepts and terminology associated with parallel computing, the topics of parallel memory architectures and programming models are then explored. These topics are followed by a discussion on a number of issues related to designing parallel programs. The last portion of the presentation is spent examining how to parallelize several different types of serial programs.

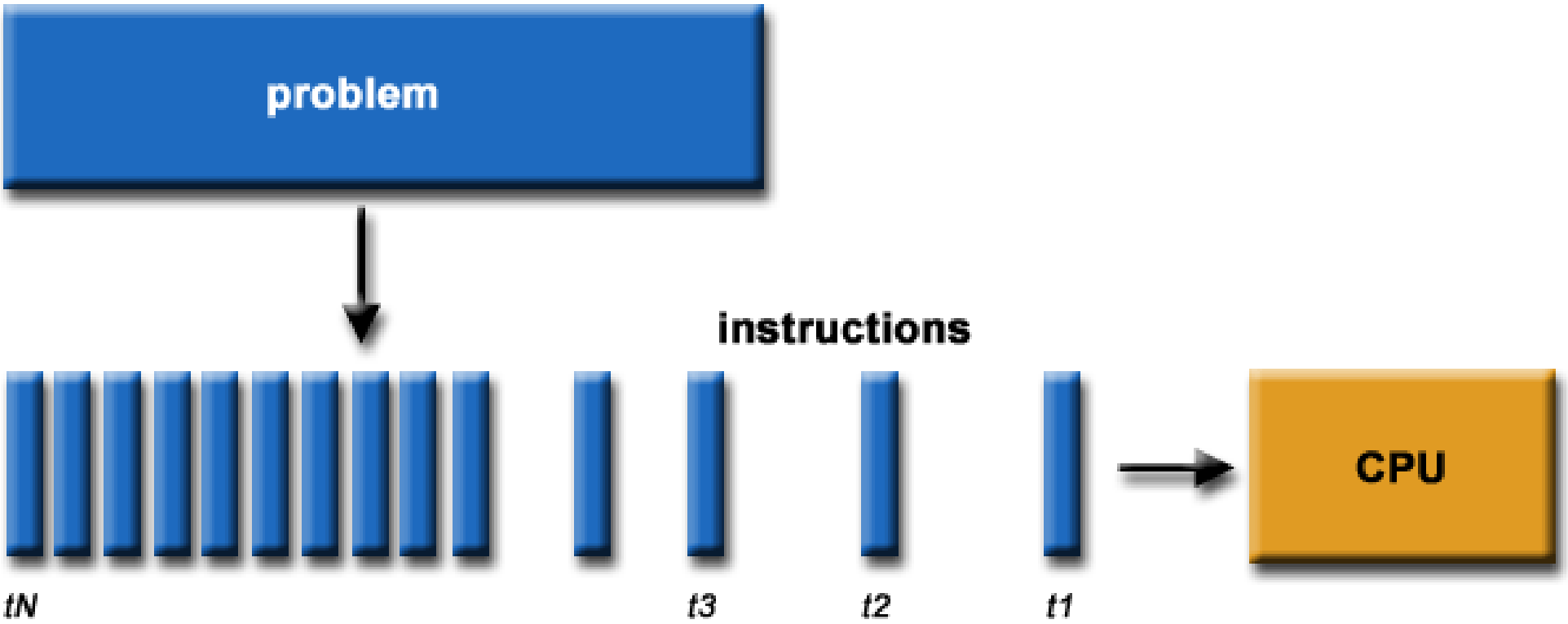
Level/Prerequisites: None

What is Parallel Computing?

Serial computation

Traditionally, software has been written for ***serial*** computation:

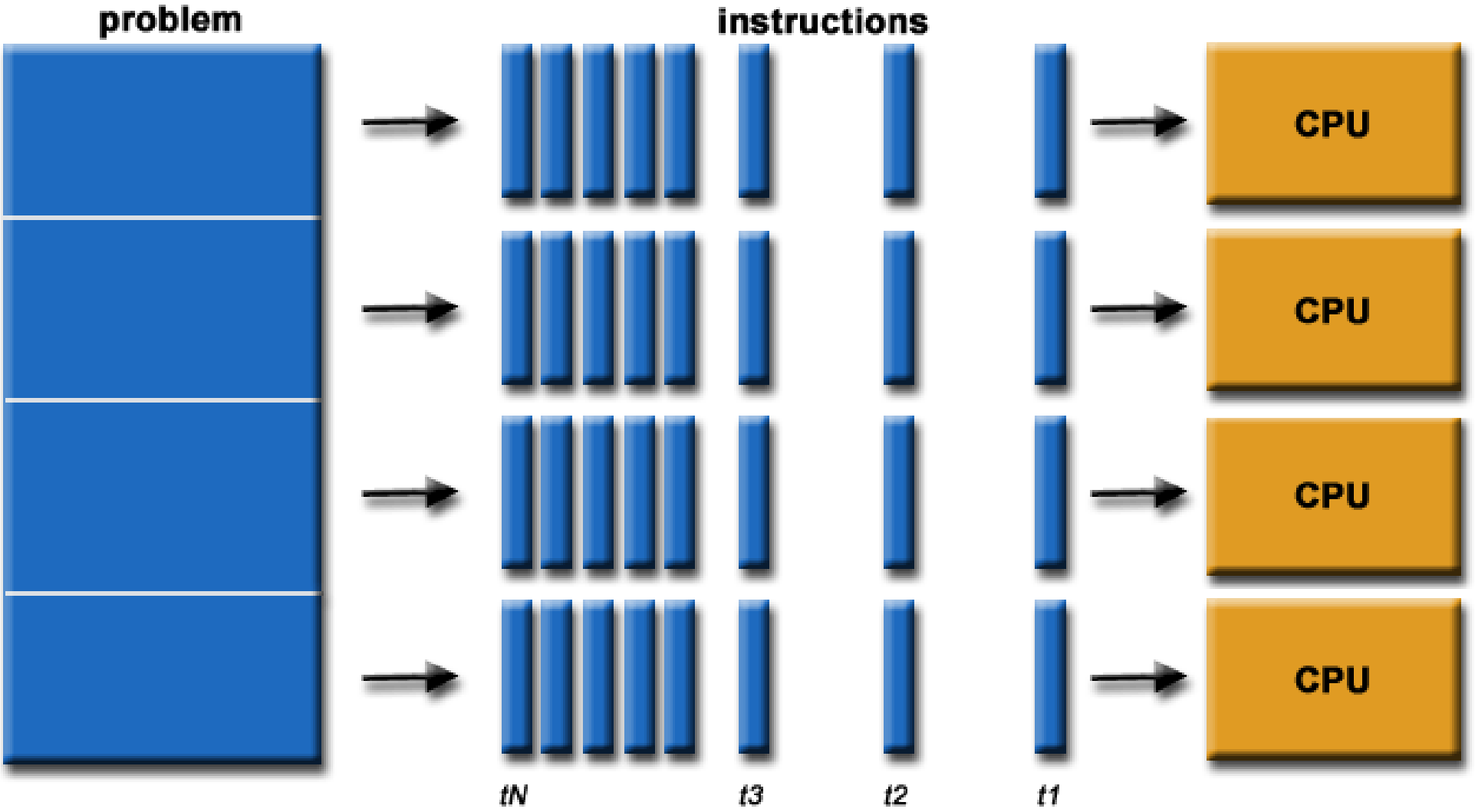
- To be run on a single computer having a single Central Processing Unit (CPU);
- A problem is broken into a discrete series of instructions.
- Instructions are executed one after another.
- Only one instruction may execute at any moment in time.


problem
instructions
CPU
tN
t3
t2
t1

Parallel computing

In the simplest sense, ***parallel computing*** is the simultaneous use of multiple compute resources to solve a computational problem.

- To be run using multiple CPUs
- A problem is broken into discrete parts that can be solved concurrently
- Each part is further broken down to a series of instructions
- Instructions from each part execute simultaneously on different CPUs


problem
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CPU
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Environment

The ***compute resources*** can include:

- A single computer with multiple processors;
- An arbitrary number of computers connected by a network;
- A combination of both.

The ***computational problem*** usually demonstrates characteristics such as the ability to be:

- Broken apart into discrete pieces of work that can be solved simultaneously;
- Execute multiple program instructions at any moment in time;
- Solved in less time with multiple compute resources than with a single compute resource.

Parallelism?

Parallel computing is an evolution of serial computing that attempts to emulate what has always been the state of affairs in the natural world: many ***complex, interrelated events happening at the same time***, yet within a sequence.

Some examples:

- Planetary and galactic orbits
- Weather and ocean patterns
- Tectonic plate drift
- Rush hour traffic in LA
- Automobile assembly line
- Daily operations within a business
- Building a shopping mall
- Ordering a hamburger at the drive through.

What for?

Traditionally, parallel computing has been considered to be "the high end of computing" and has been motivated by numerical simulations of complex systems and "Grand Challenge Problems" such as:

- weather and climate
- chemical and nuclear reactions
- biological, human genome
- geological, seismic activity
- mechanical devices - from prosthetics to spacecraft
- electronic circuits
- manufacturing processes

What for? (2)

Today, commercial applications are providing an equal or greater driving force in the development of faster computers. These applications require the ***processing of large amounts of data in sophisticated ways***. Example applications include:

- parallel databases, data mining
- oil exploration
- web search engines, web based business services
- computer-aided diagnosis in medicine
- management of national and multi-national corporations
- advanced graphics and virtual reality, particularly in the entertainment industry
- networked video and multi-media technologies
- collaborative work environments

Why Use Parallel Computing?

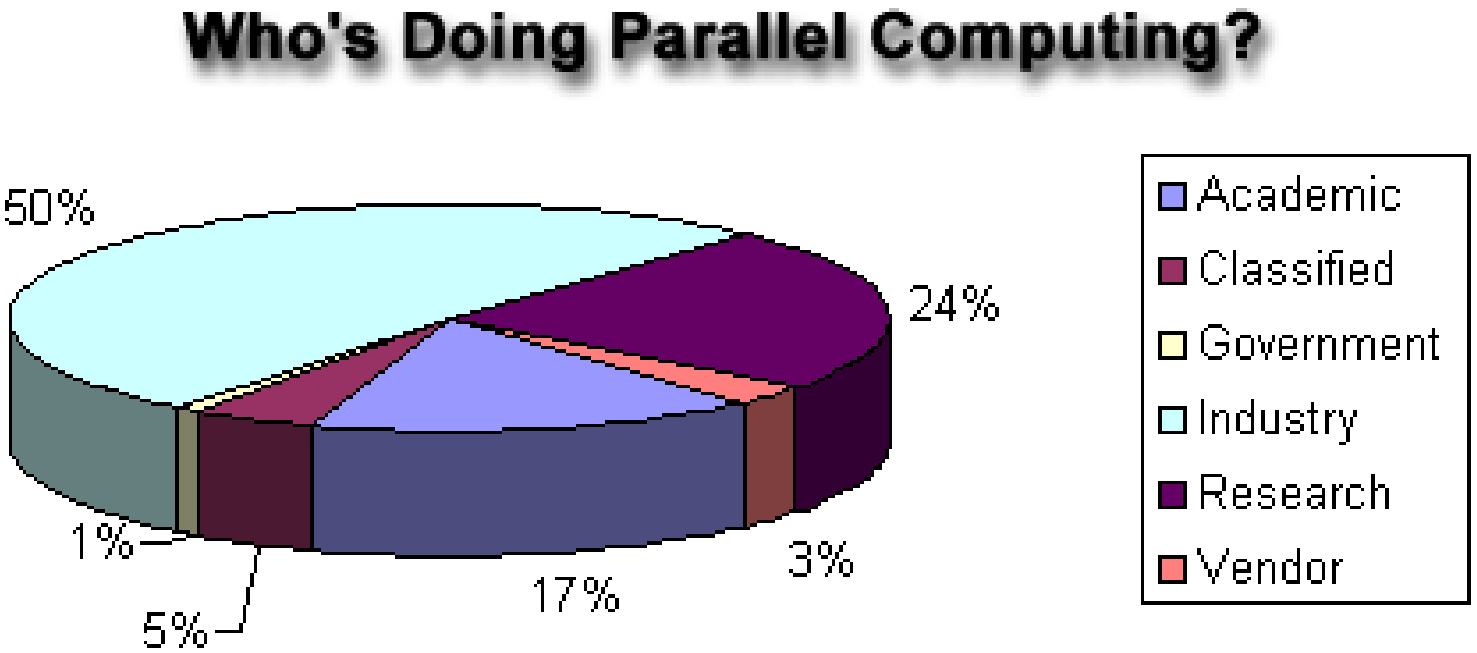
- The primary reasons for using parallel computing:
  - ***Save time - wall clock time***
  - ***Solve larger problems***
  - ***Provide concurrency*** (do multiple things at the same time)
- Other reasons might include:
  - Taking advantage of non-local resources - using available compute resources on a wide area network, or even the Internet when local compute resources are scarce.
  - Cost savings - using multiple "cheap" computing resources instead of paying for time on a supercomputer.
  - Overcoming memory constraints - single computers have very finite memory resources. For large problems, using the memories of multiple computers may overcome this obstacle.

- ***Limits to serial computing*** - both physical and practical reasons pose significant constraints to simply building ever faster serial computers:
  - Transmission speeds - the speed of a serial computer is directly dependent upon how fast data can move through hardware. Absolute limits are the speed of light (30 cm/nanosecond) and the transmission limit of copper wire (9 cm/nanosecond). Increasing speeds necessitate increasing proximity of processing elements.
  - Limits to miniaturization - processor technology is allowing an increasing number of transistors to be placed on a chip. However, even with molecular or atomic-level components, a limit will be reached on how small components can be.
  - Economic limitations - it is increasingly expensive to make a single processor faster. Using a larger number of moderately fast commodity processors to achieve the same (or better) performance is less expensive.

- ***The future***: during the past 10 years, the trends indicated by ever faster networks, distributed systems, and multi-processor computer architectures (even at the desktop level) clearly show that ***parallelism is the future of computing***.

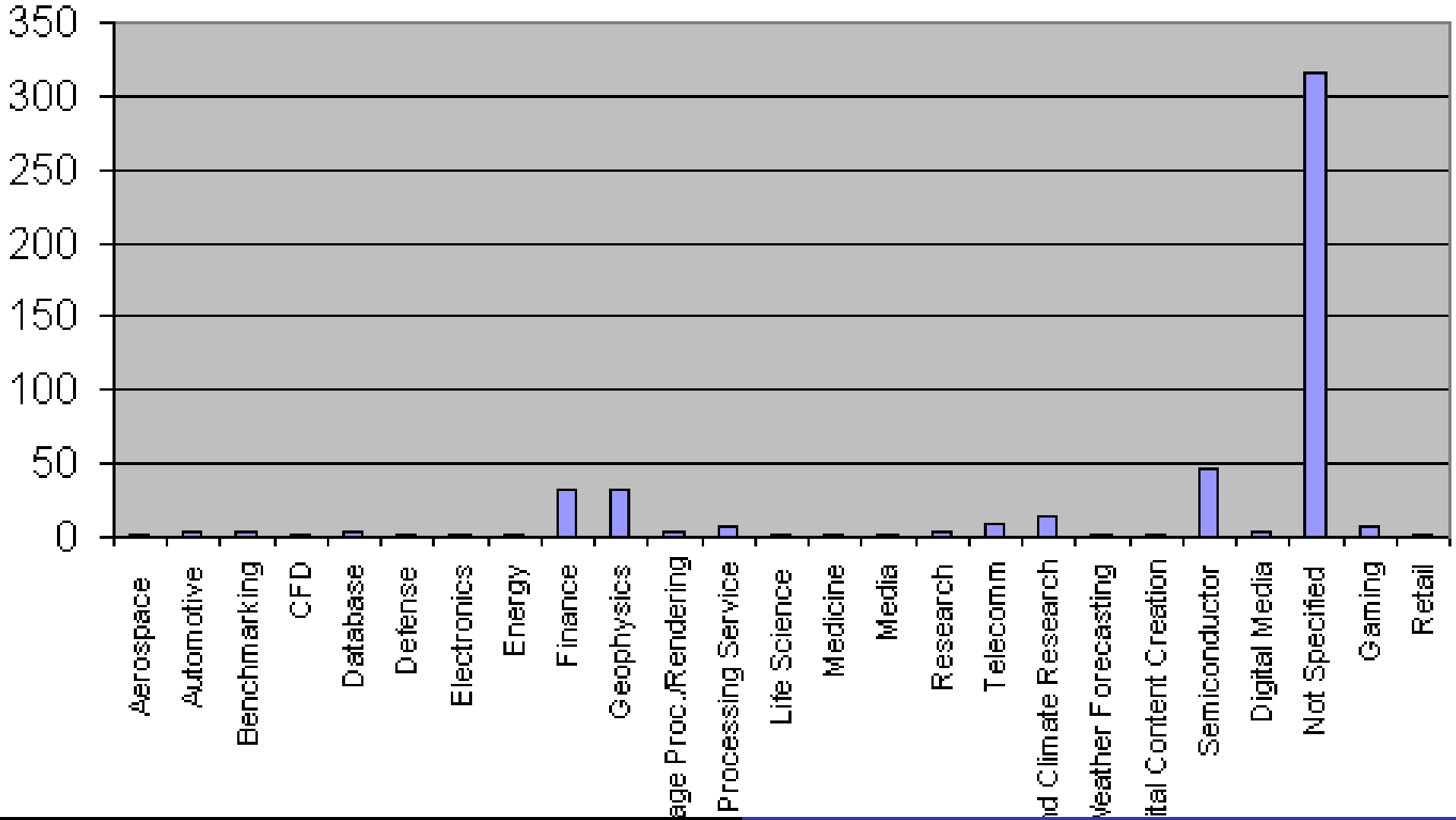
Who and What?

Top500.org[1] provides statistics on parallel computing users - the charts below are just a sample.



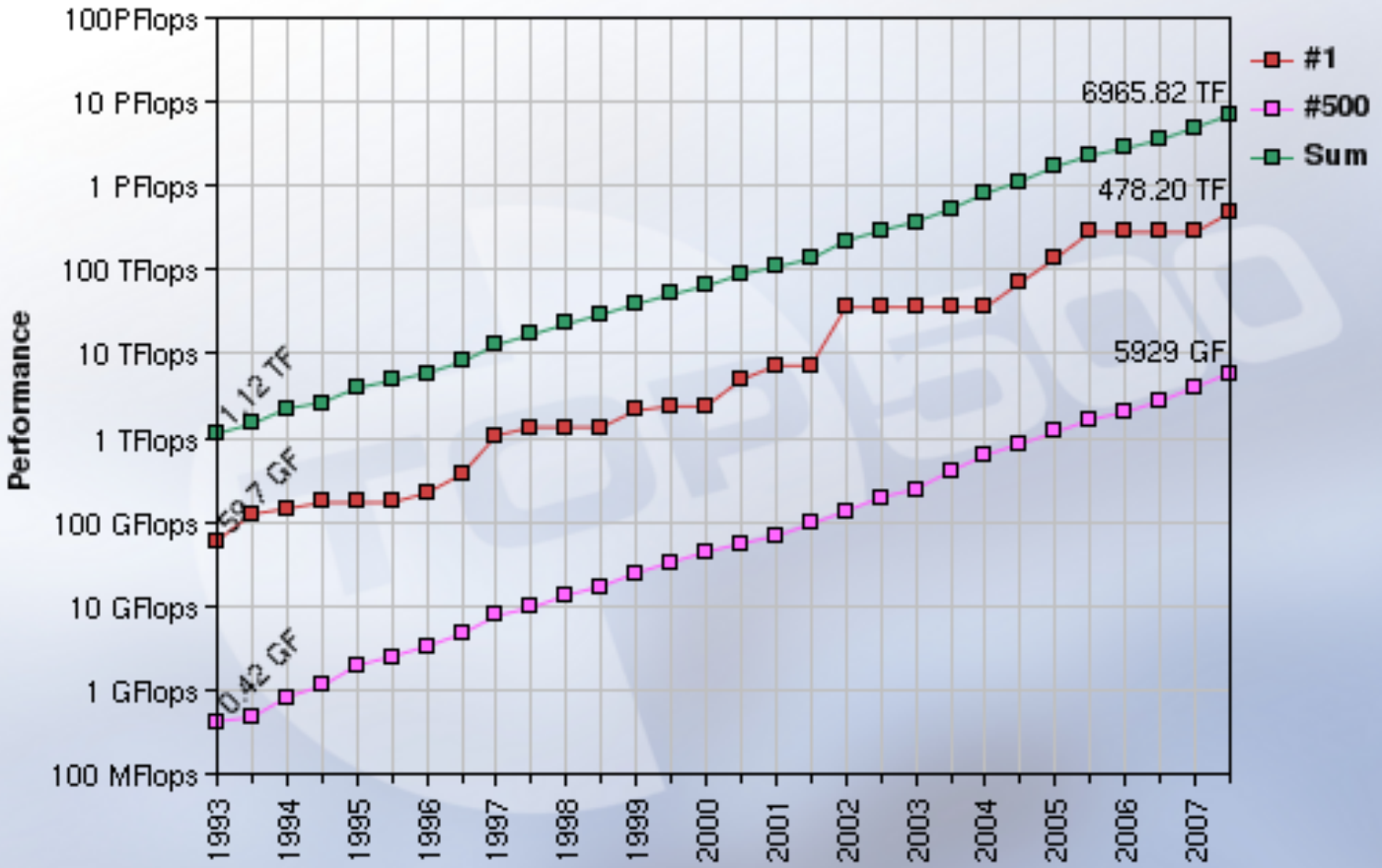
[1] See URL http://top500.org

What Are They Using it For?



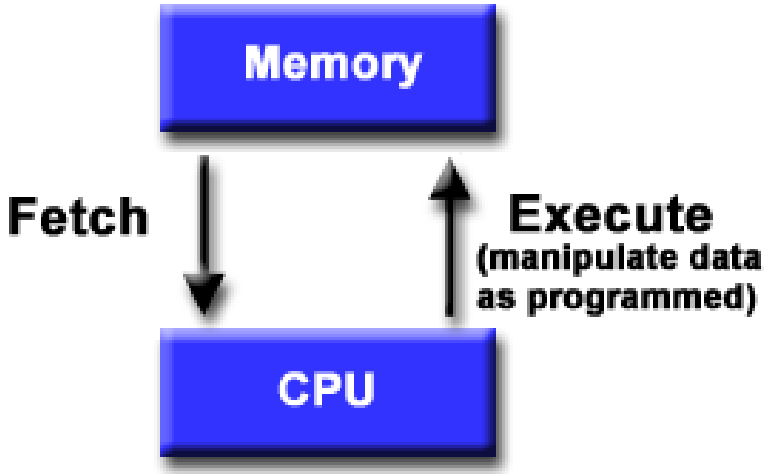
TOP500 SUPERCOMPUTER SITES

Performance Development



von Neumann Architecture

- For over 40 years, virtually all computers have followed a common machine model known as the von Neumann computer. Named after the Hungarian mathematician John von Neumann.
- A von Neumann computer uses the stored-program concept. The CPU executes a stored program that specifies a sequence of read and write operations on the memory.



Basic design:

- Memory is used to store both program and data instructions
- Program instructions are coded data which tell the computer to do something
- Data is simply information to be used by the program
- A central processing unit (CPU) gets instructions and/or data from memory, decodes the instructions and then ***sequentially*** performs them.

Flynn's Classical Taxonomy

- There are different ways to classify parallel computers. One of the more widely used classifications, in use since 1966, is called Flynn's Taxonomy.
- Flynn's taxonomy distinguishes multi-processor computer architectures according to how they can be classified along the two independent dimensions of ***Instruction*** and ***Data***. Each of these dimensions can have only one of two possible states: ***Single*** or ***Multiple***.

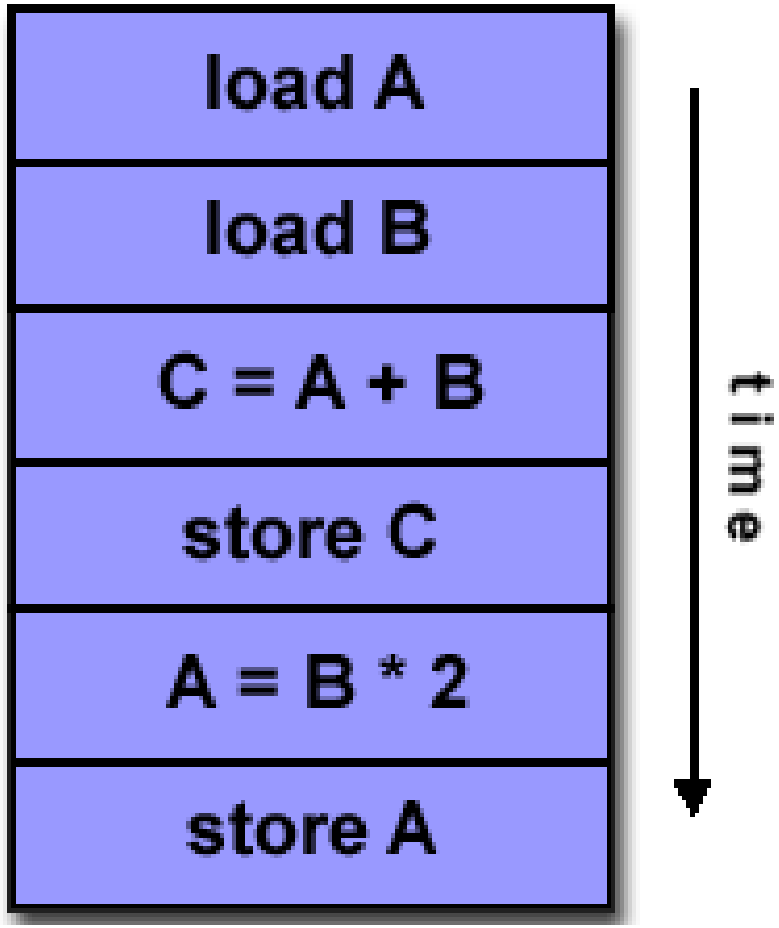
Here are the 4 possible classifications according to Flynn:

S I S D Single Instruction, Single Data	S I M D Single Instruction, Multiple Data
M I S D Multiple Instruction, Single Data	M I M D Multiple Instruction, Multiple Data

Single Instruction, Single Data (SISD)

- A serial (non-parallel) computer
- Single instruction: only one instruction stream is being acted on by the CPU during any one clock cycle
- Single data: only one data stream is being used as input during any one clock cycle
- Deterministic execution
- This is the oldest and until recently, the most prevalent form of computer
- Examples: most PCs, single CPU workstations and mainframes

SISD

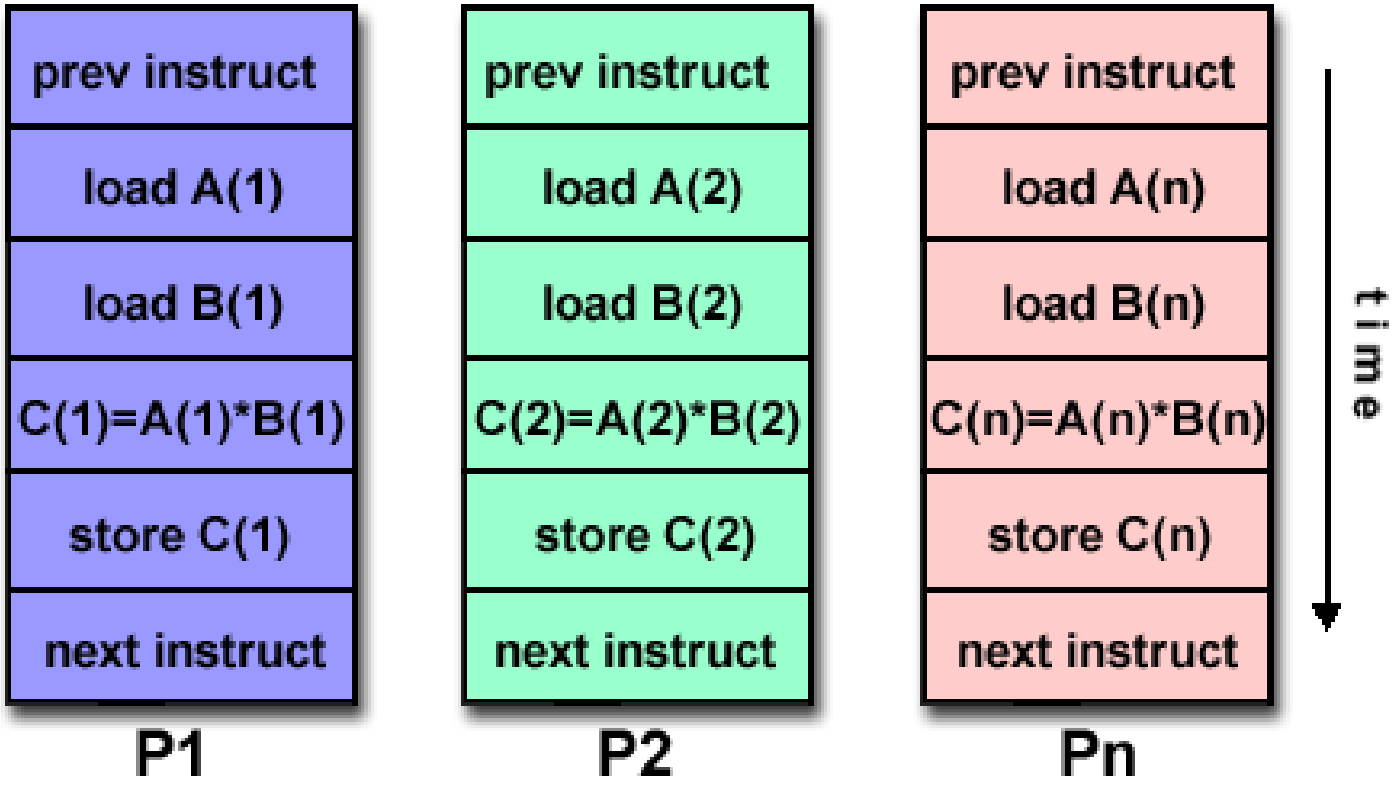


Single Instruction, Multiple Data (SIMD)

- A type of parallel computer
- Single instruction: All processing units execute the same instruction at any given clock cycle
- Multiple data: Each processing unit can operate on a different data element
- This type of machine typically has an instruction dispatcher, a very high-bandwidth internal network, and a very large array of very small-capacity instruction units.
- Best suited for specialized problems characterized by a high degree of regularity,such as image processing.
- Synchronous (lockstep) and deterministic execution
- Two varieties: Processor Arrays and Vector Pipelines

Examples of SIMD:

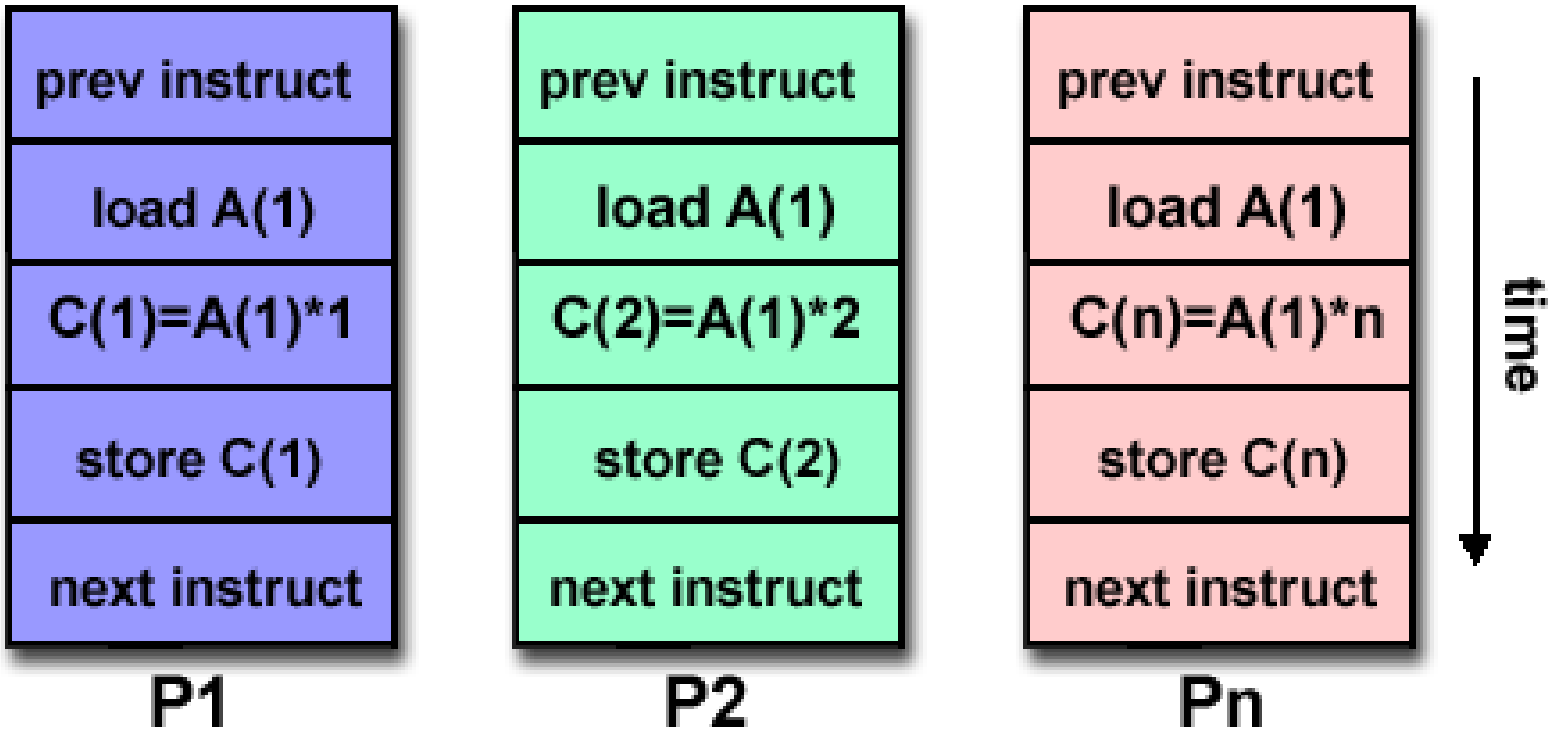
- Processor Arrays: Connection Machine CM-2, Maspar MP-1, P-2
- Vector Pipelines: IBM 9000, Cray C90, Fujitsu VP, NEC SX-2, Hitachi S820



Multiple Instruction, Single Data (MISD)

- A single data stream is fed into multiple processing units.
- Each processing unit operates on the data independently via independent instruction streams.
- Few actual examples of this class of parallel computer have ever existed. One is the experimental Carnegie-Mellon C.mmp computer (1971).
- Some conceivable uses might be:
  - multiple frequency filters operating on a single signal stream
  - multiple cryptography algorithms attempting to crack a single coded message.

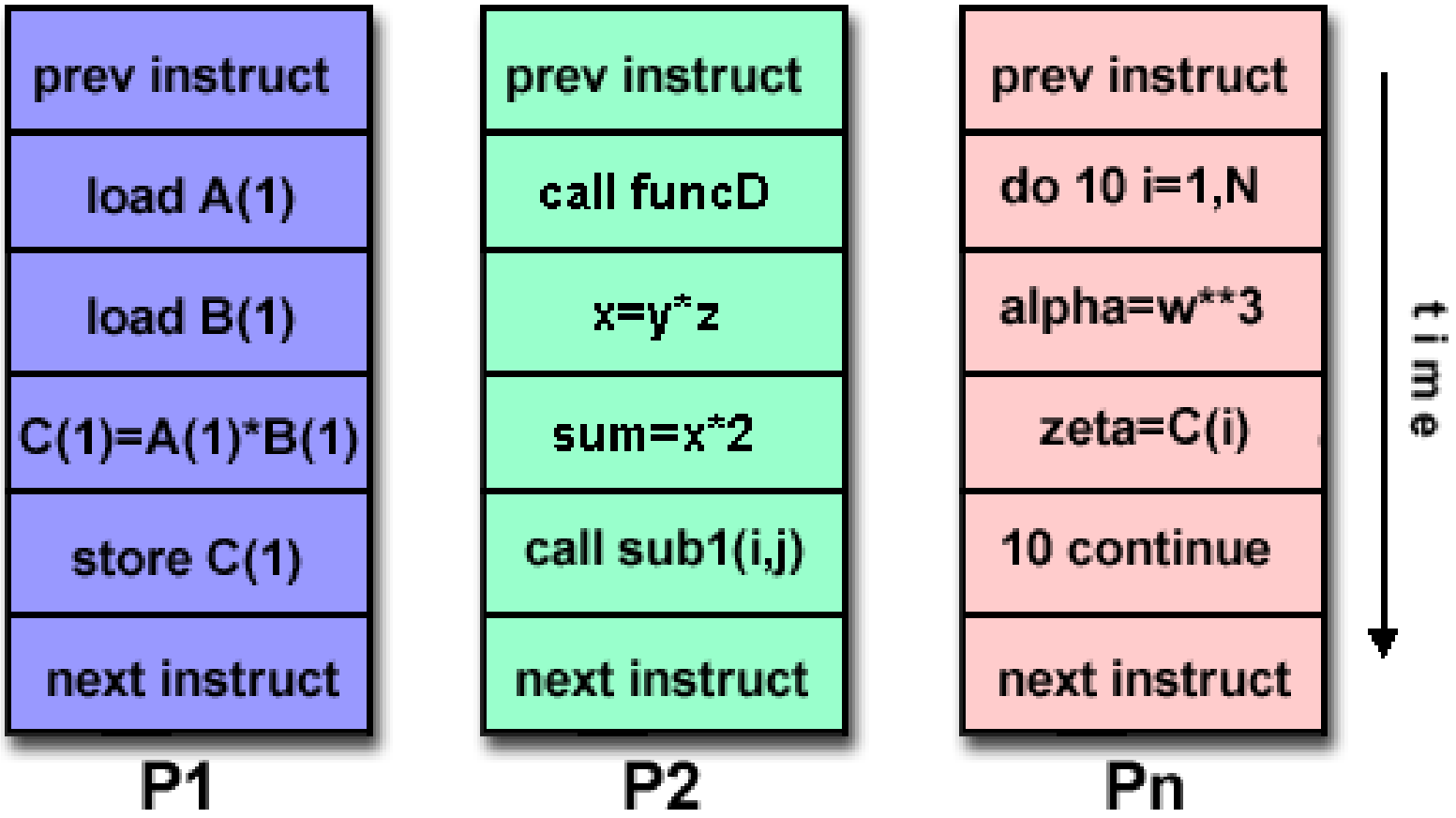
MISD


prev instruct
load A(1)
C(1)=A(1)*1
store C(1)
next instruct
P1
prev instruct
load A(1)
C(2)=A(1)*2
store C(2)
next instruct
P2
prev instruct
load A(1)
C(n)=A(1)*n
store C(n)
next instruct
Pn
time

Multiple Instruction, Multiple Data (MIMD)

- Currently, the most common type of parallel computer. Most modern computers fall into this category.
- Multiple Instruction: every processor may be executing a different instruction stream
- Multiple Data: every processor may be working with a different data stream
- Execution can be synchronous or asynchronous, deterministic or non-deterministic
- Examples: most current supercomputers, networked parallel computer "grids" and multi-processor SMP computers - including some types of PCs.

MIMD


prev instruct
load A(1)
load B(1)
C(1)=A(1)*B(1)
store C(1)
next instruct
P1
prev instruct
call funcD
x=y*z
sum=x*2
call sub1(i,j)
next instruct
P2
prev instruct
do 10 i=1,N
alpha=w**3
zeta=C(i)
10 continue
next instruct
Pn
time

Some General Parallel Terminology

Like everything else, parallel computing has its own "jargon". Some of the more commonly used terms associated with parallel computing are listed below. Most of these will be discussed in more detail later.

Task A logically discrete section of computational work. A task is typically a program or program-like set of instructions that is executed by a processor.

Parallel Task A task that can be executed by multiple processors safely (yields correct results)

Serial Execution Execution of a program sequentially, one statement at a time. In the simplest sense, this is what happens on a one processor machine. However, virtually all parallel tasks will have sections of a parallel program that must be executed serially.

Parallel Execution Execution of a program by more than one task, with each task being able to execute the same or different statement at the same moment in time.

Shared Memory From a strictly hardware point of view, describes a computer architecture where all processors have direct (usually bus based) access to common physical memory. In a programming sense, it describes a model where parallel tasks all have the same "picture" of memory and can directly address and access the same logical memory locations regardless of where the physical memory actually exists.

Distributed Memory In hardware, refers to network based memory access for physical memory that is not common. As a programming model, tasks can only logically "see" local machine memory and must use communications to access memory on other machines where other tasks are executing.

Communications Parallel tasks typically need to exchange data. There are several ways this can be accomplished, such as through a shared memory bus or over a network, however the actual event of data exchange is commonly referred to as communications regardless of the method employed.

Synchronization The coordination of parallel tasks in real time, very often associated with communications. Often implemented by establishing a synchronization point within an application where a task may not proceed further until another task(s) reaches the same or logically equivalent point.
Synchronization usually involves waiting by at least one task, and can therefore cause a parallel application's wall clock execution time to increase.

Granularity In parallel computing, granularity is a qualitative measure of the ratio of computation to communication.

- ***Coarse:*** relatively large amounts of computational work are done between communication events
- ***Fine:*** relatively small amounts of computational work are done between communication events

Observed Speedup Observed speedup of a code which has been parallelized, defined as:

$$\frac{\text{wall-clock time of serial execution}}{\text{wall-clock time of parallel execution}}$$

One of the simplest and most widely used indicators for a parallel program's performance.

Parallel Overhead The amount of time required to coordinate parallel tasks, as opposed to doing useful work. Parallel overhead can include factors such as:

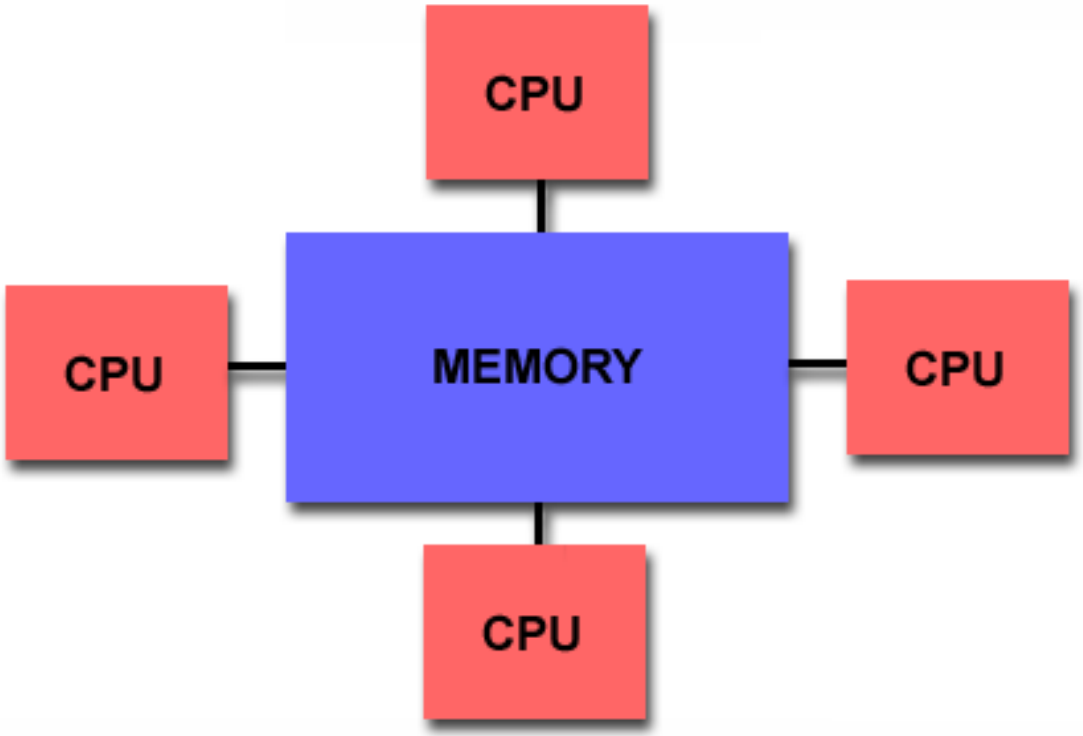
- Task start-up time
- Synchronizations
- Data communications
- Software overhead imposed by parallel compilers, libraries, tools, operating system, etc.
- Task termination time

Massively Parallel Refers to the hardware that comprises a given parallel system - having many processors. The meaning of many keeps increasing, but currently BG/L pushes this number to 6 digits.

Scalability Refers to a parallel system's (hardware and/or software) ability to demonstrate a proportionate increase in parallel speedup with the addition of more processors. Factors that contribute to scalability include:

- Hardware - particularly memory-cpu bandwidths and network communications
- Application algorithm
- Parallel overhead related
- Characteristics of your specific application and coding

Shared Memory



General Characteristics:

- Shared memory parallel computers vary widely, but generally have in common the ability for all processors to access all memory as global address space.
- Multiple processors can operate independently but share the same memory resources.
- Changes in a memory location effected by one processor are visible to all other processors.
- Shared memory machines can be divided into two main classes based upon memory access times: ***UMA*** and ***NUMA***.

UMA/NUMA

Uniform Memory Access (UMA):

- Most commonly represented today by Symmetric Multiprocessor (SMP) machines
- Identical processors
- Equal access and access times to memory
- Sometimes called CC-UMA - Cache Coherent UMA. Cache coherent means if one processor updates a location in shared memory, all the other processors know about the update. Cache coherency is accomplished at the hardware level.

UMA/NUMA (2)

Non-Uniform Memory Access (NUMA):

- Often made by physically linking two or more SMPs
- One SMP can directly access memory of another SMP
- Not all processors have equal access time to all memories
- Memory access across link is slower
- If cache coherency is maintained, then may also be called CC-NUMA - Cache Coherent NUMA

Shared Memory (...)

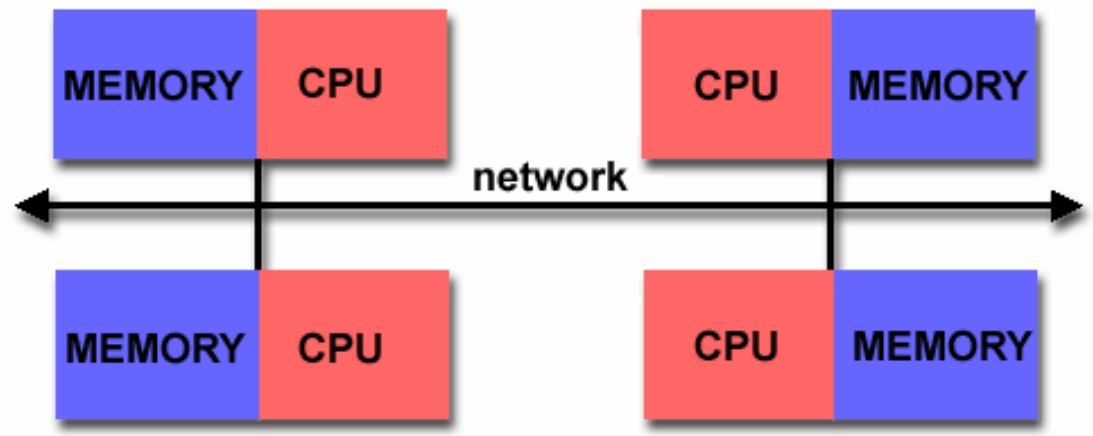
Advantages:

- Global address space provides a ***user-friendly programming*** perspective to memory
- Data sharing between tasks is both ***fast and uniform*** due to the proximity of memory to CPUs

Disadvantages:

- Primary disadvantage is the ***lack of scalability*** between memory and CPUs. Adding more CPUs can geometrically increases traffic on the shared memory-CPU path, and for cache coherent systems, geometrically increase traffic associated with cache/memory management.
- Programmer ***responsibility for synchronization*** constructs that insure "correct" access of global memory

Distributed Memory



General Characteristics:

- Like shared memory systems, distributed memory systems vary widely but share a common characteristic. Distributed memory systems ***require a communication network*** to connect inter-processor memory.

General Characteristics (...):

- Processors have their own local memory. Memory addresses in one processor do not map to another processor, so there is ***no concept of global address space*** across all processors.
- Because each processor has its own local memory, it operates independently. Changes it makes to its local memory have no effect on the memory of other processors. Hence, the ***concept of cache coherency does not apply***.
- When a processor needs access to data in another processor, it is usually the task of the programmer to explicitly define how and when data is communicated. ***Synchronization*** between tasks ***is*** likewise the ***programmer's responsibility***.
- The network "fabric" used for data transfer varies widely, though it can ***can be as simple as Ethernet***.

Distributed Memory (...)

Advantages:

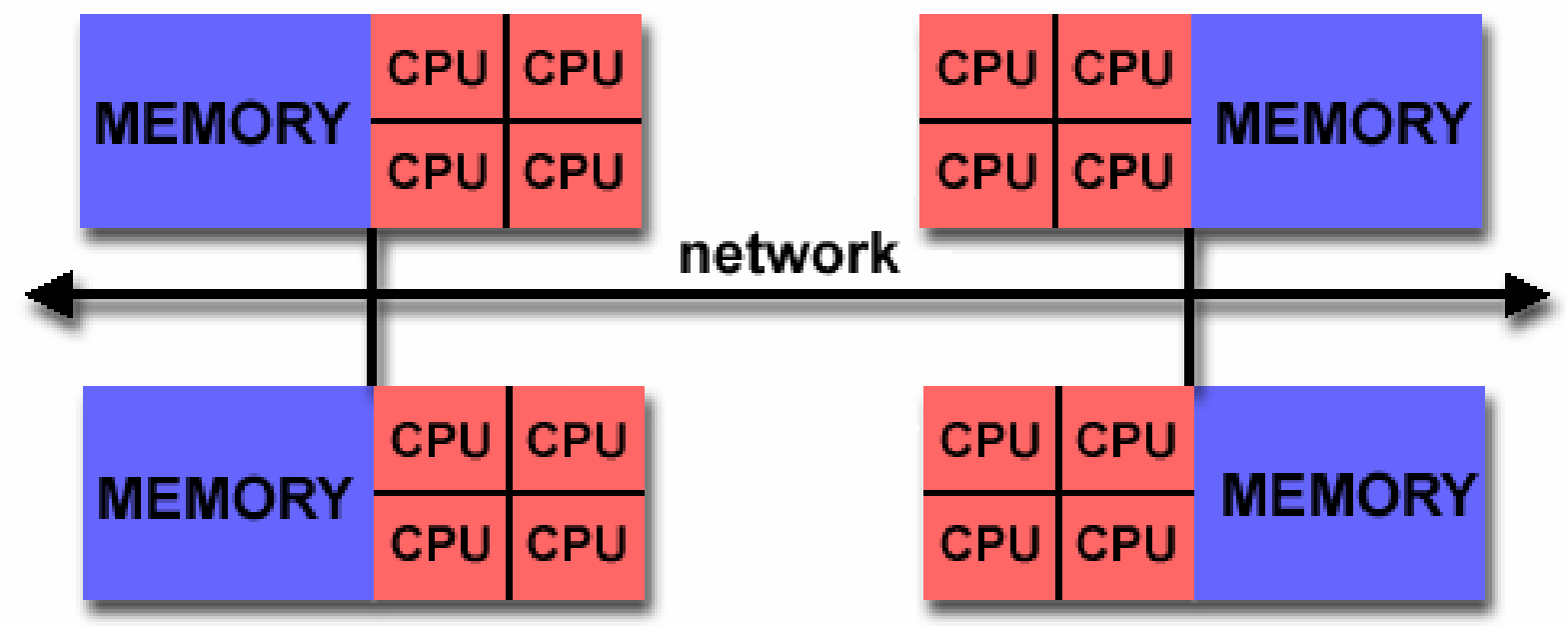
- ***Memory is scalable*** with number of processors. Increase the number of processors and the size of memory increases proportionately.
- Each processor can rapidly ***access its own memory without interference*** and without the overhead incurred with trying to maintain cache coherency.
- ***Cost effectiveness***: can use commodity, off-the-shelf processors and networking.

Distributed Memory (...)

Disadvantages:

- ***The programmer is responsible*** for many of the details associated with data communication between processors.
- It may be ***difficult to map existing data structures***, based on global memory, to this memory organization.
- ***Non-uniform memory access*** (NUMA) times

Hybrid Distributed-Shared Memory



Comparison of Shared and Distributed Memory Architectures

Architecture	CC-UMA	CC-NUMA	Distributed
Examples	SMPs, DEC/Compaq, SGI Challenge, IBM POWER3	SGI Origin, Sequent, IBM POWER4 (MCM), DEC/Compaq	Cray T3E, Maspar, IBM SP2
Communications	MPI, Threads, OpenMP, shmem	MPI, Threads, OpenMP, shmem	MPI
Scalability	to 10s of proc.	to 100s of proc.	to 1000s of proc.
Draw Backs	Memory-CPU bandwidth	Memory-CPU bandwidth, Non-uniform access times	System adm., Programming is hard to develop and maintain
Software Availability	many 1000s ISVs	many 1000s ISVs	100s ISVs

Hybrid Distributed-Shared Memory (...)

- The largest and fastest computers in the world today employ both shared and distributed memory architectures.
- The shared memory component is usually a cache coherent SMP machine. Processors on a given SMP can address that machine's memory as global.
- The distributed memory component is the networking of multiple SMPs. SMPs know only about their own memory - not the memory on another SMP. Therefore, network communications are required to move data from one SMP to another.
- Current trends seem to indicate that this type of memory architecture will continue to prevail and increase at the high end of computing for the foreseeable future.
- Advantages and Disadvantages: whatever is common to both shared and distributed memory architectures

Overview

There are several parallel programming models in common use:

- Shared Memory
- Threads
- Message Passing
- Data Parallel
- Hybrid

Parallel programming models exist as an abstraction above hardware and memory architectures.

These models are NOT specific to a particular type of machine or memory architecture. In fact, these models can (theoretically) be implemented on any underlying hardware. Two examples:

1. ***Shared memory model on a distributed memory machine***: Kendall Square Research (KSR) ALLCACHE approach. Machine memory was physically distributed, but appeared to the user as a single shared memory (global address space). Generically, this approach is referred to as "virtual shared memory".
2. ***Message passing model on a shared memory machine***: MPI on SGI Origin. The SGI Origin employed the CC-NUMA type of shared memory architecture, where every task has direct access to global memory. However, the ability to ***send and receive messages with MPI***, as is commonly done over a network of distributed memory machines, is ***is very commonly used***

Which model to use is often a combination of what is available and personal choice. There is no "best" model, although there certainly are better implementations of some models over others.

Shared Memory Model

- In the shared-memory programming model, tasks share a common address space, which they read and write asynchronously.
- Various mechanisms such as locks / semaphores may be used to control access to the shared memory.
- An advantage of this model from the programmer's point of view is that the notion of data "ownership" is lacking, so there is no need to specify explicitly the communication of data between tasks. Program development can often be simplified.
- An important disadvantage in terms of performance is that it becomes more difficult to understand and manage data locality.

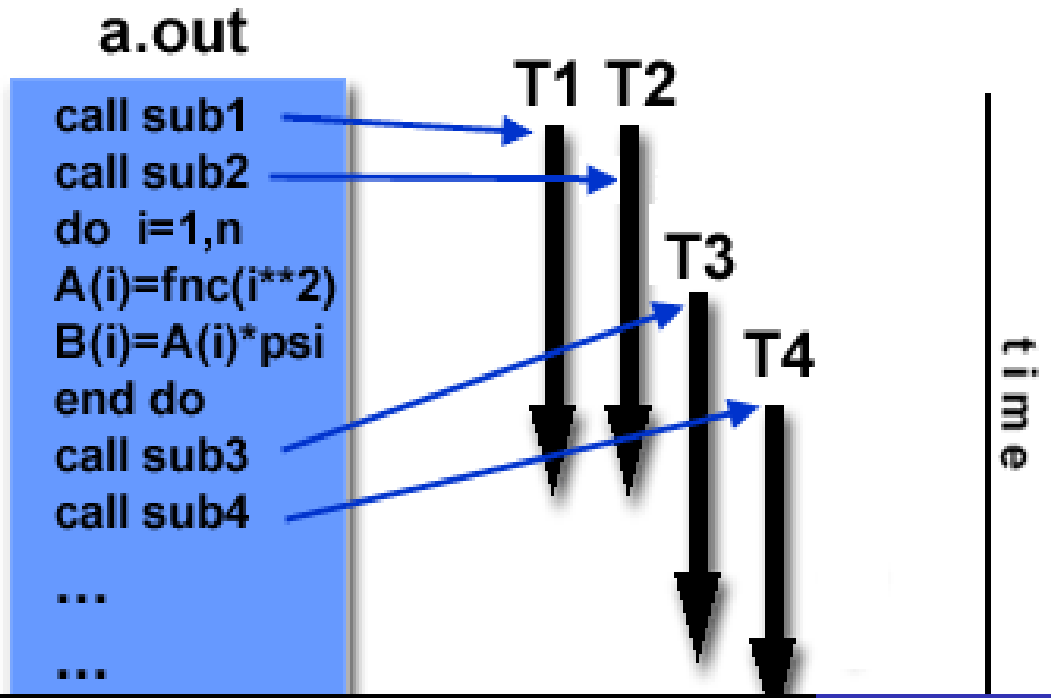
Implementations

- On shared memory platforms, the native compilers translate user program variables into actual memory addresses, which are global.
- No common distributed memory platform implementations currently exist. However, as mentioned previously in the Overview section, the KSR ALLCACHE approach provided a shared memory view of data even though the physical memory of the machine was distributed.

Threads Model

In the threads model of parallel programming, a single process can have multiple, concurrent execution paths.

An analogy to describe threads is the concept of a single program that includes a number of subroutines.



- The main program `a.out` is scheduled to run by the native OS.
- It performs some serial work, and then creates tasks (threads) that can be scheduled and run by the OS concurrently.
- Each thread has local data, but also, shares the entire resources of `a.out`. Each thread also benefits from a global memory view because it shares the memory space of `a.out`.
- A thread's work may best be described as a subroutine within the main program. Any thread can execute any subroutine at the same time as other threads.
- Threads communicate with each other through global memory This requires ***synchronization*** constructs to insure that more than one thread is not updating the same global address at any time.
- Threads can come and go, but `a.out` remains present to provide the necessary shared resources until the application has completed.

Threads are commonly associated with shared memory architectures and operating systems.

Implementations

From a programming perspective, threads implementations commonly comprise:

- A library of subroutines that are called from within parallel source code
- A set of compiler directives imbedded in either serial or parallel source code

In both cases, ***the programmer is responsible for determining all parallelism***.

Threaded implementations are not new in computing. Historically, hardware vendors have implemented their own proprietary versions of threads. These implementations differed substantially from each other making it difficult for programmers to develop portable threaded applications.

Unrelated standardization efforts have resulted in ***two very different implementations of threads***: ***POSIX Threads*** and ***OpenMP***.

POSIX Threads

- Library based; requires parallel coding
- Specified by the IEEE POSIX 1003.1c standard (1995).
- C Language only
- Commonly referred to as Pthreads.
- Most hardware vendors now offer Pthreads in addition to their proprietary threads implementations.
- Very explicit parallelism; requires significant programmer attention to detail.

OpenMP

- Compiler directive based; can use serial code
- Jointly defined and endorsed by a group of major computer hardware and software vendors. The OpenMP Fortran API was released October 28, 1997. The C/C++ API was released in late 1998.
- Portable / multi-platform, including Unix and Windows NT platforms
- Available in C/C++ and Fortran implementations
- Can be very easy and simple to use - provides for "incremental parallelism"

Microsoft has its own implementation for threads, which is not related to the UNIX POSIX standard or OpenMP.

Message Passing Model

The message passing model has the following characteristics:

- A set of tasks that use their own local memory during computation.
- Tasks exchange data through communications by sending and receiving messages.
- Data transfer usually requires cooperative operations to be performed by each process. For example, a send operation must have a matching receive operation.

Implementations

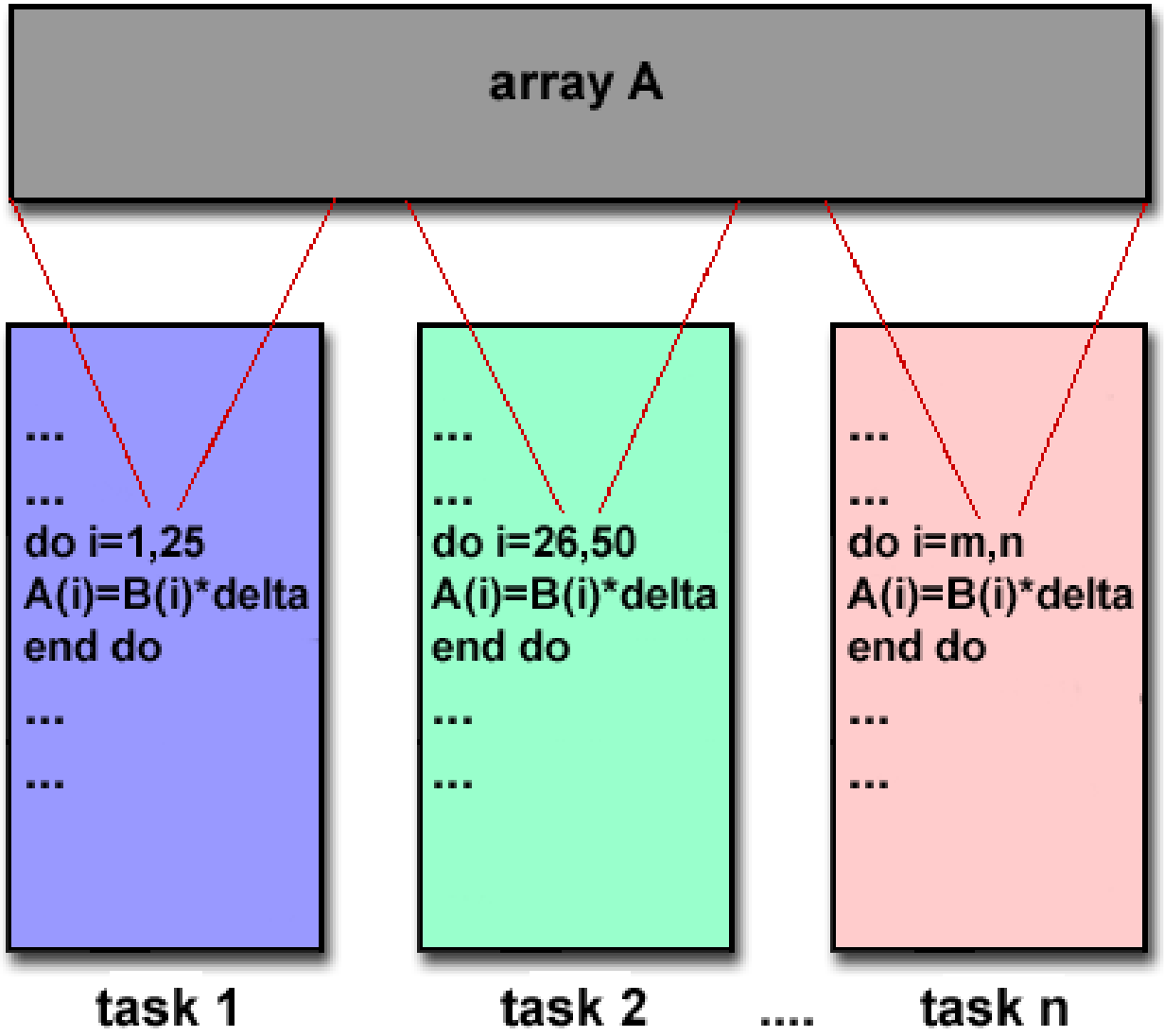
- From a programming perspective, message passing implementations commonly comprise ***a library of subroutines*** that are imbedded in source code. The programmer is responsible for determining all parallelism.
- Historically, a variety of message passing libraries have been ***available since the 1980s***. These implementations differed substantially from each other making it difficult for programmers to develop portable applications.
- In 1992, thei ***MPI Forum*** was formed with the primary goal of establishing a standard interface for message passing implementations.

- Part 1 of the **Message Passing Interface (MPI)** was released in 1994. Part 2 (MPI-2) was released in 1996. Both MPI specifications are available on the web at `www.mcs.anl.gov/Projects/mpi/standard.html`
- MPI is now the "***de facto*" *industry standard for message passing***, replacing virtually all other message passing implementations used for production work. Most, if not all of the popular parallel computing platforms offer at least one implementation of MPI. A few offer a full implementation of MPI-2.
- For shared memory architectures, MPI implementations usually don't use a network for task communications. Instead, they use shared memory (memory copies) for performance reasons.

Data Parallel Model

The data parallel model demonstrates the following characteristics:

- Most of the parallel work focuses on performing operations on ***a data set***. The data set is typically organized into a common structure, such as an array or cube.
- A set of ***tasks work collectively on the same data structure***, however, each task works on a different partition of the same data structure.
- ***Tasks perform the same operation*** on their partition of work, for example, "add 4 to every array element".


array A
...
...
do i=1,25
A(i)=B(i)*delta
end do
...
...
...
...
do i=26,50
A(i)=B(i)*delta
end do
...
...
...
...
do i=m,n
A(i)=B(i)*delta
end do
...
...
task 1
task 2
....
task n

On shared memory architectures, all tasks may have access to the data structure through global memory.

On distributed memory architectures the data structure is split up and resides as "chunks" in the loc al memory of each task.

Implementations

- Programming with the data parallel model is usually accomplished by writing a program with data parallel constructs.
- **Fortran 90 and 95 (F90, F95):** ISO/ANSI standard extensions to Fortran 77.
  - Contains everything that is in Fortran 77
  - New source code format; additions to character set
  - Additions to program structure and commands
  - Variable additions - methods and arguments
  - Pointers and dynamic memory allocation added
  - Array processing (arrays treated as objects) added
  - Recursive and new intrinsic functions added
  - Many other new features

  Implementations are available for most common parallel platforms.

- **High Performance Fortran (HPF):** Extensions to Fortran 90 to support data parallel programming.
  - Contains everything in Fortran 90
  - Directives to tell compiler how to distribute data added
  - Assertions that can improve optimization of generated code added
  - Data parallel constructs added (now part of Fortran 95)

  Implementations are available for most common parallel platforms.
- **Compiler Directives:** Allow the programmer to specify the distribution and alignment of data. Fortran implementations are available for most common parallel platforms.
- Distributed memory implementations of this model usually have the ***compiler convert the program into standard code with calls to a message passing library (MPI usually)*** to distribute the data to all the processes. All message passing is done invisibly to the programmer.

Other Models

Other parallel programming models besides those previously mentioned certainly exist, and will continue to evolve along with the ever changing world of computer hardware and software. Only three of the more common ones are mentioned here.

Hybrid

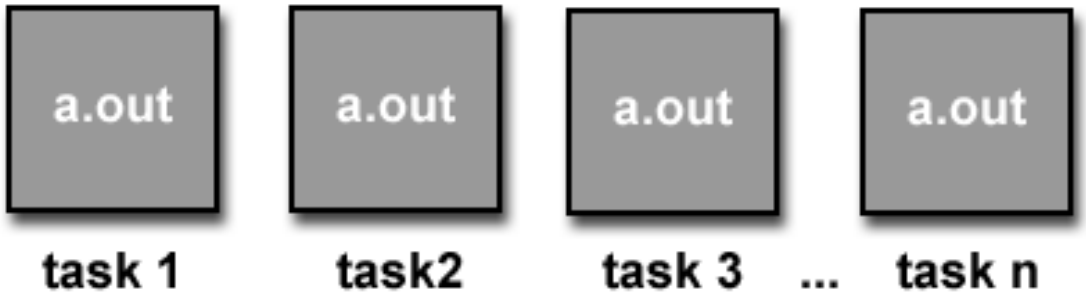
Two or more parallel programming models are combined:

- Currently, a common example of a hybrid model is the ***combination of the message passing model (MPI) with either the threads model*** (POSIX threads) or the shared memory model (OpenMP). This hybrid model lends itself well to the increasingly common hardware environment of networked SMP machines.
- Another common example of a hybrid model is ***combining data parallel with message passing***. As mentioned in the data parallel model section previously, data parallel implementations (F90, HPF) on distributed memory architectures actually use message passing to transmit data between tasks, transparently to the programmer.

Single Program Multiple Data (SPMD)

SPMD is actually ***a "high level" programming model*** that can be built upon any combination of the previously mentioned parallel programming models.

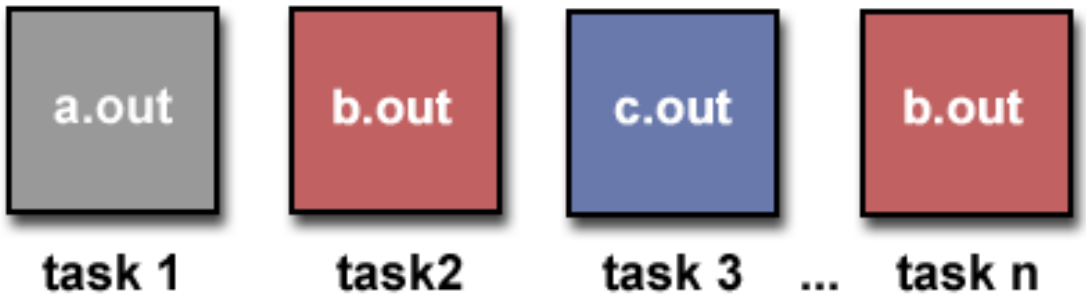
- A single program is executed by all tasks simultaneously.
- At any moment in time, tasks can be executing the same or different instructions within the same program.
- SPMD programs usually have switches to execute only part of the program.
- All tasks may use different data



Multiple Program Multiple Data (MPMD)

Like SPMD, MPMD is actually a "high level" programming model that can be built upon any combination of the previously mentioned parallel programming models.

MPMD applications typically have multiple executable object files (programs). While the application is being run in parallel, each task can be executing the same or different program as other tasks.



Automatic vs. Manual Parallelization

Designing and developing parallel programs has characteristically been a very manual process. The programmer is typically responsible for both identifying and actually implementing parallelism.

Very often, manually developing parallel codes is a time consuming, complex, error-prone and **iterative** process.

For a number of years now, various tools have been available to assist the programmer with converting serial programs into parallel programs. The most common type of tool used to automatically parallelize a serial program is a parallelizing compiler or pre-processor.

A parallelizing compiler generally works in two different ways:

- Fully Automatic
  - The compiler analyzes the source code and identifies opportunities for parallelism.
  - The analysis includes identifying inhibitors to parallelism and possibly a cost weighting on whether or not the parallelism would actually improve performance.
  - Loops (do, for) loops are the most frequent target for automatic parallelization.
- Programmer Directed
  - Using "compiler directives" or possibly compiler flags, the programmer explicitly tells the compiler how to parallelize the code.
  - May be able to be used in conjunction with some degree of automatic parallelization also.

Automatic parallelization

If you are beginning with an existing serial code and have time or budget constraints, then automatic parallelization may be the answer. However, there are several important caveats that apply to automatic parallelization:

- Wrong results may be produced
- Performance may actually degrade
- Much less flexible than manual parallelization
- Limited to a subset (mostly loops) of code
- May actually not parallelize code if the analysis suggests there are inhibitors or the code is too complex
- Most automatic parallelization tools are for Fortran

The remainder of this section applies to the manual method of developing parallel codes.

Understand the Problem and the Program

Undoubtedly, the first step in developing parallel software is to first ***understand the problem*** that you wish to solve in parallel. If you are starting with a serial program, this necessitates understanding the existing code also.

Before spending time in an attempt to develop a parallel solution for a problem, ***determine whether or not the problem is one that can actually be parallelized.***

Example of Parallelizable Problem

Calculate the potential energy for each of several thousand independent conformations of a molecule. When done, find the minimum energy conformation.

This problem is able to be solved in parallel. Each of the molecular conformations is independently determinable.

The calculation of the minimum energy conformation is also a parallelizable problem.

Example of a Non-parallelizable Problem

Calculation of the Fibonacci series (1,1,2,3,5,8,13,21,...) by use of the formula:

$$F(k+2) = F(k+1) + F(k)$$

This is a non-parallelizable problem because the calculation of the Fibonacci sequence as shown would entail dependent calculations rather than independent ones.

The calculation of the k + 2 value uses those of both k + 1 and k. These three terms cannot be calculated independently and therefore, not in parallel.

Hotspots

Identify the program's **hotspots**:

- Know where most of the real work is being done. The majority of scientific and technical programs usually accomplish most of their work in a few places.
- Profilers and performance analysis tools can help here
- Focus on parallelizing the hotspots and ignore those sections of the program that account for little CPU usage.

Bottlenecks

Identify **bottlenecks** in the program

- Are there areas that are disproportionately slow, or cause parallelizable work to halt or be deferred? For example, I/O is usually something that slows a program down.
- May be possible to restructure the program or use a different algorithm to reduce or eliminate unnecessary slow areas

Inhibitors

Identify inhibitors to parallelism. One common class of inhibitor is *data dependence*, as demonstrated by the Fibonacci sequence above.

Think different

Investigate other algorithms if possible. This may be the single most important consideration when designing a parallel application.

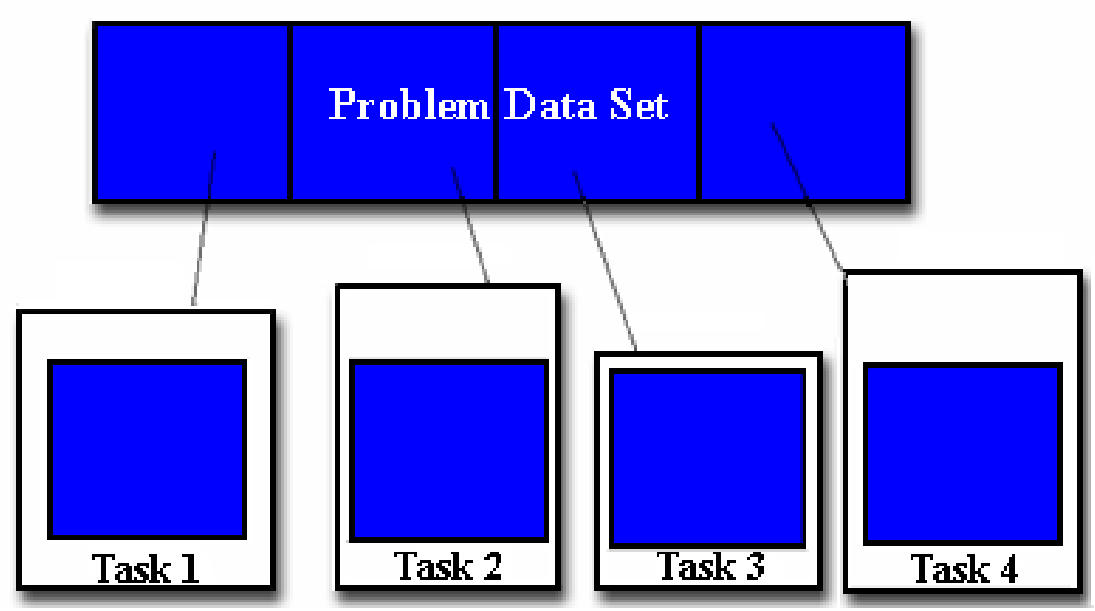
Partitioning

One of the first steps in designing a parallel program is to break the problem into discrete "chunks" of work that can be distributed to multiple tasks. This is known as decomposition or partitioning.

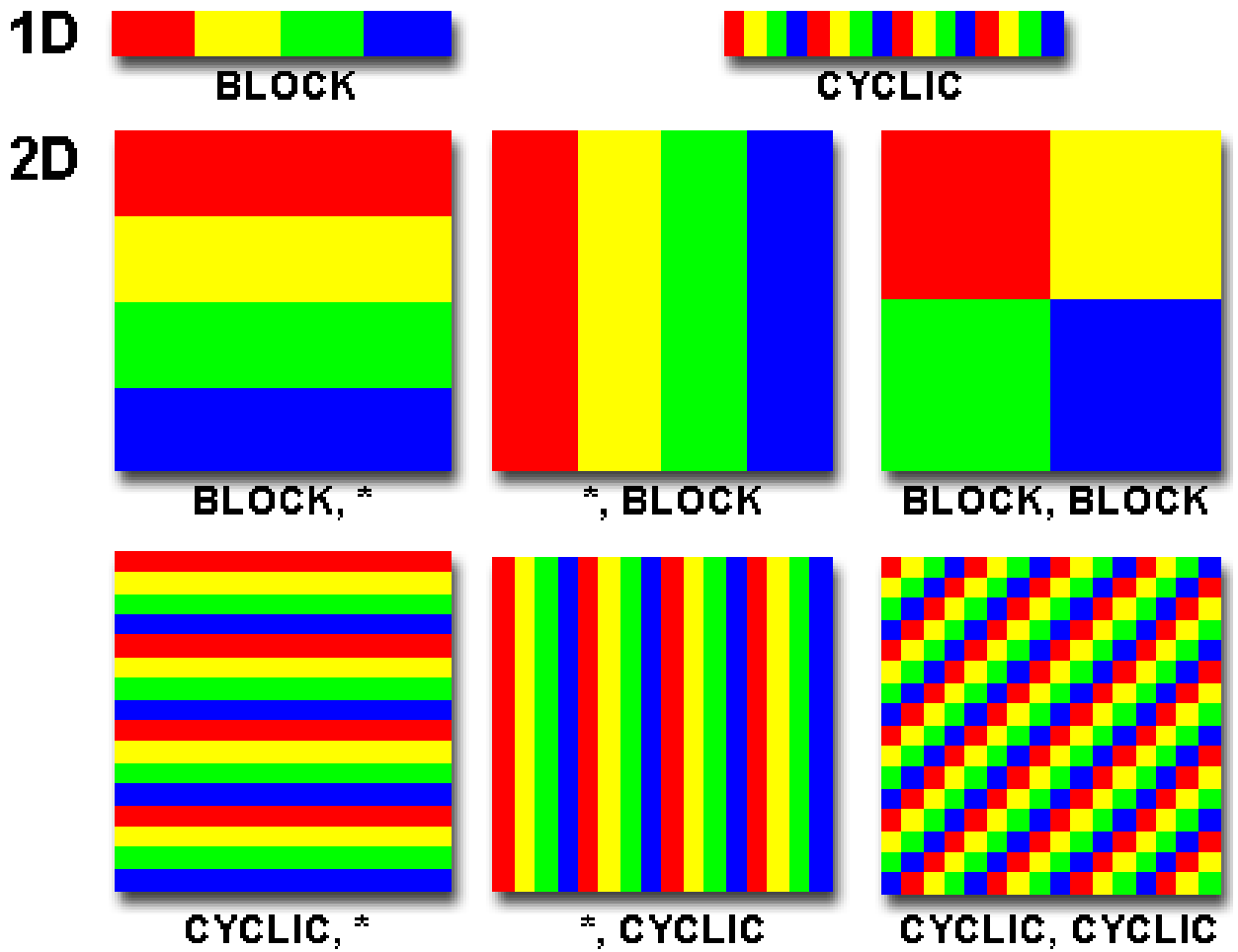
There are two basic ways to partition computational work among parallel tasks: ***domain decomposition*** and ***functional decomposition***.

Domain Decomposition

In this type of partitioning, the data associated with a problem is decomposed. Each parallel task then works on a portion of of the data.

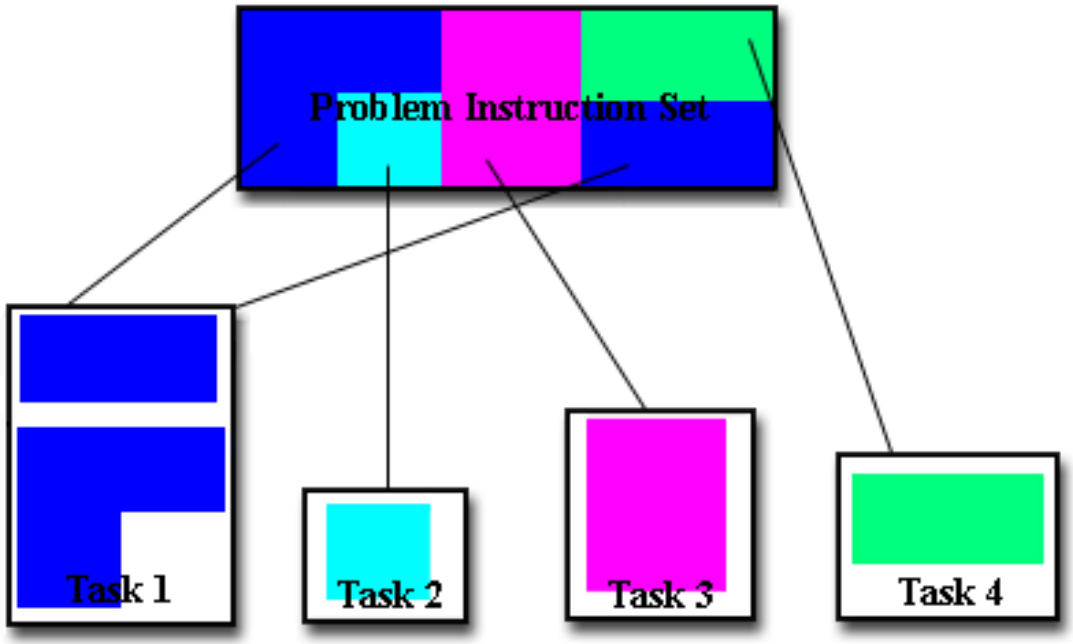


There are different ways to partition data:



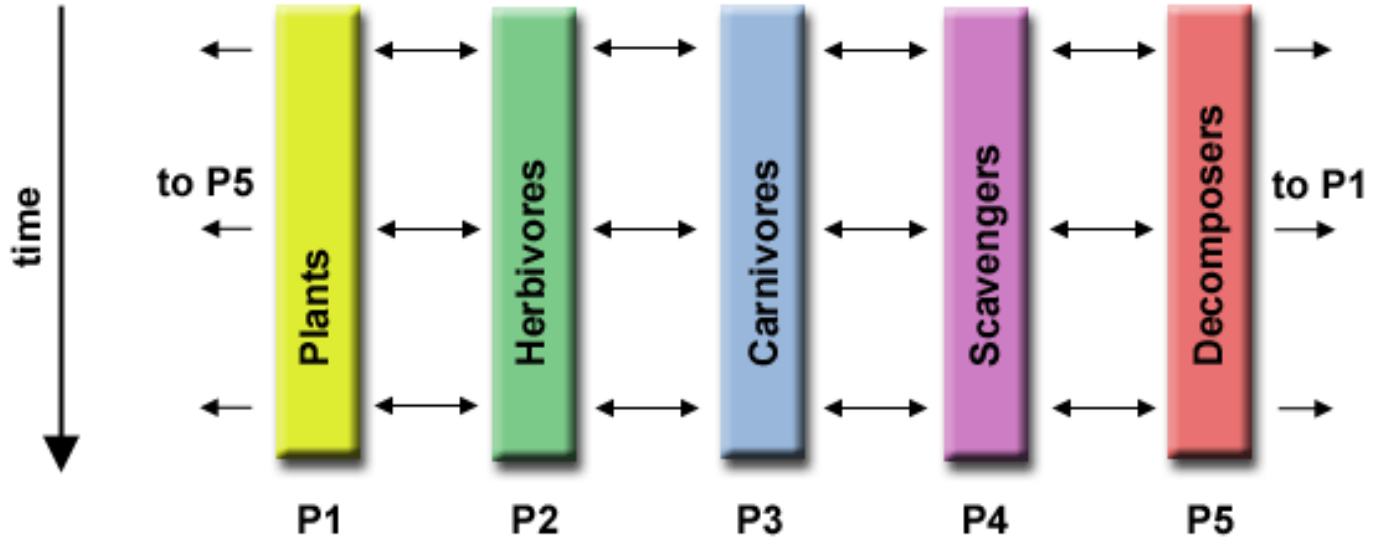
Functional Decomposition

In this approach, 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.

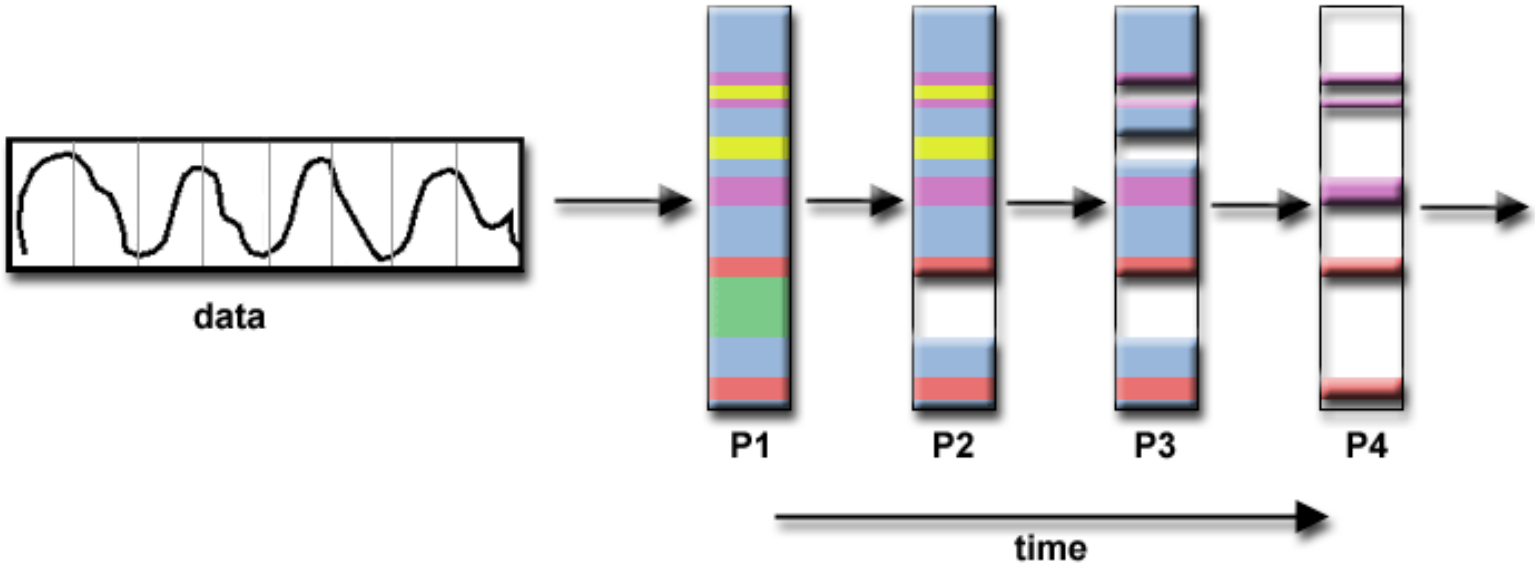


Functional decomposition lends itself well to problems that can be split into different tasks. For example:

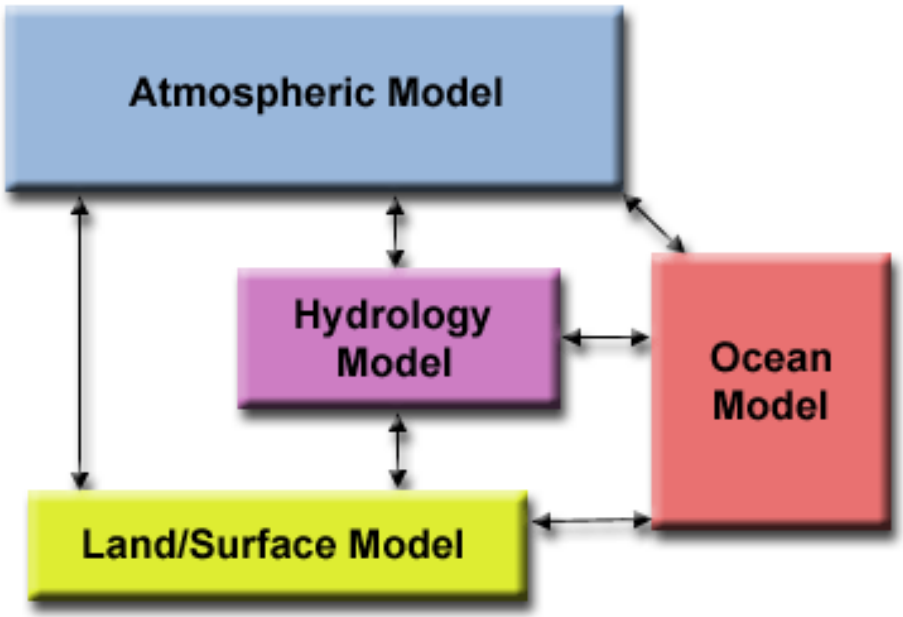
Ecosystem Modeling *Each program calculates the population of a given group, where each group's growth depends on that of its neighbors. As time progresses, each process calculates its current state, then exchanges information with the neighbor populations. All tasks then progress to calculate the state at the next time step.*



Signal Processing *An audio signal data set is passed through four distinct computational filters. Each filter is a separate process. The first segment of data must pass through the first filter before progressing to the second. When it does, the second segment of data passes through the first filter. By the time the fourth segment of data is in the first filter, all four tasks are busy.*



Climate Modeling *Each model component can be thought of as a separate task. Arrows represent exchanges of data between components during computation: the atmosphere model generates wind velocity data that are used by the ocean model, the ocean model generates sea surface temperature data that are used by the atmosphere model, and so on.*



Combining domain decomposition and functional decomposition is common and natural.

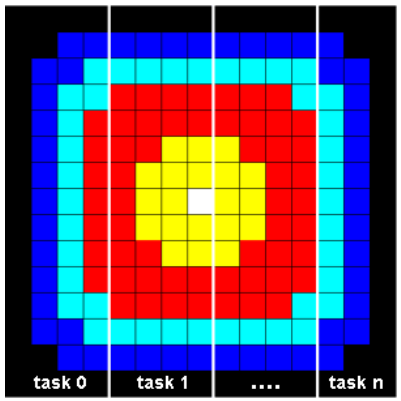
Communications

Who Needs Communications?

The need for communications between tasks depends upon your problem:

You DO need communications

Most parallel applications are not quite so simple, and do require tasks to share data with each other.



For example, a 2-D heat diffusion problem requires a task to know the temperatures calculated by the tasks that have neighboring data. Changes to neighboring data has a direct effect on that task's data.

You DON'T need communications

- Some types of problems can be decomposed and executed in parallel with virtually no need for tasks to share data.
- These types of problems are often called ***embarrassingly parallel*** because they are so straight-forward. Very little inter-task communication is required.

Factors to Consider

Cost of communications

- Inter-task communication virtually always implies overhead.
- Machine cycles and resources that could be used for computation are instead used to package and transmit data.
- Communications frequently require some type of synchronization between tasks, which can result in tasks spending time "waiting" instead of doing work.
- Competing communication traffic can saturate the available network bandwidth, further aggravating performance problems.

Factors to Consider (2)

Latency vs. Bandwidth

- ***latency*** is the time it takes to send a minimal (0 byte) message from point A to point B. Commonly expressed as microseconds.
- ***bandwidth*** is the amount of data that can be communicated per unit of time. Commonly expressed as megabytes/sec.
- Sending many small messages can cause latency to dominate communication overheads. Often it is more efficient to package small messages into a larger message, thus increasing the effective communications bandwidth.

Factors to Consider (3)

Visibility of communications

- With the Message Passing Model, communications are explicit and generally quite visible and under the control of the programmer.
- With the Data Parallel Model, communications often occur transparently to the programmer, particularly on distributed memory architectures. The programmer may not even be able to know exactly how inter-task communications are being accomplished.

Factors to Consider (4)

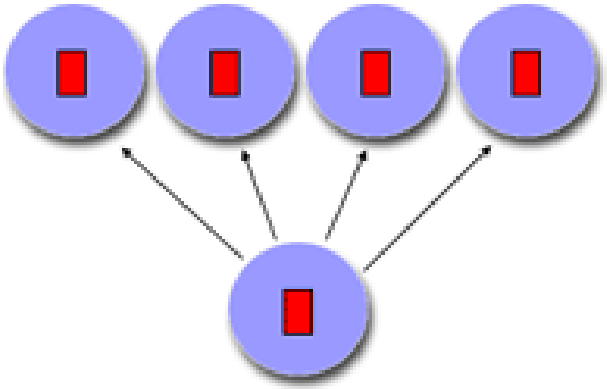
Synchronous vs. asynchronous communications

- Synchronous communications require some type of "handshaking" between tasks that are sharing data.
- Synchronous communications are often referred to as ***blocking*** communications since other work must wait until the communications have completed.
- Asynchronous communications allow tasks to transfer data independently from one another.
- Asynchronous communications are often referred to as ***non-blocking*** communications since other work can be done while the communications are taking place.
- Interleaving computation with communication is the single greatest benefit for using asynchronous communications.

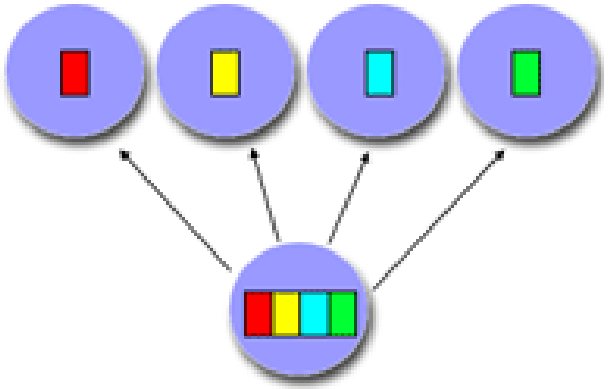
Factors to Consider (5)

Scope of communications

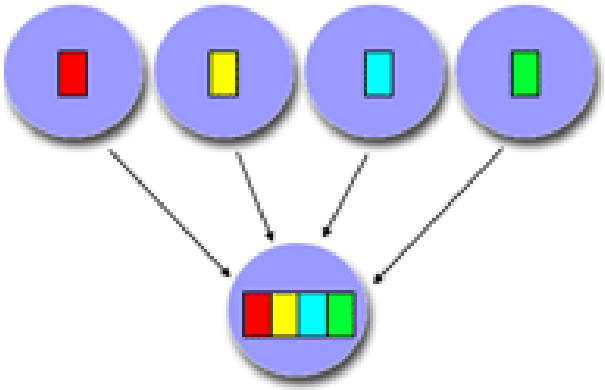
- Knowing which tasks must communicate with each other is critical during the design stage of a parallel code. Both of the two scopings described below can be implemented synchronously or asynchronously.
- ***Point-to-point*** - involves two tasks with one task acting as the sender/producer of data, and the other acting as the receiver/consumer.
- ***Collective*** - involves data sharing between more than two tasks, which are often specified as being members in a common group, or collective. Some common variations (there are more):



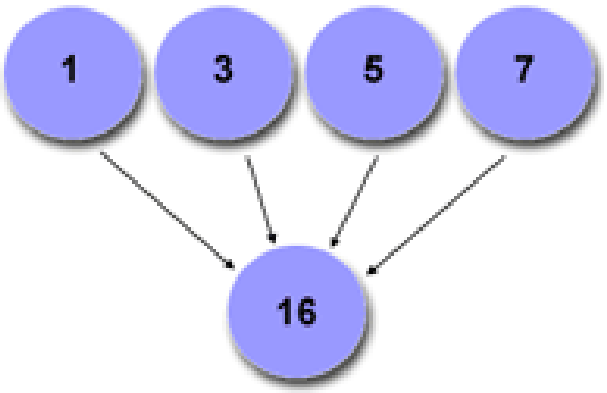
broadcast



scatter



gather



reduction

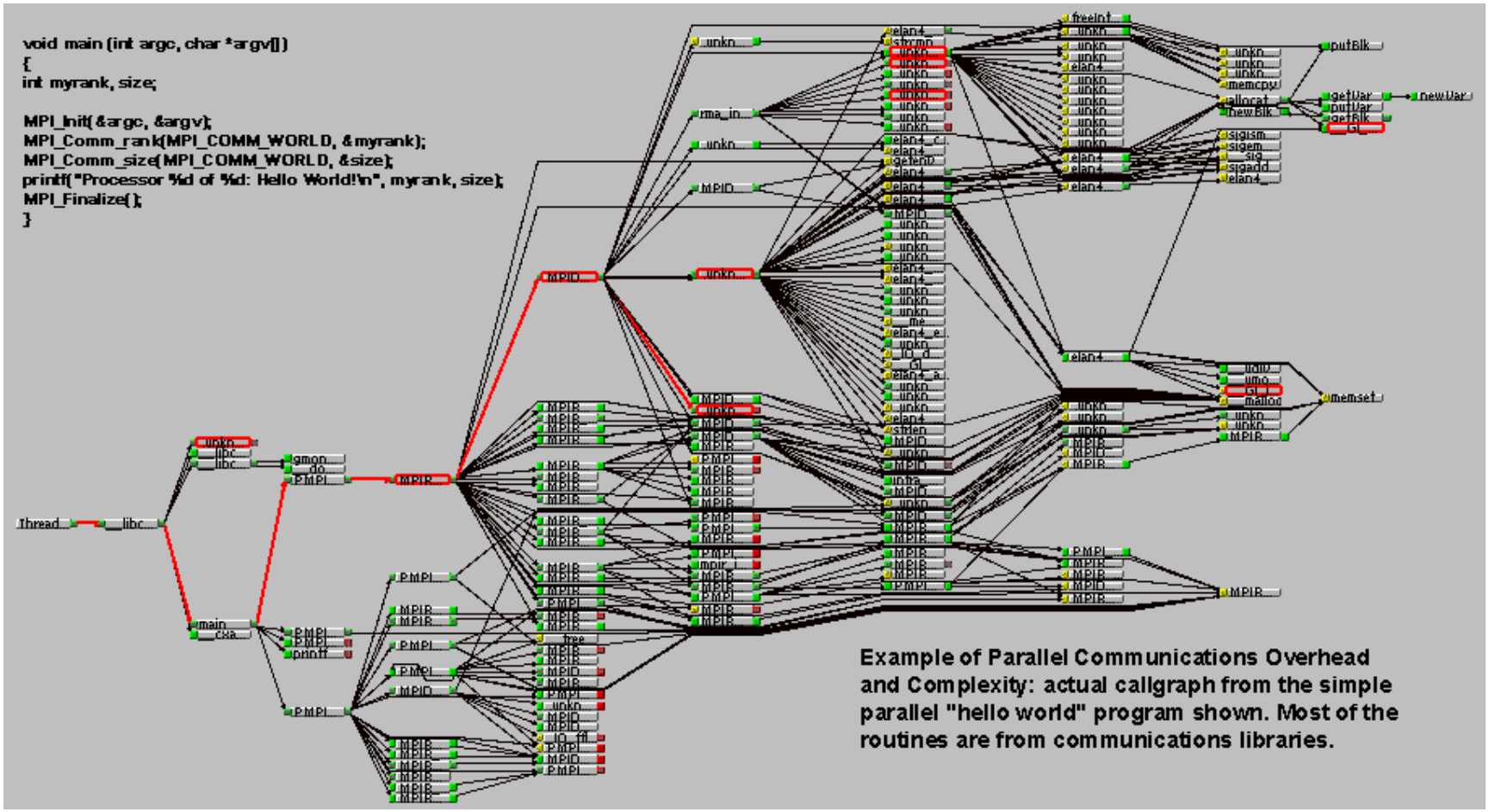
Factors to Consider (6)

Efficiency of communications

- Very often, the programmer will have a choice with regard to factors that can affect communications performance. Only a few are mentioned here.
- Which implementation for a given model should be used? Using the Message Passing Model as an example, one MPI implementation may be faster on a given hardware platform than another.
- What type of communication operations should be used? As mentioned previously, asynchronous communication operations can improve overall program performance.
- Network media - some platforms may offer more than one network for communications. Which one is best?

Factors to Consider (7)

Overhead and Complexity



Example of Parallel Communications Overhead and Complexity: actual callgraph from the simple parallel "hello world" program shown. Most of the routines are from communications libraries.

Factors to Consider (8)

Realize that this is only a partial list of things to consider!!!

Synchronization

Types of Synchronization

- Barrier
- Lock / semaphore
- Synchronous communication operations

Barrier

- Usually implies that all tasks are involved
- Each task performs its work until it reaches the barrier. It then stops, or "blocks".
- When the last task reaches the barrier, all tasks are synchronized.
- What happens from here varies. Often, a serial section of work must be done. In other cases, the tasks are automatically released to continue their work.

Lock / semaphore

- Can involve any number of tasks
- Typically used to serialize (protect) access to global data or a section of code. Only one task at a time may use (own) the lock / semaphore / flag.
- The first task to acquire the lock "sets" it. This task can then safely (serially) access the protected data or code.
- Other tasks can attempt to acquire the lock but must wait until the task that owns the lock releases it.
- Can be blocking or non-blocking

Synchronous communication operations

- Involves only those tasks executing a communication operation
- When a task performs a communication operation, some form of coordination is required with the other task(s) participating in the communication. For example, before a task can perform a send operation, it must first receive an acknowledgment from the receiving task that it is OK to send.
- Discussed previously in the Communications section.

Data Dependencies

Definition:

- A ***dependence*** exists between program statements 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.
- Dependencies are important to parallel programming because they are one of the primary inhibitors to parallelism.

Examples of Data Dependencies

Loop carried data dependence

```
DO 500 J = MYSTART,MYEND
   A(J) = A(J-1) * 2.0
500 CONTINUE
```

The value of A(J-1) must be computed before the value of A(J), therefore A(J) exhibits a data dependency on A(J-1). Parallelism is inhibited.

If Task 2 has A(J) and task 1 has A(J-1), computing the correct value of A(J) necessitates:

- Distributed memory architecture - task 2 must obtain the value of A(J-1) from task 1 after task 1 finishes its computation
- Shared memory architecture - task 2 must read A(J-1) after task 1 updates it

Examples of Data Dependencies (2)

Loop independent data dependence

```
task 1      task 2
------      ------

X = 2       X = 4
  .           .
  .           .
Y = X*2     Y = X*3
```

As with the previous example, parallelism is inhibited. The value of Y is dependent on:

- Distributed memory architecture - if or when the value of X is communicated between the tasks.
- Shared memory architecture - which task last stores the value of X.

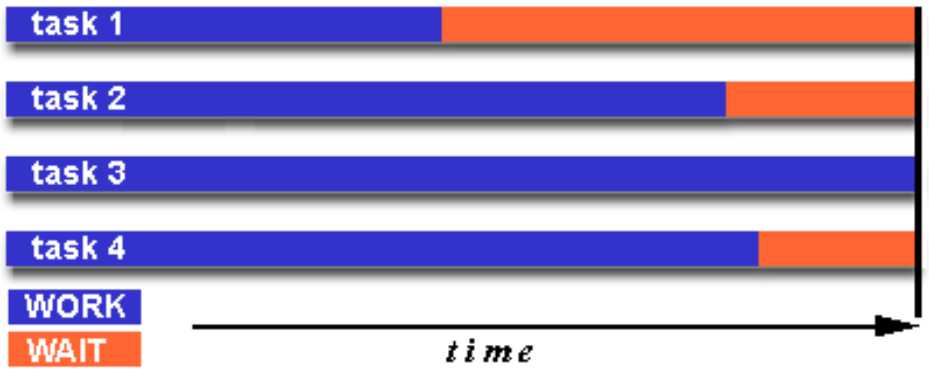
Although all data dependencies are important to identify when designing parallel programs, loop carried dependencies are particularly important since ***loops are possibly the most common target of parallelization efforts***.

How to Handle Data Dependencies

- Distributed memory architectures - communicate required data at synchronization points.
- Shared memory architectures - synchronize read/write operations between tasks.

Load Balancing

- Load balancing refers to the practice of distributing work among tasks so that ***all*** tasks are kept busy ***all*** of the time. It can be considered a ***minimization of task idle time***.
- Load balancing is important to parallel programs for performance reasons. *For example, if all tasks are subject to a barrier synchronization point, the slowest task will determine the overall*



How to Achieve Load Balance

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.
- If a heterogeneous mix of machines with varying performance characteristics are being used, be sure to use some type of performance analysis tool to detect any load imbalances. Adjust work accordingly.

How to Achieve Load Balance (2)

Use dynamic work assignment

- Certain classes of problems result in ***load imbalances even if data is evenly distributed*** among tasks:
  - Sparse arrays - some tasks will have actual data to work on while others have mostly "zeros".
  - Adaptive grid methods - some tasks may need to refine their mesh while others don't.
- When the amount of work each task will perform is intentionally variable, or is ***unable to be predicted***, it may be helpful to use a ***scheduler*** - ***task pool*** approach. As each task finishes its work, it queues to get a new piece of work.
- It may become necessary to design an algorithm which detects and handles load imbalances as they occur dynamically within the code.

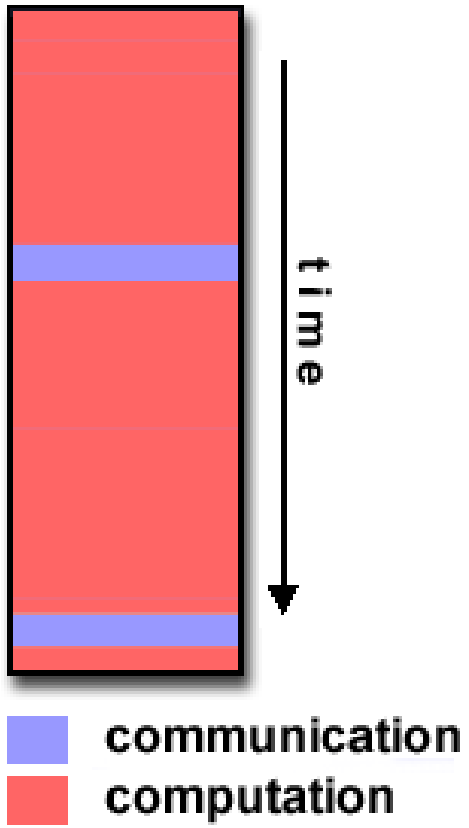
Granularity

Computation / Communication Ratio

- In parallel computing, granularity is a qualitative measure of the ratio of computation to communication.
- Periods of computation are typically separated from periods of communication by synchronization events.

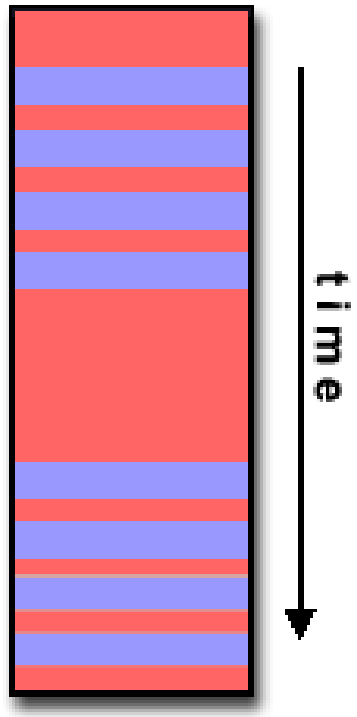
Coarse-grain Parallelism

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



Fine-grain Parallelism

- Relatively small amounts of computational work are done between communication events
- Low computation to communication ratio
- Facilitates load balancing
- Implies high communication overhead and less opportunity for performance enhancement
- If granularity is too fine it is possible that the overhead required for communications and synchronization between tasks takes longer than the computation.



Which is Best?

- The most efficient granularity is dependent on the algorithm and the hardware environment in which it runs.
- In most cases the overhead associated with communications and synchronization is high relative to execution speed so it is advantageous to have coarse granularity.
- Fine-grain parallelism can help reduce overheads due to load imbalance.

I/O

The Bad News

- I/O operations are generally regarded as inhibitors to parallelism
- Parallel I/O systems are immature or not available for all platforms
- In an environment where all tasks see the same filespace, write operations will result in file overwriting
- Read operations will be affected by the fileserver's ability to handle multiple read requests at the same time
- I/O that must be conducted over the network (NFS, non-local) can cause severe bottlenecks

The Good News

- Some parallel file systems are available. For example:
  - GPFS: General Parallel File System for AIX (IBM)
  - Lustre: for Linux clusters (Cluster File Systems, Inc.)
  - PVFS/PVFS2: Parallel Virtual File System for Linux clusters (Clemson/Argonne/Ohio State/others)
  - PanFS: Panasas ActiveScale File System for Linux clusters (Panasas, Inc.)
  - HP SFS: HP StorageWorks Scalable File Share. Lustre based parallel file system (Global File System for Linux) product from HP
- The parallel I/O programming interface specification for MPI has been available since 1996 as part of MPI-2. Vendor and "free" implementations are now commonly available.

Some options

- If you have access to a parallel file system, investigate using it.
- Rule #1: Reduce overall I/O as much as possible
- Confine I/O to specific serial portions of the job, and then use parallel communications to distribute data to parallel tasks. *For example, Task 1 could read an input file and then communicate required data to other tasks.*
- For distributed memory systems with shared filespace, perform I/O in local, non-shared filespace. *For example, each processor may have /tmp filespace which can used.*
- Create unique filenames for each tasks' input/output file(s)

Limits and Costs of Parallel Programming

Amdahl's Law

Amdahl's Law states that ***potential program speedup*** is defined by the fraction of code (P) that can be parallelized (S beeing the serial fraction):

$$\text{speedup} = \frac{1}{1 - P} = \frac{1}{S}$$

If none of the code can be parallelized, P = 0 and the speedup = 1 (no speedup). If all of the code is parallelized, P = 1 and the speedup is infinite (in theory).

If 50% of the code can be parallelized, maximum speedup = 2, meaning the code will run twice as fast.

Introducing the number of processors performing the parallel fraction of work, the relationship can be modeled by:

$$\text{speedup} = \frac{1}{\frac{P}{N} + S}$$

where P = parallel fraction, N = number of processors and S = serial fraction.

It soon becomes obvious that there are limits to the scalability of parallelism. For example, at P = .50, .90 and .99 (50%, 90% and 99% of the code is parallelizable):

	speedup		
N	P = .50	P = .90	P = .99
10	1.82	5.26	9.17
100	1.98	9.17	50.25
1000	1.99	9.91	90.99
10000	1.99	9.91	99.02

However, certain problems demonstrate increased performance by increasing the problem size. For example:

2D Grid Calculations	85 seconds	85%
Serial fraction	15 seconds	15%

We can increase the problem size by doubling the grid dimensions and halving the time step. This results in four times the number of grid points and twice the number of time steps. The timings then look like:

2D Grid Calculations	680 seconds	97.84%
Serial fraction	15 seconds	2.16%

Problems that increase the percentage of parallel time with their size are more ***scalable*** than problems with a fixed percentage of parallel time.

Complexity

In general, parallel applications are much more complex than corresponding serial applications, perhaps ***an order of magnitude***. Not only do you have multiple instruction streams executing at the same time, but you also have data flowing between them.

The costs of complexity are measured in programmer time in virtually every aspect of the software development cycle:

- Design
- Coding
- Debugging
- Tuning
- Maintenance

Adhering to "good" software development practices is essential when when working with parallel applications - especially if somebody besides you will have to work with the software.

Portability

Thanks to standardization in several APIs, such as MPI, POSIX threads, HPF and OpenMP, portability issues with parallel programs are not as serious as in years past. However...

All of the usual portability issues associated with serial programs apply to parallel programs. For example, if you use vendor "enhancements" to Fortran, C or C++, portability will be a problem.

Even though standards exist for several APIs, implementations will differ in a number of details, sometimes to the point of requiring code modifications in order to effect portability.

Operating systems can play a key role in code portability issues.

Hardware architectures are characteristically highly variable and can affect portability.

Resource Requirements

The primary intent of parallel programming is to decrease execution ***wall clock time***, however in order to accomplish this, ***more CPU time*** is required. For example, a parallel code that runs in 1 hour on 8 processors actually uses 8 hours of CPU time.

The ***amount of memory*** required can be greater for parallel codes than serial codes, due to the need to replicate data and for overheads associated with parallel support libraries and subsystems.

For short running parallel programs, there can actually be a decrease in performance compared to a similar serial implementation. The ***overhead costs*** associated with setting up the parallel environment, task creation, communications and task termination can comprise a significant portion of the total execution time for short runs.

Scalability

The ability of a parallel program's performance to scale is a result of a number of interrelated factors. Simply adding more machines is rarely the answer.

The algorithm may have inherent limits to scalability. ***At some point, adding more resources causes performance to decrease***. Most parallel solutions demonstrate this characteristic at some point.

Hardware factors play a significant role in scalability. Examples:

- Memory-cpu bus bandwidth on an SMP machine
- Communications network bandwidth
- Amount of memory available on any given machine or set of machines
- Processor clock speed

Parallel support libraries and subsystems software can limit scalability independent of your application.