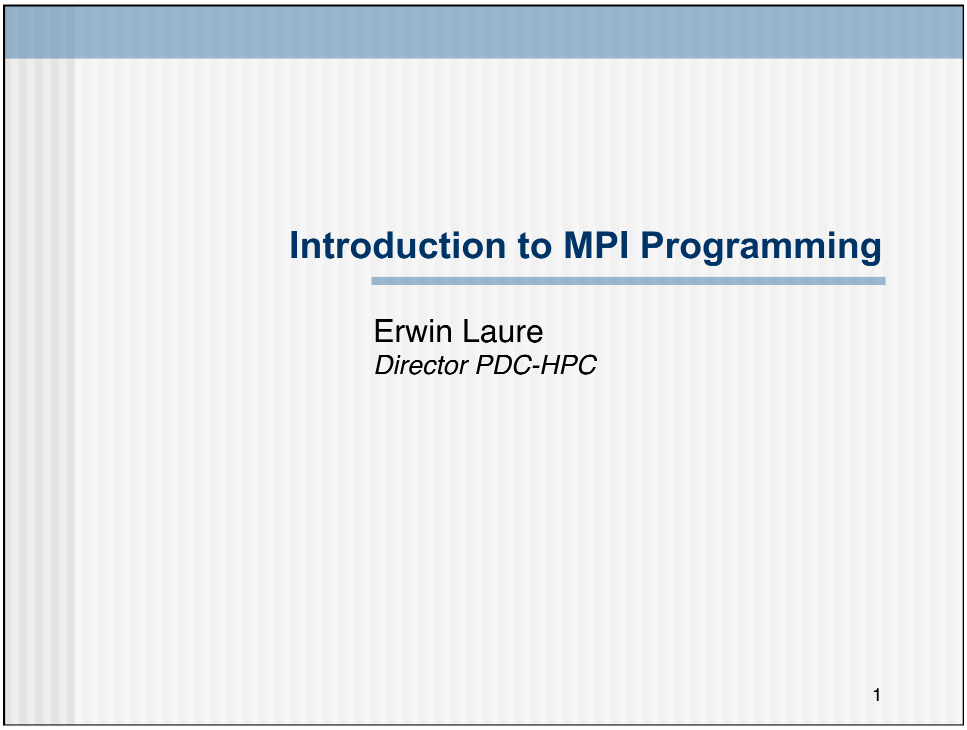
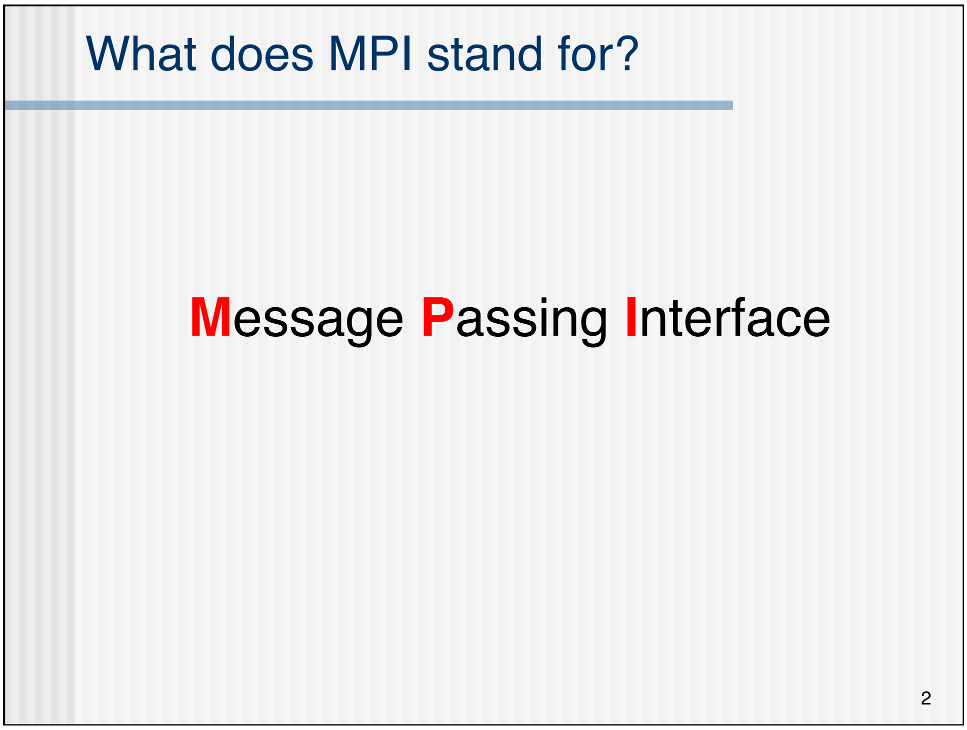


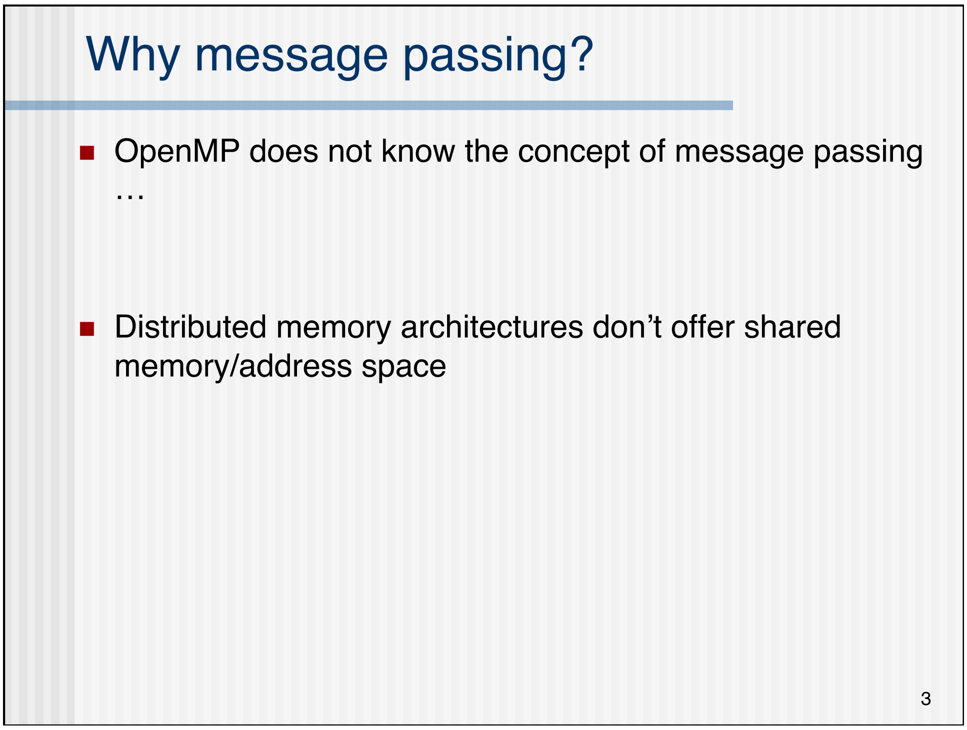
# Introduction to MPI Programming

Erwin Laure
*Director PDC-HPC*



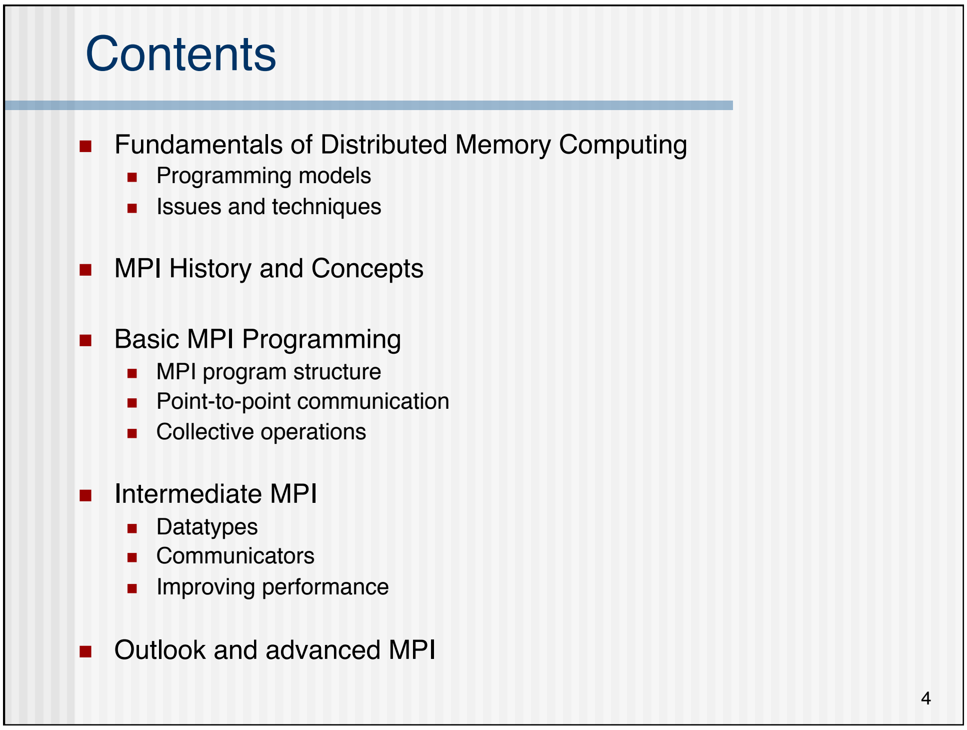
## What does MPI stand for?

**M**essage **P**assing **I**nterface



## Why message passing?

- OpenMP does not know the concept of message passing …
- Distributed memory architectures don’t offer shared memory/address space



## Contents

- Fundamentals of Distributed Memory Computing
  - Programming models
  - Issues and techniques
- MPI History and Concepts
- Basic MPI Programming
  - MPI program structure
  - Point-to-point communication
  - Collective operations
- Intermediate MPI
  - Datatypes
  - Communicators
  - Improving performance
- Outlook and advanced MPI

## Material

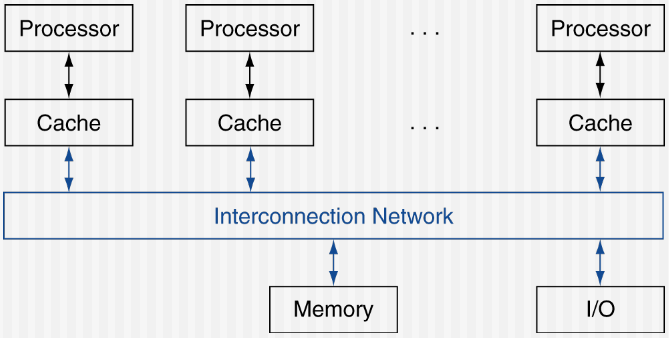
- This course is mainly based on
- Using MPI – Portable Parallel Programming with the Message-Passing Interface, W. Gropp, E. Lusk and A. Skjellum, MIT Press, 1994
- Several online tutorials:
  - http://www.mcs.anl.gov/research/projects/mpi/tutorial/
  - https://computing.llnl.gov/tutorials/mpi/
  - http://www.nccs.nasa.gov/tutorials/mpi1.pdf.gz
  - http://www.citutor.org/index.php
- Lecture notes by Michael Hanke, CSC, KTH

## Recap: Computer Architecture

# Shared Memory

## Shared Memory Multiprocessor

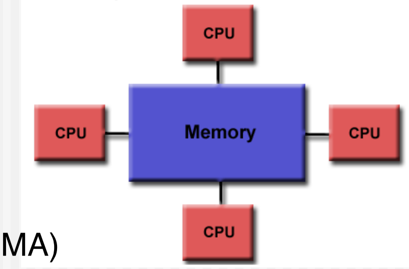
- Hardware provides single physical address space for all processors
- Global physical address space and symmetric access to all of main memory (*symmetric multiprocessor - SMP*)
- All processors and memory modules are attached to the same interconnect (bus or switched network)



## Differences in Memory Access

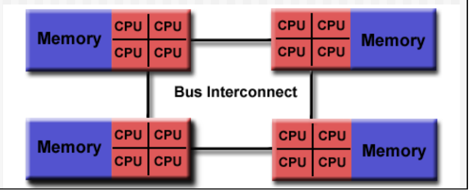
- Uniform Memory Access (UMA)

  Memory access takes about the same time independent of data location and requesting processor



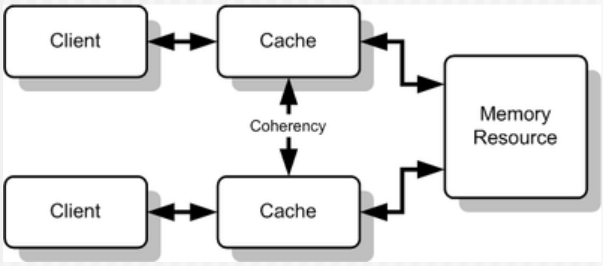
- Nonuniform memory access (NUMA)

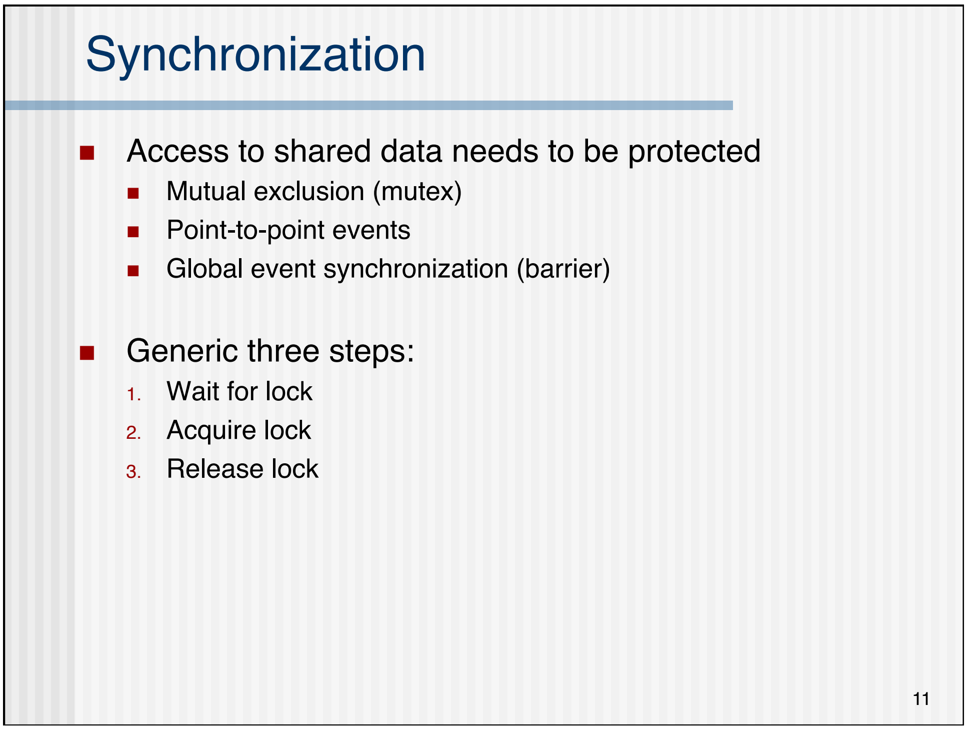
  Memory access can differ depending on where the data is located and which processor requests the data



## Cache coherence

- While main memory is shared, caches are local to individual processors
- Client B's cache might have old data since updates in client A's cache are not yet propagated
- Different cache coherency protocols to avoid this problem





## Synchronization

- Access to shared data needs to be protected
  - Mutual exclusion (mutex)
  - Point-to-point events
  - Global event synchronization (barrier)
- Generic three steps:
  1. Wait for lock
  2. Acquire lock
  3. Release lock

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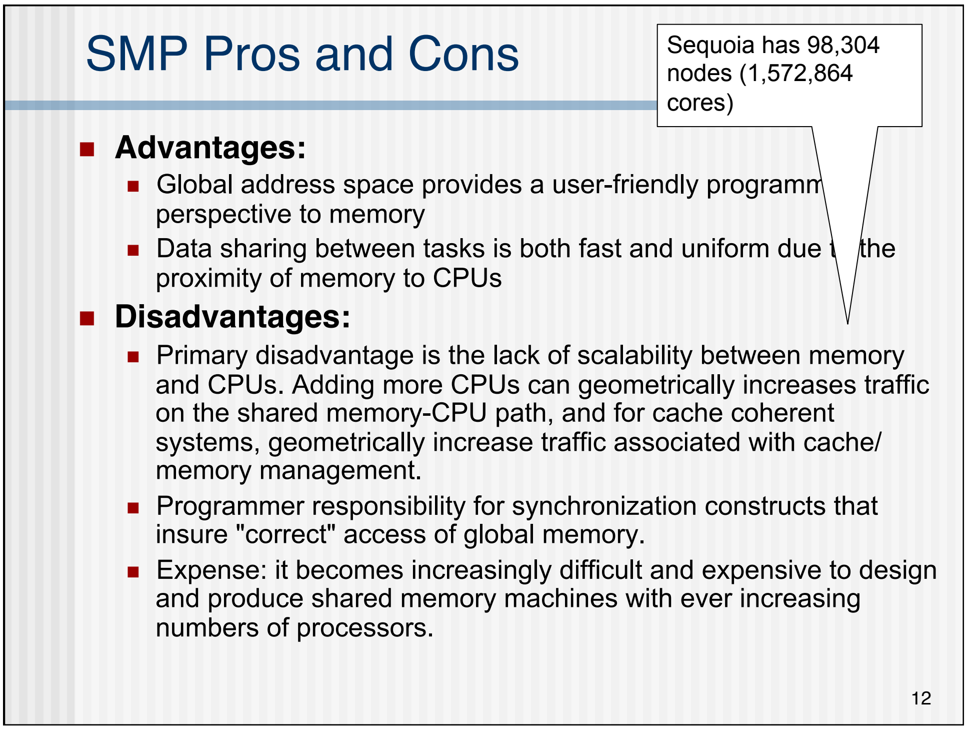

## SMP Pros and Cons

Sequoia has 98,304 nodes (1,572,864 cores)

- **Advantages:**
  - Global address space provides a user-friendly programm perspective to memory
  - Data sharing between tasks is both fast and uniform due t 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.
  - Expense: it becomes increasingly difficult and expensive to design and produce shared memory machines with ever increasing numbers of processors.

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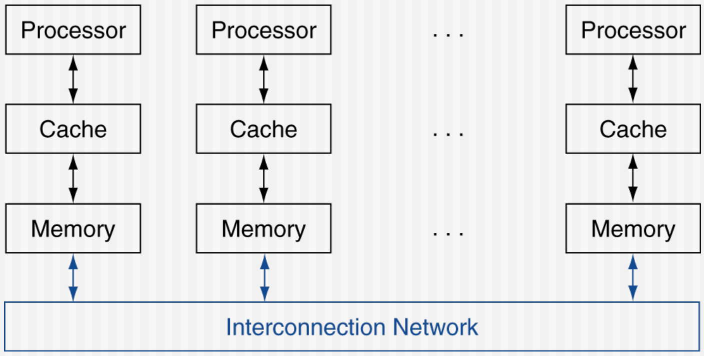
# Distributed Memory Multiprocessors

## DMMPs

- Each processor has private physical address space
  - No cache coherence problem
- Hardware sends/receives messages between processors
  - Message passing

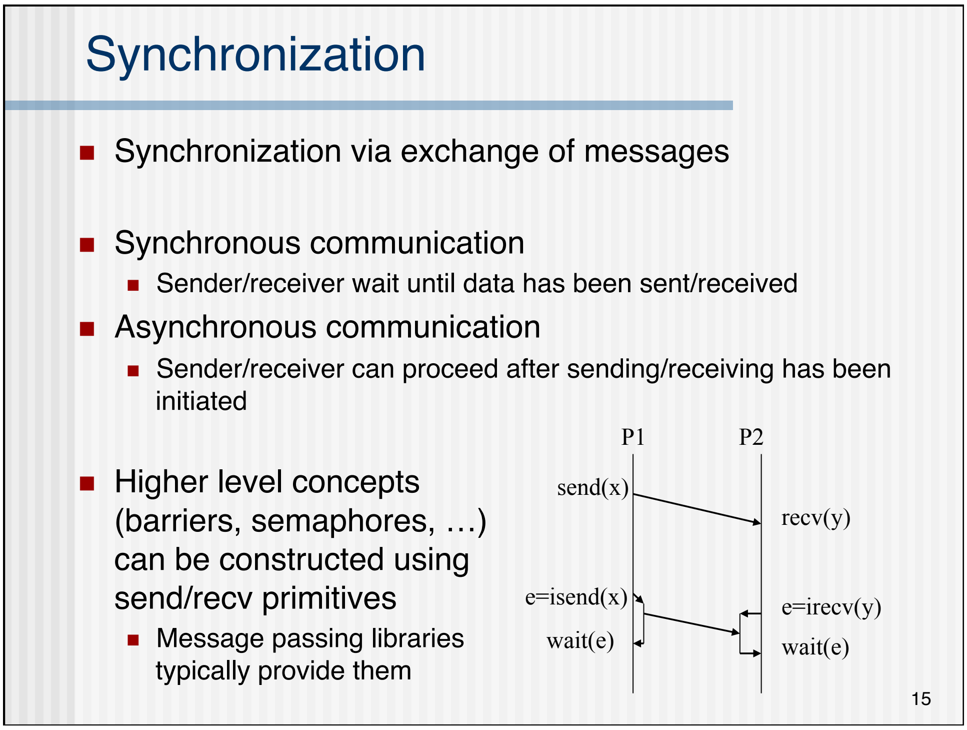


Processor Processor . . . Processor

Cache Cache . . . Cache

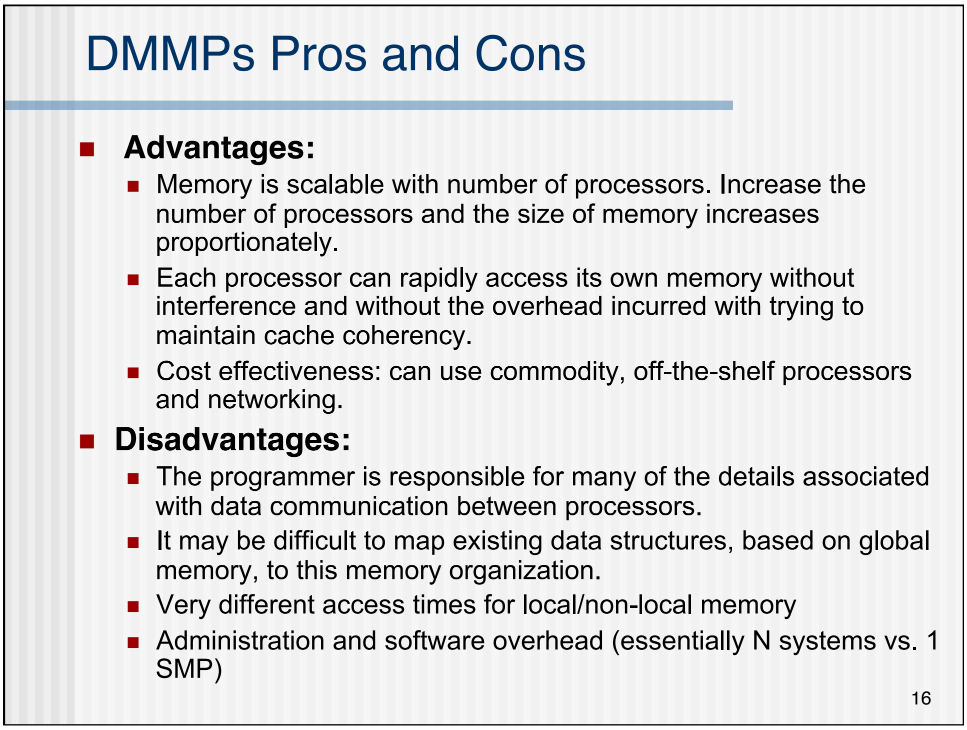
Memory Memory . . . Memory

Interconnection Network



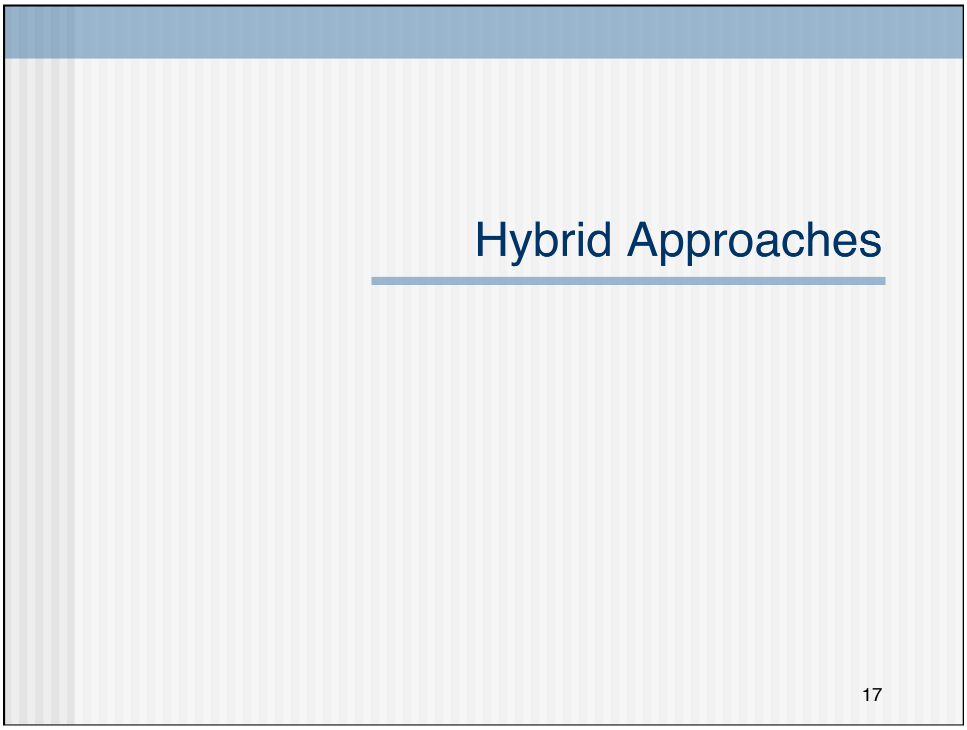
## Synchronization

- Synchronization via exchange of messages
- Synchronous communication
  - Sender/receiver wait until data has been sent/received
- Asynchronous communication
  - Sender/receiver can proceed after sending/receiving has been initiated
- Higher level concepts (barriers, semaphores, …) can be constructed using send/recv primitives
  - Message passing libraries typically provide them



## DMMPs Pros and Cons

- **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.
- **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.
  - Very different access times for local/non-local memory
  - Administration and software overhead (essentially N systems vs. 1 SMP)



# Hybrid Approaches

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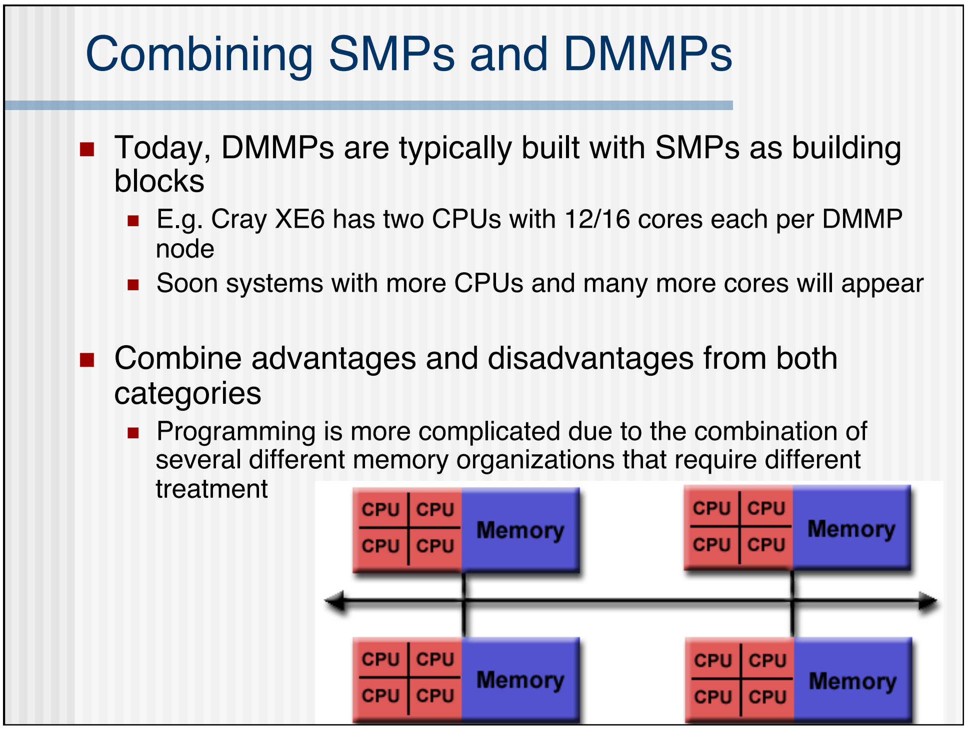


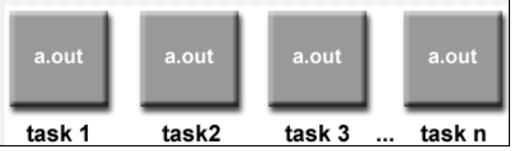
## Combining SMPs and DMMPs

- Today, DMMPs are typically built with SMPs as building blocks
  - E.g. Cray XE6 has two CPUs with 12/16 cores each per DMMP node
  - Soon systems with more CPUs and many more cores will appear
- Combine advantages and disadvantages from both categories
  - Programming is more complicated due to the combination of several different memory organizations that require different treatment

# Programming DMMPs

## Single Program Multiple Data (SPMD)

- DMMPs are typically programmed following the SPMD model
- 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. All tasks may use different data. (MIMD)
- SPMD programs usually have the necessary logic programmed into them to allow different tasks to branch or conditionally execute only those parts of the program they are designed to execute. That is, tasks do not necessarily have to execute the entire program - perhaps only a portion of it.

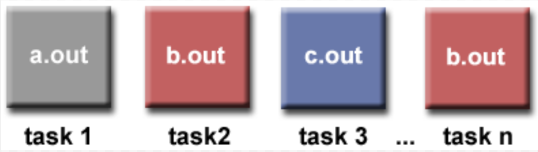


a.out a.out a.out a.out

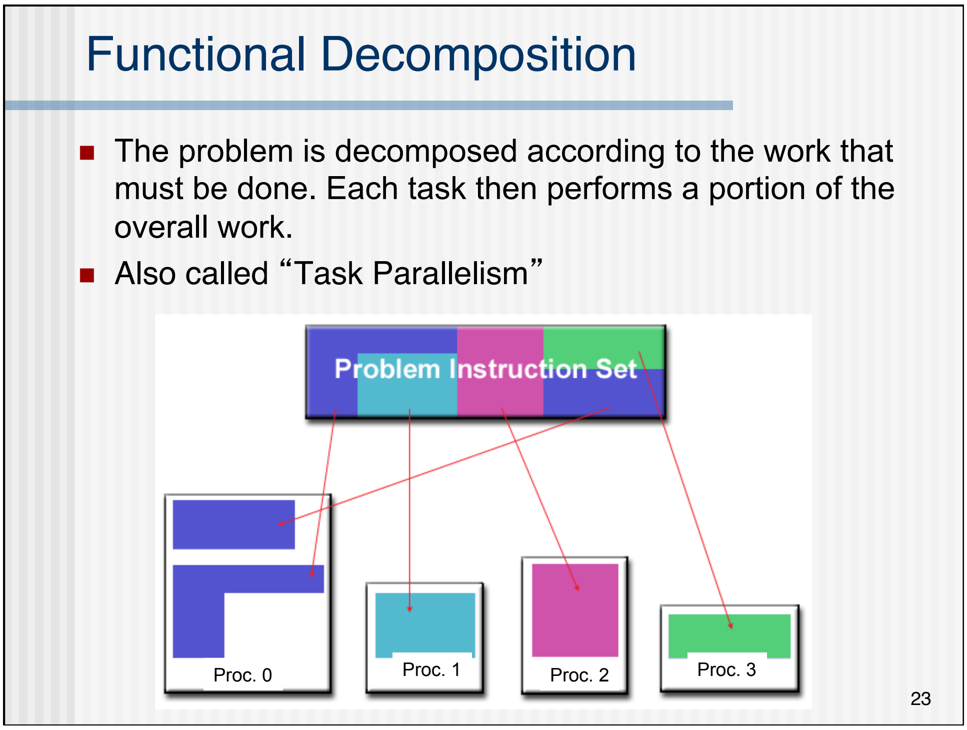
task 1 task2 task 3 ... task n

## Multiple Program Multiple Data (MPMD)

- 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.
- All tasks may use different data
- Workflow applications, multidisciplinary optimization, combination of different models



## How to decompose a problem in SPMD?



## Functional Decomposition

- The problem is decomposed according to the work that must be done. Each task then performs a portion of the overall work.
- Also called “Task Parallelism”

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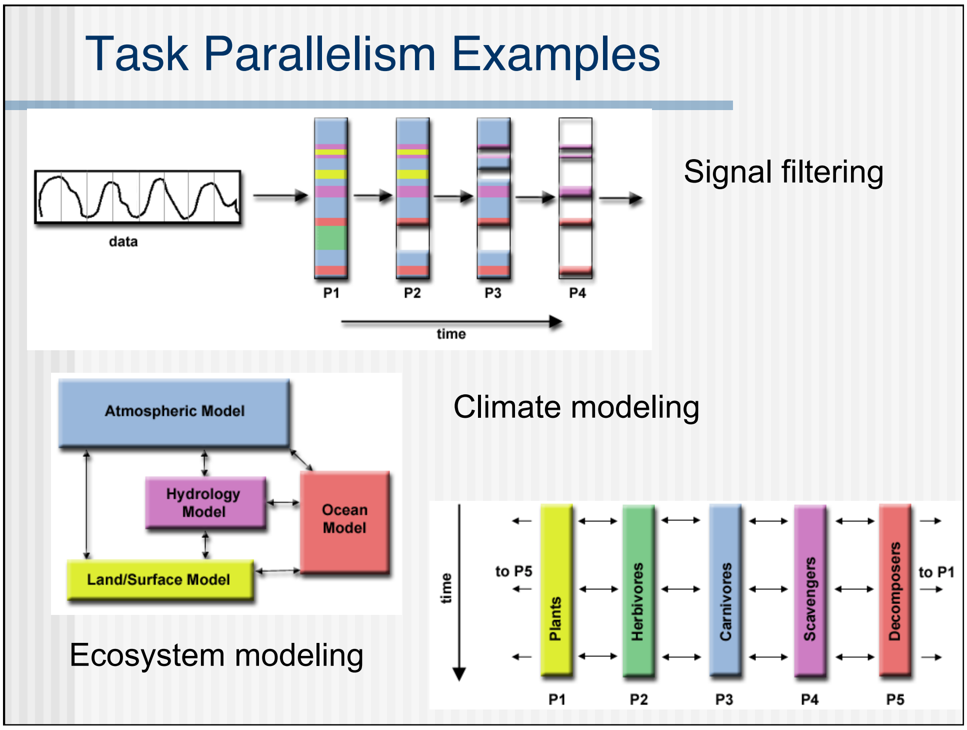


## Task Parallelism Examples

Signal filtering

Climate modeling

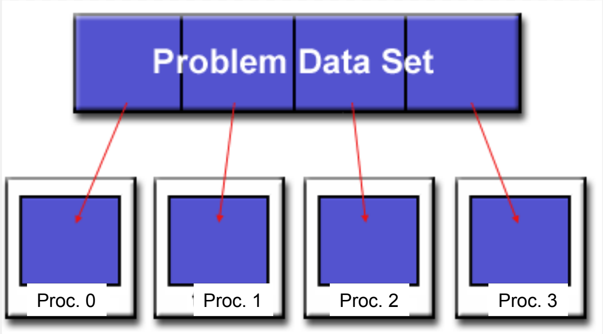
Ecosystem modeling

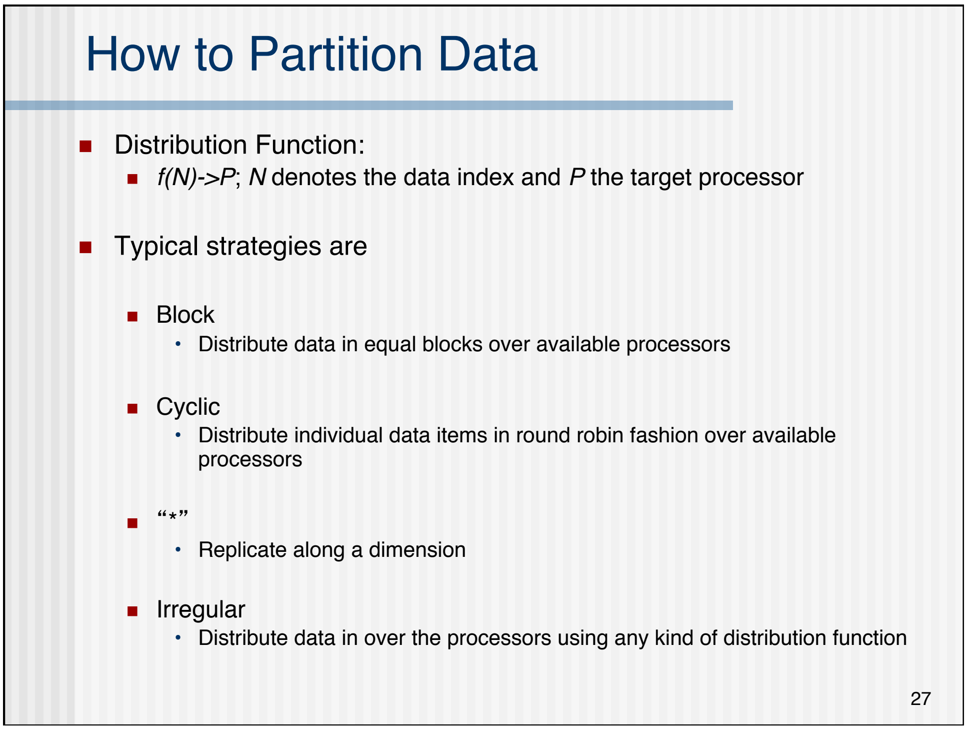
## Task Parallelism Summary

- Often pipelined approaches or Master/Slave
  - Master assigns work items to its slaves
- “Natural” approach to parallelism
- Typically good efficiency
  - Tasks proceed without interactions
  - Synchronization/communication needed at the end
- In practice scalability is limited
  - Problem can by split only into a finite set of different tasks

## Domain Decomposition

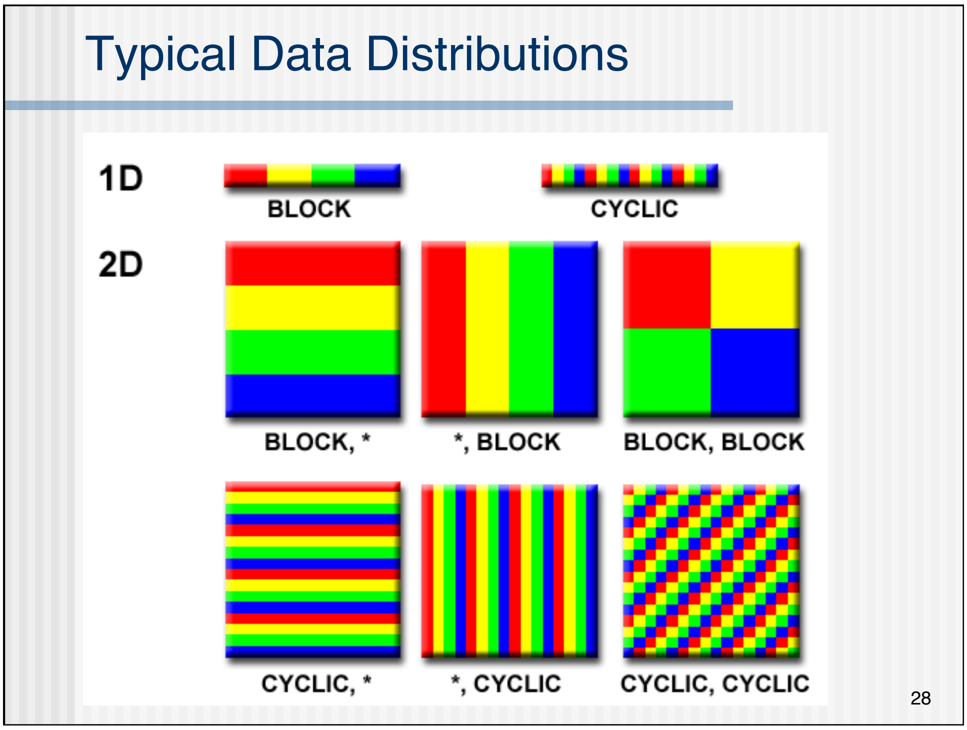
- The data associated with a problem is decomposed. Each parallel task then works on a portion of of the data.
- Also called “Data Parallelism”



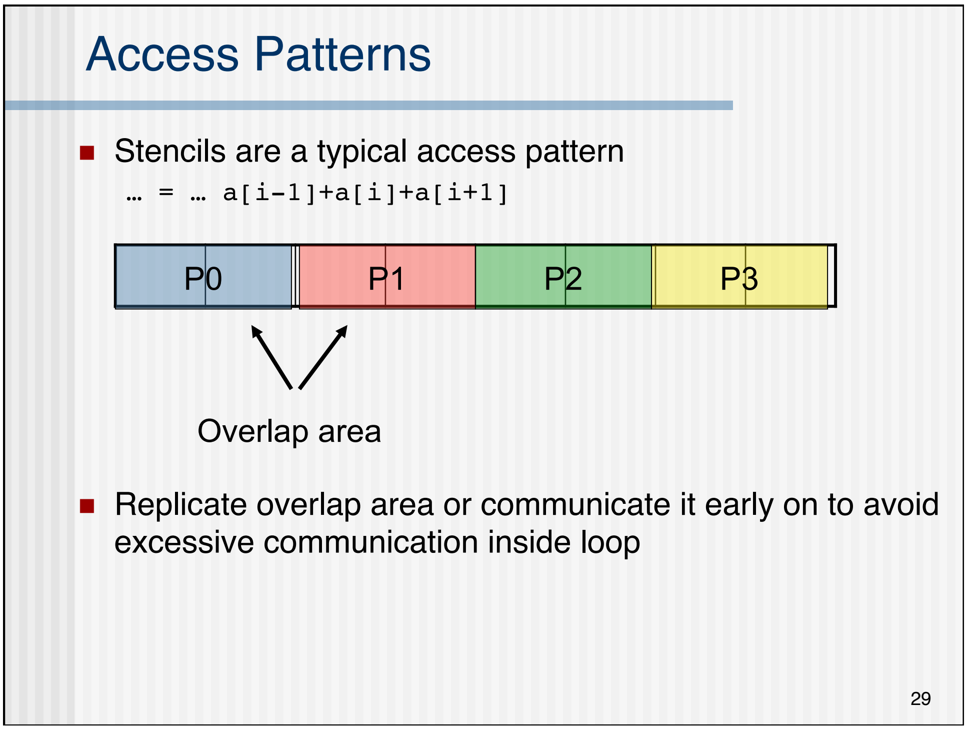


## How to Partition Data

- Distribution Function:
  - *f(N)->P*; *N* denotes the data index and *P* the target processor
- Typical strategies are
  - Block
    - Distribute data in equal blocks over available processors
  - Cyclic
    - Distribute individual data items in round robin fashion over available processors
  - “*”
    - Replicate along a dimension
  - Irregular
    - Distribute data in over the processors using any kind of distribution function



## Typical Data Distributions



# Access Patterns

- Stencils are a typical access pattern

```
… = … a[i-1]+a[i]+a[i+1]
```

- Replicate overlap area or communicate it early on to avoid excessive communication inside loop

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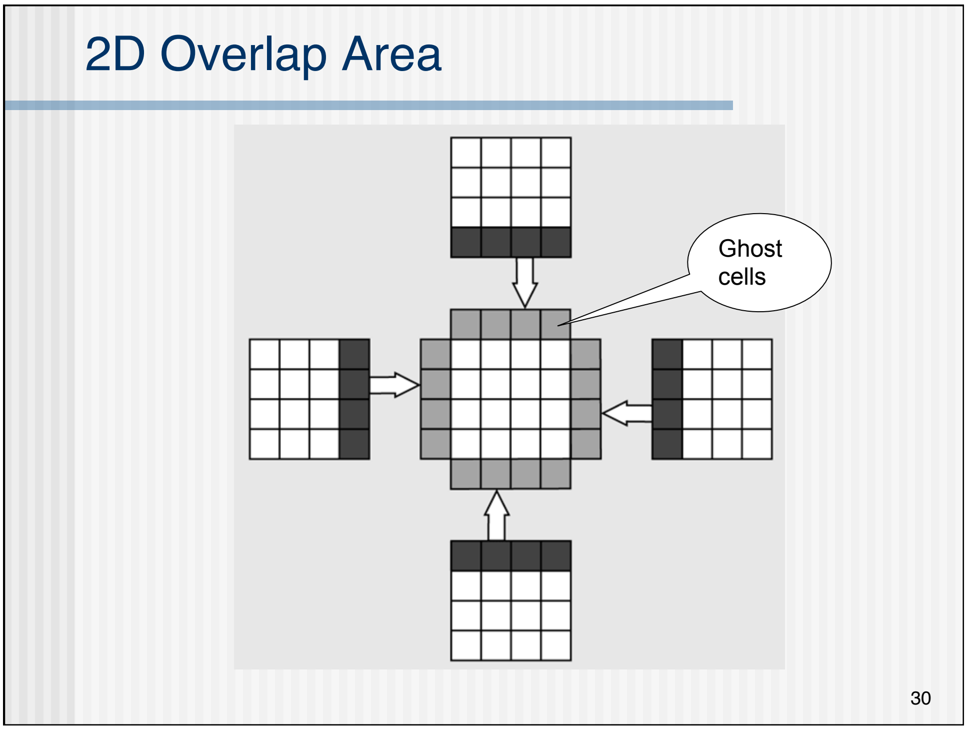

# 2D Overlap Area

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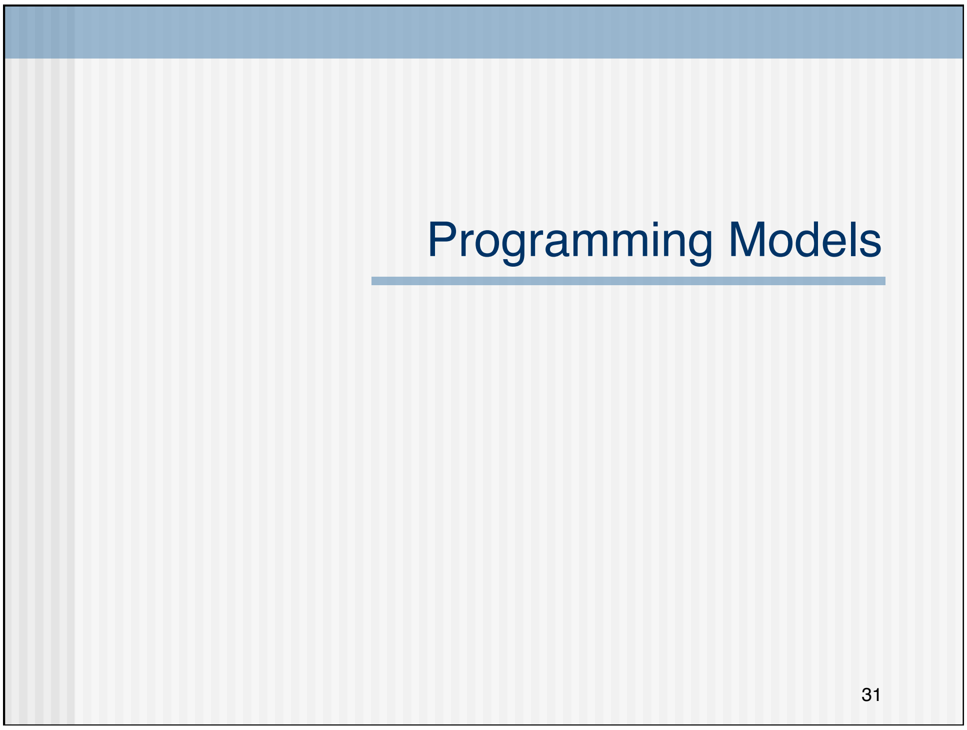
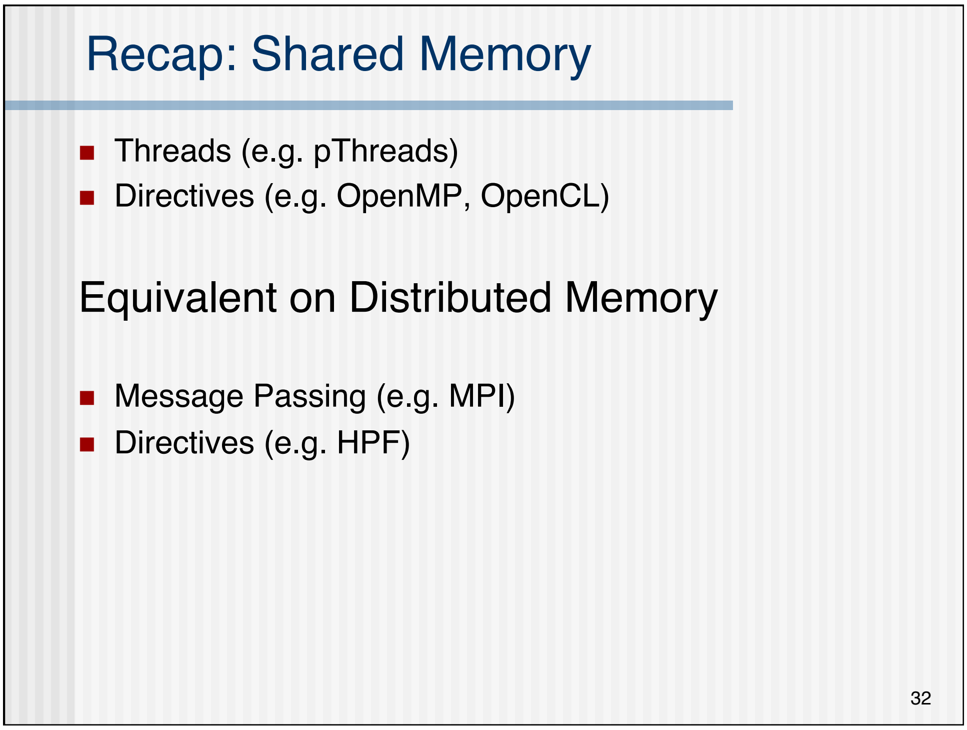


# Programming Models

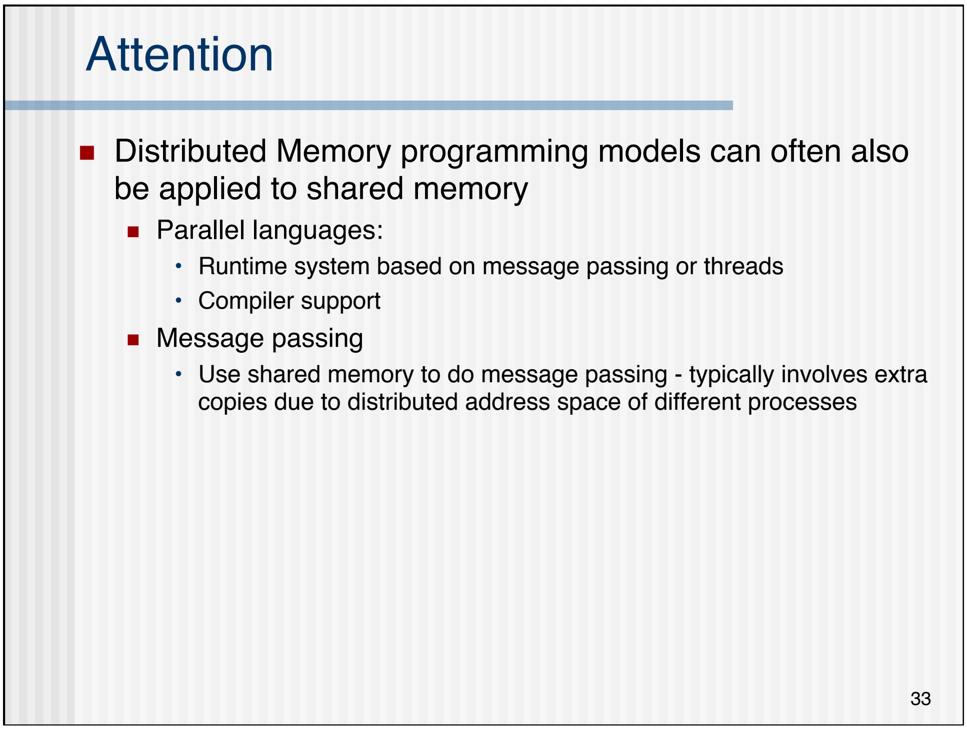


## Recap: Shared Memory

- Threads (e.g. pThreads)
- Directives (e.g. OpenMP, OpenCL)

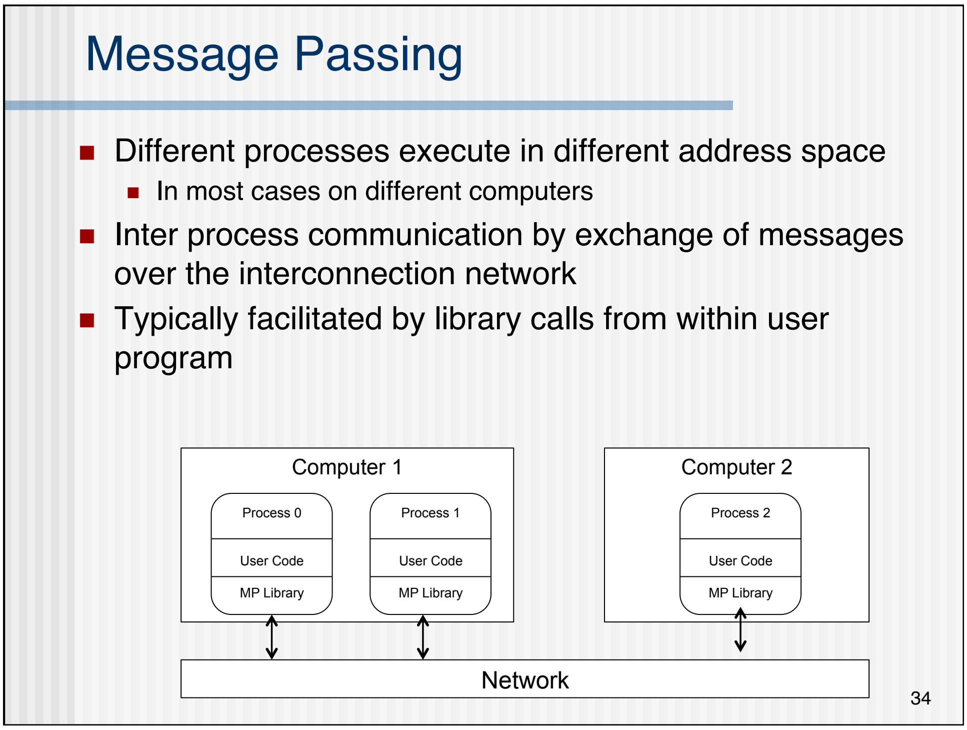
Equivalent on Distributed Memory

- Message Passing (e.g. MPI)
- Directives (e.g. HPF)



# Attention

- Distributed Memory programming models can often also be applied to shared memory
  - Parallel languages:
    - Runtime system based on message passing or threads
    - Compiler support
  - Message passing
    - Use shared memory to do message passing - typically involves extra copies due to distributed address space of different processes



# Message Passing

- Different processes execute in different address space
  - In most cases on different computers
- Inter process communication by exchange of messages over the interconnection network
- Typically facilitated by library calls from within user program

Computer 1

Process 0

User Code

MP Library

Process 1

User Code

MP Library

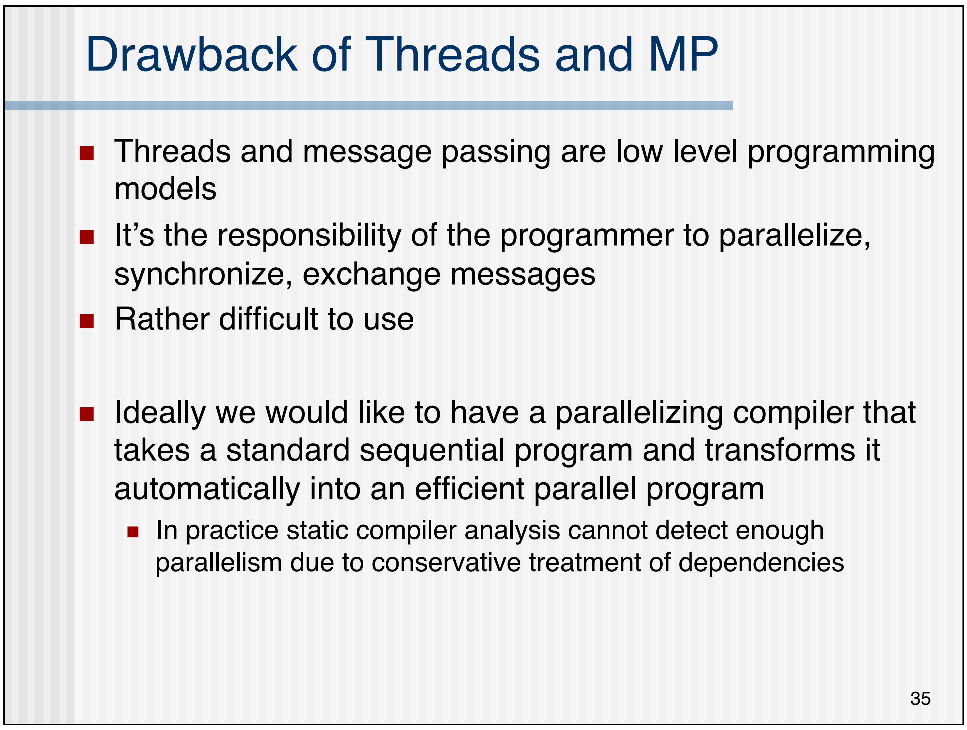
Computer 2

Process 2

User Code

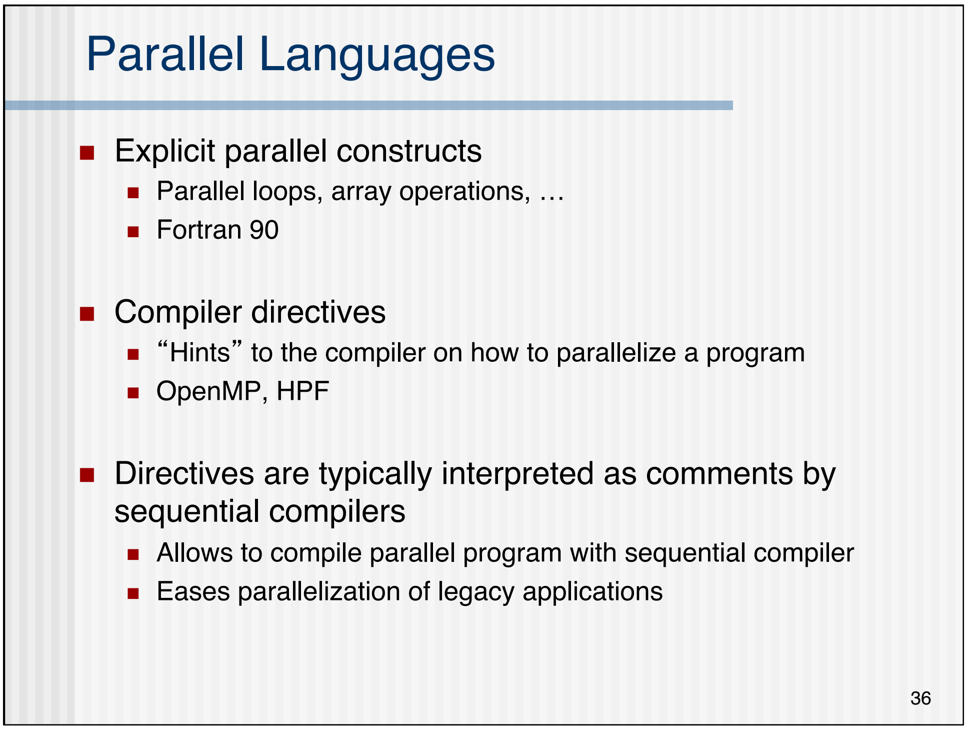
MP Library

Network



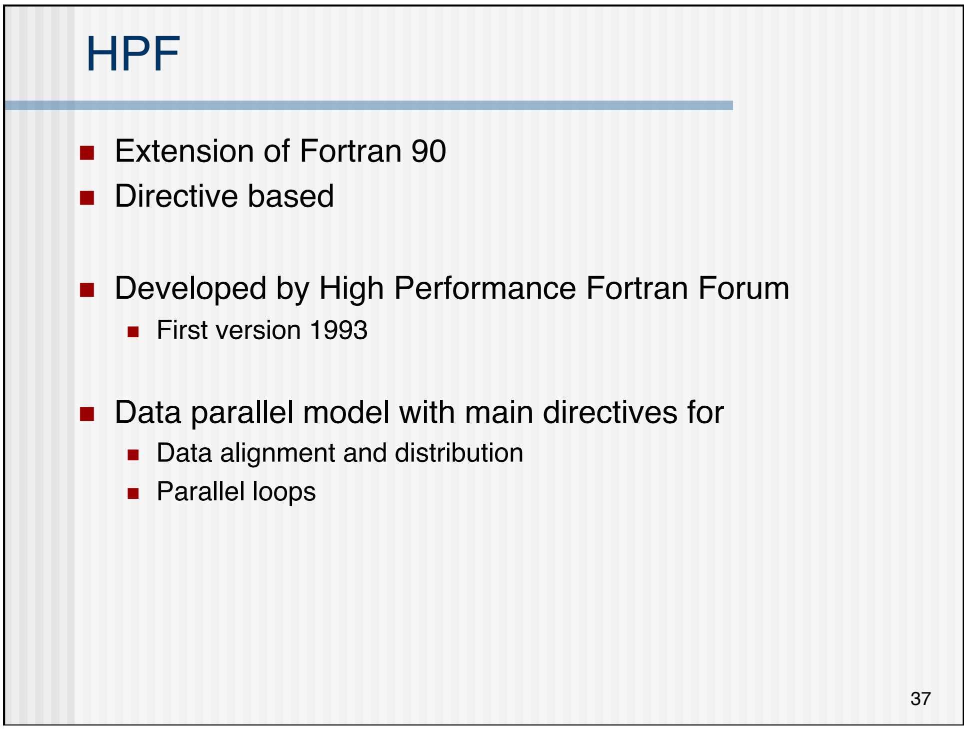
## Drawback of Threads and MP

- Threads and message passing are low level programming models
- It's the responsibility of the programmer to parallelize, synchronize, exchange messages
- Rather difficult to use
- Ideally we would like to have a parallelizing compiler that takes a standard sequential program and transforms it automatically into an efficient parallel program
  - In practice static compiler analysis cannot detect enough parallelism due to conservative treatment of dependencies



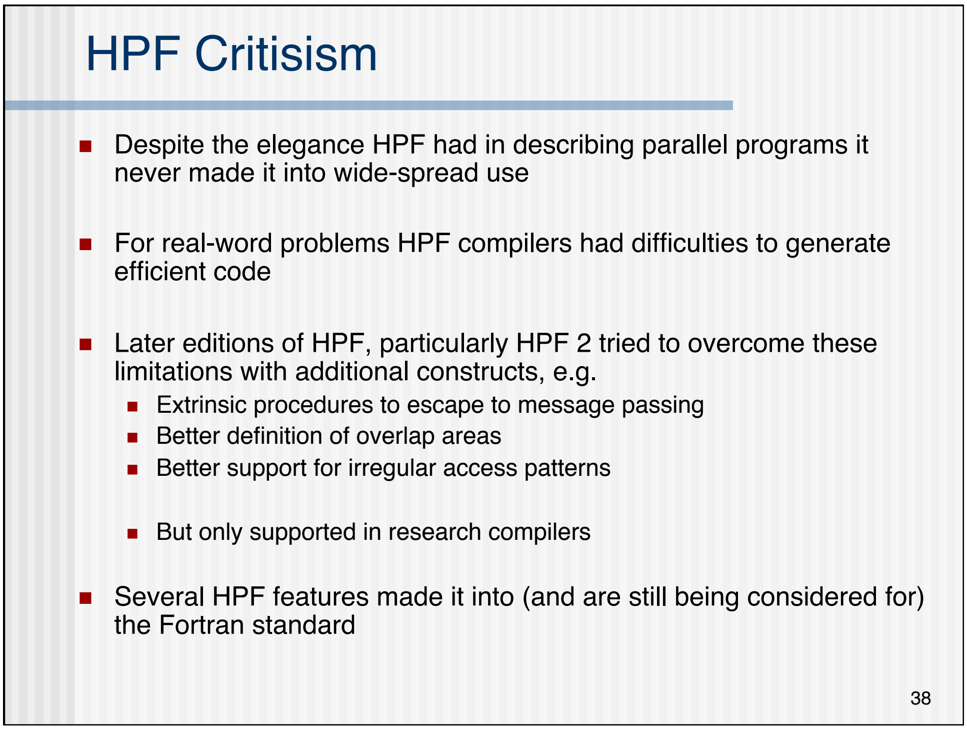
## Parallel Languages

- Explicit parallel constructs
  - Parallel loops, array operations, …
  - Fortran 90
- Compiler directives
  - "Hints" to the compiler on how to parallelize a program
  - OpenMP, HPF
- Directives are typically interpreted as comments by sequential compilers
  - Allows to compile parallel program with sequential compiler
  - Eases parallelization of legacy applications



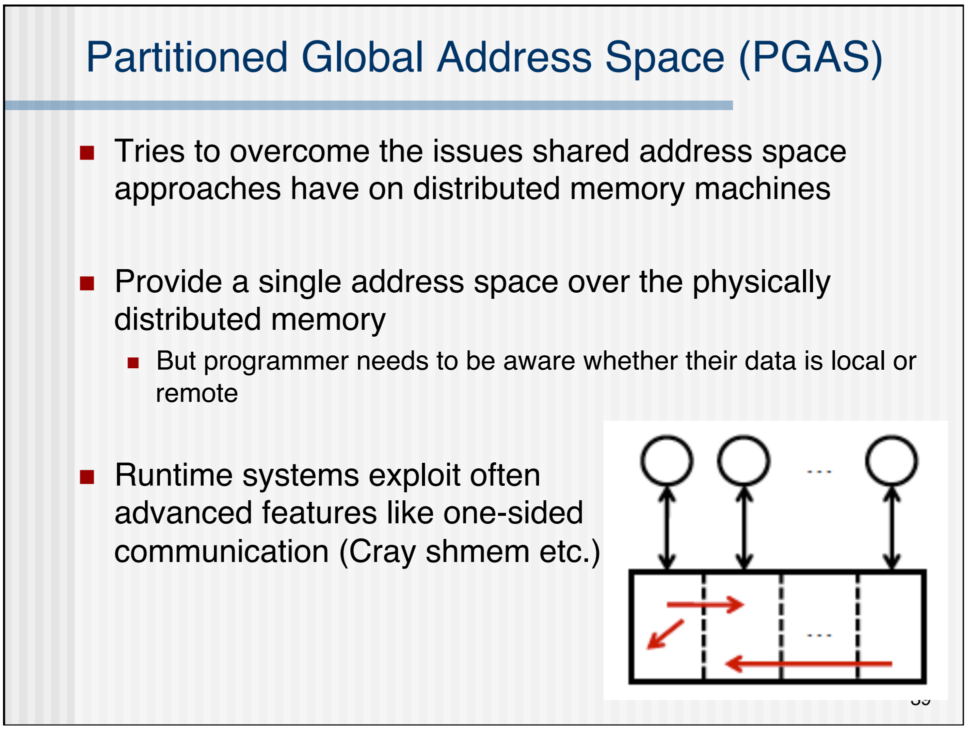
# HPF

- Extension of Fortran 90
- Directive based
- Developed by High Performance Fortran Forum
  - First version 1993
- Data parallel model with main directives for
  - Data alignment and distribution
  - Parallel loops



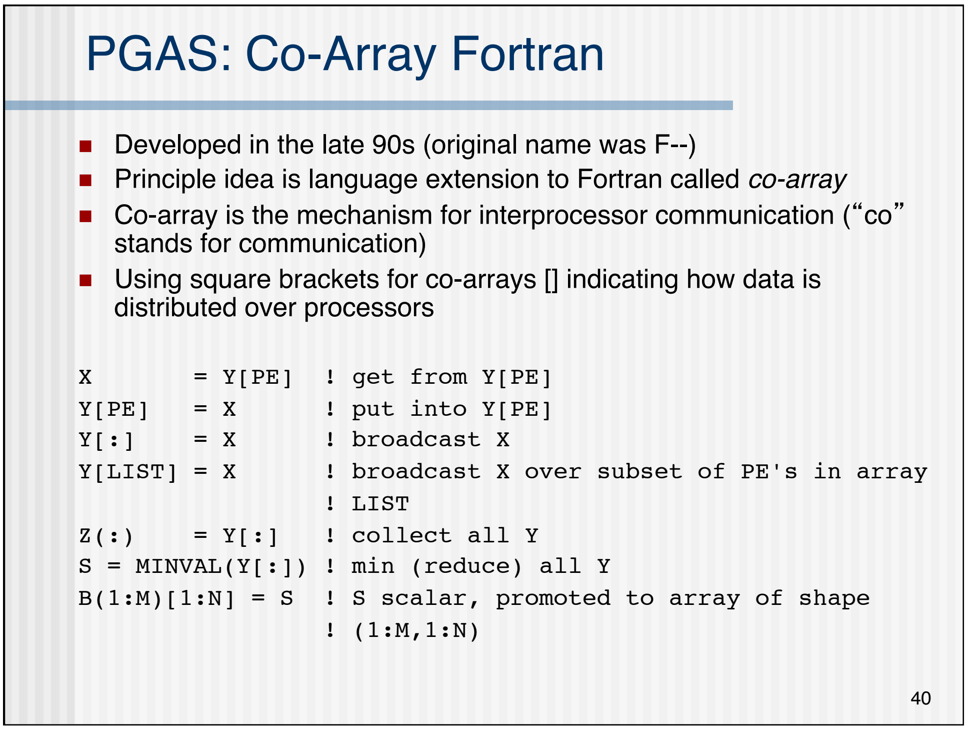
# HPF Critisism

- Despite the elegance HPF had in describing parallel programs it never made it into wide-spread use
- For real-word problems HPF compilers had difficulties to generate efficient code
- Later editions of HPF, particularly HPF 2 tried to overcome these limitations with additional constructs, e.g.
  - Extrinsic procedures to escape to message passing
  - Better definition of overlap areas
  - Better support for irregular access patterns
  - But only supported in research compilers
- Several HPF features made it into (and are still being considered for) the Fortran standard



## Partitioned Global Address Space (PGAS)

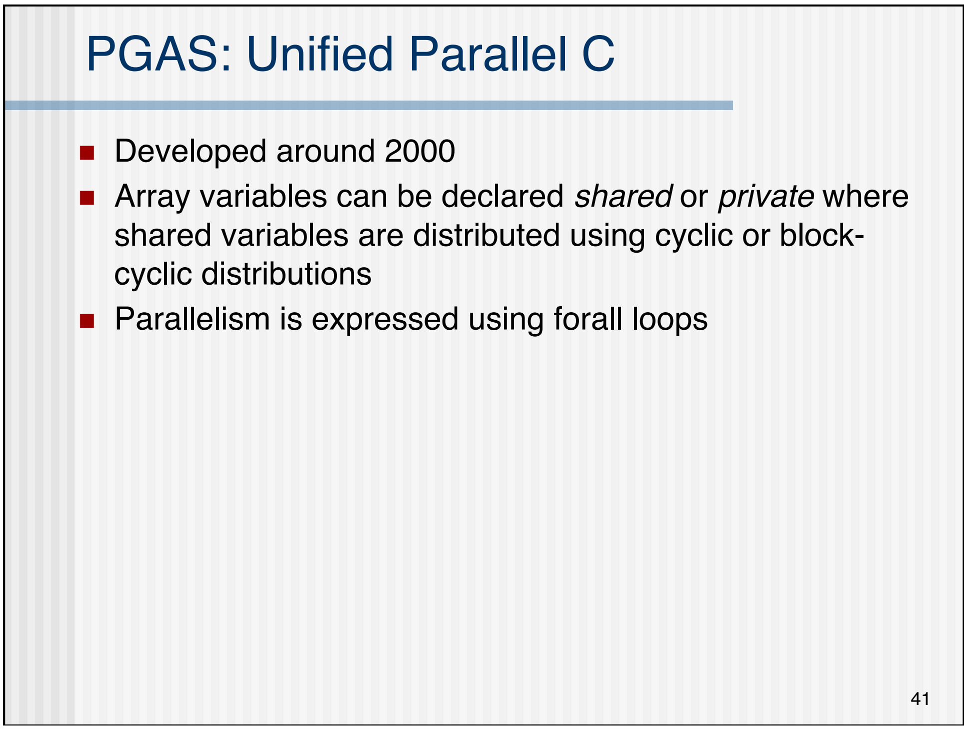
- Tries to overcome the issues shared address space approaches have on distributed memory machines
- Provide a single address space over the physically distributed memory
  - But programmer needs to be aware whether their data is local or remote
- Runtime systems exploit often advanced features like one-sided communication (Cray shmem etc.)



## PGAS: Co-Array Fortran

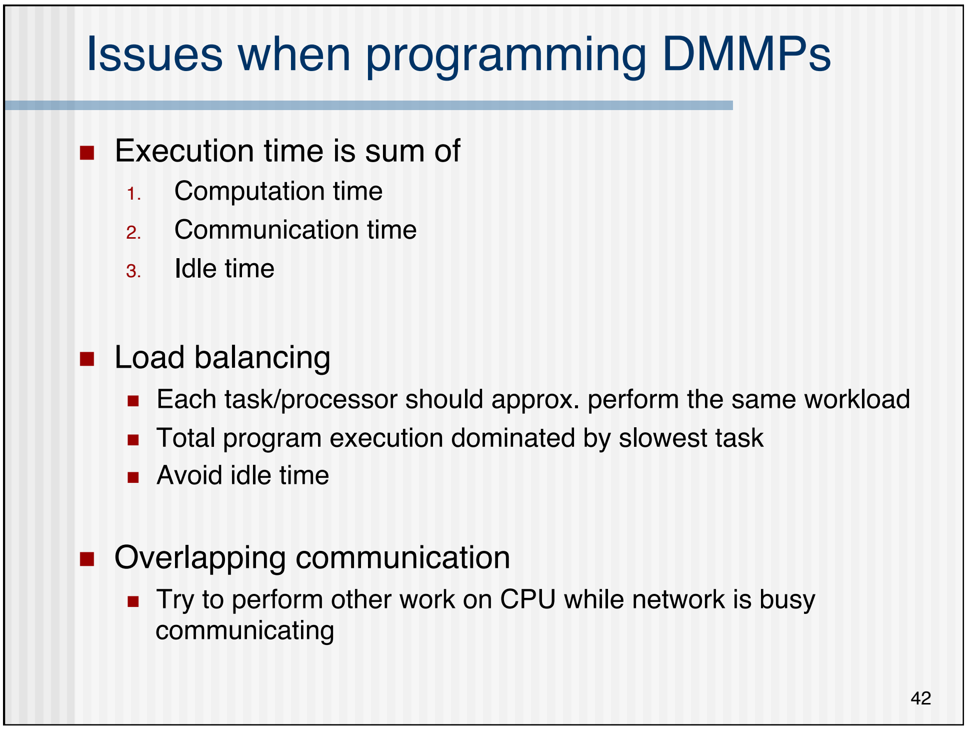
- Developed in the late 90s (original name was F--)
- Principle idea is language extension to Fortran called *co-array*
- Co-array is the mechanism for interprocessor communication ("co" stands for communication)
- Using square brackets for co-arrays [] indicating how data is distributed over processors

```
X       = Y[PE]  ! get from Y[PE]
Y[PE]   = X      ! put into Y[PE]
Y[:]    = X      ! broadcast X
Y[LIST] = X      ! broadcast X over subset of PE's in array
                 ! LIST
Z(:)    = Y[:]   ! collect all Y
S = MINVAL(Y[:]) ! min (reduce) all Y
B(1:M)[1:N] = S  ! S scalar, promoted to array of shape
                 ! (1:M,1:N)
```



## PGAS: Unified Parallel C

- Developed around 2000
- Array variables can be declared *shared* or *private* where shared variables are distributed using cyclic or block-cyclic distributions
- Parallelism is expressed using forall loops



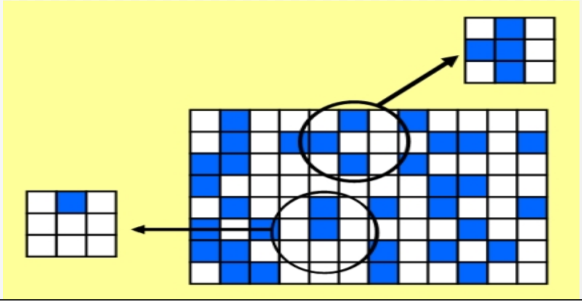
## Issues when programming DMMPs

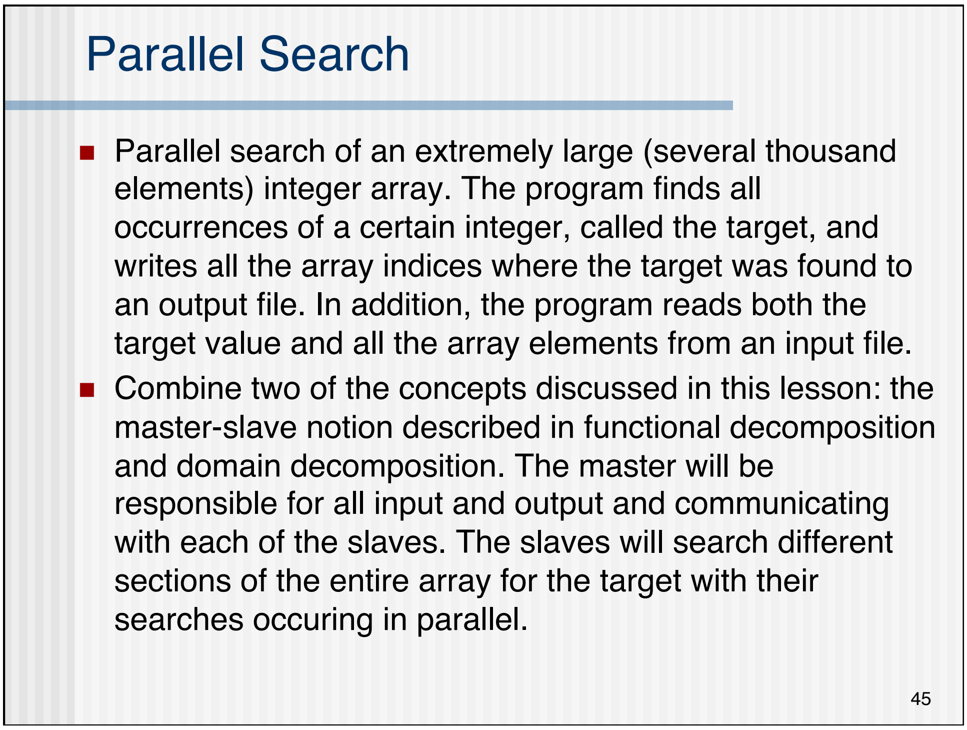
- Execution time is sum of
  1. Computation time
  2. Communication time
  3. Idle time
- Load balancing
  - Each task/processor should approx. perform the same workload
  - Total program execution dominated by slowest task
  - Avoid idle time
- Overlapping communication
  - Try to perform other work on CPU while network is busy communicating

# Running Examples

## Game of Life

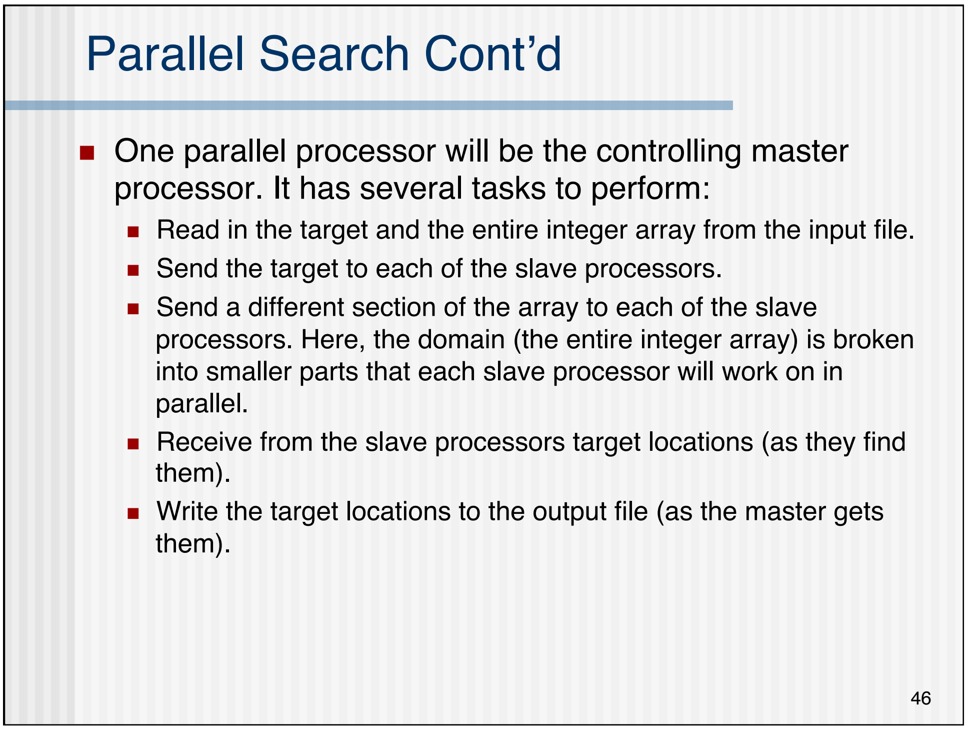
- In the "Game of Life" the domain is a 2-dimensional array of cells, and each cell can have one of two possible states, usually referred to as "alive" or "dead." At each time step, each cell may or may not change its state, based on the number of adjacent alive cells, including diagonals. There are three rules:
  1. If a cell has three neighbors that are alive, the cell will be alive. If it was already alive, it will remain so, and if it was dead, it will become alive.
  2. If a cell has two neighbors that are alive, there is no change to the cell. If it was dead, it will remain dead, and if it was alive, it will remain alive.
  3. In all other cases — the cell will be dead. If it was alive it becomes dead and if it was dead it remains dead.





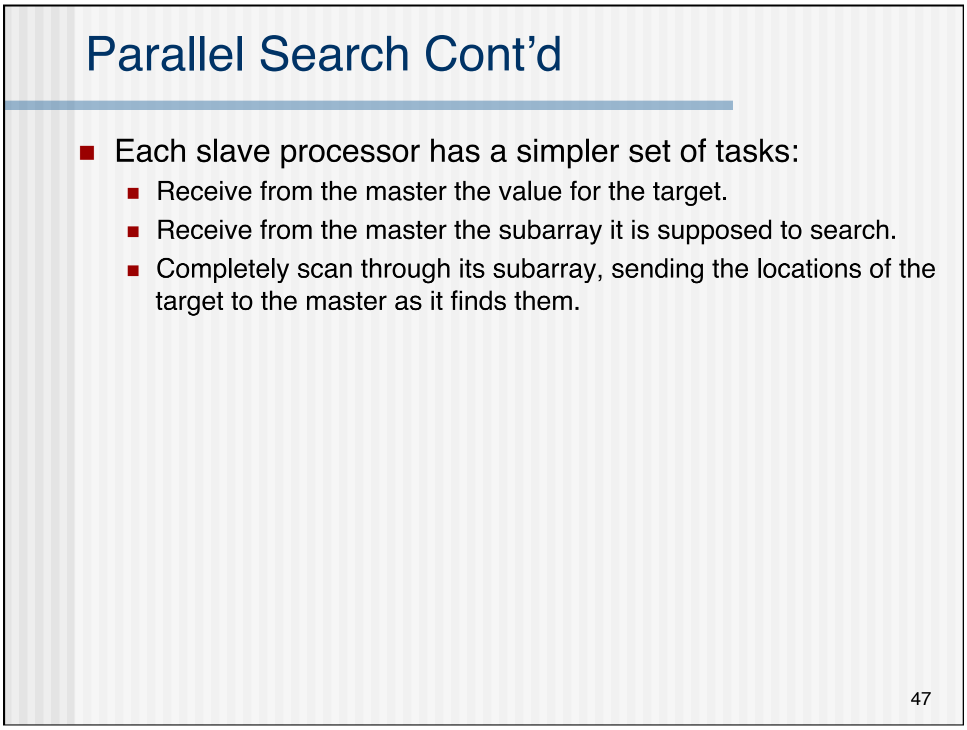
## Parallel Search

- Parallel search of an extremely large (several thousand elements) integer array. The program finds all occurrences of a certain integer, called the target, and writes all the array indices where the target was found to an output file. In addition, the program reads both the target value and all the array elements from an input file.
- Combine two of the concepts discussed in this lesson: the master-slave notion described in functional decomposition and domain decomposition. The master will be responsible for all input and output and communicating with each of the slaves. The slaves will search different sections of the entire array for the target with their searches occuring in parallel.



## Parallel Search Cont’d

- One parallel processor will be the controlling master processor. It has several tasks to perform:
  - Read in the target and the entire integer array from the input file.
  - Send the target to each of the slave processors.
  - Send a different section of the array to each of the slave processors. Here, the domain (the entire integer array) is broken into smaller parts that each slave processor will work on in parallel.
  - Receive from the slave processors target locations (as they find them).
  - Write the target locations to the output file (as the master gets them).



## Parallel Search Cont’d

- Each slave processor has a simpler set of tasks:
  - Receive from the master the value for the target.
  - Receive from the master the subarray it is supposed to search.
  - Completely scan through its subarray, sending the locations of the target to the master as it finds them.