Introduction to High Performance Computing

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Thank you

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This presentation borrows heavily from information freely available on the web by Ian Foster and Blaise Barney (see references)

Outline

- Introduction
- Thinking in Parallel
- Parallel Computer Architectures
- Parallel Programming Models
- References

Introduction

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Disclaimer: High Performance Computing (HPC) is valuable to a variety of applications over a very wide range of fields. Many of my examples will come from the world of physics, but I will try to present them in a general sense

Why Use Parallel Computing?

- Single processor speeds are reaching their ultimate limits

- Multi-core processors and multiple processors are the most promising paths to performance improvements

Definition of a parallel computer:

A set of independent processors that can work cooperatively to solve a problem.

Introduction

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The March towards Petascale Computing

- Computing performance is defined in terms of FLoating-point OPerations per Second (FLOPS)

GigaFLOP $1\ \mathrm{GF} = 10^9\ \mathrm{FLOPS}$

TeraFLOP $1\ \mathrm{TF} = 10^{12}\ \mathrm{FLOPS}$

PetaFLOP $1\ \mathrm{PF} = 10^{15}\ \mathrm{FLOPS}$

- Petascale computing also refers to extremely large data sets

PetaByte $1\ \mathrm{PB} = 10^{15}\ \mathrm{Bytes}$

Introduction

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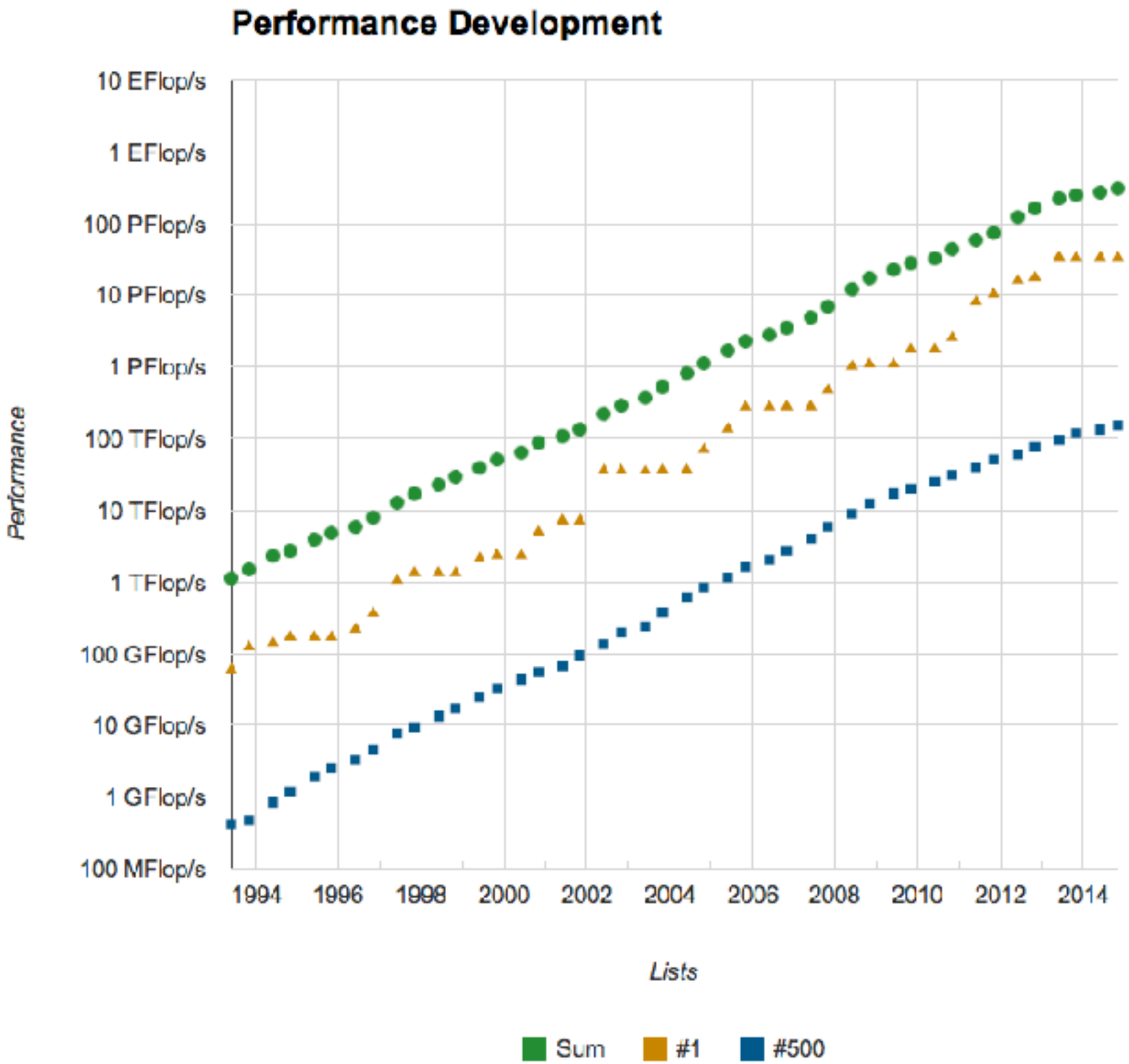
Performance improves by factor of ~10 every 4 years!



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Thinking in Parallel

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DEFINITION Concurrency: The property of a parallel algorithm that a number of operations can be performed by separate processors at the same time.

Concurrency is the key concept in the design of parallel algorithms:

- Requires a different way of looking at the strategy to solve a problem
- May require a very different approach from a serial program to achieve high efficiency

Thinking in Parallel

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DEFINITION Scalability: The ability of a parallel algorithm to demonstrate a speedup proportional to the number of processors used.

DEFINITION Speedup: The ratio of the serial wallclock time to the parallel wallclock time required for execution.

$$S = \frac{\text{wallclock time}_{serial}}{\text{wallclock time}_{parallel}}$$

• An algorithm that has good scalability will take half the time with double the number of processors

• Parallel Overhead, the time required to coordinate parallel tasks and communicate information between processors, degrades scalability.

Example: Numerical Integration

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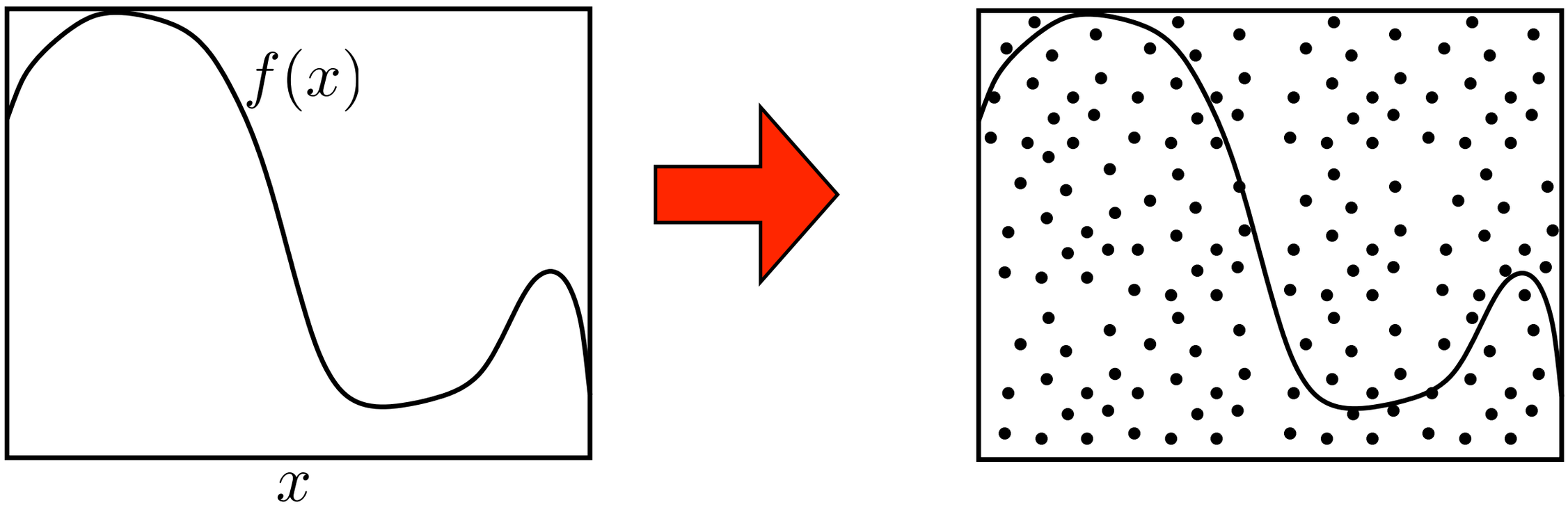
Numerical Integration: Monte Carlo Method

- Choose N points within the box of total area A
- Determine the number of points n falling below $f(x)$
- Integral value is $I = \frac{n}{N} A$



How do we do this computation in parallel?

Example: Numerical Integration

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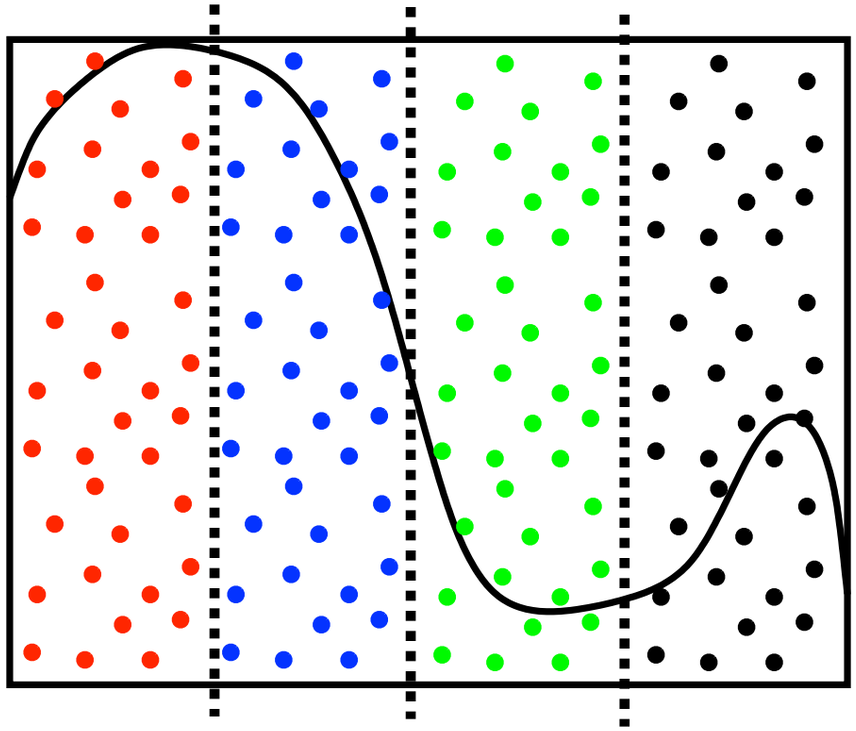
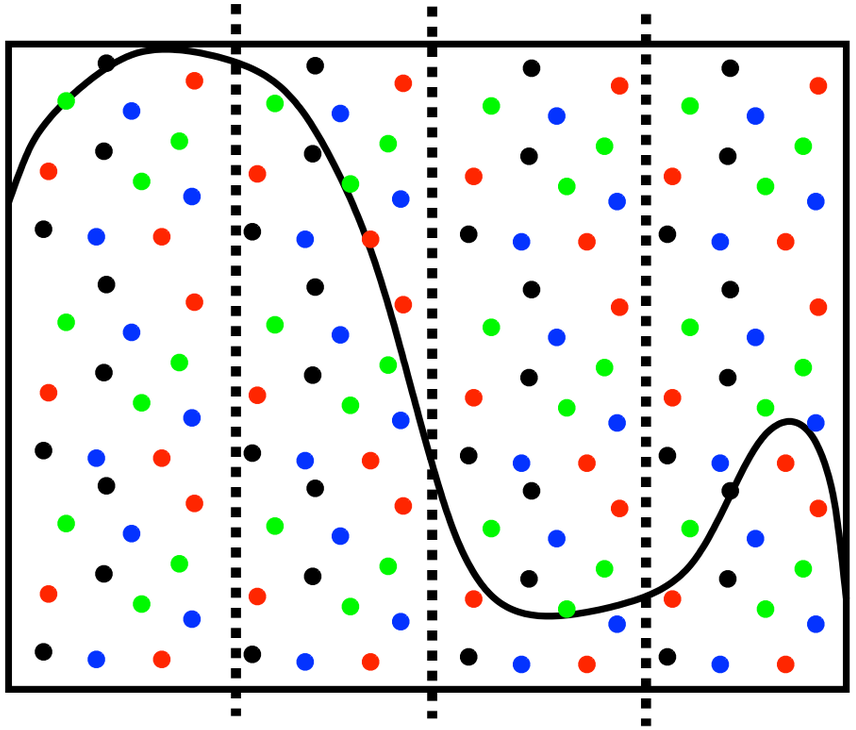
Strategies for Parallel Computation of the Numerical Integral:

1) Give different ranges of x to different processors and sum results



2) Give $N/4$ points to each processor and sum results



Example: Fibonacci Series

The Fibonacci series is defined by:

$$f(k+2) = f(k+1) + f(k) \quad \text{with } f(1) = f(2) = 1$$

The Fibonacci series is therefore $(1, 1, 2, 3, 5, 8, 13, 21, \ldots)$

The Fibonacci series can be calculated using the loop

```
f(1)=1
f(2)=1
do i=3, N
      f(i)=f(i-1)+f(i-2)
enddo
```

How do we do this computation in parallel?

This calculation cannot be made parallel.

- We cannot calculate $f(k+2)$ until we have $f(k+1)$ and $f(k)$

- This is an example of data dependence that results in a non-parallelizable problem

Example: Protein Folding

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- Protein folding problems involve a large number of independent calculations that do not depend on data from other calculations
- Concurrent calculations with no dependence on the data from other calculations are termed Embarrassingly Parallel
- These embarrassingly parallel problems are ideal for solution by HPC methods, and can realize nearly ideal concurrency and scalability

Unique Problems Require Unique Solutions

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- Each scientific or mathematical problem will, in general, require a unique strategy for efficient parallelization

Thus, each of you may require a different parallel implementation of your numerical problem to achieve good performance.

- Flexibility in the way a problem is solved is beneficial to finding a parallel algorithm that yields a good parallel scaling.

- Often, one has to employ substantial creativity in the way a parallel algorithm is implemented to achieve good scalability.

Understand the Dependencies

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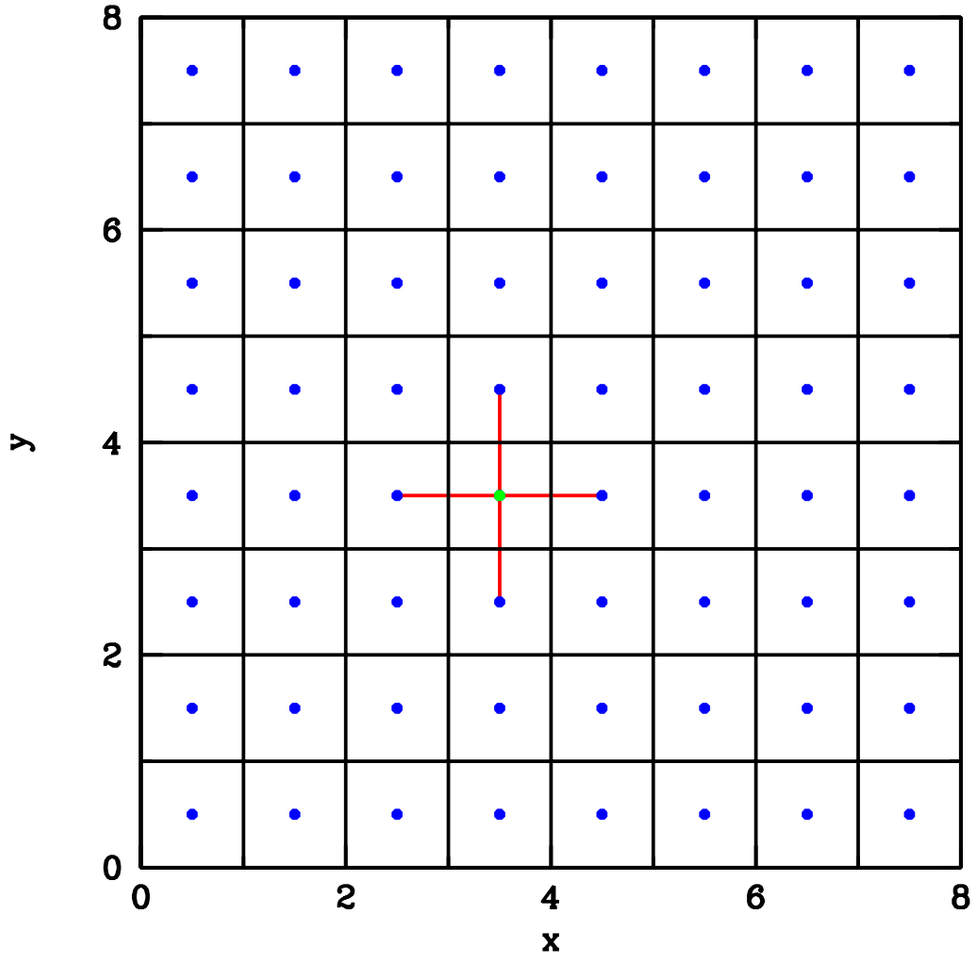
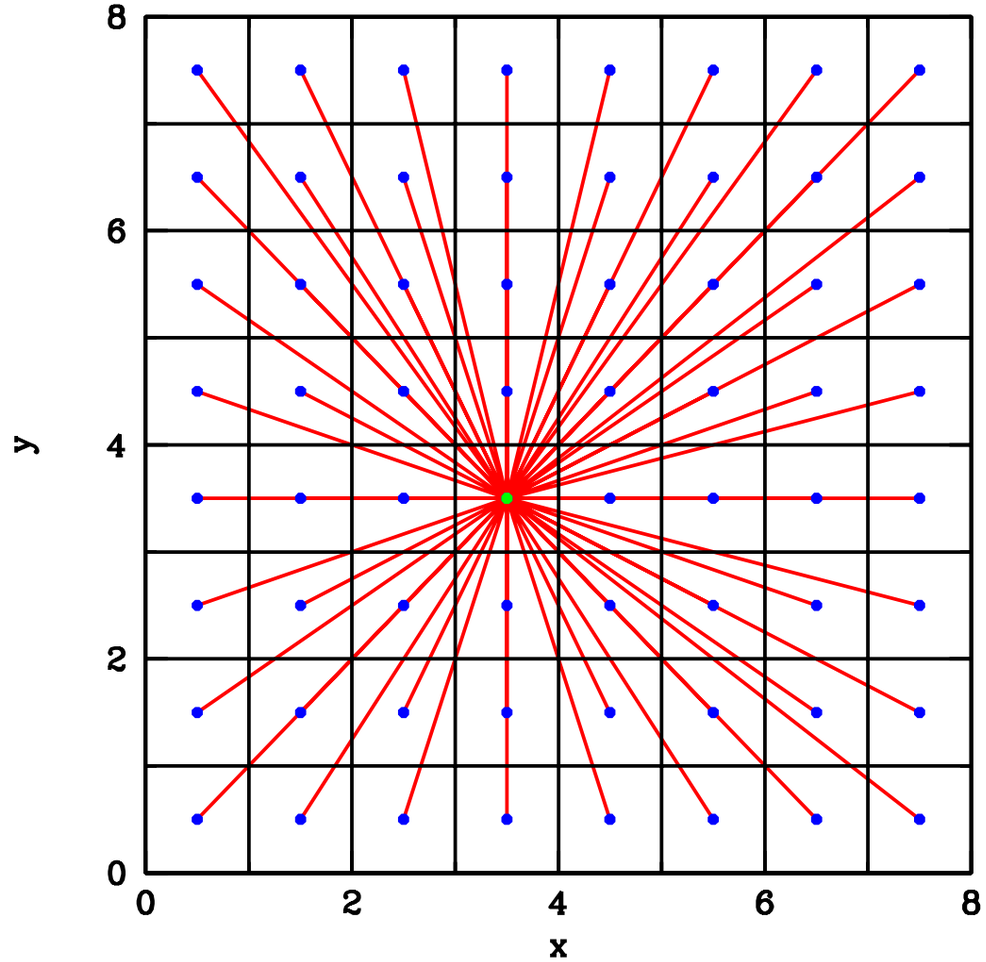
- One must understand all aspects of the problem to be solved, in particular the possible dependencies of the data.

- It is important to understand fully all parts of a serial code that you wish to parallelize.

Example: Pressure Forces (Local) vs. Gravitational Forces (Global)





Rule of Thumb

When designing a parallel algorithm, always remember:

Computation is FAST

Communication is SLOW

Input/Output (I/O) is INCREDIBLY SLOW

Other Issues

In addition to concurrency and scalability, there are a number of other important factors in the design of parallel algorithms:

Locality

Granularity

Modularity

Flexibility

Load balancing

We'll learn about these when we discuss the design of parallel algorithms.

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The Von Neumann Architecture

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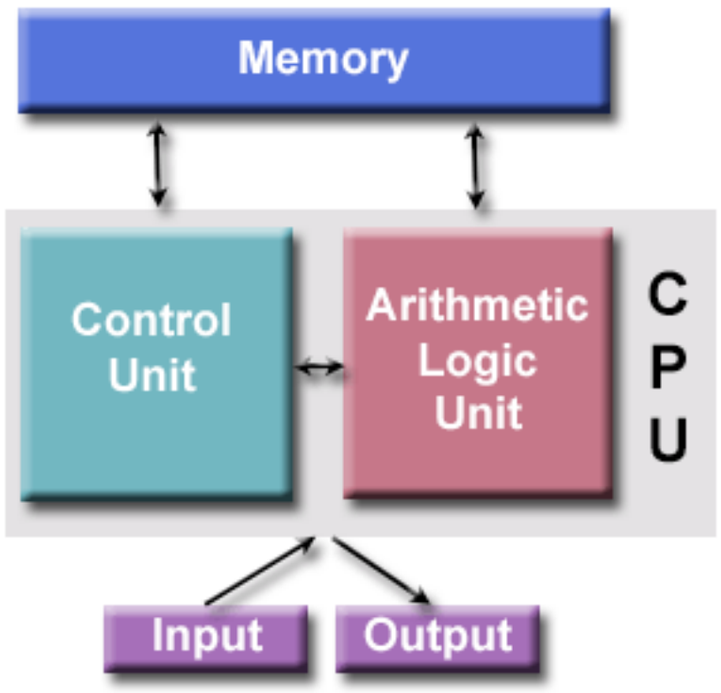
Virtually all computers follow this basic design



- Memory stores both instructions and data
- Control unit fetches instructions from memory, decodes instructions, and then sequentially performs operations to perform programmed task
- Arithmetic Unit performs mathematical operations
- Input/Output is interface to the user

Flynn's Taxonomy

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

- SISD: This is a standard serial computer: one set of instructions, one data stream

- SIMD: All units execute same instructions on different data streams (vector)
  - Useful for specialized problems, such as graphics/image processing
  - Old Vector Supercomputers worked this way, also moderns GPUs

- MISD: Single data stream operated on by different sets of instructions, not generally used for parallel computers

- MIMD: Most common parallel computer, each processor can execute different instructions on different data streams
  -Often constructed of many SIMD subcomponents

Parallel Computer Memory Architectures

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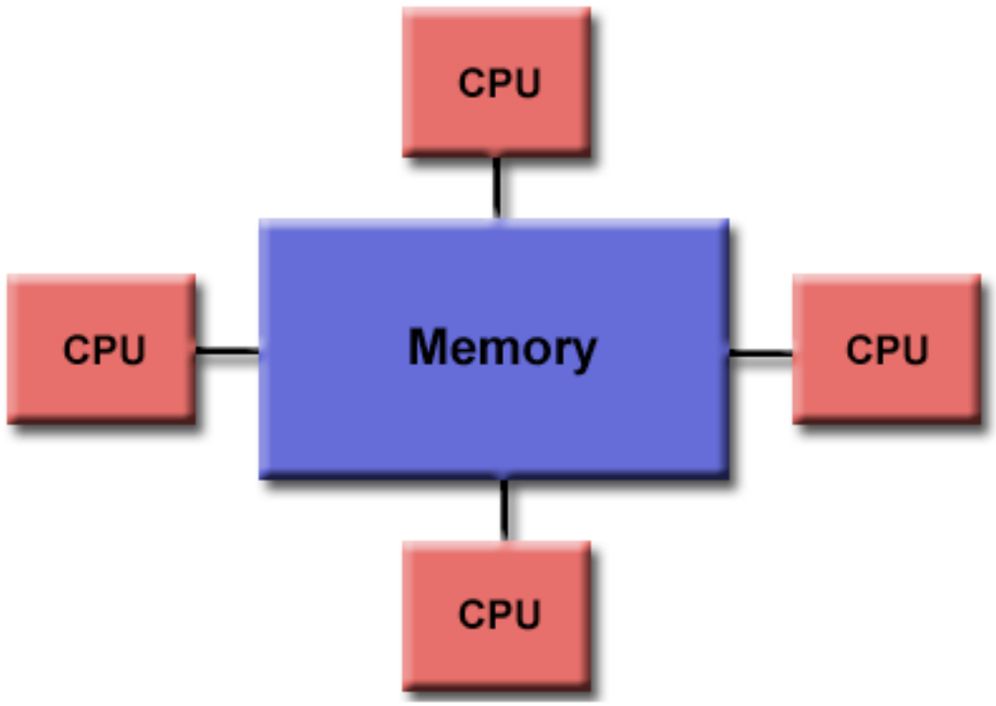
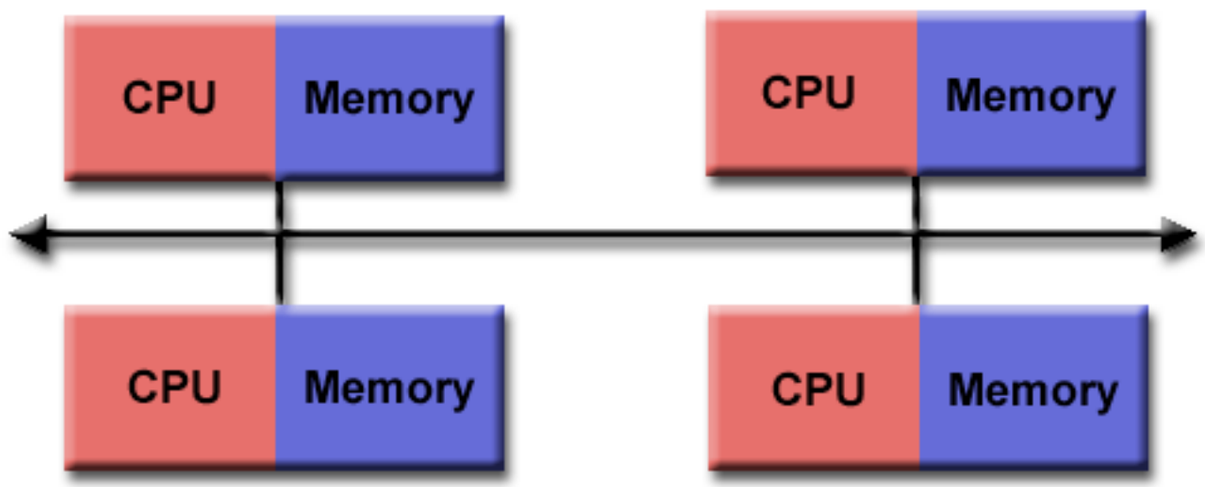
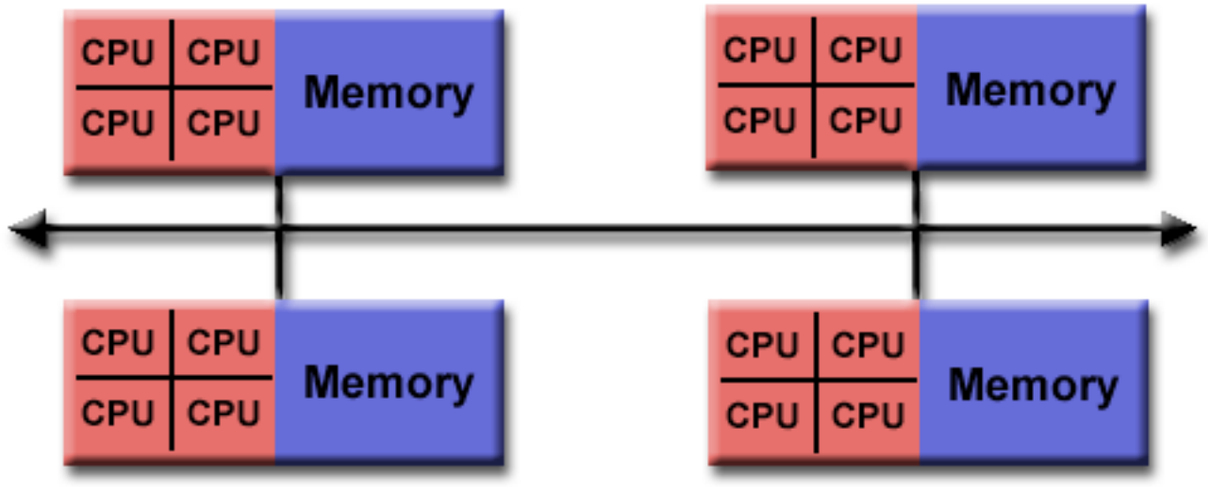
Shared Memory



Distributed Memory



Hybrid Distributed Shared Memory



Relation to Parallel Programming Models

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• OpenMP: Multi-threaded calculations occur within shared-memory components of systems, with different threads working on the same data.

• MPI: Based on a distributed-memory model, data associated with another processor must be communicated over the network connection.

• GPUs: Graphics Processing Units (GPUs) incorporate many (hundreds) of computing cores with single Control Unit, so this is a shared-memory model.

• Processors vs. Cores: Most common parallel computer, each processor can execute different instructions on different data streams

  -Often constructed of many SIMD subcomponents

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Parallel Programming Models

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- Embarrassingly Parallel
- Master/Slave
- Threads
- Message Passing
- Single Program-Multiple Data (SPMD)
  vs. Multiple Program-Multiple Data (MPMD)
- Other Parallel Implementations: GPUs and CUDA

Embarrassingly Parallel

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- Refers to an approach that involves solving many similar but independent tasks simultaneously

- Little to no coordination (and thus no communication) between tasks

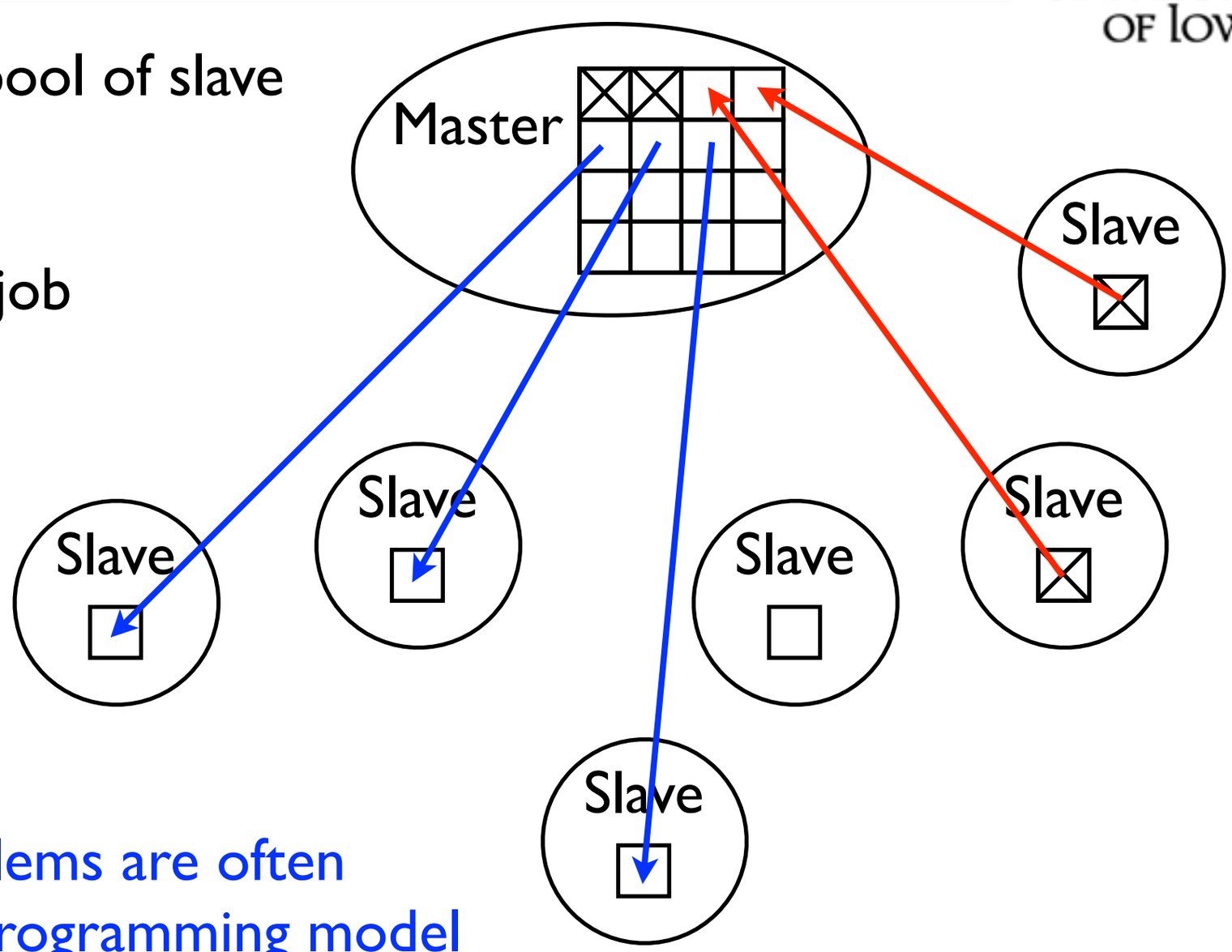
- Each task can be a simple serial program

- This is the "easiest" type of problem to implement in a parallel manner. Essentially requires automatically coordinating many independent calculations and possibly collating the results.

- Examples:
  - Computer Graphics and Image Processing
  - Protein Folding Calculations in Biology
  - Geographic Land Management Simulations in Geography
  - Data Mining in numerous fields
  - Event simulation and reconstruction in Particle Physics

Master/Slave

- Master Task assigns jobs to pool of slave tasks
- Each slave task performs its job independently
- When completed, each slave returns its results to the master, awaiting a new job



- Emabarrasingly parallel problems are often well suited to this parallel programming model

Multi-Threading

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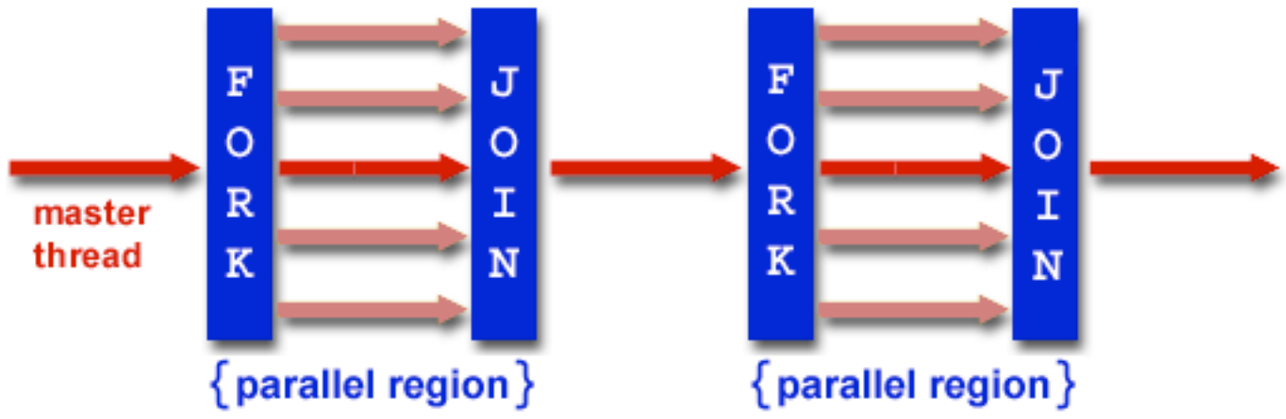
• Threading involves a single process that can have multiple, concurrent execution paths

• Works in a shared memory architecture

• Most common implementation is OpenMP (Open Multi-Processing)

```
serial code
        .
        .
        .

!$OMP PARALLEL DO
do i = 1,N
  A(i)=B(i)+C(i)
enddo
!$OMP END PARALLEL DO
        .
        .
        .
serial code
```



• Relatively easy to make inner loops of a serial code parallel and achieve substantial speedups with modern multi-core processors

Message Passing

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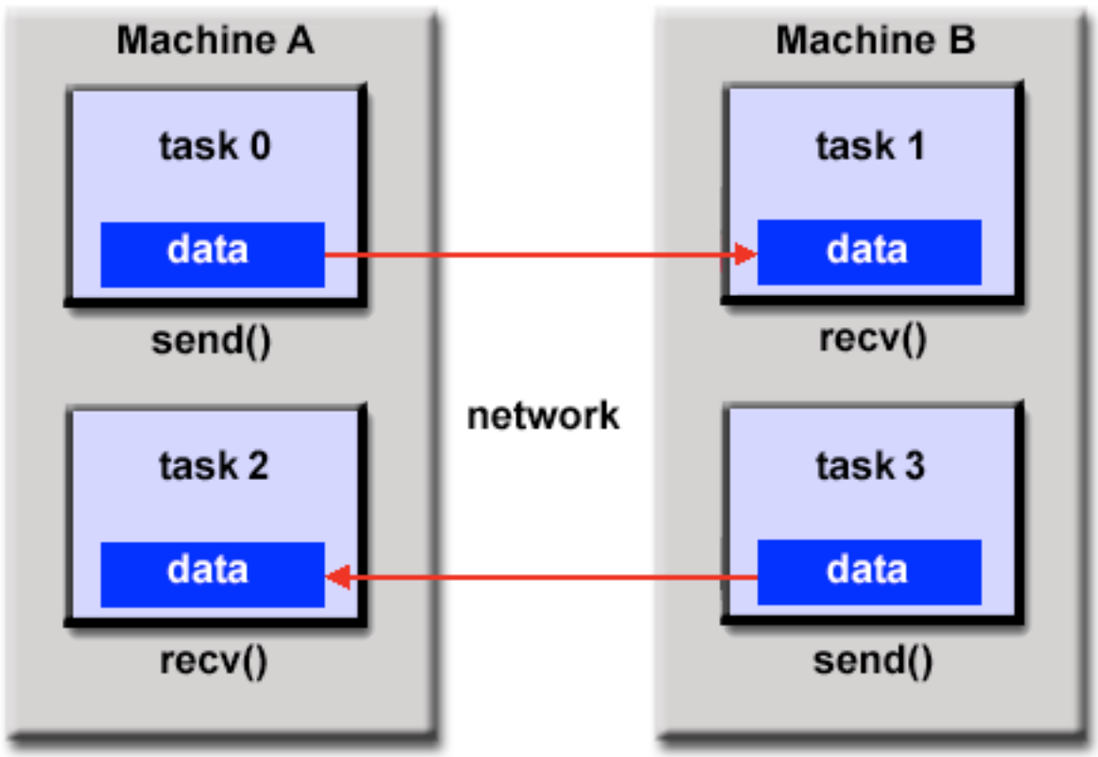
- The most widely used model for parallel programming

- Message Passing Interface (MPI) is the most widely used implementation

- A set of tasks have their own local memory during the computation (distributed-memory, but can also be used on shared-memory machines)

- Tasks exchange data by sending and receiving messages, requires programmer to coordinate explicitly all sends and receives.



- One aim of this course will focus on the use of MPI to write parallel programs.

SPMD vs. MPMD

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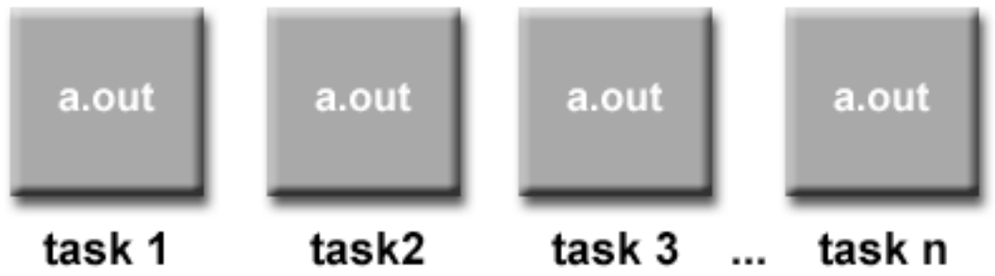
Single Program-Multiple Data (SPMD)

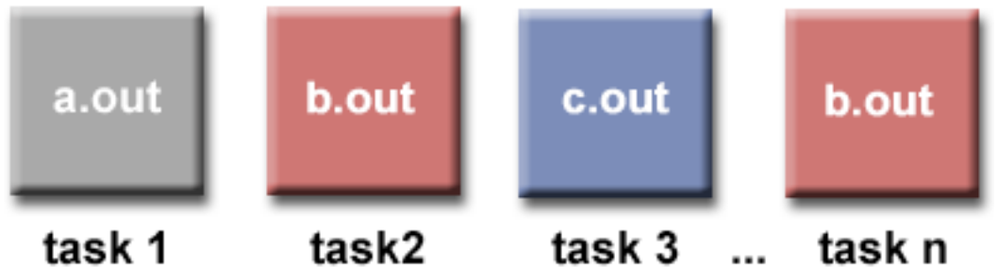
- A single program executes on all tasks simultaneously



- At a single point in time, different tasks may be executing the same or different instructions (logic allows different tasks to execute different parts of the code)

Multiple Program-Multiple Data (MPMD)

- Each task may be executing the same or different programs than other tasks



- The different executable programs may communicate to transfer data

Other Parallel Programming Models

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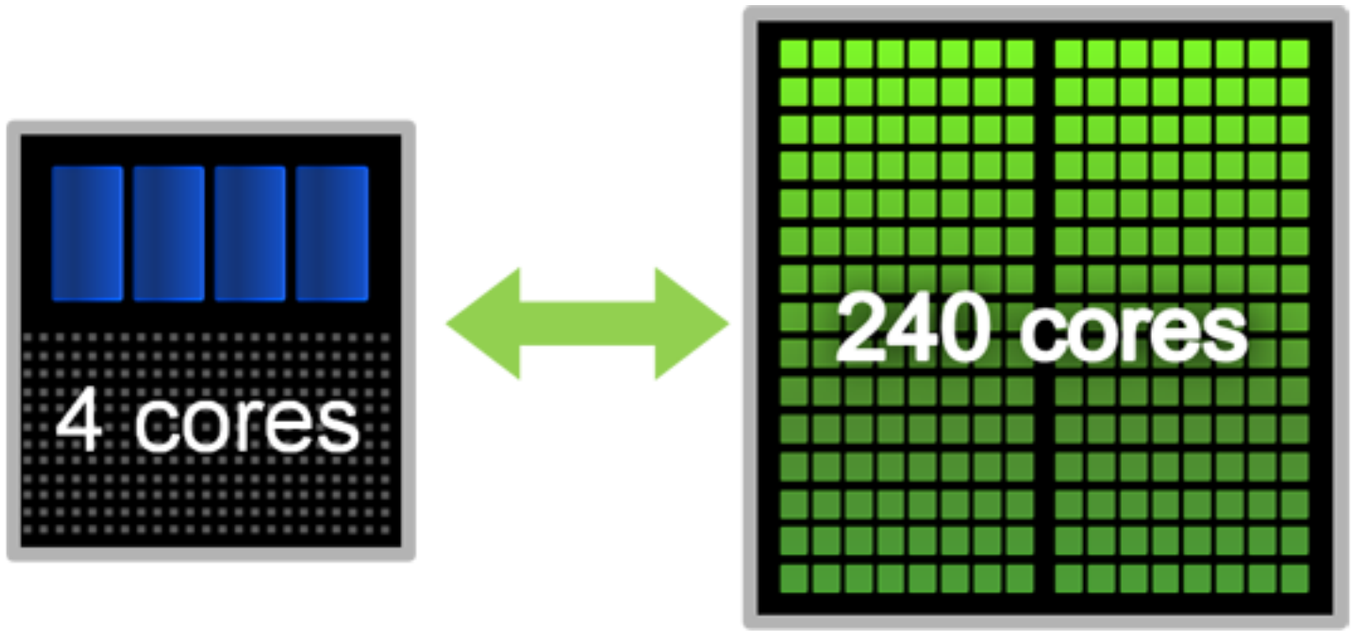
- GPUs (Graphics Processing Units) contain many (hundreds) of processing cores, allowing for rapid vector processing (Single Instruction, Multiple Data)



• CUDA (Compute Unified Device Architecture) programming allows one to call on this powerful computing engine from codes written in C, Fortran, Python, Java, and Matlab.

• This is an exciting new way to achieve massive computing power for little hardware cost, but memory access bandwidth limitations constrain the possible applications.

Parting Thoughts

• Part of the challenge of parallel computing is that the most efficient parallelization strategy for each problem generally requires a unique solution.

• It is generally worthwhile spending significant time considering alternative algorithms to find an optimal one, rather than just implementing the first thing that comes to mind

• But, consider the time required to code a given parallel implementation
  - You can use a less efficient method if the implementation is much easier.
  - You can always improve the parallelization scheme later. Just focus on making the code parallel first.

TIME is the ultimate factor is choosing a parallelization strategy---Your Time!

References

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Introductory Information on Parallel Computing

- Designing and Building Parallel Programs, Ian Foster
  http://www.mcs.anl.gov/~itf/dbpp/
  -Somewhat dated (1995), but an excellent online textbook with detailed discussion about many aspects of HPC. This presentation borrowed heavily from this reference
- Introduction to Parallel Computing, Blaise Barney
  https://computing.llnl.gov/tutorials/parallel_comp/
  -Up to date introduction to parallel computing with excellent links to further information
- MPICH2: Message Passage Inteface (MPI) Implementation
  http://www.mcs.anl.gov/research/projects/mpich2/
  -The most widely used Message Passage Interface (MPI) Implementation
- OpenMP
  http://openmp.org/wp/
  -Application Program Interface (API) supports multi-platform shared-memory parallel programming in C/C++ and Fortran
- Numerical Recipes
  http://www.nr.com/
  -Incredibly useful reference for a wide range of numerical methods, though not focused on parallel algorithms.
- The Top 500 Computers in the World
  http://www.top500.org/
  -Updated semi-annually list of the Top 500 Supercomputers

References

Introductory Information on Parallel Computing

- Message Passing Interface (MPI), Blaise Barney
  https://computing.llnl.gov/tutorials/mpi/
  -Excellent tutorial on the use of MPI, with both Fortran and C example code

- OpenMP, Blaise Barney
  https://computing.llnl.gov/tutorials/openMP/
  -Excellent tutorial on the use of OpenMP, with both Fortran and C example code

- High Performance Computing Training Materials, Lawrence Livermore National Lab
  https://computing.llnl.gov/?set=training&page=index
  -An excellent online set of webpages with detailed tutorials on many aspects of high performance computing.