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
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

The March towards Petascale Computing

• Computing performance is defined in terms of Floating-point Operations per Second (FLOPS)

\[
\begin{align*}
\text{GigaFLOP} & : 1 \text{ GF} = 10^9 \text{ FLOPS} \\
\text{TeraFLOP} & : 1 \text{ TF} = 10^{12} \text{ FLOPS} \\
\text{PetaFLOP} & : 1 \text{ PF} = 10^{15} \text{ FLOPS}
\end{align*}
\]

• Petascale computing also refers to extremely large data sets

\[
\begin{align*}
\text{PetaByte} & : 1 \text{ PB} = 10^{15} \text{ Bytes}
\end{align*}
\]
Introduction

Performance improves by factor of ~10 every 4 years!
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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
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.

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

- 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.
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

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
The Fibonacci series is defined by:

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

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

The Fibonacci series can be calculated using the loop

\[
\begin{align*}
  f(1) &= 1 \\
  f(2) &= 1 \\
  \text{do } i &= 3, N \\
  \quad f(i) &= f(i-1) + f(i-2) \\
  \text{enddo}
\end{align*}
\]

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

• 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

• 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

• 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

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

- **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

Shared Memory

Distributed Memory

Hybrid Distributed Shared Memory
Relation to Parallel Programming Models

- **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

- 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

• 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
- Embarrassingly parallel problems are often well suited to this parallel programming model
Multi-Threading

- 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)

```plaintext
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

• 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 summer school will focus on the use of MPI to write parallel programs.
**SPMD vs. MPMD**

**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

- 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!
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 Interface (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/](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/](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](https://computing.llnl.gov/?set=training&page=index)
  
  - An excellent online set of webpages with detailed tutorials on many aspects of high performance computing.