Beginner Parallel Computing

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Questions? #RC_Meetups

Link to survey on this topic: http://goo.gl/forms/8VidcwOhRT

Slides: https://github.com/ResearchComputing/Final_Tutorials

Outline

- Serial vs. Parallel processing
- Shared vs. Distributed Memory
- OpenMP vs. MPI
- Matlab
- Overhead

What Is Parallelism?

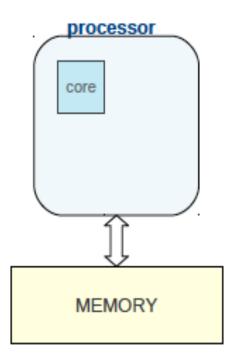
- What is parallelism?
 - Idea where many instructions are carried out simultaneously across a computing system
 - Can divide a large problem up into many smaller problems
 - The idea of splitting up mowing the lawn with your spouse
 - Or of you and your spouse mowing your lawn and your neighbor's lawn
 - Potentially faster, more efficient

Why Parallelize?

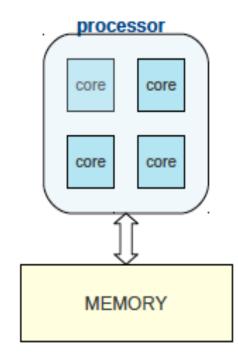
- Single core too slow for solving the problem in a "reasonable" time
 - "Reasonable" time: overnight, over lunch, duration of a PhD thesis
- Memory requirements
 - Larger problem
 - More physics
 - More particles

Basic Architecture

Older processor had only one cpu core to execute instructions



Modern processors have 4 or more independent cpu cores to execute instructions



Source: http://people.math.umass.edu/~johnston/PHI_WG_2014/OpenMPSlides_tamu_sc.pdf

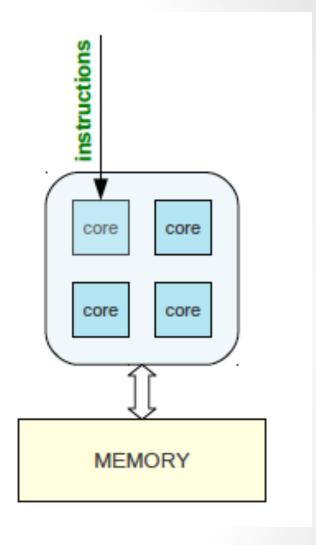
Serial Processing – Thought Experiment

- Jigsaw puzzle analogy**
- Have a 1000 piece jigsaw puzzle
 - You can do it yourself, maybe it will take 1 hour to do
 - Serial processing
- Maybe you have three friends sitting nearby willing to help, but you won't let them
 - Wasted resources

^{**}from Henry Neeman, OSCER, "Supercomputing in Plain English"

Serial Processing

- Instructions are executed on one core
- The other cores sit idle
- If a task is running, Task
 2 waits for Task 1 to
 complete, etc.
- Wasting resources
- Want to instead parallelize and use all cores



Source: http://people.math.umass.edu/~johnston/PHI_WG_2014/OpenMPSlides_tamu_sc.pdf

Shared Memory Parallel Processing – Thought Experiment

- Jigsaw puzzle analogy**
 - Let's say you decide to let one of your friends, Stacey, join you
 - Stacey and you sit at a table and each work on half the puzzle
 - In theory you reduce the puzzle time completion by half
 - However, other time sinks
 - Reaching for the same puzzle pieces
 - Resource contention
 - Communicating about puzzle interfaces
 - Might take 35 minutes instead of 30

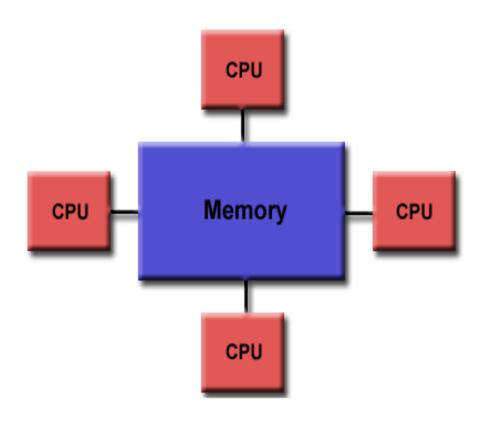
^{**}from Henry Neeman, OSCER, "Supercomputing in Plain English"

Shared Memory Parallel Processing – Thought Experiment

- Jigsaw puzzle analogy**
 - Now you let your other two friends, Fred and Jim, join in
 - Now conceivably could finish in ¼ the time (15 minutes)
 - But there's even more contention for resources
 - More communication
 - Slows down the process even more (maybe takes 23 minutes to complete instead)
 - Too many people slows down the process too much to make it worthwhile
 - Eventually have a "diminishing return"

^{**}from Henry Neeman, OSCER, "Supercomputing in Plain English"

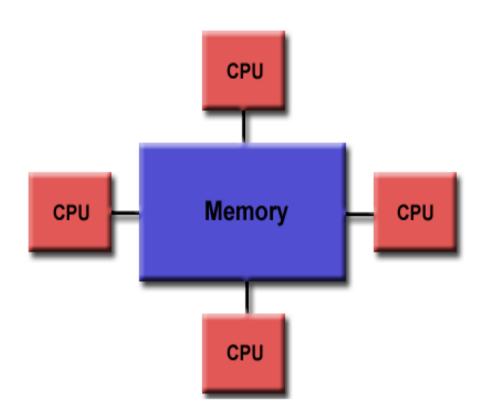
Shared-memory Model



The concept is that all processors can access all memory available

Multiple processors can perform tasks on their own but share the same memory

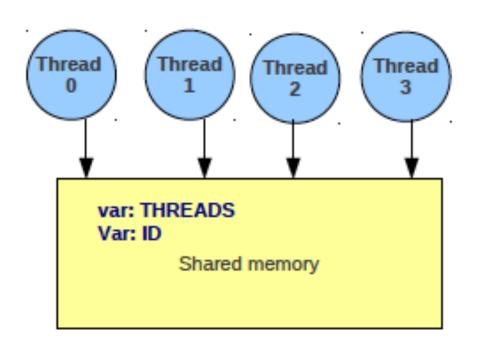
Shared-memory Model



Advantage: data sharing is fast and uniform

Disadvantage: adding more processors can cause performance issues when accessing the same shared memory resource

Shared-memory Model



A thread is a block of code with one entry and one exit that is abstract and is mapped onto a physical core. Multiple threads can be mapped onto one core.

Threads communicate by depositing contents in shared memory area

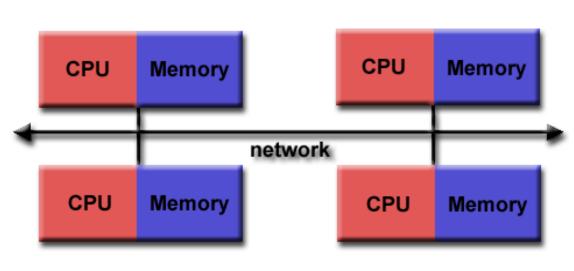
Source: http://people.math.umass.edu/~johnston/PHI_WG_2014/OpenMPSlides_tamu_sc.pdf

Distributed Memory Parallel Processing – Thought Experiment

- Jigsaw puzzle analogy**
 - Now we have two tables with one person at each table doing the puzzle
 - We split the puzzle equally between tables
 - Each person works completely independently
 - But to communicate costs more
 - How do you work out connecting the puzzle?
 - Can you really divide up the puzzle evenly?

^{**}from Henry Neeman, OSCER, "Supercomputing in Plain English"

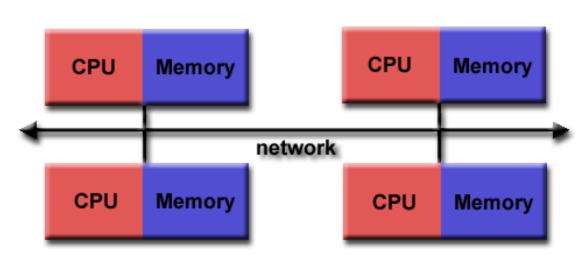
Distributed-memory Model



Distributed memory requires a communication network to connect memory

Processors have own memory and don't map globally

Distributed-memory Model



Programmers
explicitly define how
processors access
other processor's
memory

Advantage: scalable

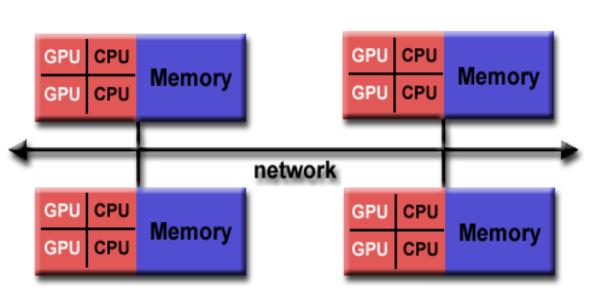
memory

Disadvantage: need to

know parallel

programming!

Distributed-Shared Memory



Most large and fast computers now

Shared memory machines connected to other shared memory machines

Programming to Use Parallelism

Parallelism across processors/threadsOpenMP

 Parallelism across multiple nodes -MPI



Linux micro OS



www.scan.co.uk

OpenMP

- OpenMP: An application programming interface (API) for parallel programming on multiprocessors
- Uses shared memory
- OpenMP is used through compiler directives embedded in Fortran, C, or C++ code
- Directs multi-threaded, shared memory parallelism
- Can do a lot with only a handful of commands
- Intended to be easy to use

Source: https://computing.llnl.gov/tutorials/openMP/#Introduction

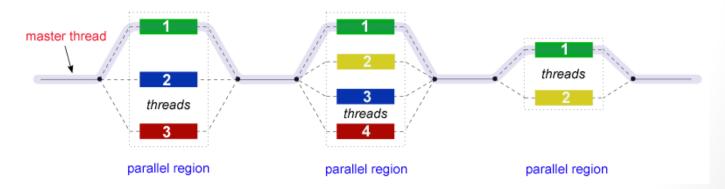
Multi-Threaded, Shared Memory Parallelism

- Have a main program that loads all needed resources
- Main program does many things, including run subroutines
 - Threads that can be run concurrently
 - Share the same resources from the main program, but also has local data
 - Threads communicate through global memory
 - Must ensure multiple threads don't update concurrently
 - Where OpenMP and programmers come

a.out call sub1() call sub2() do i=1.n A(i)=fnc(i**2) B(i)=A(i)*psi end do call sub3() call sub4() private private a.out Memory

OpenMP – Fork/Join

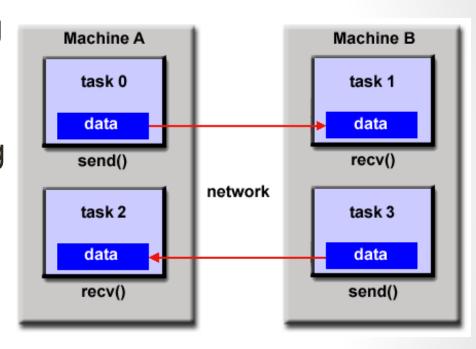
- OpenMP programs start with a single thread (master)
- Then Master creates a team of parallel "worker" threads (FORK)
- Statements in block are executed in parallel by every thread
- At end, all threads synchronize and join master thread



Source: https://computing.llnl.gov/tutorials/openMP/#Introduction

Distributed Memory

- Tasks use own local memory when computing
- Can reside on one or many machines
- Communicate by sending and receiving messages
- Have an inter-connect, such as Infiniband



http://www.ee.ryerson.ca/~courses/ee8218/mpi_openmp.pdf

MPI

- MPI is a library specification for message passing Based on consensus of many organizations
 - Provides widely used standard for writing message passing programs
- Operates on a distributed model
- Exchange data through communication between tasks – send and receive data
- MPI can get complicated
- Programmers must explicitly implement parallelism using MPI constructs

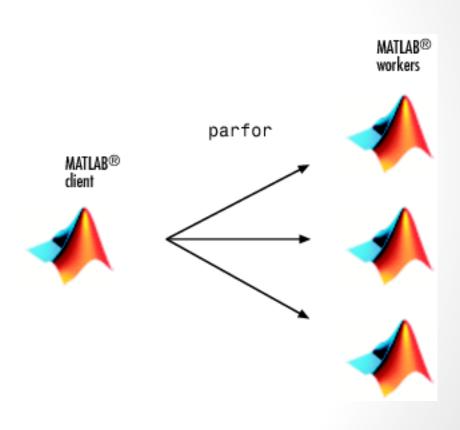
https://computing.llnl.gov/tutorials/mpi/

MPI or OpenMP?

- OpenMP
 - Don't understand parallel programming
 - Only need to run on one node
 - Just want to speed up application
 - Program is not complicated
- MPI
 - Multiple nodes
 - Running out of memory and need to use more nodes

Running Matlab in Parallel

- Mimics OpenMP or MPI
 - Depends on toolbox you have
 - Easiest to get the Parallel Computing Toolbox
 - Mimics OpenMP
- Easy to convert code from serial to parallel
 - parfor
 - spmd
- Workers: copies of the original client created to assist in computation



Parallel Overhead

- Should you convert your serial code to parallel?
- Usually do it to speed up
- But need to consider things like overhead
- Overhead because of
 - Startup time
 - Synchronizations
 - Communication
 - Overhead by libraries, compilers
 - Termination time

Questions?

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- Twitter: @CUBoulderRC
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- Questions? #RC_Meetup