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

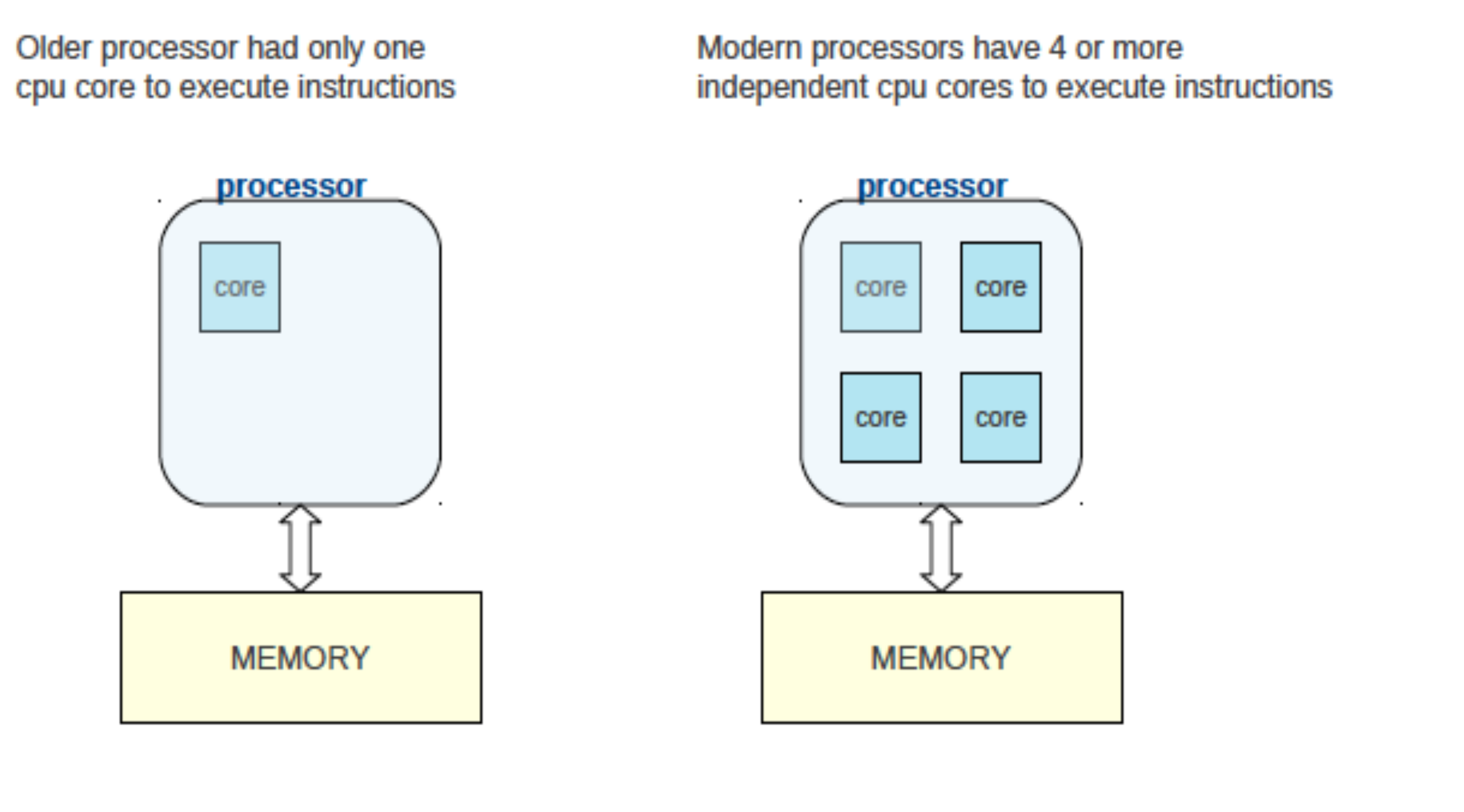
What Is Parallelism?

- 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

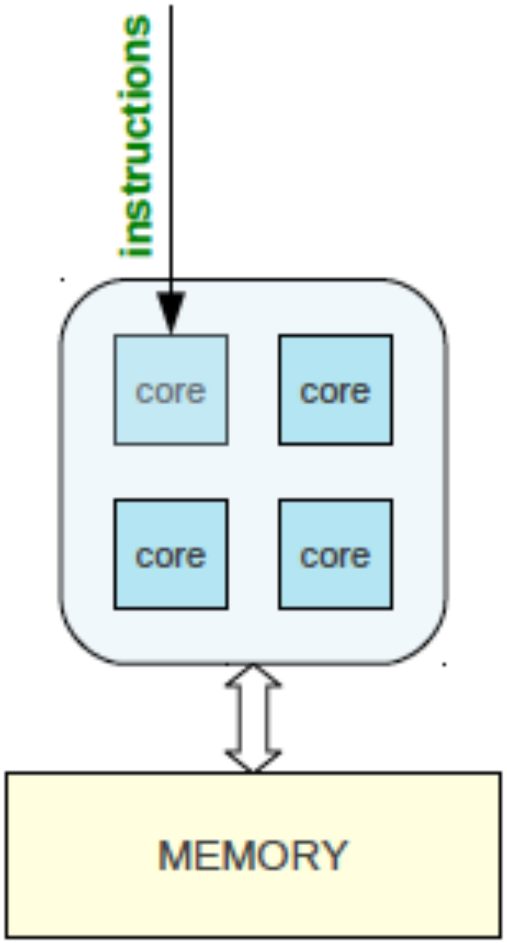
Serial Processing – Thought Experiment

- 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



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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

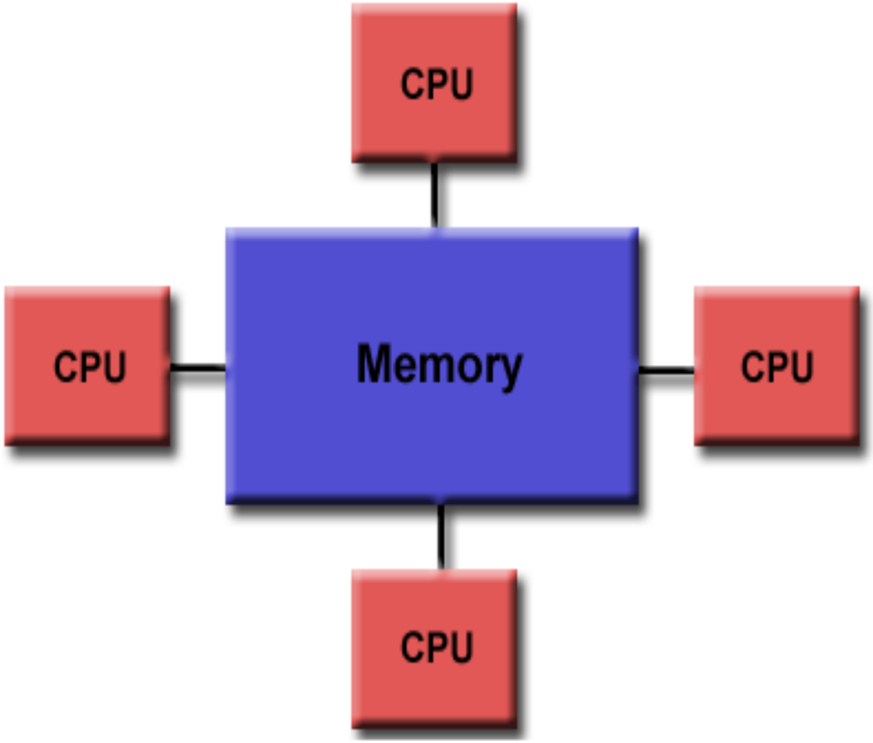
**from Henry Neeman, OSCER, “Supercomputing in Plain English”

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

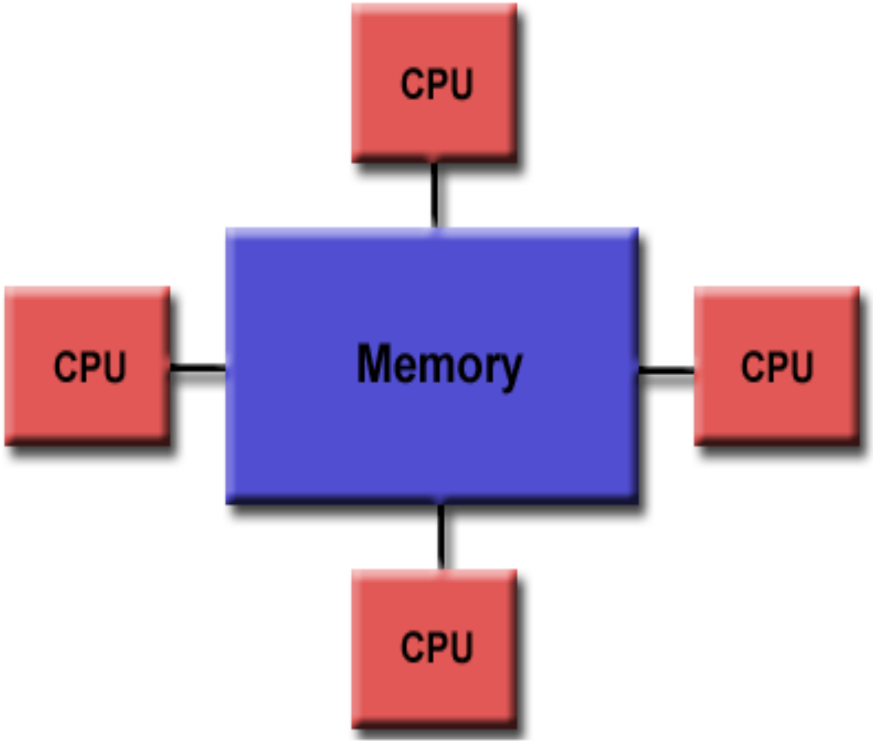


The concept is that all processors can access all memory available

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

Source: https://computing.llnl.gov/tutorials/parallel_comp/#ModelsShared

Shared-memory Model

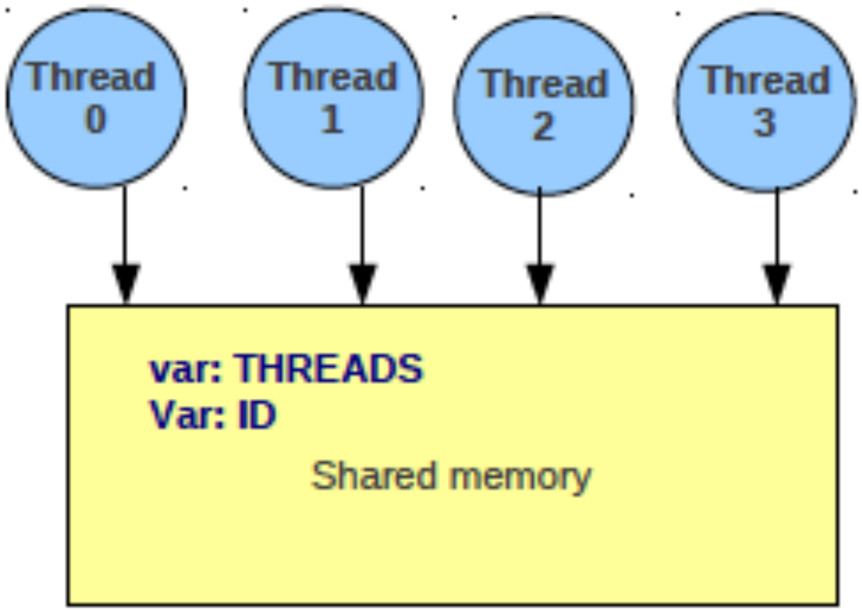


Advantage: data sharing is fast and uniform

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

Source: https://computing.llnl.gov/tutorials/parallel_comp/#ModelsShared

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

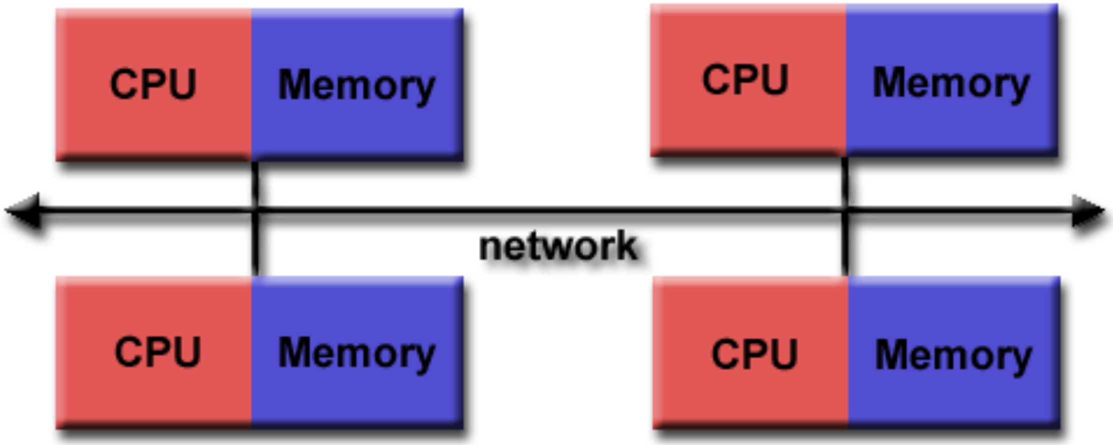
Source: http://people.math.umass.edu/~johnston/PHI_WG_2014/OpenMPSlides_tamu_sc.pdf

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

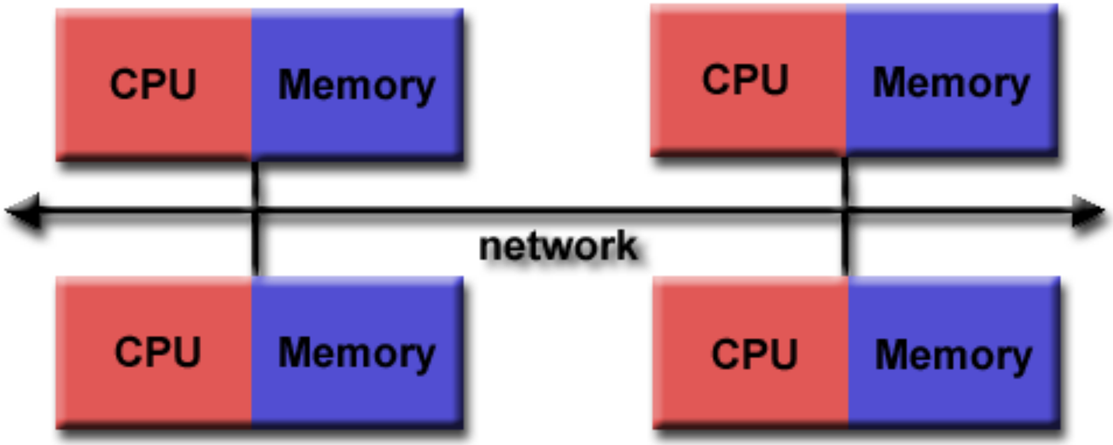


Distributed memory requires a communication network to connect memory

Processors have own memory and don’t map globally

Source: https://computing.llnl.gov/tutorials/parallel_comp/#ModelsShared

Distributed-memory Model



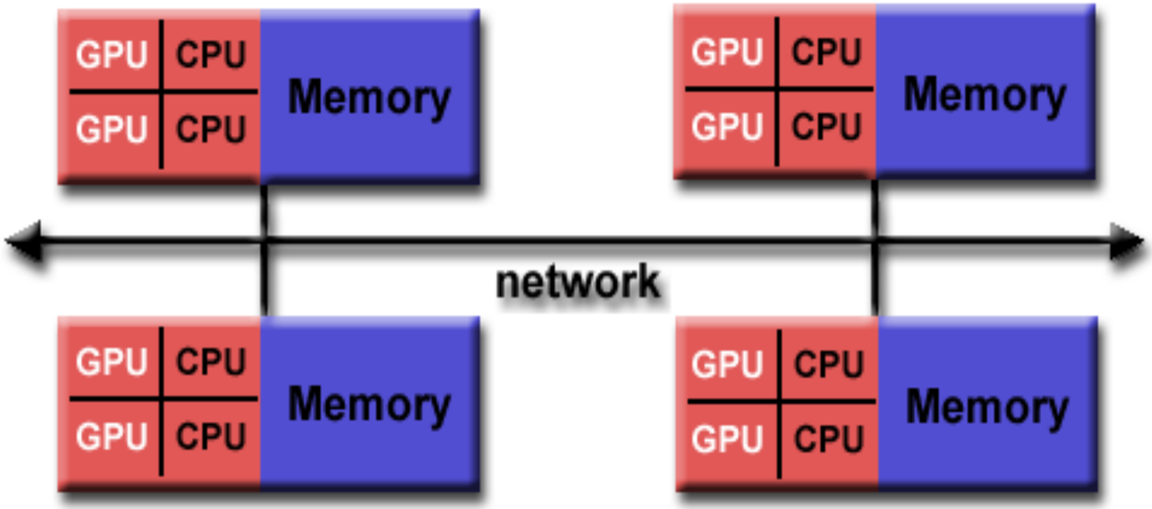
Programmers explicitly define how processors access other processor's memory

Advantage: scalable memory

Disadvantage: need to know parallel programming!

Source: https://computing.llnl.gov/tutorials/parallel_comp/#ModelsShared

Distributed-Shared Memory



Most large and fast computers now

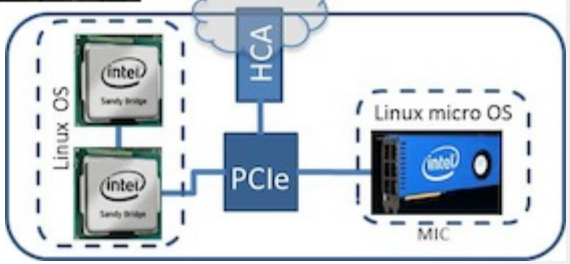
Shared memory machines connected to other shared memory machines

Source: https://computing.llnl.gov/tutorials/parallel_comp/#ModelsShared

Programming to Use Parallelism

- Parallelism across processors/threads - OpenMP

- Parallelism across multiple nodes - MPI



www.scan.co.uk

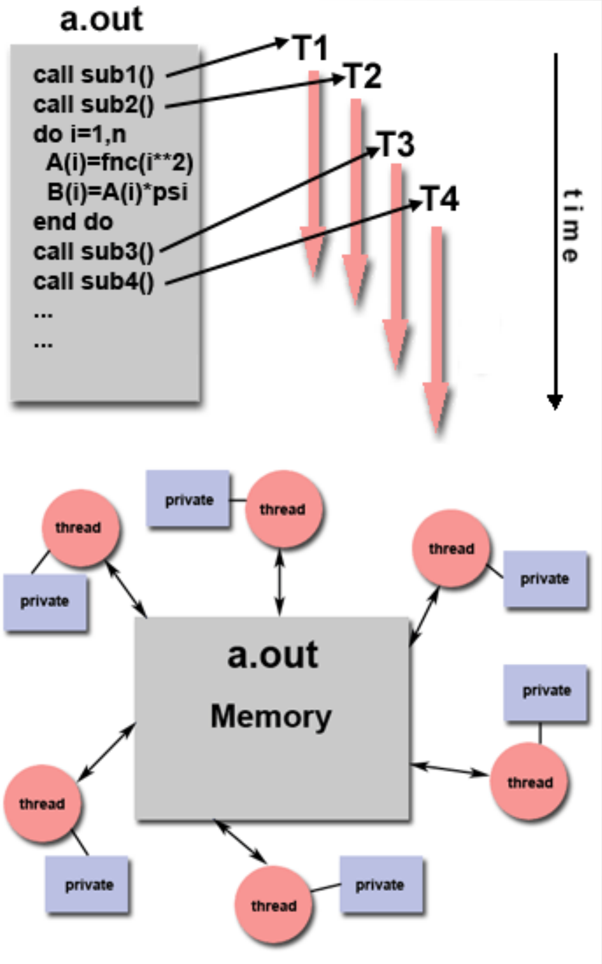
OpenMP

- 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 in

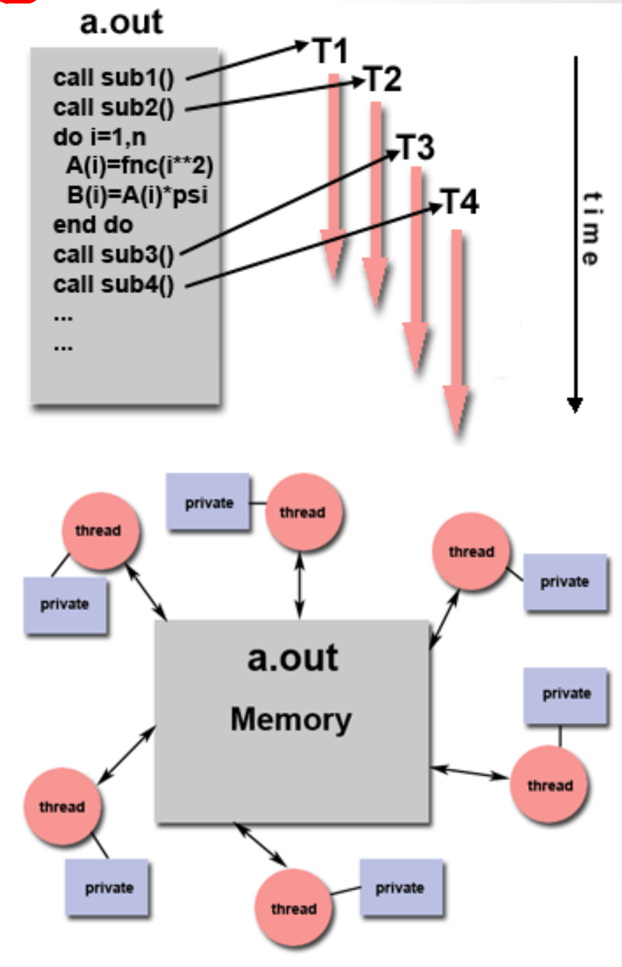


```
call sub1()
call sub2()
do i=1,n
  A(i)=fnc(i**2)
  B(i)=A(i)*psi
end do
call sub3()
call sub4()
...
...
```

Source: https://computing.llnl.gov/tutorials/parallel_comp/#ModelsShared

OpenMP Programming

- Implementing threaded code consists of
  - Library of subroutines called within parallel source code
  - Compiler directives
- The programmer is responsible for this
- OpenMP can be used to accomplish this



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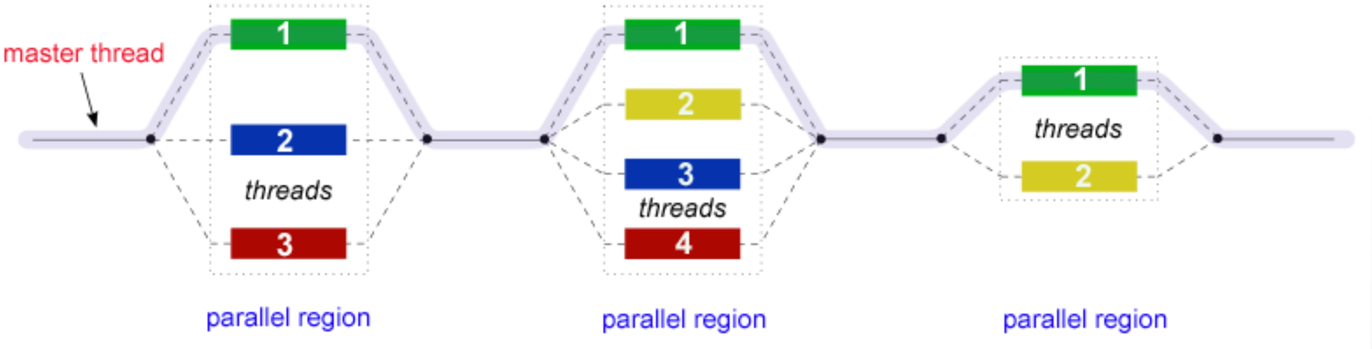
OpenMP – Fork/Join

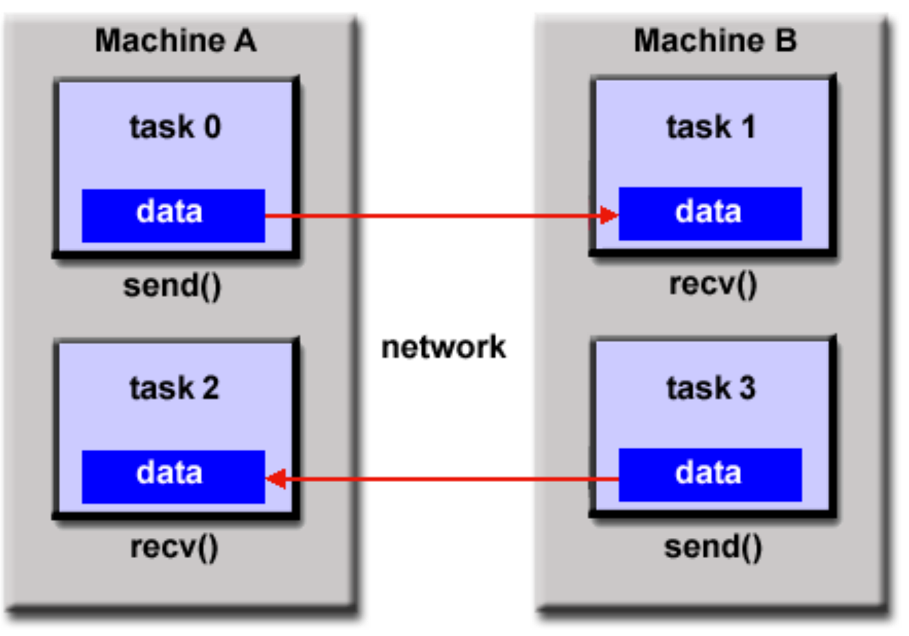
- OpenMP programs start with a single thread (master)
- Then Master creates a team of parallel "worker" threads (FORK)
- Statements in block are executed in parallel by every thread
- At end, all threads synchronize and join master thread



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/

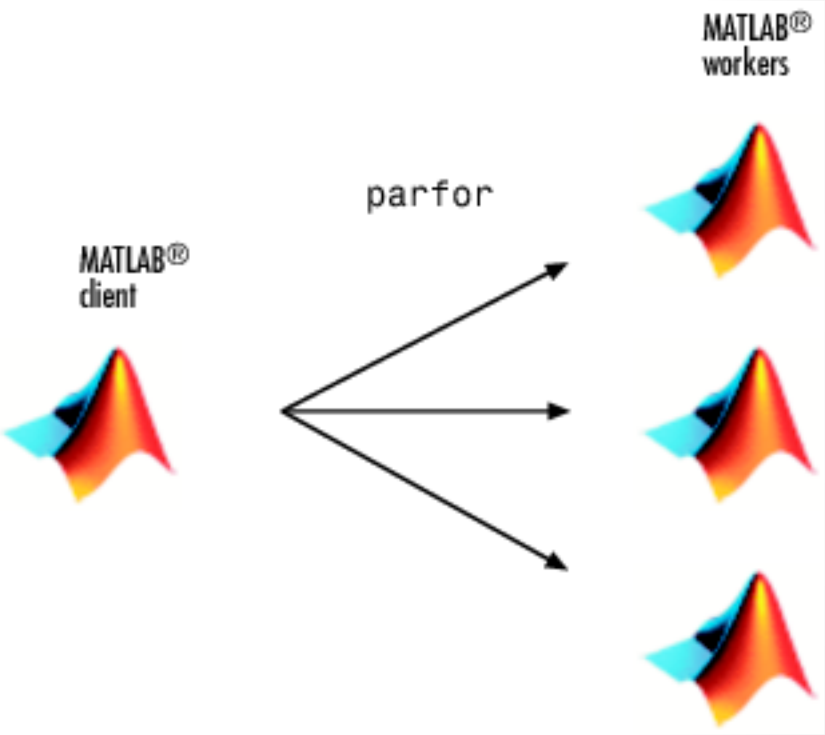
MPI or OpenMP?

- 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

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