Introduction to MPI

EAS 520
High Performance Scientific Computing

University of Massachusetts Dartmouth

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References

This presentation is almost an exact copy of Dartmouth College's Introduction to MPI tutorial. The link can be found in:

http://www.dartmouth.edu/~rc/classes/intro_mpi/

Changes from the original document are related to compilers and job submissions for UMass Dartmouth clusters.
Advantages of Parallel Programming

- Need to solve larger problems
  - more memory intensive
  - more computation
  - more data intensive

- Parallel programming provides
  - more CPU resources
  - more memory resources
  - solve problems that were not possible with serial program
  - solve problems more quickly
Parallel Computer Architectures

Two Basic Architectures

- Distributed Memory (ex. Compute cluster)
  - collection of nodes which have multiple cores
  - each node uses its own local memory
  - work together to solve a problem
  - communicate between nodes and cores via messages
  - nodes are networked together

- Shared Memory Computer
  - multiple cores
  - share a global memory space
  - cores can efficiently exchange/share data
Parallel Programming Models

- Directives-based parallel programming language
  - OpenMP (most widely used)
  - High Performance Fortran (HPF)
  - directives tell processor how to distribute data and work across the processors
  - directives appear as comments in the serial code
  - implemented on shared memory architectures

- Message Passing (MPI)
  - pass messages to send/receive data between processes
  - each process has its own local variables
  - can be used on either shared or distributed memory architectures
  - outgrowth of PVM software
Pros and Cons of MPI

- **Pros of MPI**
  - runs on either shared or distributed memory architectures
  - can be used on a wider range of problems than OpenMP
  - each process has its own local variables
  - distributed memory computers are less expensive than large shared memory computers

- **Cons of MPI**
  - requires more programming changes to go from serial to parallel version
  - can be harder to debug
  - performance is limited by the communication network between the nodes
Pros and Cons of OpenMP

• Pros of OpenMP
  • easier to program and debug than MPI
  • directives can be added incrementally - gradual parallelization
  • can still run the program as a serial code
  • serial code statements usually don't need modification
  • code is easier to understand and maybe more easily maintained

• Cons of OpenMP
  • can only be run in shared memory computers
  • requires a compiler that supports OpenMP
  • mostly used for loop parallelization
Parallel Programming Issues

- Goal is to reduce execution time
  - computation time
  - idle time - waiting for data from other processors
  - communication time - time the processors take to send and receive messages
- Load Balancing
  - divide the work equally among the available processors
- Minimizing Communication
  - reduce the number of messages passed
  - reduce amount of data passed in messages
- Where possible - overlap communication and computation
- Many problems scale well to only a limited number of processors
Problem Decomposition

Two kinds of decompositions:

- **Domain decomposition**
  - data divided into pieces of same size and mapped to different processors
  - processor works only on data assigned to it
  - communicates with other processors when necessary
  - examples of domain (data) decomposition
    - embarrassingly parallel applications (Monte Carlo simulations)
    - finite difference calculations
    - numerical integration

- **Functional decomposition**
  - used when pieces of data require different processing times
  - performance limited by the slowest process
  - program decomposed into a number of small tasks
  - tasks assigned to processors as they become available
  - implemented in a master/slave paradigm
  - examples of functional decomposition
    - surface reconstruction from a finite element mesh
    - searching images or data bases
What is MPI?

- MPI stands for Message Passing Interface
- library of functions (C/C++) or subroutines (Fortran)

**History**
- Early message passing Argonne's P4 and Oak Ridge PVM in 1980s
- MPI-1 completed in May 1994
- MPI-2 completed in 1998
  - parallel I/O
  - C++/F90 bindings
  - dynamic process management
- full MPI-2 implementations only recently
- MPI-2 features gradually added to MPI implementations
Differences between versions of MPI

- Examples of Different Implementations
  - MPICH - developed by Argonne Nationa Labs (freeware)
  - MPI/LAM - developed by Indiana, OSC, Notre Dame (freeware)
  - MPI/Pro - commercial product
  - Apple's X Grid
  - **OpenMPI** - MPI-2 compliant, thread safe

- Similarities in Various Implementations
  - source code compatibility (except parallel I/O)
  - programs should compile and run as is
  - support for heterogeneous parallel architectures
    - clusters, groups of workstations, SMP computers, grids

- Difference in Various Implementations
  - commands for compiling and linking
  - how to launch an MPI program
  - parallel I/O (from MPI-2)
  - debugging

- Programming Approaches
  - SPMD - Single Program Multiple Data (same program on all processors)
  - MPMD- Multiple Program Multiple Data (different programs on different processors)