Overview

- **Lengthy Computer Simulations**
  - Engineering Computational Design
  - Scientific High Performance Computing
  - Financial Computing
- **What is Parallel Computing**
  - Message Passing Interface
  - Open Source Solutions
- **What is Sun Grid Engine**
  - Resource manager
  - Costs
- **Why use either**
Simulations That Take Time

- Programs need resources to run
  - Large programs require more memory than others
  - Output of executed program can exceed available memory
  - Need to organize and efficiently use resources of computational clusters

- Large Networks of Nodes
  - System needs organization
  - Needs Queue for managing large number of jobs

Solution

Parallel computing

Using Sun Grid Engine
Implementation

- Create a computational cluster for use on parallel computing
- Install MPI onto Linux machines
- Install SGE onto cluster machines

Parallel Computing Structure

- Parallel computing environment
  - Work with multiple processor environment
  - Programmer's responsibility to write MPI code
- SGE manages resources efficiently
- Higher productivity when system allows tight control of distributed parallel processes
MPI Software Available

- Commercial versions
  - ChaMPion/Pro
  - Alpha Data MPI
  - Hitachi MPI
  - HP MPI
  - MPI/SX

- Open Source versions
  - MPICH
  - DISI
  - LAM/MPI
  - MPI/FM
  - OPEN_MP

Our Choices

- Use MPICH
  - Developed by Argonne National Laboratory
  - Readily available with instructions on how to compile
  - Open source
  - Can be used with various platforms, including RedHat Linux 9.0
  - Other newer commercial releases only worked on certain platforms
Configuring MPICH

• Working knowledge of Linux systems administration
  • Network Information Services
  • Network File Transfer
  • RSH
  • A bit of shell scripting
  “Rsync” for synchronizing installation

Configuring MPICH (continued)

• Compilation of code and configuration
  • Use Modified Configuration Script
    #!/bin/bash
    export RSHCOMMAND=rsh
    ./configure -comm=shared
    Note shared memory usage
Configuring MPICH (Continued)

• **Network Information Services**
  - Required for use with MPI and for parallel environment.
  - Synchronize user information between the nodes; sharing accounts over NIS. Highly efficient when large number of users.
  - Can also use Lightweight Directory Access Protocol or Synchronize passwords files. Usually done with few number of users.

Configuring MPICH (Continued)

• **Network File System**
  - Also a requirement for MPI operation and for parallel environment
  - Executable need only be present in one file system on one computer then be mounted to the other computers
  - NFS is slow, advance cluster used PVFS or Lustre for sharing files
  - Using Automount
    - Shares particular system file over nodes
    - Unlike Standard mount, Automount provides on demand form of mounting file system and then un-mounts automatically
Configuring MPICH (Continued)

- RSH – Remote SHell client
  - Managing nodes
  - Starts parallel processes
  - Modify /etc/hosts.equiv for rsh between computational nodes

Problems

- Could not kill the process easily
  - "ctrl+C" will end only one process, but since the program is running on multiple processor must kill each independently
  - Not very clean
Solution: Use SGE

- SGE will organize resources and also make execution and termination of programs more manageable in multi-user and multi-process environment
- Add simplicity to the user. SGE will take the file, find available resources and submit them, making the process of running parallel simulation more user friendly

Sun Grid Engine

- Software Available
  - OpenPBS
  - MauiME
  - Sun Grid Engine 5.3
- Used SunGrid Engine
  - Sun is most efficient
  - Forerunner in Grid Technology
Sun Grid Engine Configuration

Configure master node/administrator and then configure the computational
• Requires setting up queue for all of the computational nodes
• Specify number of processors in each node
• Need to specify parallel environment to MPI

SGE Configuration [tight] (continued)

• Modifying the startmpi.sh script
  – Must make sure that the mpi local file path is correct
  – Must also specify location of the SGE local files
• Modifying the stopmpi.sh script
  – Must make sure that the mpi local file path is correct
  – Must also specify location of the SGE local files
SGE Submission of Executable

- **Use mpi_submi.sh**
  - Name if file is specified in shell script
    - myjob=rkftwobody
  - Single line initiates MPI and submits the job to the queue system
    - $SGE_ROOT/mpi/watchMPI.sh &
    - $MPIR_HOME/bin/mpirun -np $NSLOTS -machinefile TMPDIR/machines $myjob

Observations

- Program ran slower as parallel simulation
  - Removal of pointer
  - Addition of many lines of MPI_Bcast
  - Shows that communication between processors slows things down

- MPI not best for System of Ordinary Differential Equations
Comparison of Code

• Manual use of MPI is tedious
  • Options to specify
    ▪ Machine file name
    ▪ Number of processors
  • Using submit script and SGE we can increase the efficiency of dealing with not only multiple processors, but also multiple processor JOBS
• Queue is great way to supervise the running jobs
Conclusion

- MPI is a powerful tool for producing scientific data from computer simulations
- Software that uses MPI
  - FLUENT (CFD)
  - GASP (Gas Dynamics)
  - AMBER (Molecular Dynamics)
  - NAMD (Molecular Dynamics)
- Areas of Research where MPI is used
  - Automotive design
  - Financial modeling
  - Computational physics
  - Computational Fluid Dynamics
  - Materials Research

Conclusion (continued)

- Sun Grid Engine does an exemplary job of managing the resources available in a computational cluster
- As more and more advances in parallel computing with multiple processor nodes and network parallel computing continues, development of Grid Engine technology will become essential in managing these resources
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