Hybrid MPI and OpenMP Parallel Programming

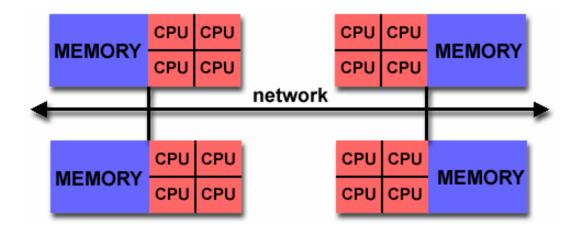
Jemmy Hu

SHARCNET HPTC Consultant July 8, 2015

Objectives

- difference between message passing and shared memory models (MPI, OpenMP)
- why or why not hybrid?
- a common model for utilizing both MPI and OpenMP approaches to parallel programming
- example hybrid code
- compile and execute hybrid code on SHARCNET clusters

Hybrid Distributed-Shared Memory Architecture



- Employ both shared and distributed memory architectures
- The shared memory component is usually a cache coherent SMP node. Processors on a given SMP node can address that node's memory as global.
- The distributed memory component is the networking of multiple SMP nodes. SMPs know only about their own memory not the memory on another SMP. Therefore, network communications are required to move data from one SMP to another.
- Current trends seem to indicate that this type of memory architecture will continue to prevail: more cpus per SMP node, less memory or bandwidth ratio per cpu.

MPI

- standard for distributed memory communications
- provides an explicit means to use message passing on distributed memory clusters
- specializes in packing and sending complex data structures over the network
- data goes to the process
- synchronization must be handled explicitly due to the nature of distributed memory

OpenMP

- a shared memory paradigm, implicit intra-node communication
- efficient utilization of shared memory SMP systems
- easy threaded programming, supported by most major compilers
- the process goes to the data, communication among threads is implicit

MPI vs. OpenMP

- Pure MPI Pros:

- Portable to distributed and shared memory machines.
- Scales beyond one node
- No data placement problem

– Pure MPI Cons:

- Explicit communication
- High latency, low bandwidth
- Difficult load balancing

- Pure OpenMP Pros:

- Easy to implement parallelism
- Implicit Communication
- Low latency, high bandwidth
- Dynamic load balancing

– Pure OpenMP Cons:

- Only on shared memory nodes/machines
- Scale within one node
- data placement problem

Why Hybrid: employ the best from both worlds

- MPI makes inter-node communication relatively easy
- MPI facilitates efficient inter-node scatters, reductions, and sending of complex data structures
- Since program state synchronization is done explicitly with messages, correctness issues are relatively easy to avoid

- OpenMP allows for high performance, and relatively straightforward, intra-node threading
- OpenMP provides an interface for the concurrent utilization of each SMP's shared memory, which is much more efficient that using message passing
- Program state synchronization is implicit on each SMP node, which eliminates much of the overhead associated with message passing

Overall Goal:

to reduce communication needs and memory consumption, or improve load balance

Why not Hybrid?

- OpenMP code performs worse than pure MPI code within node
 - all threads are idle except one while MPI communication
 - data placement, cache coherence
 - critical section for shared variables
- Possible waste of effort

A Common Hybrid Approach

- From sequential code, parallel with MPI first, then try to add OpenMP.
- From MPI code, add OpenMP
- From OpenMP code, treat as serial code.
- Simplest and least error-prone way is to use MPI outside parallel region, and allow only master thread to communicate between MPI tasks.
- Could use MPI inside parallel region with thread-safe MPI.

Hybrid – Program Model

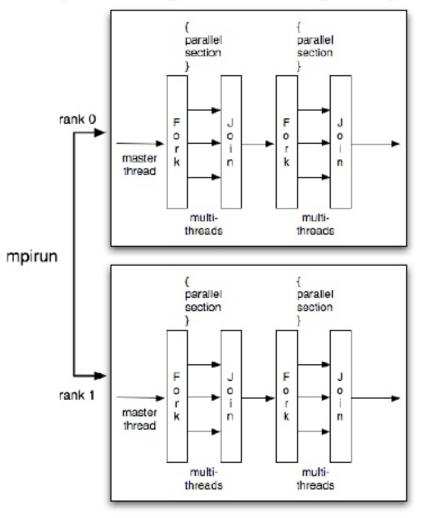
- Start with MPI initialization
- Create OMP parallel regions within MPI task (process).
 - Serial regions are the master thread or MPI task.
 - MPI rank is known to all threads
- Call MPI library in serial and parallel regions.
- Finalize MPI

Program hybrid

```
call MPI INIT (ierr)
call MPI COMM RANK (...)
call MPI_COMM_SIZE (...)
 ... some computation and MPI
communication
 ... start OpenMP within node
!$OMP PARALLEL DO PRIVATE(i)
!$OMP&
                    SHARED(n)
  do i=1,n
    ... computation
  enddo
 !$OMP END PARALLEL DO
 ... some computation and MPI
communication
call MPI FINALIZE (ierr)
end
```

Hybrid MPI+OpenMP Programming

Each MPI process spawns multiple OpenMP threads



MPI vs. MPI+OpenMP

work	P P P P		work	Pt t t t
Interconnection Network	P P P P		Interconnection Network	Pt t t t
	P P P P			Pt t t t
Inter	P P P P		Interc	Pt t t t
MPI		Node		MPI+OpenMP

16 cpus across 4 nodes 16 MPI processes 16 cpus across 4 nodes 1 MPI process and 4 threads per node

Example: Calculating π

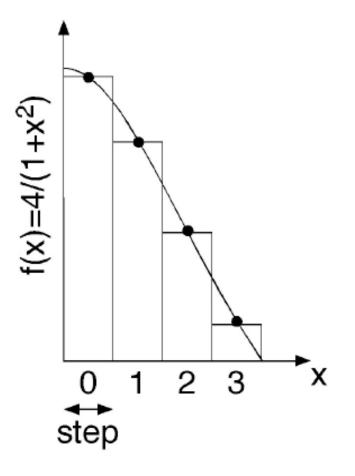
Numerical integration

$$\int_{0}^{1} \frac{4}{1+x^2} dx = \pi$$

- Discretization:
 - $\Delta = 1/N: \text{step} = 1/\text{NBIN}$ $x_i = (i+0.5)\Delta \ (i = 0, \dots, N-1)$

$$\sum_{i=0}^{N-1} \frac{4}{1+x_i^2} \Delta \cong \pi$$

```
#include <stdio.h>
#define NBIN 100000
void main() {
    int i; double step,x,sum=0.0,pi;
    step = 1.0/NBIN;
    for (i=0; i<NBIN; i++) {
        x = (i+0.5)*step;
        sum += 4.0/(1.0+x*x);}
    pi = sum*step;
    printf("PI = %f\n",pi);
}</pre>
```



pi – MPI version

#include <stdio.h>
#include <stdlib.h>
#include <mpi.h> /* MPI header file */
#define NUM_STEPS 10000000

```
int main(int argc, char *argv[]) {
    int nprocs;
    int myid;
    double start_time, end_time;
    int i;
    double x, pi;
    double sum = 0.0;
    double step = 1.0/(double) NUM_STEPS;
```

/* initialize for MPI */
MPI_Init(&argc, &argv); /* starts MPI */
/* get number of processes */
MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
/* get this process's number (ranges from 0 to nprocs - 1) */
MPI_Comm_rank(MPI_COMM_WORLD, &myid);

```
/* do computation */
  for (i=myid; i < NUM_STEPS; i += nprocs) { /* changed */
    x = (i+0.5)*step;
    sum = sum + 4.0/(1.0+x*x);
  }
                                      /* changed */
  sum = step * sum;
  MPI_Reduce(&sum, &pi, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);/* added */
/* print results */
  if (myid == 0) {
    printf("parallel program results with %d processes:\n", nprocs);
    printf("pi = %g (%17.15f)\n",pi, pi);
  }
  /* clean up for MPI */
```

MPI_Finalize();

return 0;

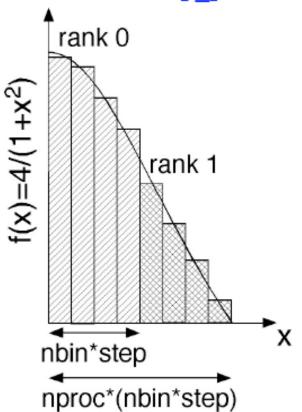
}

OpenMP, **reduction** clause

```
#include <stdio.h>
#include <omp.h>
#define NBIN 100000
int main(int argc, char *argv[ ]) {
  int I, nthreads;
  double x, pi;
  double sum = 0.0;
  double step = 1.0/(double) NUM_STEPS;
  /* do computation -- using all available threads */
  #pragma omp parallel
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    #pragma omp for private(x) reduction(+:sum) schedule(runtime)
    for (i=0; i < NUM_STEPS; ++i) {
       x = (i+0.5)*step;
       sum = sum + 4.0/(1.0+x*x);
    #pragma omp master
       pi = step * sum;
  printf("PI = %f\n",pi);
```

MPI+OpenMP Calculation of π

- Each MPI process integrates over a range of width 1/nproc, as a discrete sum of nbin bins each of width step
- Within each MPI process, nthreads OpenMP threads perform part of the sum as in omp_pi.c



MPI_OpenMP version

#include <stdio.h> #include <stdlib.h> #include <mpi.h> /* MPI header file */ #include <omp.h> **I*** OpenMP header file */ #define NUM STEPS 10000000 #define MAX THREADS 4 int main(int argc, char *argv[]) { int nprocs, myid; int tid, nthreads, nbin; double start time, end time; double pi, Psum=0.0, sum[MAX_THREADS]={0.0}; double step = 1.0/(double) NUM STEPS; /* initialize for MPI */ MPI_Init(&argc, &argv); /* starts MPI */ /* get number of processes */

MPI_Comm_size(MPI_COMM_WORLD, &nprocs); /* get this process's number (ranges from 0 to nprocs - 1) */ MPI_Comm_rank(MPI_COMM_WORLD, &myid);

nbin= NUM_STEPS/nprocs;

```
#pragma omp parallel private(tid)
```

```
int i;
    double x:
    nthreads=omp_get_num_threads();
    tid=omp get thread num();
    for (i=nbin*myid+tid; i < nbin*(myid+1); i+= nthreads) { /* changed*/
      x = (i+0.5)*step;
      sum[tid] += 4.0/(1.0+x*x);
    }
for(tid=0; tid<nthreads; tid++) /*sum by each mpi process*/
    Psum += sum[tid]*step;
```

MPI_Reduce(&Psum, &pi, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);/* added */

```
if (myid == 0) {
  printf("parallel program results with %d processes:\n", nprocs);
  printf("pi = %g (%17.15f)\n",pi, pi);
MPI Finalize();
```

```
return 0;
```

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}

Compile and Run

- Compile (default intel compilers on SHARCNT systems)
 mpicc -o pi-mpi pi-mpi.c
 cc -openmp -o pi-omp pi-omp.c
 mpicc -openmp -o pi-hybrid pi-hybrid.c
- Run (sqsub)

sqsub -q mpi -n 8 --ppn=4 -r 10m -o pi-mpi.log ./pi-mpi sqsub -q threaded -n 8 -r 10m -o pi-omp.log ./pi-omp sqsub -q mpi -n 8 --ppn=1 --tpp=4 -r 10m -o pi-hybrid.log ./pi-hybrid

Example codes and results are in: /home/jemmyhu/CES706/Hybrid/pi/

Results

MPI MPI uses 8 processes: pi = 3.14159 (3.141592653589828)

- OpenMP
 OpenMP uses 8 threads:
 pi = 3.14159 (3.141592653589882)
- Hybrid mpi process 0 uses 4 threads mpi process 1 uses 4 threads mpi process 1 sum is 1.287 (1.287002217586605) mpi process 0 sum is 1.85459 (1.854590436003132) Total MPI processes are 2 pi = 3.14159 (3.141592653589738)

Summary

- Computer systems in High-performance computing (HPC) feature a hierarchical hardware design (multi-core nodes connected via a network)
- OpenMP can take advantage of shared memory to reduce communication overhead
- Pure OpenMP performs better than pure MPI within node is a necessity to have hybrid code better than pure MPI across node.
- Whether the hybrid code performs better than MPI code depends on whether the communication advantage outcomes the thread overhead, etc. or not.
- There are more positive experiences of developing hybrid MPI/OpenMP parallel paradigms now. It's encouraging to adopt hybrid paradigm in your own application.

References

- http://openmp.org/sc13/HybridPP_Slides.pdf
- https://www.cct.lsu.edu/~estrabd/intro-hybrid-mpi-openmp.pdf
- http://www.cac.cornell.edu/education/Training/parallelMay2011/Hybrid_T alk-110524.pdf