Hybrid MPI and OpenMP Parallel Programming

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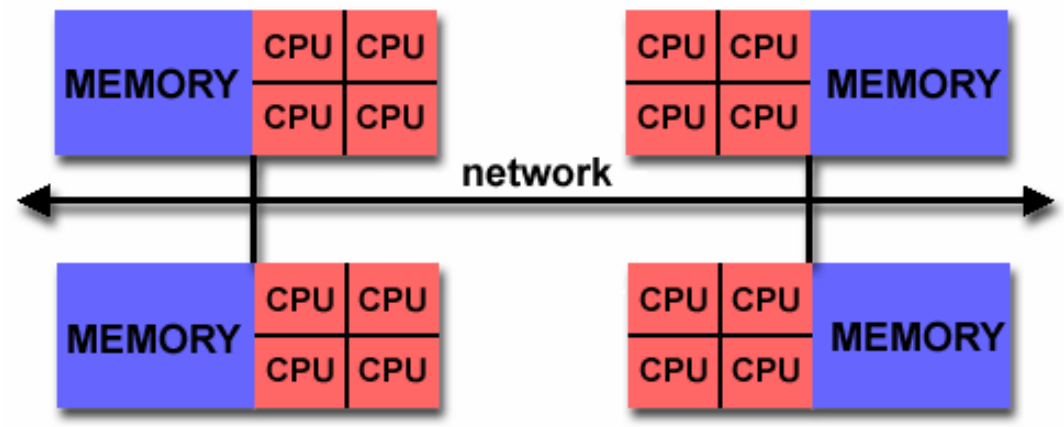
Objectives

- difference between message passing (MPI) and shared memory (OpenMP) approaches
- why or why not hybrid?
- a straightforward approach to combine both MPI and OpenMP in parallel programming
- example hybrid code, compile and execute hybrid code on SHARCNET clusters

Hybrid Distributed-Shared Memory Architecture



- Computer cluster basics, 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.

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 node or machine
  - Scale within one node
  - data placement problem

Why Hybrid: employ the best from both approaches

- 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.

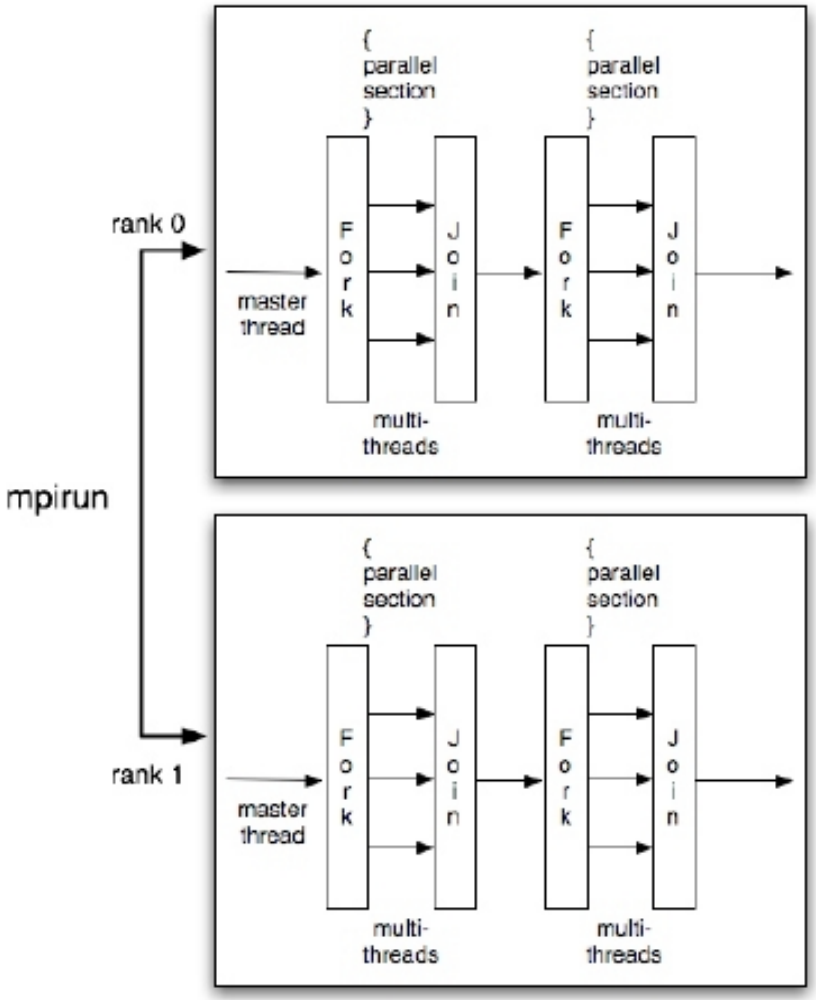
Hybrid – Program Model

- 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

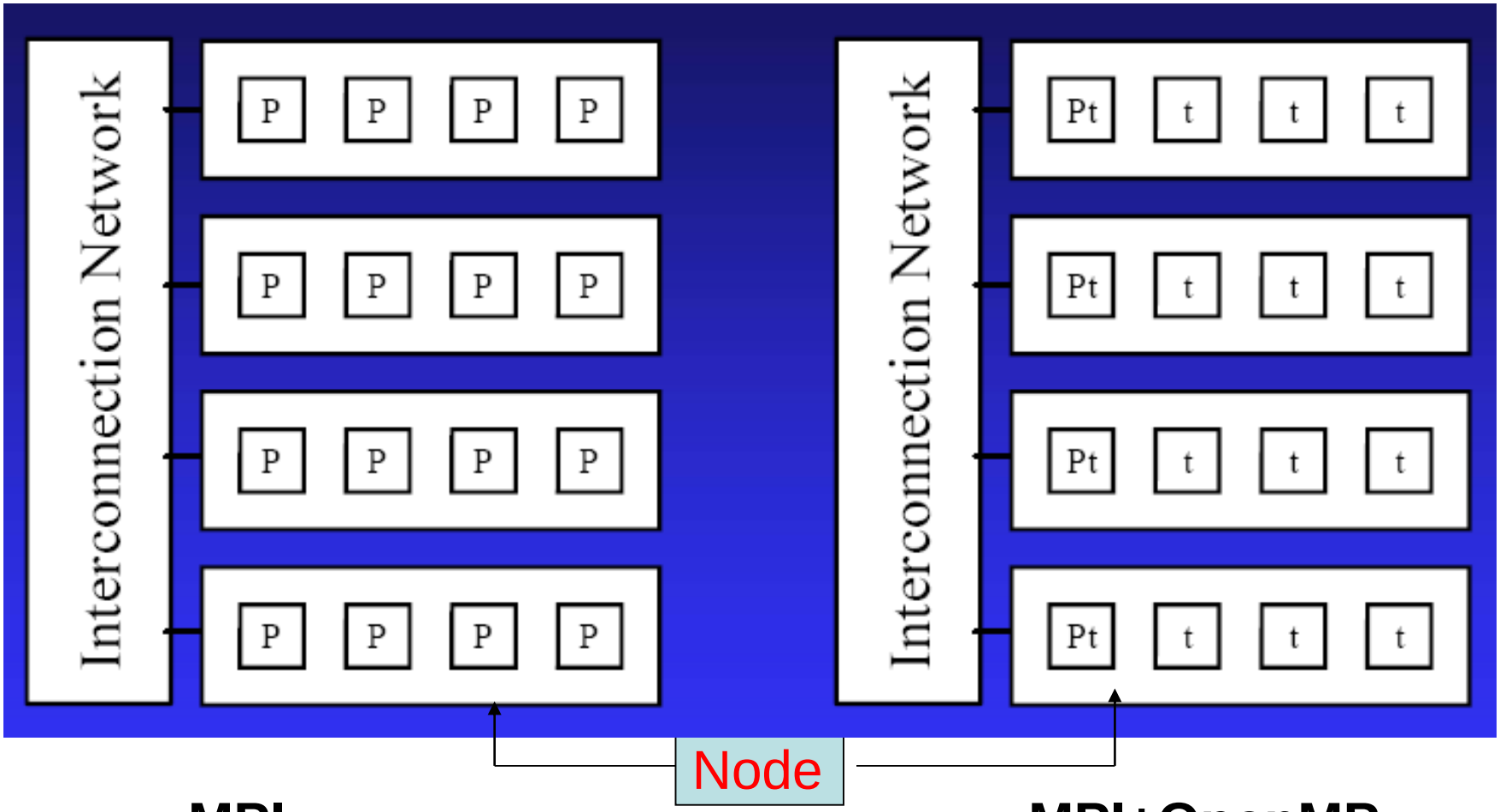
```
Program hybrid
call MPI_INIT (ierr)
call MPI_COMM_RANK (…)
call MPI_COMM_SIZE (…)
 …  some computation and MPI communication
 …  start OpenMP within node
!$OMP PARALLEL DO PRIVATE(i)
!$OMP&                    SHARED(n)
   do i=1,n
      … computation
   enddo
 !$OMP END PARALLEL DO
 …  some computation and MPI communication
call MPI_FINALIZE (ierr)
end
```

Hybrid MPI+OpenMP Programming

Each MPI process spawns multiple OpenMP threads



MPI vs. MPI+OpenMP



MPI

16 cpus across 4 nodes
4 MPI processes per node

MPI+OpenMP

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

Example: Calculating π

- **Numerical integration**

$$\int_0^1 \frac{4}{1+x^2}\,dx = \pi$$

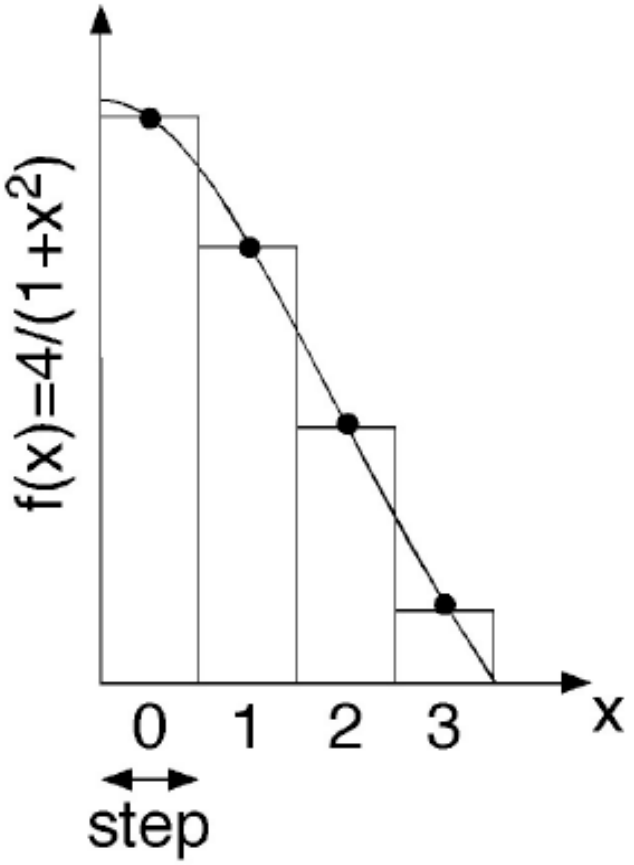
- **Discretization:**

$\Delta = 1/N$: `step = 1/NBIN`

$x_i = (i+0.5)\Delta$ $(i = 0,\ldots,N\text{-}1)$

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

```
#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);
}
```



pi – MPI version

```
#include <stdio.h>
#include <stdlib.h>
#include <mpi.h>              /* MPI header file */
#define NUM_STEPS 100000000

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);
    }
    sum = step * sum;                               /* changed */
    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;
}
```

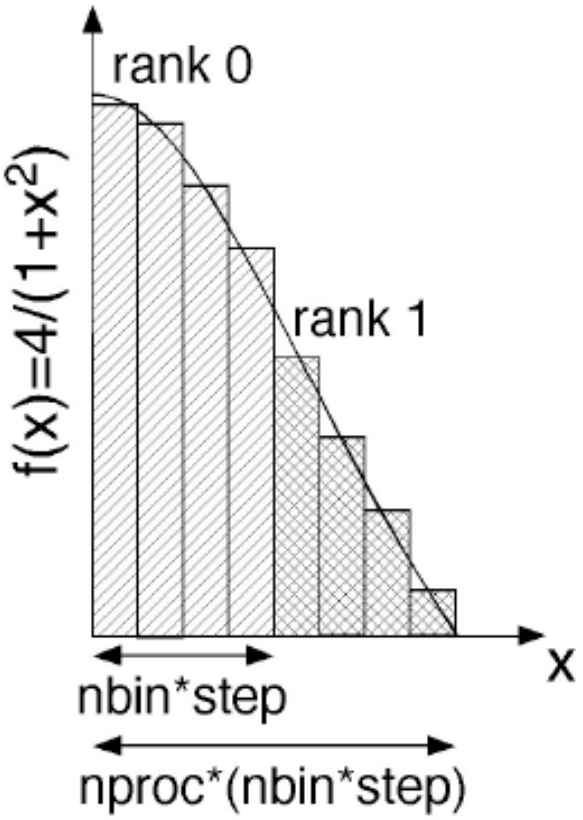
OpenMP, reduction clause

```
#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
   {
      #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>              /* OpenMP header file */
#define NUM_STEPS 100000000
#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;
}
```

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 (1.28700221758660 5)
  mpi process 0 sum is 1.85459 (1.85459043600313 2)
  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_Talk-110524.pdf