Hybrid Programming with MPI and OpenMP

B. Estrade

<estrabd@lsu.edu>

Objectives

- understand the difference between message passing and shared memory models;
- learn of basic models for utilizing both message passing and shared memory approaches to parallel programming;
- learn how to program a basic hybrid program and execute it on local resources;
- learn of basic issues regarding the *hybridization* of existing serial, all-MPI, or all-OpenMP codes;

What is *Hybridization*?

- the use of inherently different models of programming in a complimentary manner, in order to achieve some benefit not possible otherwise;
- a way to use different models of parallelization in a way that takes advantage of the good points of each;

How Does Hybridization Help?

- introducing MPI into OpenMP applications can help scale across multiple SMP nodes;
- introducing OpenMP into MPI applications can help make more efficient use of the shared memory on SMP nodes, thus mitigating the need for explicit intra-node communication;
- introducing MPI *and* OpenMP during the design/coding of a *new* application can help maximize efficiency, performance, and scaling;

When Does Hybridization Make Sense?

- when one wants to scale a shared memory OpenMP application for use on multiple SMP nodes in a cluster;
- when one wants to reduce an MPI application's sensitivity to becoming communication bound;
- when one is designing a parallel program from the very beginning;

Hybridization Using MPI and OpenMP

- facilitates cooperative shared memory (OpenMP) programming across clustered SMP nodes;
- MPI facilitates communication among SMP nodes;
- OpenMP manages the workload on each SMP node;
- MPI and OpenMP are used in tandem to manage the overall concurrency of the application;

MPI

- provides a familiar and explicit means to use message passing on distributed memory clusters;
- has implementations on many architectures and topologies;
- is the defacto standard for distributed memory communications;
- requires that program state synchronization must be handled explicitly due to the nature of distributed memory;
- data goes *to* the process;
- program correctness is an issue, but not big compared to those inherent to OpenMP;

OpenMP

- allows for implicit intra-node communication, which is a *shared memory* paradigm;
- provides for efficient utilization of shared memory SMP systems;
- facilitates relatively easy threaded programming;
- does not incur the overhead of message passing, since communication among threads is implicit;
- is the defacto standard, and is supported by most major compilers (Intel, IBM, gcc, etc);
- the process goes *to* the data
- program correctness is an issue since all threads can update shared memory locations;

The Best From Both Worlds

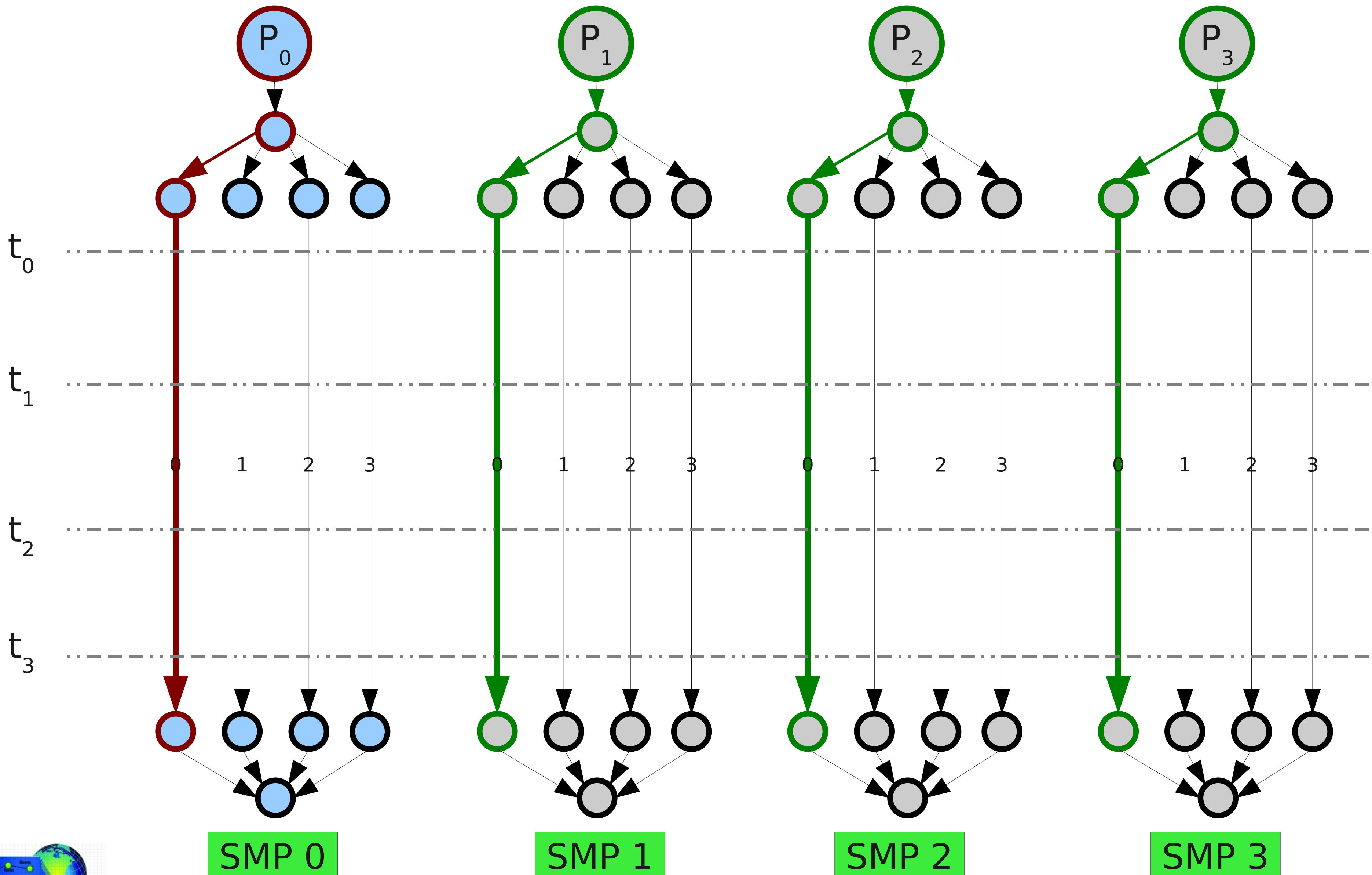
- MPI allows for inter-node communication;
- MPI facilitates efficient inter-node reductions and sending of complex data structures;
- Program state synchronization is explicit;

- OpenMP allows for high performance intra-node threading;
- OpenMP provides an interface for the concurrent utilization of each SMP's shared memory;
- Program state synchronization is implicit;

A Common Execution Scenario

1) a single MPI process is launched on each SMP node in the cluster;
2) each process spawns N threads on each SMP node;
3) at some global sync point, the *master thread* on each SMP communicate with one another;
4) the threads belonging to each process continue until another sync point or completion;

What Does This Scenario Look Like?



Basic Hybrid "*Stub*"

```c
#include <omp.h>
#include "mpi.h"
#include <stdio.h>
#define _NUM_THREADS 4

/*  Each MPI process spawns a distinct OpenMP
 *  master thread; so limit the number of MPI
 *  processes to one per node
 */

int main (int argc, char *argv[]) {
  int p,my_rank,c;

  /* set number of threads to spawn */
  omp_set_num_threads(_NUM_THREADS);

  /* initialize MPI stuff */
  MPI_Init(&argc, &argv);
  MPI_Comm_size(MPI_COMM_WORLD,&p);
  MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);

  /* the following is a parallel OpenMP
   * executed by each MPI process
   */

  #pragma omp parallel reduction(+:c)
  {
    c = omp_get_num_threads();
  }

  /* expect a number to get printed for each MPI process */
  printf("%d\n",c);
  /* finalize MPI */
  MPI_Finalize();
  return 0;
}
```

Compiling

- IBM p5 575s:
  - mpcc_r, mpCC_r, mpxlf_r, mpxlf90_r, mpxlf95_r

bash

```
%mpcc_r -qsmp=omp test.c
%OMP_NUM_THREADS=4 poe ./a.out -rmpool 1 -nodes 1 -procs 2
```

- x86 Clusters:
  - mpicc, mpiCC, mpicxx, mpif77, mpif90

bash

```
%mpicc -openmp test.c
```

PBS (Linux)

```
#!/bin/bash
#PBS -q checkpt
#PBS -A your_allocation
#PBS -l nodes=4:ppn=8
#PBS -l cput=2:00:00
#PBS -l walltime=2:00:00
#PBS -o /work/yourdir/myoutput2
#PBS -j oe # merge stdout and stderr
#PBS -N myhybridapp
export WORK_DIR=/work/yourdir
# create a new machinefile file which only contains unique nodes
cat $PBS_NODEFILE | uniq > hostfile
# get number of MPI processes and create proper machinefile
export NPROCS=`wc -l hostfile | gawk '//{print $1}'`
ulimit -s hard
# setting number of OpenMP threads
cd $WORK_DIR
export OMP_NUM_THREADS=8
mpirun -machinefile ./hostfile -np $NPROCS ./hybrid.x
```

**Shangli Ou, https://docs.loni.org/wiki/Running_a_MPI/OpenMP_hybrid_Job*

LoadLeveler (AIX)

```
#!/usr/bin/ksh
# @ job_type = parallel
# @ input = /dev/null
# @ output = /work/default/ou/flower/output/out.std
# @ error = /work/default/ou/flower/output/out.err
# @ initialdir = /work/default/ou/flower/run
# @ notify_user = ou@baton.phys.lsu.edu
# @ class = checkpt
# @ notification = always
# @ checkpoint = no
# @ restart = no
# @ wall_clock_limit = 10:00:00
# @ node = 4,4
# @ network.MPI = sn_single,shared,US
# @ requirements = ( Arch == "Power5" )
# @ node_usage = not_shared
# @ tasks_per_node = 1
# @ environment=MP_SHARED_MEMORY=yes; COPY_ALL
# @ queue
# the following is run as a shell script
export OMP_NUM_THREADS=8
mpirun -NP 4 ./hybrid.x
```

**Shangli Ou, https://docs.loni.org/wiki/Running_a_MPI/OpenMP_hybrid_Job*

Retro-fitting MPI Apps With OpenMP

- involves most commonly the work-sharing of simple looks;
- is the easiest of the two “retro-fit” options because the program state synchronization is already handled in an explicit way; adding OpenMP directives admits the need for implicit state synchronization, which is *easier*;
- benefits depend on how many simple loops may be work-shared; otherwise, the effects tend towards using *fewer* MPI processes;
- the number of MPI processes per SMP node will depend on how many threads one wants to use per process;
- most beneficial for communication bound applications, since it reduces the number of MPI processes needing to communicate; however, CPU processor utilization on each node becomes an issue;

Information Technology Services

Retro-fitting OpenMP Apps With MPI

- not as straightforward as retro-fitting an MPI application with OpenMP because global program state must be explicitly handled with MPI;
- requires careful thought about how each process will communicate amongst one another;
- may require a complete reformulation of the parallelization, with a need to possibly redesign it from the ground up;
- successful retro-fitting of OpenMP applications with MPI will usually yield greater improvement in performance and scaling, presumably because the original shared memory program takes great advantage of the entire SMP node;

General Retro-fitting Guidelines

- adding OpenMP to MPI applications is fairly straightforward because the distributed memory of multiple SMP nodes has already been handled;
- MPI applications that are communication bound *and* have <u>many</u> simple loops that may be work-shared will benefit greatly due to the reduction in need for communication among SMP nodes;
- adding MPI to OpenMP applications is not very straightforward, but will yield better scaling and higher performing application in many cases;
- OpenMP applications handle program state implicitly, thus introducing MPI requires the explicit handling of program state – which is not easy do “bolt on” after the fact;
- in general, adding MPI to OpenMP applications should initiate a redesign of the application from the ground up in order to handle the need for explicit synchronizations across distribute memory;
- fortunately, much of the old OpenMP application code may be reused;

Designing Hybrid Apps From Scratch

- redesigning an application, whether originally using OpenMP or MPI, is the ideal situation; although, this is not always possible or desired;
- benefits are greatest when considering the introduction of MPI into shared memory programs;
- great care should be taken to find the right balance of MPI computation and OpenMP “work”; it is the shared memory parts that do the work; MPI is used to simply keep everyone on the same page;
- Prioritized list of some considerations
  i. the ratio of communication among nodes and time spend keeping the processors on a single node should be minimized in order to maximize scaling;
  ii. the shared memory computations on each node should utilize as many threads as possible during the computation parts;
  iii. MPI is most efficient at communicating a small number of larger data structures; therefore, many small messages will introduce a communication overhead unnecessarily;

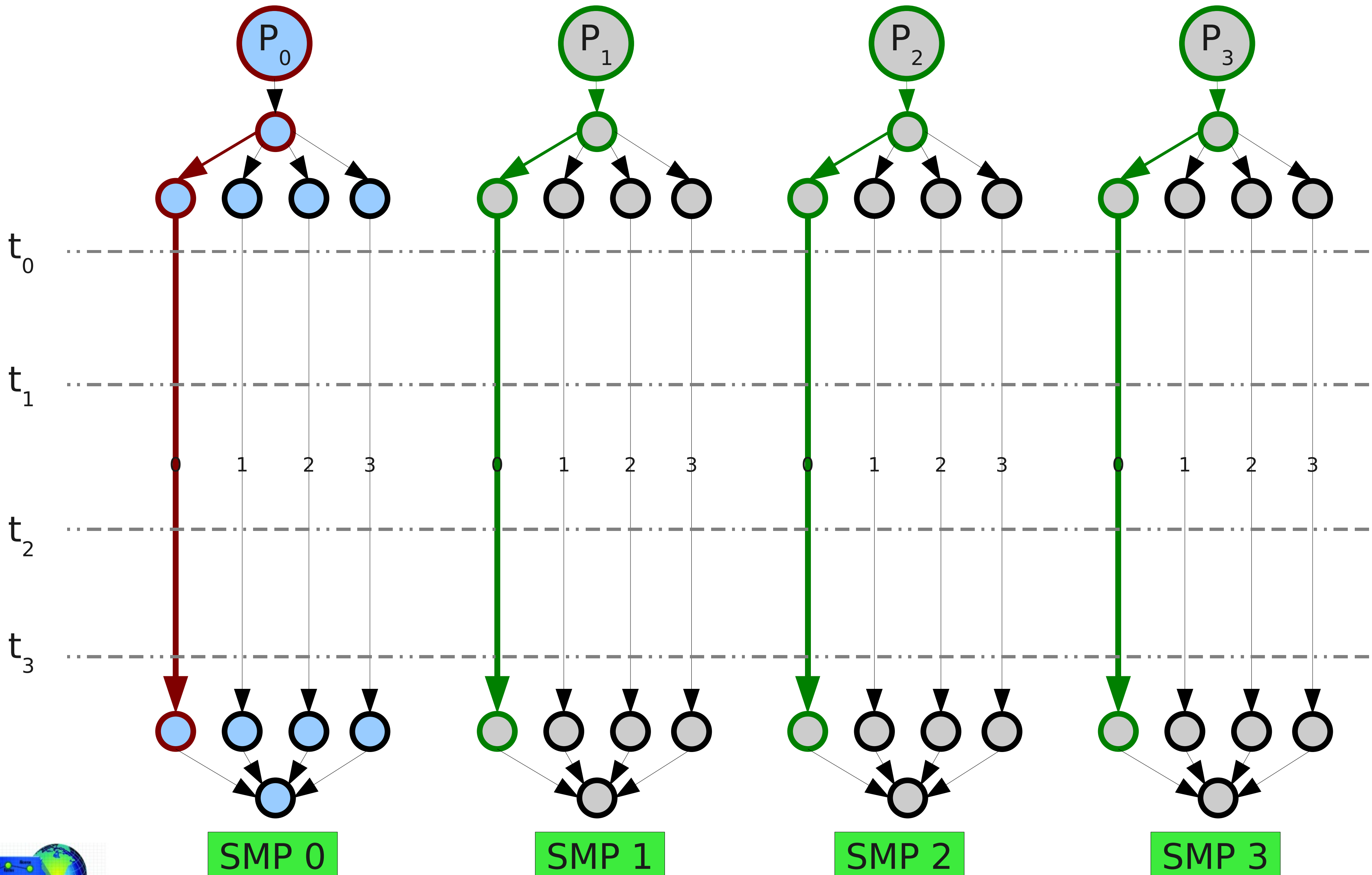
Example Concept 1

ROOT MPI Process Controls All Communications

- most straightforward paradigm;
- maps one MPI process to one SMP node;
- each MPI process spawns a fixed number of shared memory threads;
- communication among MPI processes is handled by the *main MPI process* only, at fixed predetermined intervals;
- allows for tight control of all communications;

```
// do only if master thread, else wait
#pragma omp master
{ if (0 == my_rank)
     // some MPI_ call as ROOT process
  else
     // some MPI_ call as non-ROOT process
}
// end of omp master
```

What Does Example 1 Look Like?



Example 1 Code Stub

```
#include <omp.h>
#include "mpi.h"
#include <stdio.h>

#define _NUM_THREADS 4

int main (int argc, char *argv[]) {
  int p,my_rank,c;

  /* set number of threads to spawn */
  omp_set_num_threads(_NUM_THREADS);

  /* initialize MPI stuff */
  MPI_Init(&argc, &argv);
  MPI_Comm_size(MPI_COMM_WORLD,&p);
  MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);

  /* the following is a parallel OpenMP
   * executed by each MPI process
   */
  #pragma omp parallel reduction(+:c)
  {
    #pragma omp master
    {
      if ( 0 == my_rank)
        // some MPI_ call as ROOT process
        c = 1;
      else
        // some MPI_ call as non-ROOT process
        c = 2
    }
  }
  /* expect a number to get printed for each MPI process */
  printf("%d\n",c);
  /* finalize MPI */
  MPI_Finalize();
  return 0;
}
```

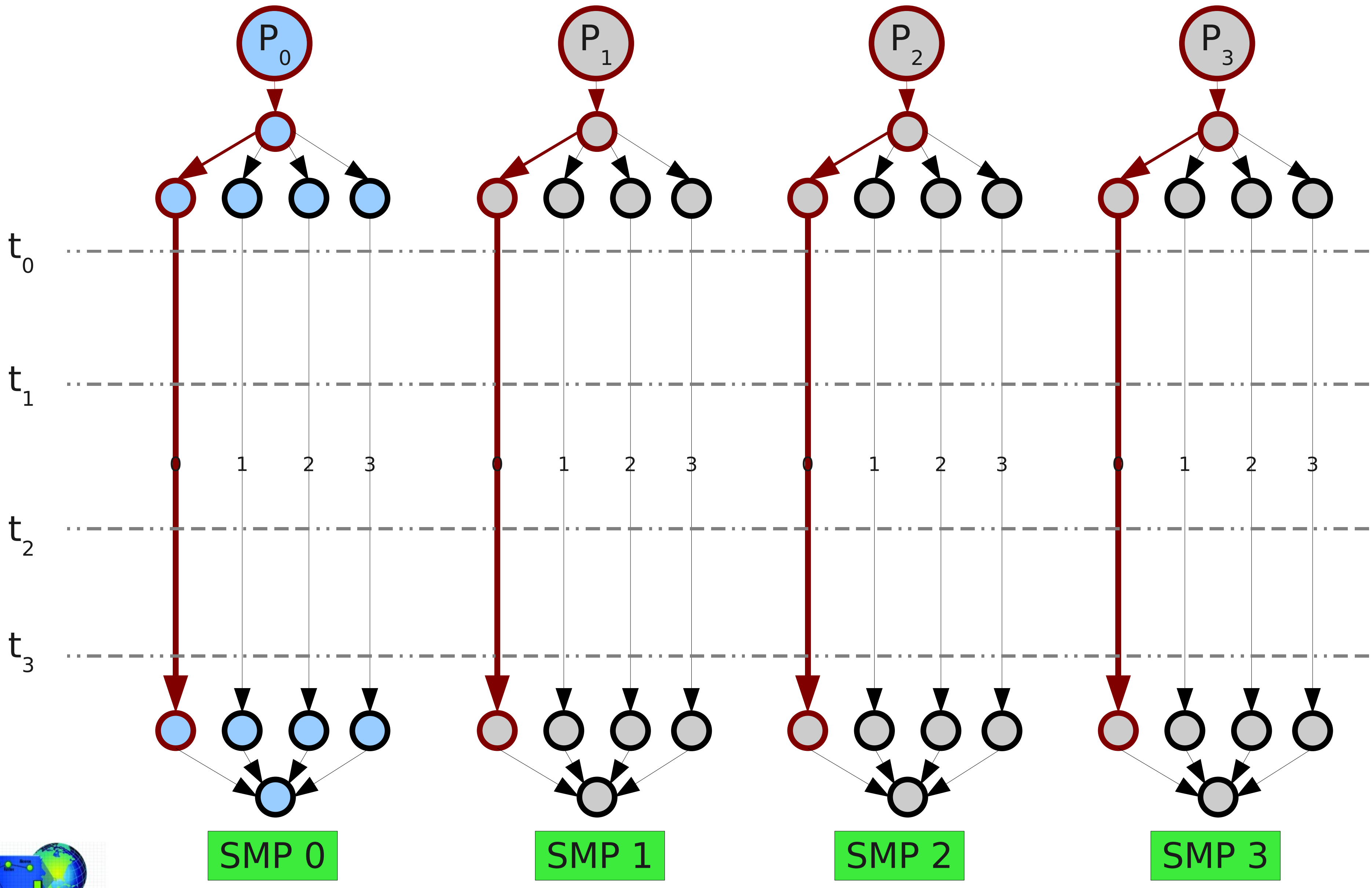
Example Concept 2

Master OpenMP Thread Controls All Communications

- each MPI process uses its own OpenMP *master thread* (1 per SMP node) to communicate;
- allows for more *asynchronous* communications;
- not nearly as rigid as example 1;
- more care needs to be taken to ensure efficient communications, but the flexibility may yield efficiencies elsewhere;

```
// do only if master thread, else wait
#pragma omp master
{
 // some MPI_ call as an MPI process
}
// end of omp master
```

What Does a Example 2 Look Like?



Example 2 Code Stub

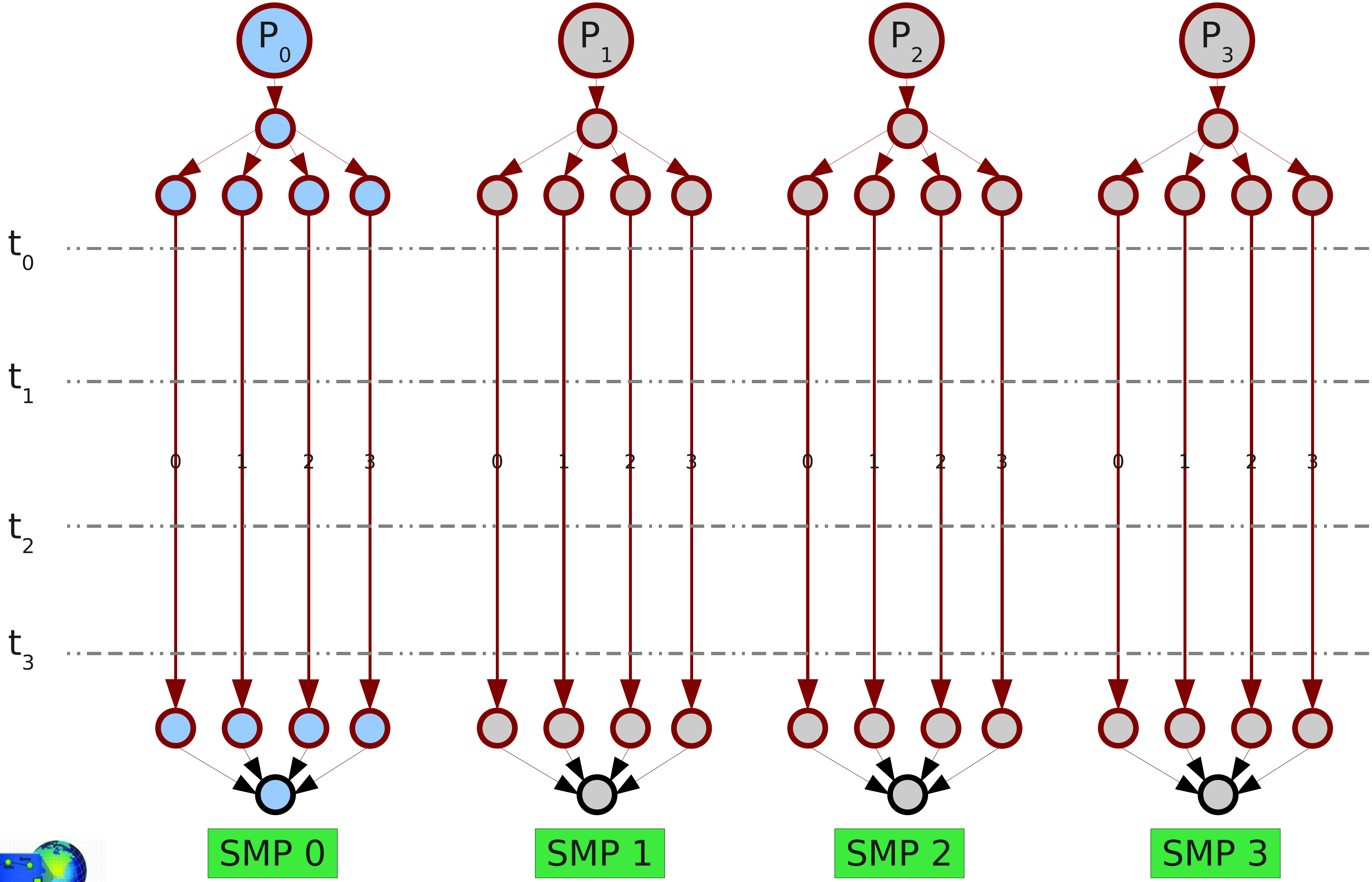
```
#include <omp.h>
#include "mpi.h"
#include <stdio.h>
#define _NUM_THREADS 4

int main (int argc, char *argv[]) {
  int p,my_rank;
  int c = 0;
  /* set number of threads to spawn */
  omp_set_num_threads(_NUM_THREADS);

  /* initialize MPI stuff */
  MPI_Init(&argc, &argv);
  MPI_Comm_size(MPI_COMM_WORLD,&p);
  MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);

  /* the following is a parallel OpenMP
   * executed by each MPI process
   */
  #pragma omp parallel
  {
    #pragma omp master
    {
      // some MPI_ call as an MPI process
      c = 1;
    }
  }

  /* expect a number to get printed for each MPI process */
  printf("%d\n",c);
  /* finalize MPI */
  MPI_Finalize();
  return 0;
}
```

Example Concept 3

All OpenMP Threads May Use MPI Calls

- this is by far the most flexible communication scheme;
- enables true *distributed* behavior similar to that which is possible using pure MPI;
- the greatest risk of inefficiencies are contained using this approach;
- great care must be made in explicitly accounting for which thread of which MPI process is communication;
- requires a addressing scheme that denotes the *tuple* of which MPI processes participating in communication and which thread of the MPI process is involved; e.g., *<my_rank,omp_thread_id>;*
- *neither MPI nor OpenMP have built-in facilities for tracking this;*
- *critical sections, potentially named, may be utilized for some level of control and correctness;*

What Does Example 3 Look Like?



Example 3 Code Stub

```
#include <omp.h>
#include "mpi.h"
#include <stdio.h>
#define _NUM_THREADS 4

int main (int argc, char *argv[]) {
  int p,my_rank;
  int c = 0;
  /* set number of threads to spawn */
  omp_set_num_threads(_NUM_THREADS);

  /* initialize MPI stuff */
  MPI_Init(&argc, &argv);
  MPI_Comm_size(MPI_COMM_WORLD,&p);
  MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);

  /* the following is a parallel OpenMP
   * executed by each MPI process
   */
  #pragma omp parallel
  {
    #pragma omp critical /* not required */
    {
      // some MPI_ call as an MPI process
      c = 1;
    }
  }

  /* expect a number to get printed for each MPI process */
  printf("%d\n",c);
  /* finalize MPI */
  MPI_Finalize();
  return 0;
}
```

Comparison of Examples

1.

```
// do only if master thread, else wait
#pragma omp master
{ if (0 == my_rank)
    // some MPI_ call as ROOT process
  else
    // some MPI_ call as non-ROOT process
}
// end of omp master
```

2.

```
// do only if master thread, else wait
#pragma omp master
{
 // some MPI_ call as an MPI process
}
// end of omp master
```

3.

```
// each thread makes a call; can utilize
// critical sections for some control
#pragma omp critical
{
 // some MPI_ call as an MPI process
}
```

General Design Guidelines

- the ratio of communications to time spent computing on each SMP node should be *minimized* in order to improve the scaling characteristics of the hybrid code;
- introducing OpenMP into MPI is much easier, but the benefits are not as great or likely as vice-versa;
- the greatest benefits are seen when an application is redesigned from scratch; fortunately, much of the existing code is salvageable;
- there are many, many communication paradigms that may be employed; we covered just 3; it is prudent to investigate all options;
- great care must be taken to ensure program correctness and efficient communications;

Summary

- simply compiling MPI and OpenMP into the same program is easy;
- adding OpenMP to an MPI app is easy, but the benefits may not be that great (but give it a shot!);
- adding MPI to an OpenMP app is hard, but usually worth it;
- designing a hybrid application from scratch is ideal, and allows one to best balance the strengths of both MPI and OpenMP to create an optimal performing and scaling application;
- there are a lot of schemes that incorporate both shared and distributed memory, so it is worth the time to investigate them wrt the intended applications;

Additional Resources

- http://docs.loni.org
  - *https://docs.loni.org/wiki/Running_a_MPI/OpenMP_hybrid_Job*
- sys-help@loni.org
- otrs@loni.org