OpenMP* / MPI Hybrid Programming

Agenda

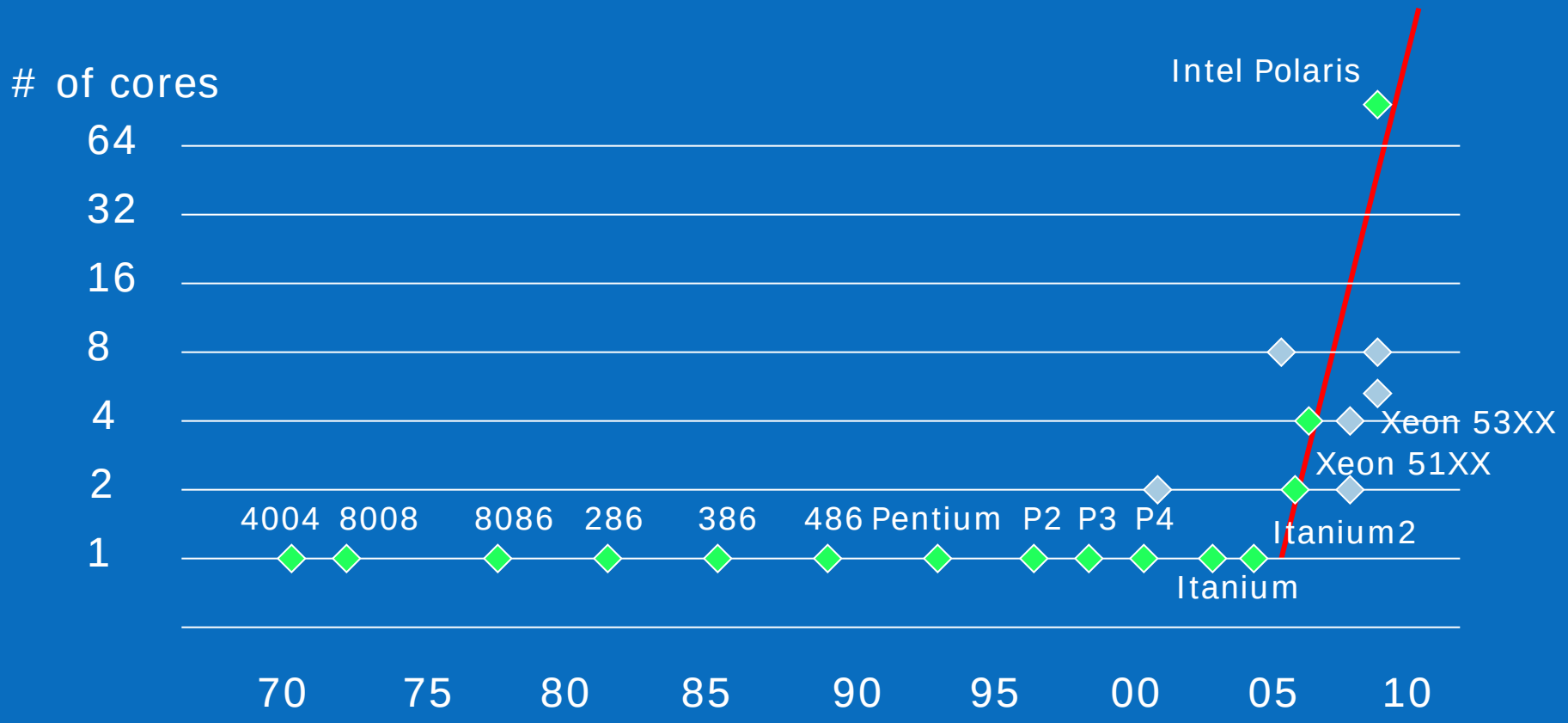
Why Hybrid Programming?

Testing Thread-safety of MPI Implementations

Master Communication

Multi-threaded Communication

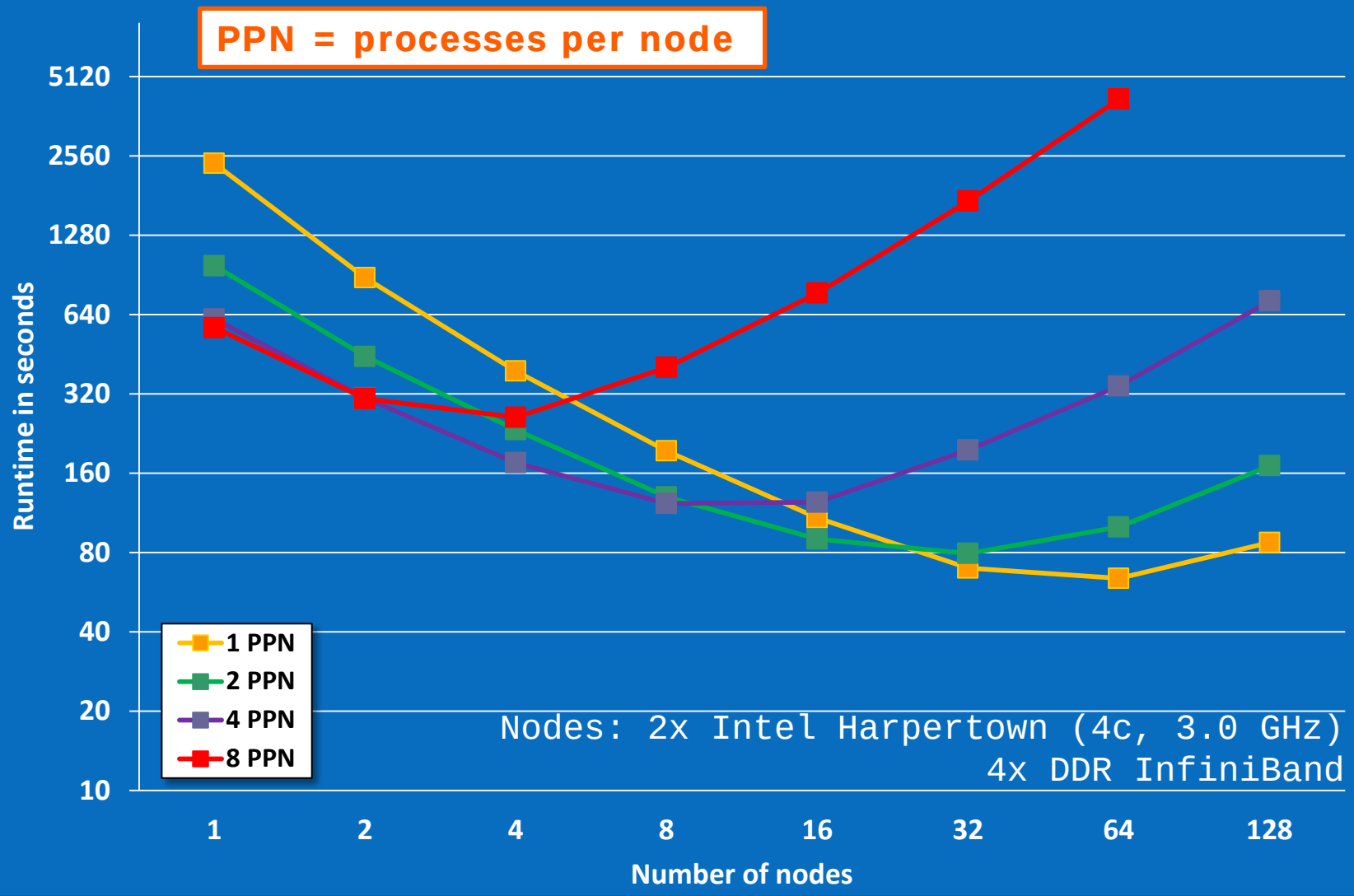
Why Hybrid Programming?



Core counts will steadily increase during the next years.

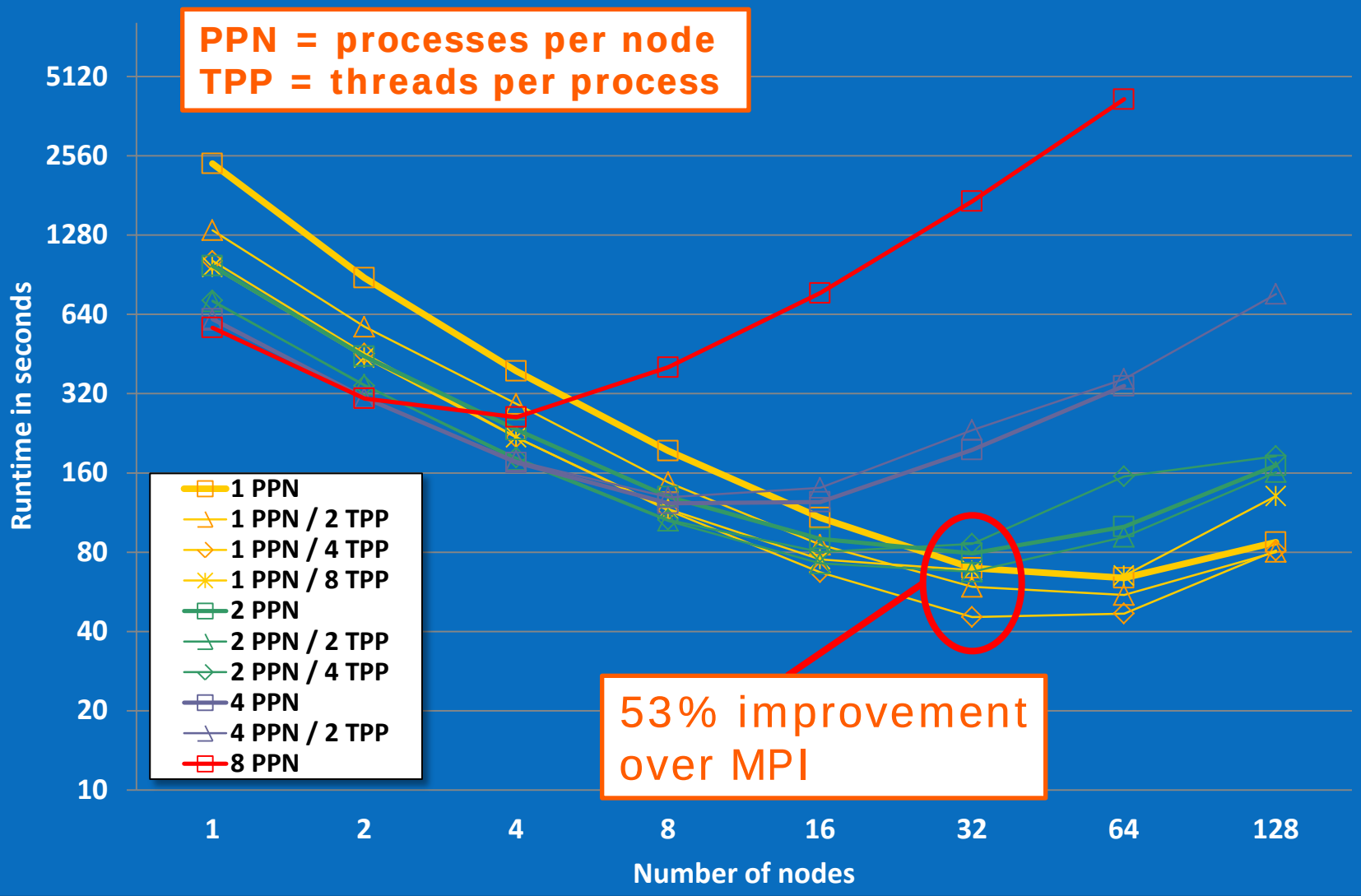
Cluster nodes will become highly parallel machines.

Why Hybrid Programming? MPI only



Simulation of Free-Surface Flows, Finite Element CFD solver written in Fortran and C
Figure kindly provided by HPC group of the Center of Computing and Communication, RWTH Aachen, Germany

Why Hybrid Programming? OpenMP / MPI



Simulation of Free-Surface Flows, Finite Element CFD solver written in Fortran and C
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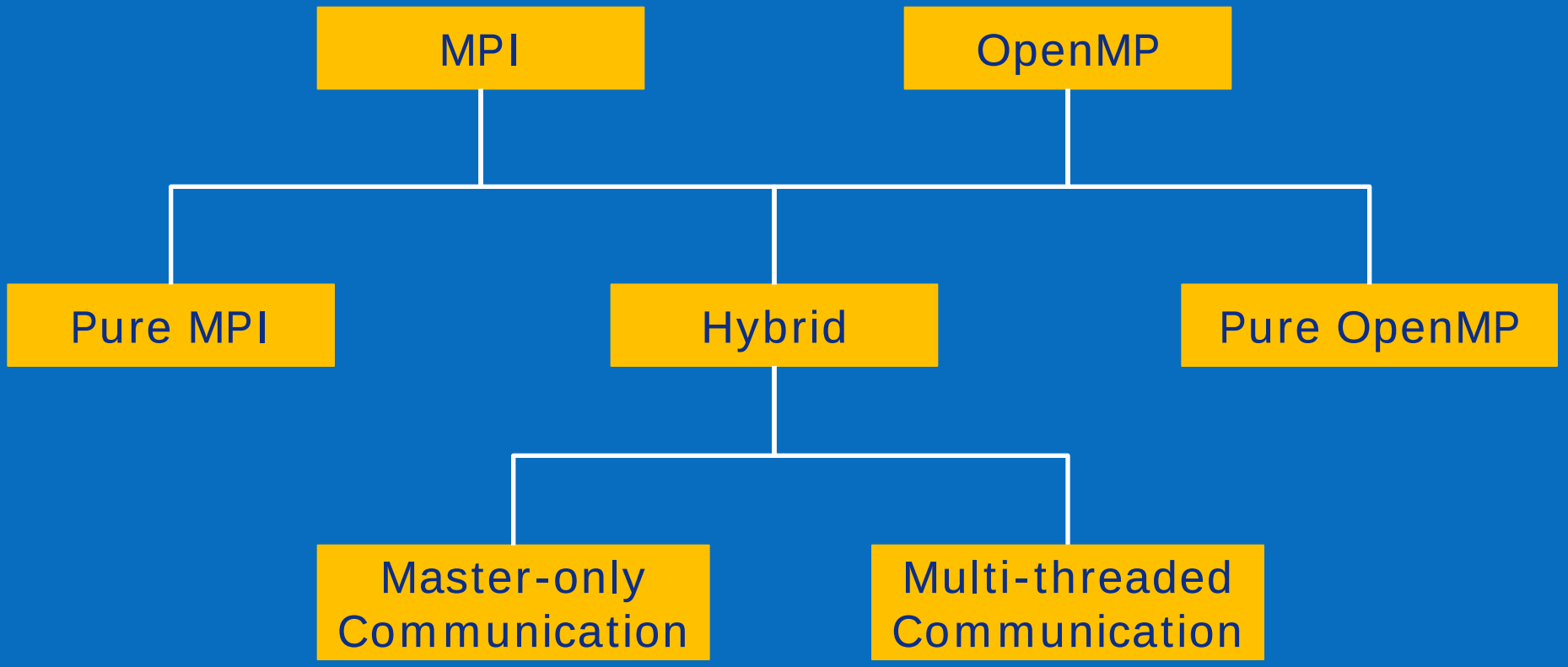
Hybrid Programming with OpenMP and MPI



Using OpenMP Together with MPI

OpenMP and MPI blend well with each other

- OpenMP statements express multi-threading in processes
- MPI interconnects processes to form a distributed application

Notes:

- Not all MPI implementations are thread-safe.
- In older MPI implementations, only the OpenMP master thread should invoke MPI primitives.
- Implementations conforming to MPI 2.1 offer an API to query threading capabilities.

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MPI_Init_thread

```
int MPI_Init_thread(int *argc, char ***argv,
                    int required, int *provided)

MPI_INIT_THREAD(REQUIRED, PROVIDED, IERROR)
        INTEGER REQUIRED, PROVIDED, IERROR
```

Initialize the MPI runtime and prepare for threaded execution

- Should be called instead of MPI_Init in multi-threaded applications
- Programmer specifies threading level *needed* for execution
- MPI library responds with threading level *supported*.

MPI_Init_thread

argc	C: `argc` argument of `main`
argv	C: `argv` argument of `main`
required	Threading level required (see below)
provided	Threading level supported (see below)

MPI_THREAD_SINGLE	Application only uses one thread
MPI_THREAD_FUNNELED	Application is multi-threaded, but only the master thread calls MPI routines
MPI_THREAD_SERIALIZED	Application is multi-threaded, but only one thread at a time calls MPI routines
MPI_THREAD_MULTIPLE	Multiple threads call MPI routines without restrictions

Note: MPI_THREAD_SINGLE < MPI_THREAD_FUNNELED < MPI_THREAD_SERIALIZED < MPI_THREAD_MULTIPLE

MPI_Is_thread_main & MPI_Query_thread

```
int MPI_Query_thread(int *provided)

MPI_QUERY_THREAD(PROVIDED, IERROR)
        INTEGER PROVIDED, IERROR
```

Queries the level of threading support of the MPI library.

```
int MPI_Is_thread_main(int *flag)

MPI_IS_THREAD_MAIN(FLAG, IERROR)
        LOGICAL FLAG
        INTEGER IERROR
```

Tests if the calling thread is the main thread.

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Master-only Communication – Pattern 1 (MPI_THREAD_FUNNELED)

Only the sequential code invokes MPI routines.

```
void example() {
    /* main/master thread */
    MPI_Recv(/* receive data */);
#pragma omp parallel
    {
        /* multi-threaded execution */
    }

    /* main/master thread */
    MPI_Send(/* send back data */);
}
```

Master-only Communication – Pattern 2 (MPI_THREAD_FUNNELED)

Only the master thread invokes MPI routines.

```
void example() {
   #pragma omp parallel
        {
   #pragma omp master
            {
                MPI_Recv(/* receive data */);
            }
   #pragma omp barrier

            /* multi-threaded execution */

   #pragma omp master
            {
                MPI_Send(/* send back data */);
            }
   #pragma omp barrier
        }
   }
```

Discussion of MPI_THREAD_FUNNELED

Limited degree of parallelism when communication occurs:

- Only the master thread of the process communicates.
- Parallel OpenMP execution has to be stopped while communicating.

Performance suffers:

- The additional barrier needed introduces overheads and causes additional cache flushes.
- On NUMA architectures with first-touch policies, the master thread “touches” data when receiving a message.
- OpenMP threads might frequently access data stored remotely on the NUMA node of the master thread.

But: Easy to use and implement even with MPI libraries that are not fully multi-threaded.

Global Barriers

Global barriers involve a 2-stage barrier synchronization:

- intra-process OpenMP barrier
- inter-process MPI barrier

```
void barrier() {
   #pragma omp parallel
        {
             /* multi-threaded execution */

   #pragma omp barrier
   #pragma omp master
             {
                  MPI_Barrier(/* arguments */);
             }
   #pragma omp barrier

             /* multi-threaded execution */
        }
   }
```

Intra-process OpenMP barrier

Inter-process MPI barrier

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Serialized Communication (MPI_THREAD_SERIALIZED)

Any thread invokes MPI calls, but communication is serialized by means of critical regions.

```
void example() {
   #pragma omp parallel
        {
   #pragma omp critical (MPI)
            {
                MPI_Recv(/* receive data */);
            }

        /* multi-threaded execution */

   #pragma omp critical (MPI)
            {
                MPI_Send(/* send back data */);
            }
        }
   }
```

Specify name for critical region to associate it with MPI communication.

Note: OpenMP lock routines could be used as well.

Discussion of MPI_THREAD_SERIALIZED

Limited degree of parallelism when communication occurs:

- OpenMP execution does not need to stop while communicating.
- However, only one thread of the process communicates at a time.

Performance does not suffer as with MPI_THREAD_FUNNELED

- Expensive barrier synchronization is avoided.
- Lock operations are not as expensive, but cache flushes still occur.
- On NUMA architectures with first-touch policies, the communicating threads “touch” the data received and cause allocation on the local NUMA node.

Multi-threaded Communication (MPI_THREAD_MULTIPLE)

Any thread invokes MPI calls and communicates with other threads of other processes.

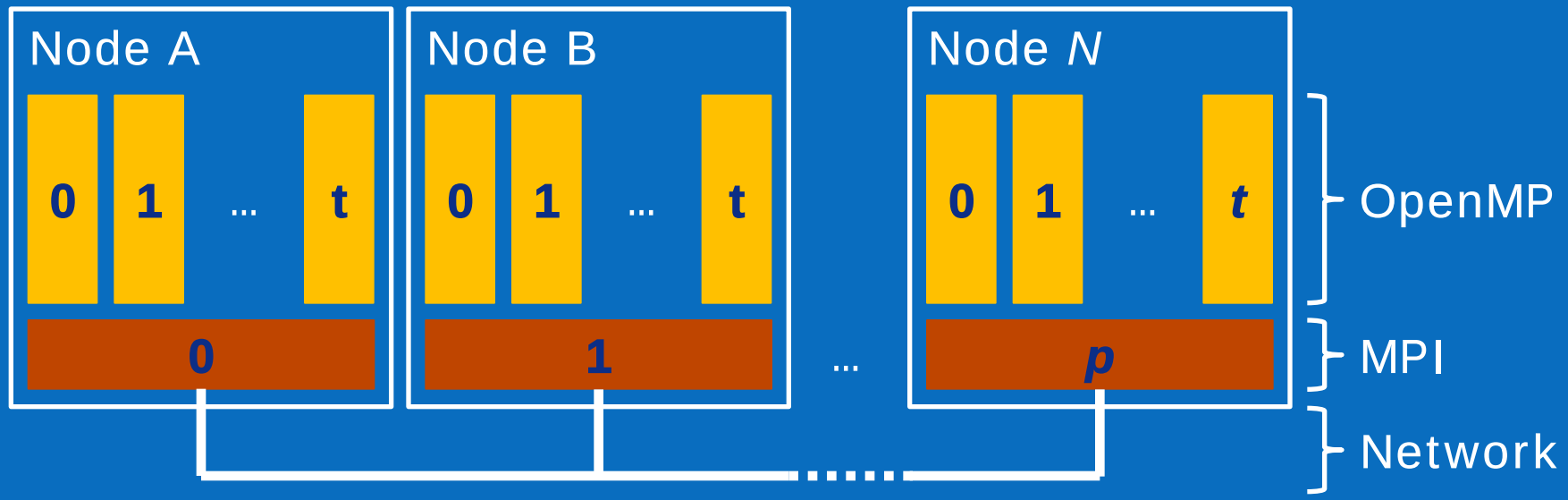
```
void example() {
   #pragma omp parallel
       {
           MPI_Recv(/* receive data */);

           /* multi-threaded execution */

           MPI_Send(/* send back data */);
       }
   }
```

How to address OpenMP threads?

Addressing OpenMP Threads



OpenMP and MPI use different numbering schemes.

- OpenMP threads IDs are not recognized as valid MPI ranks.
- Programmers need to work around this restriction.
- Solution: Use message tags to address threads.

Addressing OpenMP Threads

Sending messages:

```
MPI_Send(buf, count, dtype, dest, threadID, comm)

call MPI_SEND(BUF, COUNT, DTYPE, DEST, THREADID, COMM, ERR)
```

Receiving messages:

```
MPI_Recv(buf, count, dtype, source, omp_get_thread_num(),
         comm, status)

call MPI_Recv(BUF, COUNT, DTYPE, SOURCE, OMP_GET_THREAD_NUM(),
              COMM, STATUS, ERR)
```

Addressing OpenMP Threads

If tags are needed to distinguish message types, thread IDs and message tags need to be fused to a single value:

```
#define THREADID(id, tag) (((id) << 16) | (tag))

#define THISTHREAD(tag) (omp_get_thread_num() << 16 | (tag))
```

(These macros leave 16 bits for the message tags.)

Usage examples:

```
MPI_Send(buf, count, dtype, dest, THREADID(1, 42), comm)

MPI_Recv(buf, count, dtype, source, THISTHREAD(42),
         comm, status)
```

Global Barriers

Global barriers still involve a 2-stage barrier synchronization:

- intra-process OpenMP barrier
- inter-process MPI barrier

```
void barrier() {
   #pragma omp parallel
        {
            /* multi-threaded execution */

            MPI_Barrier(/* arguments */);

            /* multi-threaded execution */
        }
   }
```

This does not establish a barrier for OpenMP threads!

Collective operations need to be performed by one thread only.

The Good, the Bad, and the Ugly

The Good

- OpenMP and MPI blend well with each other if certain rules are respected by programmers.
- Hybrid programs can greatly improve performance of parallel codes.

The Bad

- Programmers need to be aware of the issues of hybrid programming.
- Not all MPI implementations are thread-safe (but situation improves)

The Ugly

- Work-arounds needed to make things work.
- Hybrid programming does not automatically lead to efficient programs. What's the best setting for PPN and TPP for a given machine?

References

Message Passing Interface (MPI) Forum, *MPI: A Message-Passing Interface Standard*, Version 2.1, 2008, available at www.mpi-forum.org.

The OpenMP Architecture Review Board, *OpenMP Application Program Interface*, Version 3.0, 2008, available at www.openmp.org.

Michael J. Quinn, *Parallel Programming in C with MPI and OpenMP*, McGraw-Hill, 2004.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