MPI and OpenMP

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Overview

- Motivation
- Potential advantages of MPI + OpenMP
- Problems with MPI + OpenMP
- Styles of MPI + OpenMP programming
  - MPI's thread interface
- MPI Endpoints

Motivation

- With the ubiquity of multicore chips, almost all current CPU systems are *clustered architectures*
- Distributed memory systems, where each node consist of a shared memory multiprocessor (SMP).
- Single address space within each node, but separate nodes have separate address spaces.

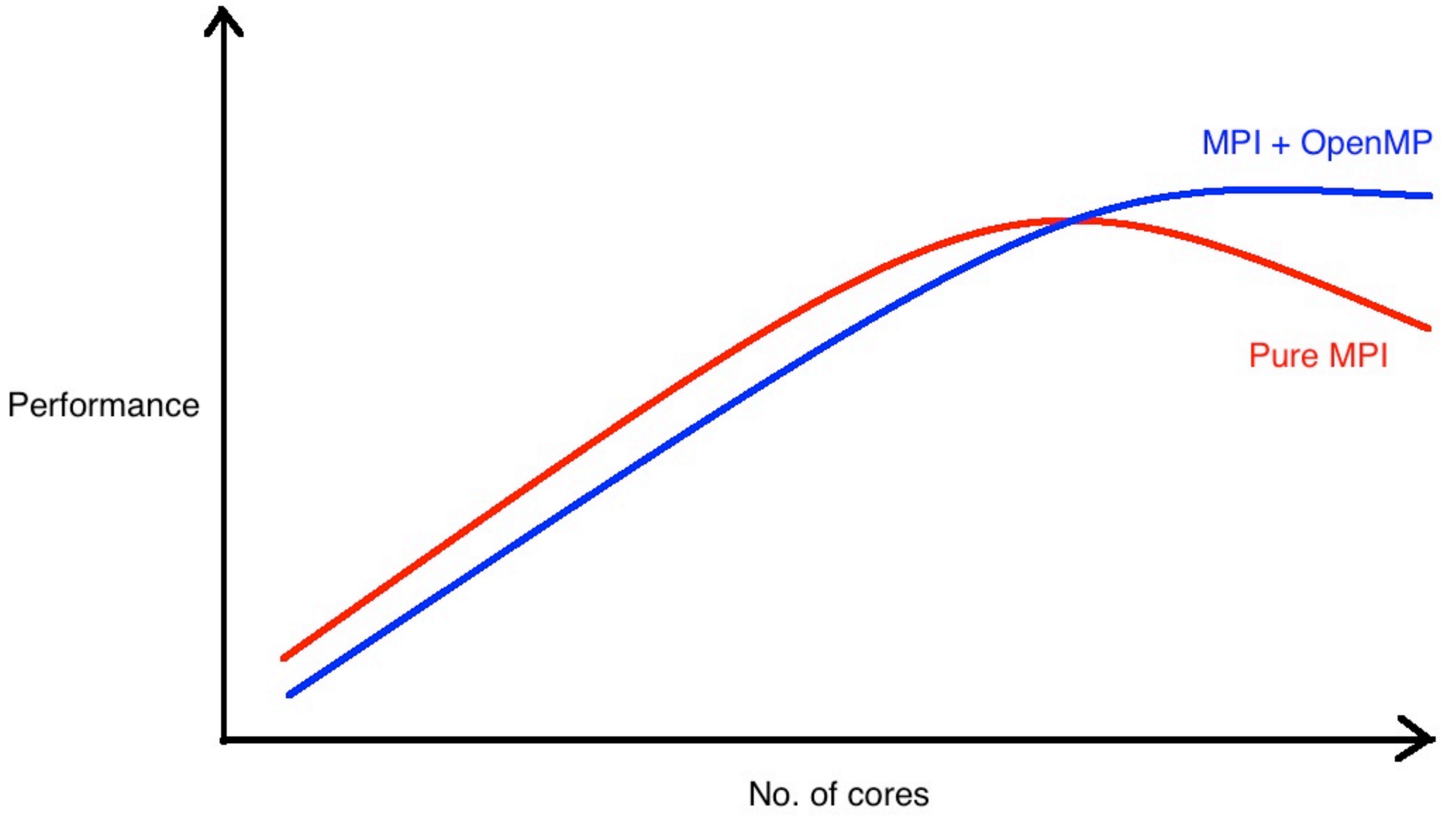
Programming clusters

- How should we program such a machine?
- Could use MPI across whole system
- Cannot (in general) use OpenMP/threads across whole system
  - requires support for single address space
  - this is possible in software, but inefficient
  - also possible in hardware, but expensive
- Could use OpenMP/threads within a node and MPI between nodes
  - is there any advantage to this?

Expectations

- In general, MPI + OpenMP does not improve performance (and may be worse!) in the regime where the MPI application is scaling well.
- Benefits come when MPI scalability (either in time or memory) starts to run out
- MPI +OpenMP may extend scalability to larger core counts

Typical performance curves



Potential advantages of MPI + OpenMP

- Reducing memory usage
- Exploiting additional levels of parallelism
- Reducing load imbalance
- Reducing communication costs

Reducing memory usage

- Some MPI codes use a replicated data strategy
  - all processes have a copy of a major data structure
- Classical domain decomposition codes have replication in halos
- MPI internal message buffers can consume significant amounts of memory
- A pure MPI code needs one copy per process/core.
- A mixed code would only require one copy per node
  - data structure can be shared by multiple threads within a process
  - MPI buffers for intra-node messages no longer required
- Will be increasingly important
  - amount of memory per core is not likely to increase in future

Effect of domain size on halo storage

- Typically, using more processors implies a smaller domain size per processor
  - unless the problem can genuinely weak scale
- Although the amount of halo data does decrease as the local domain size decreases, it eventually starts to occupy a significant amount fraction of the storage
  - even worse with deep halos or >3 dimensions

Local domain size	Halos	% of data in halos
$50^3 = 125000$	$52^3 – 50^3 = 15608$	11%
$20^3 = 8000$	$22^3 – 20^3 = 2648$	25%
$10^3 = 1000$	$12^3 – 10^3 = 728$	42%

Exploiting additional levels of parallelism

- Some MPI codes do not scale beyond a certain core count because they run of of available parallelism at the top level.
- However, there may be additional lower levels of parallelism that can be exploited.
- In principle, this could also be done using MPI.
- In practice this can be hard
    - The lower level parallelism may be hard to load balance, or have irregular (or runtime determined) communication patterns.
    - May be hard to work around design decisions in the original MPI version.

- It may, for practical reasons, be easier to exploit the additional level(s) of parallelism using OpenMP threads.
- Can take an incremental (e.g. loop by loop) approach to adding OpenMP
  - maybe not performance optimal, but keeps development cost/time to a minimum.
- Obviously OpenMP parallelism cannot extend beyond a single node, but this may be enough
  - future systems seem likely to have more cores per nodes, rather than many more nodes

Reducing load imbalance

- Load balancing between MPI processes can be hard
  - need to transfer both computational tasks and data from overloaded to underloaded processes
  - transferring small tasks may not be beneficial
  - having a global view of loads may not scale well
  - may need to restrict to transferring loads only between neighbours
- Load balancing between threads is much easier
  - only need to transfer tasks, not data
  - overheads are lower, so fine grained balancing is possible
  - easier to have a global view
- For applications with load balance problems, keeping the number of MPI processes small can be an advantage

Reducing communication costs

- It is natural to suppose that communicating data inside a node is faster between OpenMP threads between MPI processes.
    - no copying into buffers, no library call overheads
- True, but there are lots of caveats – see later.
- In some cases, MPI codes actually communicate more data than is actually required
    - where actual data dependencies may be irregular and/or data-dependent
    - makes implementation easier

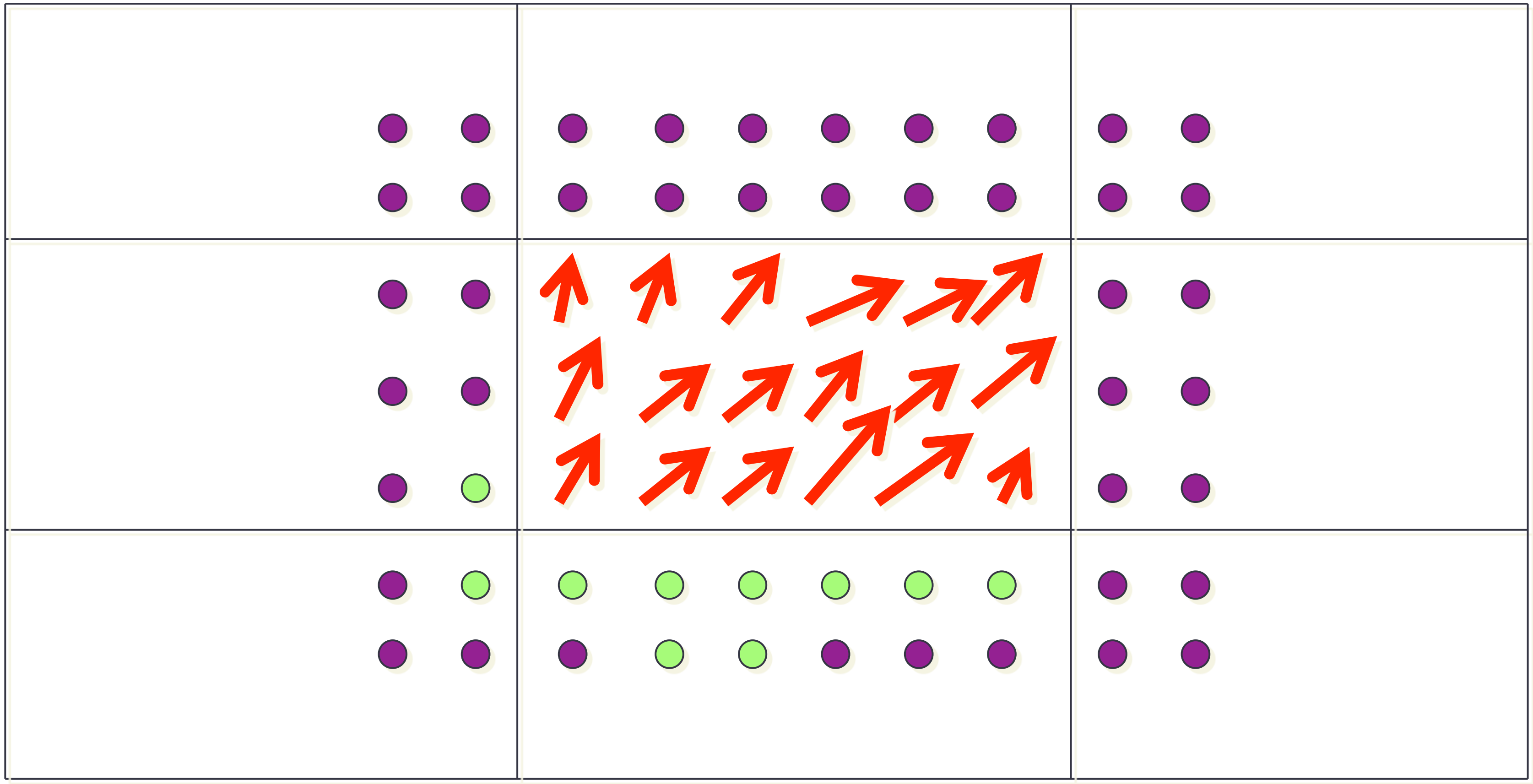
Collective communication

- In some circumstances, collective communications can be improved by using MPI + OpenMP
  - e.g. AllReduce, AlltoAll
- In principle, the MPI implementation ought to be well optimised for clustered architectures, but this isn't always the case.
  - hard to do for AlltoAllv, for example
- Can be cases where MPI + OpenMP transfers less data
  - e.g. AllReduce where every thread contributes to the sum, but only the master threads uses the result

Example

- ECMWF IFS weather forecasting code
- Semi-Lagrangian advection: require data from neighbouring grid cells only in an upwind direction.
- MPI solution – communicate all the data to neighbouring processors that *could possibly* be needed.
- MPI + OpenMP solution – within a node, only read data from other threads' grid point if it is actually required
  - Significant reduction in communication costs

IFS example



Problems with MPI + OpenMP

- Development/maintenance costs
- Portability
- Libraries
- Performance pitfalls

Development / maintenance costs

- In most cases, development and maintenance will be harder than for a pure MPI code.

- OpenMP programming is easier than MPI (in general), but it’s still parallel programming, and therefore hard!
  - application developers need yet another skill set

- OpenMP (as with all threaded programming) is subject to subtle race conditions and non-deterministic bugs
  - correctness testing can be hard

Portability

- Both OpenMP and MPI are themselves highly portable (but not perfect).

- Combined MPI/OpenMP is less so
  - main issue is thread safety of MPI
  - if maximum thread safety is assumed, portability will be reduced

- Desirable to make sure code functions correctly (maybe with conditional compilation) as stand-alone MPI code (and as stand-alone OpenMP code?)

Libraries

- If the pure MPI code uses a distributed-memory library, need to replace this with a hybrid version.
- If the pure MPI code uses a sequential library, need to replace this with either a threaded version called from the master thread, or a thread-safe version called inside parallel regions.
- If thread/hybrid library versions use something other than OpenMP threads internally, can get problems with oversubscription.
  - Both the application an the library may create threads that might not idle nicely when not being used

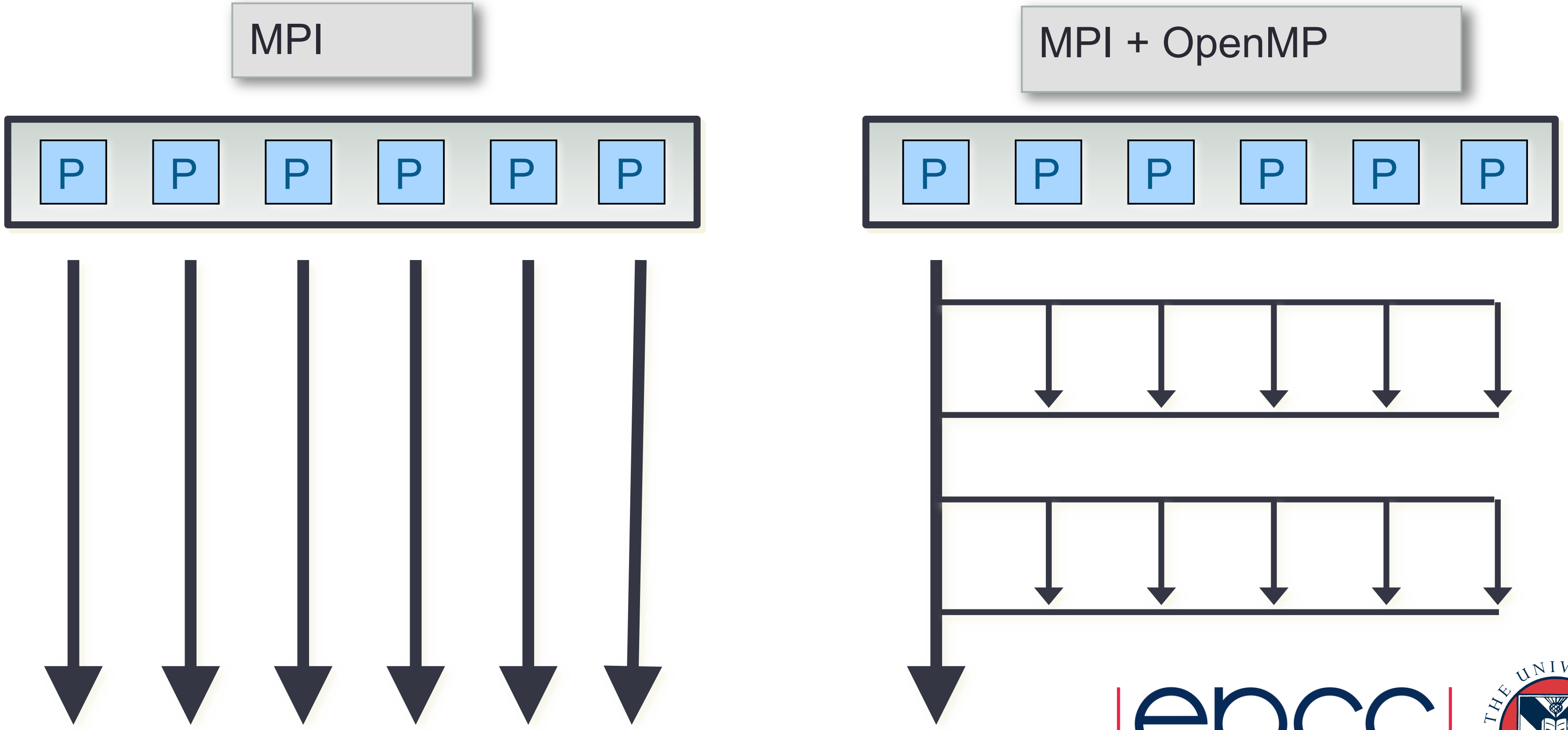
Performance pitfalls

- Adding OpenMP may introduce additional overheads not present in the MPI code (e.g. synchronisation, false sharing, sequential sections, NUMA effects).

- Adding OpenMP introduces a tunable parameter – the number of threads per MPI process
  - optimal value depends on hardware, compiler, input data
  - hard to guess the right value without experiments

- Placement of MPI processes and their associated OpenMP threads within a node can have performance consequences.

- An incremental, loop by loop approach to adding OpenMP is easy to do, but it can be hard to get sufficient parallel coverage.
  - just Amdahl's law applied inside the node



More pitfalls...

- The mixed implementation may require more synchronisation than a pure OpenMP version, if non-thread-safety of MPI is assumed.
- Implicit point-to-point synchronisation via messages may be replaced by (more expensive) barriers.
  - loose thread to thread synchronisation is hard to do in OpenMP
- In the pure MPI code, the intra-node messages will often be naturally overlapped with inter-node messages
  - harder to overlap inter-thread communication with inter-node messages – see later
- OpenMP codes can suffer from false sharing (cache-to-cache transfers caused by multiple threads accessing different words in the same cache block)
  - MPI naturally avoids this

NUMA effects

- Nodes which have multiple sockets are NUMA: each socket has it's own block of RAM.
- OS allocates virtual memory pages to physical memory locations
  - has to choose a socket for every page
- Common policy (default in Linux) is *first touch* – allocate on socket where the first read/write comes from
  - right thing for MPI
  - worst possible for OpenMP if data initialisation is not parallelised
  - all data goes onto one socket
- NUMA effects can limit the scalability of OpenMP: it may be advantageous to run one MPI process per NUMA domain, rather than one MPI process per node.

Process/thread placement

- On NUMA nodes need to make sure that:
  - MPI processes are spread out across sockets
  - OpenMP threads are on the same socket as their parent process

- Not all batch systems do a good job of this....
  - can be hard to fix this as a user
  - gets even more complicated if SMT (e.g. Hyperthreads) is used.

Styles of MPI + OpenMP programming

- Can identify 4 different styles of MPI + OpenMP programming, depending on when/how OpenMP threads are permitted to make MPI library calls
- Each has its advantages and disadvantages
- MPI has a threading interface which allow the programmer to request and query the level of thread support

The 4 styles

- Master-only
  - all MPI communication takes place in the sequential part of the OpenMP program (no MPI in parallel regions)
- Funneled
  - all MPI communication takes place through the same (master) thread
  - can be inside parallel regions
- Serialized
  - only one thread makes MPI calls at any one time
  - distinguish sending/receiving threads via MPI tags or communicators
  - be very careful about race conditions on send/recv buffers etc.
- Multiple
  - MPI communication simultaneously in more than one thread
  - some MPI implementations don't support this
  - …and those which do mostly don't perform well

OpenMP Master-only

Fortran

```
!$OMP parallel
 work…
!$OMP end parallel

call MPI_Send(…)

!$OMP parallel
 work…
!$OMP end parallel
```

C

```
#pragma omp parallel
{
   work…
}
ierror=MPI_Send(…);
#pragma omp parallel
{
   work…
}
```

OpenMP Funneled

Fortran

```
!$OMP parallel
… work
!$OMP barrier
!$OMP master
  call MPI_Send(…)
!$OMP end master
!$OMP barrier
.. work
!$OMP end parallel
```

C

```
#pragma omp parallel
{
  … work
  #pragma omp barrier
  #pragma omp master
  {
    ierror=MPI_Send(…);
  }
 #pragma omp barrier
  … work
}
```

OpenMP Serialized

Fortran

```
!$OMP parallel
… work
!$OMP critical
  call MPI_Send(…)
!$OMP end critical
… work
!$OMP end parallel
```

C

```
#pragma omp parallel
{
  … work
  #pragma omp critical
  {
    ierror=MPI_Send(…);
  }
  … work
}
```

OpenMP Multiple

Fortran

```
!$OMP parallel
… work
call MPI_Send(…)
… work
!$OMP end parallel
```

C

```
#pragma omp parallel
{
  … work
  ierror=MPI_Send(…);
  … work
}
```

Thread Safety

- Making MPI libraries thread-safe is difficult
  - lock access to data structures
  - multiple data structures: one per thread
  - …

- Adds significant overheads
  - which may hamper standard (single-threaded) codes

- MPI defines various classes of thread usage
  - library can supply an appropriate implementation

MPI_Init_thread

- MPI_Init_thread works in a similar way to MPI_Init by initialising MPI on the main thread.
- It has two integer arguments:
  - Required ([in] Level of desired thread support)
  - Provided ([out] Level of provided thread support)

- C syntax

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

- Fortran syntax

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

MPI_Init_thread

- MPI_THREAD_SINGLE
  - Only one thread will execute.
- MPI_THREAD_FUNNELED
  - The process may be multi-threaded, but only the main thread will make MPI calls (all MPI calls are funneled to the main thread).
- MPI_THREAD_SERIALIZED
  - The process may be multi-threaded, and multiple threads may make MPI calls, but only one at a time: MPI calls are not made concurrently from two distinct threads (all MPI calls are serialized).
- MPI_THREAD_MULTIPLE
  - Multiple threads may call MPI, with no restrictions.

MPI_Init_thread

- These integer values are monotonic; i.e.,
  - MPI_THREAD_SINGLE < MPI_THREAD_FUNNELED < MPI_THREAD_SERIALIZED < MPI_THREAD_MULTIPLE
- Note that these values do not strictly map on to the four MPI/OpenMP Mixed-mode styles as they are more general (i.e. deal with Posix threads where we don’t have “parallel regions”, etc.)
  - e.g. no distinction here between Master-only and Funneled
  - see MPI standard for full details

MPI_Query_thread()

- MPI_Query_thread() returns the current level of thread support
  - Has one integer argument: provided [in] as defined for MPI_Init_thread()

- C syntax

```
int MPI_query_thread(int *provided);
```

- Fortran syntax

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

- Need to compare the output manually, i.e.

```
If (provided < requested) {
 printf("Not a high enough level of thread support!\n");
 MPI_Abort(MPI_COMM_WORLD,1)
    …etc.
}
```

Master-only

- Advantages
  - simple to write and maintain
  - clear separation between outer (MPI) and inner (OpenMP) levels of parallelism
  - no concerns about synchronising threads before/after sending messages
- Disadvantages
  - threads other than the master are idle during MPI calls
  - all communicated data passes through the cache where the master thread is executing.
  - inter-process and inter-thread communication do not overlap.
  - only way to synchronise threads before and after message transfers is by parallel regions which have a relatively high overhead.
  - packing/unpacking of derived datatypes is sequential.

Example

```
!$omp parallel do
       DO I=1,N * nthreads
          A(I) = B(I) + C(I)
       END DO

       CALL MPI_BSEND(A(N),1,.....)
       CALL MPI_RECV(A(0),1,.....)

!$omp parallel do
       DO I = 1,N * nthreads
          D(I) = A(I-1) + A(I)
       END DO
```

Implicit barrier added here

Intra-node messages overlapped with inter-node

Inter-thread communication occurs here

Funneled

- Advantages
  - relatively simple to write and maintain
  - cheaper ways to synchronise threads before and after message transfers
  - possible for other threads to compute while master is in an MPI call
- Disadvantages
  - less clear separation between outer (MPI) and inner (OpenMP) levels of parallelism
  - all communicated data still passes through the cache where the master thread is executing.
  - inter-process and inter-thread communication still do not overlap.

OpenMP Funneled with overlapping (1)

```
#pragma omp parallel
{
  … work
  #pragma omp barrier
  if (omp_get_thread_num() == 0)  {
    ierror=MPI_Send(…);
  }
  else {
    do some computation
  }
 #pragma omp barrier
  … work
}
```

Can’t using worksharing here!

OpenMP Funneled with overlapping (2)

```
#pragma omp parallel num_threads(2)
{
if (omp_get_thread_num() == 0)  {
    ierror=MPI_Send(…);
  }
  else {
#pragma omp parallel
    {
       do some computation
    }
  }
}
```

Higher overheads and harder to synchronise between teams

Serialised

- Advantages
  - easier for other threads to compute while one is in an MPI call
  - can arrange for threads to communicate only their “own” data (i.e. the data they read and write).
- Disadvantages
  - getting harder to write/maintain
  - more, smaller messages are sent, incurring additional latency overheads
  - need to use tags or communicators to distinguish between messages from or to different threads in the same MPI process.

Distinguishing between threads

- By default, a call to MPI_Recv by any thread in an MPI process will match an incoming message from the sender.
- To distinguish between messages intended for different threads, we can use MPI tags
  - if tags are already in use for other purposes, this gets messy
- Alternatively, different threads can use different MPI communicators
  - OK for simple patterns, e.g. where thread N in one process only ever communicates with thread N in other processes
  - more complex patterns also get messy

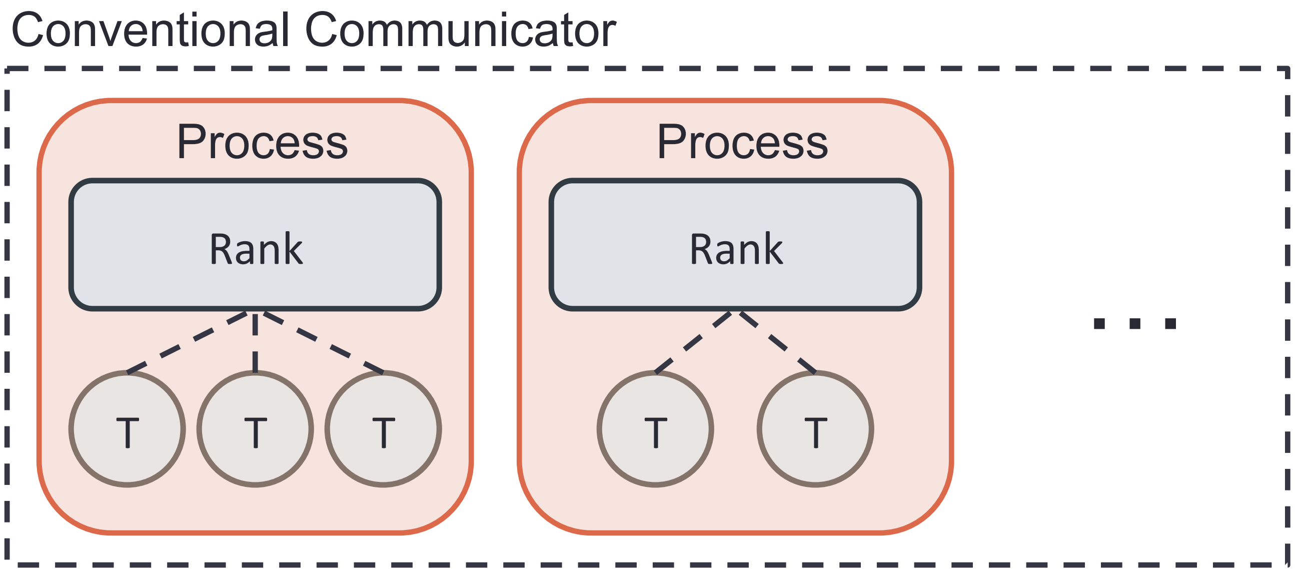
Multiple

- Advantages
  - Messages from different threads can (in theory) overlap
    - many MPI implementations serialise them internally.
  - Natural for threads to communicate only their “own” data
  - Fewer concerns about synchronising threads (responsibility passed to the MPI library)
- Disdavantages
  - Hard to write/maintain
  - Not all MPI implementations support this – loss of portability
  - Most MPI implementations don’t perform well like this
    - Thread safety implemented crudely using global locks.

Endpoints proposal for MPI 4.0

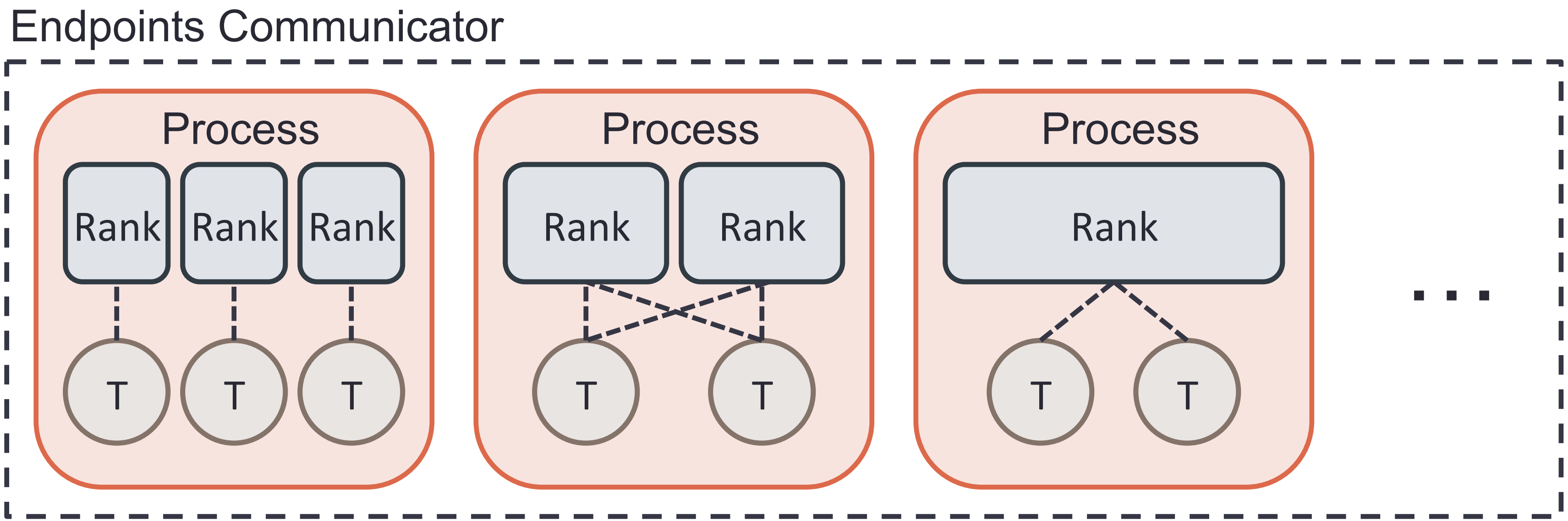
- Idea is to make Multiple style easier to use and easier to implement efficiently.
- Not yet available in implementations, but likely to appear in the fairly near future...

Mapping of Ranks to Processes in MPI



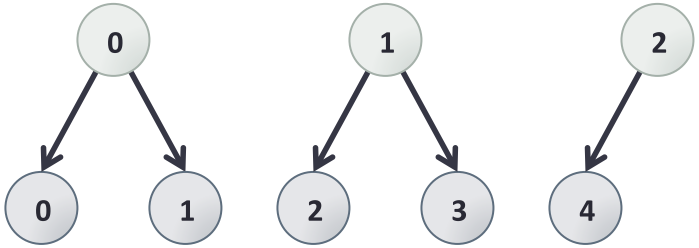
- MPI provides a 1-to-1 mapping of ranks to processes
- Programmers use many-to-one mapping of threads to processes

Flexible Mapping of Ranks to Processes



- Provide a many-to-one mapping of ranks to processes
  - Allows threads to act as first-class participants in MPI operations
  - Improve programmability of MPI + node-level and MPI + system-level models
  - Potential for improving performance of hybrid MPI + X
- A rank represents a communication “endpoint”
  - Set of resources that supports the independent execution of MPI communications

Endpoints: Proposed Interface



```
int MPI_Comm_create_endpoints(
        MPI_Comm parent_comm,
        int my_num_ep,
        MPI_Info info,
        MPI_Comm *out_comm_hdls[])
```

- Each rank in *parent_comm* gets *my_num_ep* ranks in *out_comm*
  - *My_num_ep* can be different at each process
  - Rank order: process 0’s ranks, process 1’s ranks, etc.
- Output is an array of communicator handles
  - *i*th handle corresponds to *i*th endpoint create by parent process
  - To use that endpoint, use the corresponding handle

Endpoints example

```
int main(int argc, char **argv) {
    int world_rank, tl;
    int max_threads = omp_get_max_threads();
    MPI_Comm ep_comm[max_threads];

    MPI_Init_thread(&argc, &argv, MULTIPLE, &tl);
    MPI_Comm_rank(MPI_COMM_WORLD, &world_rank);

#pragma omp parallel
    {
        int nt = omp_get_num_threads();
        int tn = omp_get_thread_num();
        int ep_rank;
#pragma omp master
        {
            MPI_Comm_create_endpoints(MPI_COMM_WORLD,
                nt, MPI_INFO_NULL, ep_comm);
        }
#pragma omp barrier
        MPI_Comm_attach(ep_comm[tn]);
        MPI_Comm_rank(ep_comm[tn], &ep_rank);
        ... // divide up work based on 'ep_rank'
        MPI_Allreduce(..., ep_comm[tn]);

        MPI_Comm_free(&ep_comm[tn]);
    }
    MPI_Finalize();
}
```

Summary

- MPI + OpenMP programming is becoming standard practice
  - ~30% of consumed CPU hours on ARCHER
- Many see it as the key to exascale, however …
  - may require MPI_THREAD_MULTIPLE style to reduce overheads
  - ... and end points to make this usable?
- Achieving correctness is hard
  - have to consider race conditions on message buffers
- Achieving performance is hard
  - entire application must be threaded (efficiently!)
- Must optimise choice of
  - numbers of processes/threads
  - placement of processes/threads on NUMA architectures

Practical session

Copy source code using:

```
cp /home/z01/shared/advomp.tar .
```

and unpack with

```
tar xvf advomp.tar
```

Code is in **`Advanced/C/Traffic`** or **`Advanced/Fortran90/Traffic`**

See Practical Notes sheet on course materials page and go straight to Exercise 2.