

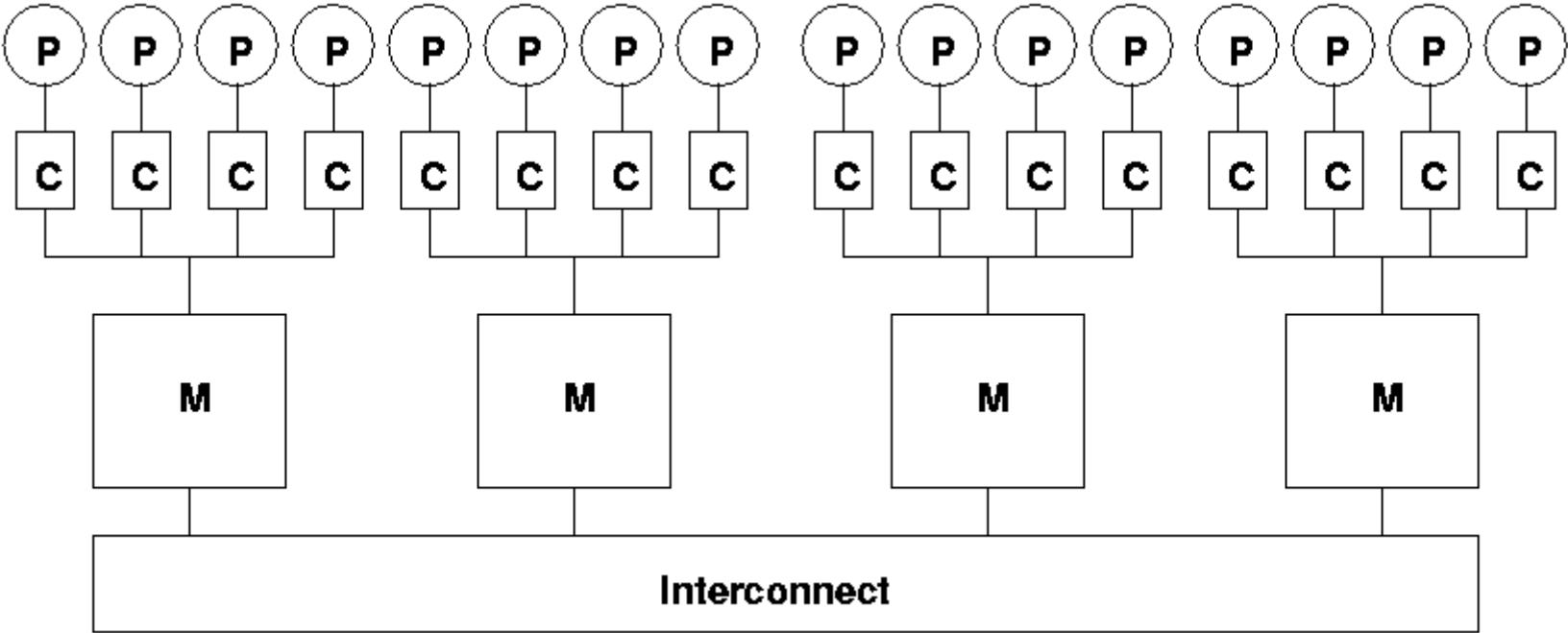


Advanced OpenMP

Lecture 4: OpenMP and MPI

- In recent years there has been a trend towards *clustered architectures*
- Distributed memory systems, where each node consist of a traditional shared memory multiprocessor (SMP).
 - with the advent of multicore chips, every cluster is like this
- Single address space within each node, but separate nodes have separate address spaces.

Clustered architecture



- 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?

We need to consider:

- Development / maintenance costs
- Portability
- Performance

- In most cases, development and maintenance will be harder than for an MPI code, and much harder than for an OpenMP code.
- If MPI code already exists, addition of OpenMP may not be *too* much overhead.
- In some cases, it may be possible to use a simpler MPI implementation because the need for scalability is reduced.
 - e.g. 1-D domain decomposition instead of 2-D

- 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?)

- Making libraries thread-safe can be 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
 - see later

Four possible performance reasons for mixed OpenMP/MPI codes:

1. Replicated data
2. Poorly scaling MPI codes
3. Limited MPI process numbers
4. MPI implementation not tuned for SMP clusters

- Some MPI codes use a replicated data strategy
 - all processes have a copy of a major data structure
 - classical domain decomposition code have replication in halos
 - MPI 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
- Halo regions are a type of replicated data
 - can become significant for small domains (i.e. many processes)

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%

- If the MPI version of the code scales poorly, then a mixed MPI/OpenMP version *may* scale better.
- May be true in cases where OpenMP scales better than MPI due to:
 1. Algorithmic reasons.
 - e.g. adaptive/irregular problems where load balancing in MPI is difficult.
 2. Simplicity reasons
 - e.g. 1-D domain decomposition

- 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

- MPI library implementation may not be able to handle millions of processes adequately.
 - e.g. limited buffer space
 - Some MPI operations are hard to implement without $O(p)$ computation, or $O(p)$ storage in one or more processes
 - e.g. AlltoAllv, matching wildcards
- Likely to be an issue on very large systems.
- Mixed MPI/OpenMP implementation will reduce number of MPI processes.

- Some MPI implementations are not well optimised for SMP clusters
 - less of a problem these days
- Especially true for collective operations (e.g. reduce, alltoall)
- Mixed-mode implementation naturally does the right thing
 - reduce within a node via OpenMP reduction clause
 - then reduce across nodes with MPI_Reduce
- Mixed-mode code also tends to aggregate messages
 - send one large message per node instead of several small ones
 - reduces latency effects, and contention for network injection

- 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

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...
}
```

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
}
```


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
}
```

Fortran

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

C

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

- 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_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.

- 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.  
}
```

- The OpenMP implementation may introduce additional overheads not present in the MPI code (e.g. synchronisation, false sharing, sequential sections).
- 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 may be replaced by (more expensive) barriers.
- 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.
- 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 placement becomes very important

- 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
```

Implicit barrier added here

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

Intra-node messages overlapped with inter-node

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

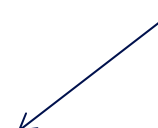
Inter-thread communication occurs here

- 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

- 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.

- 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

- 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)

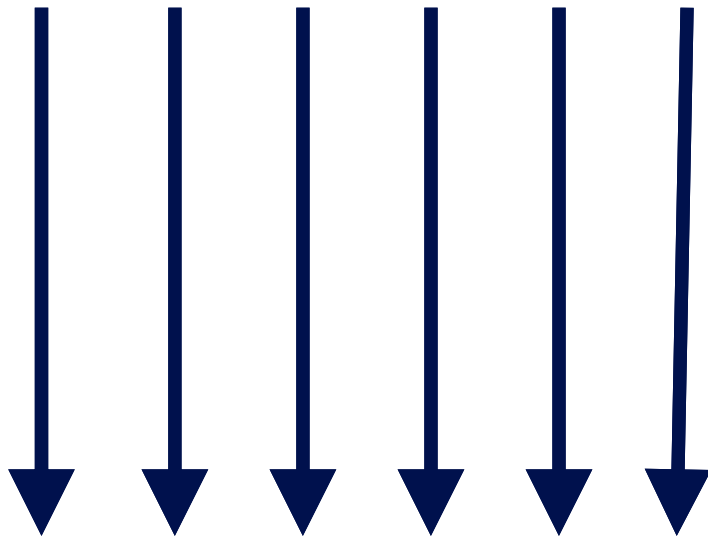
- Disadvantages

- 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.

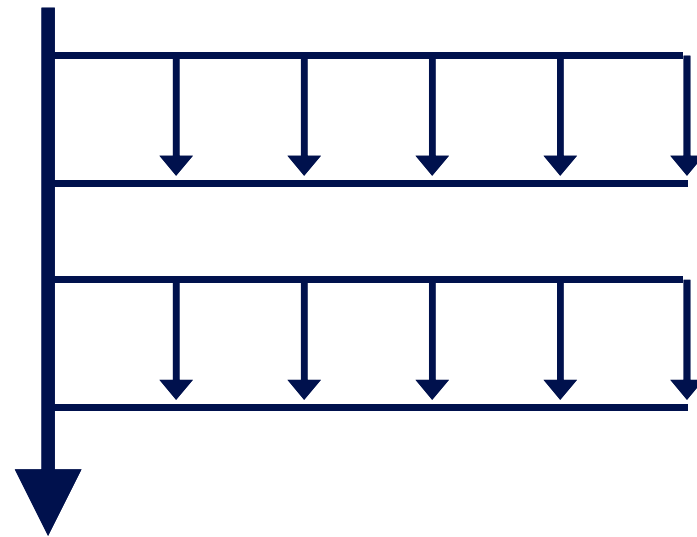
- A possible solution to permit more easier use and efficient implementations of Multiple is to extend MPI so that an MPI rank may have multiple source and destination identifiers (end points)
- e.g. if we want 4 threads per MPI process we could create an MPI communicator with 4 end points per rank
 - each thread can use a different end point
- Avoids need to use tags to identify threads
- Currently under discussion in MPI Forum
 - might appear in MPI 4.0?

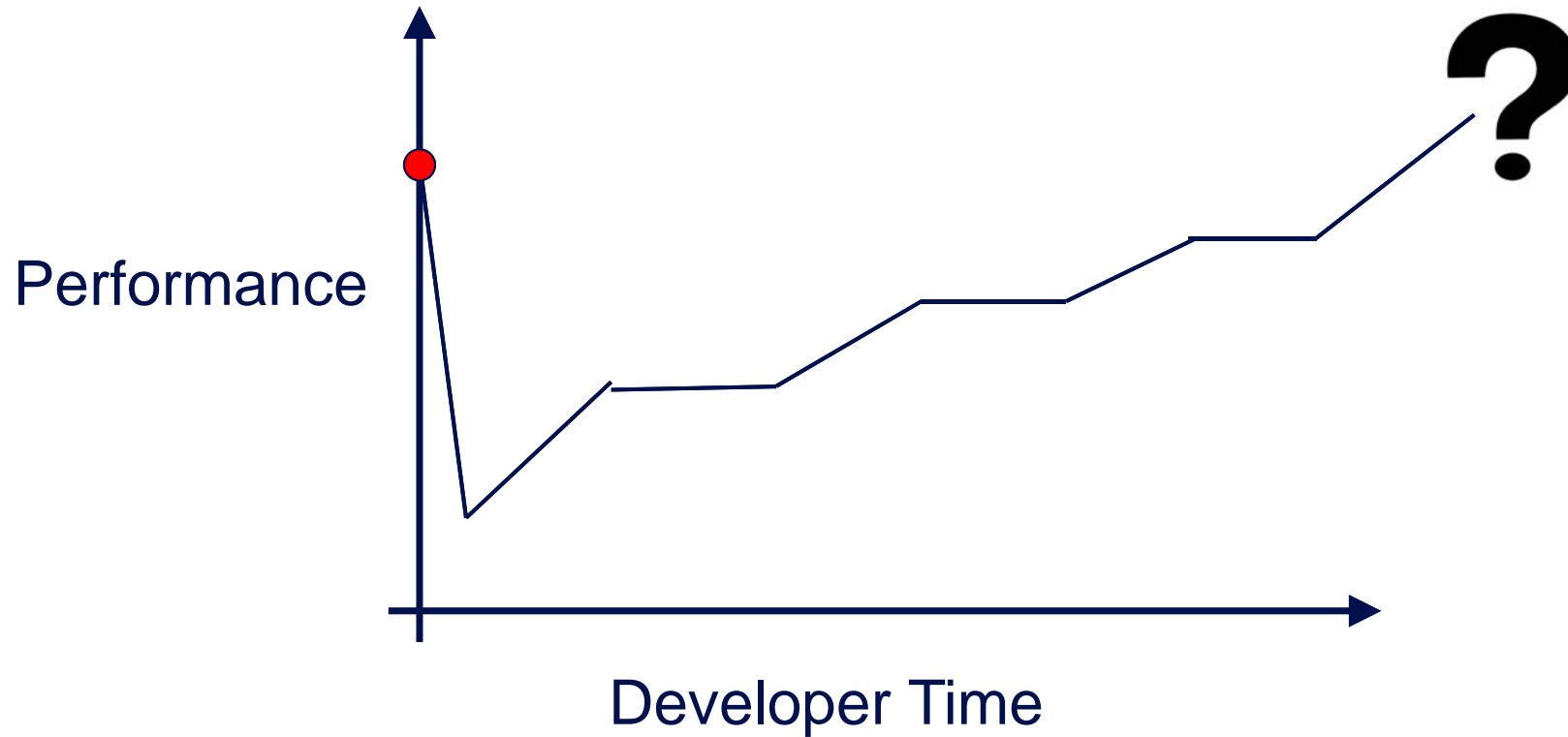
- Conceptually easy to write
 - rather messy
 - hard to get good performance: cannot just concentrate on key kernels

MPI



MPI + OpenMP





- Hybrid programming still a major current research topic
- Many see it as the key to exascale, however ...
 - will require MPI_THREAD_MULTIPLE style to avoid synchronisation
 - ... and end points to make this usable?
- Achieving correctness is hard
 - have to consider race conditions on messages
- 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