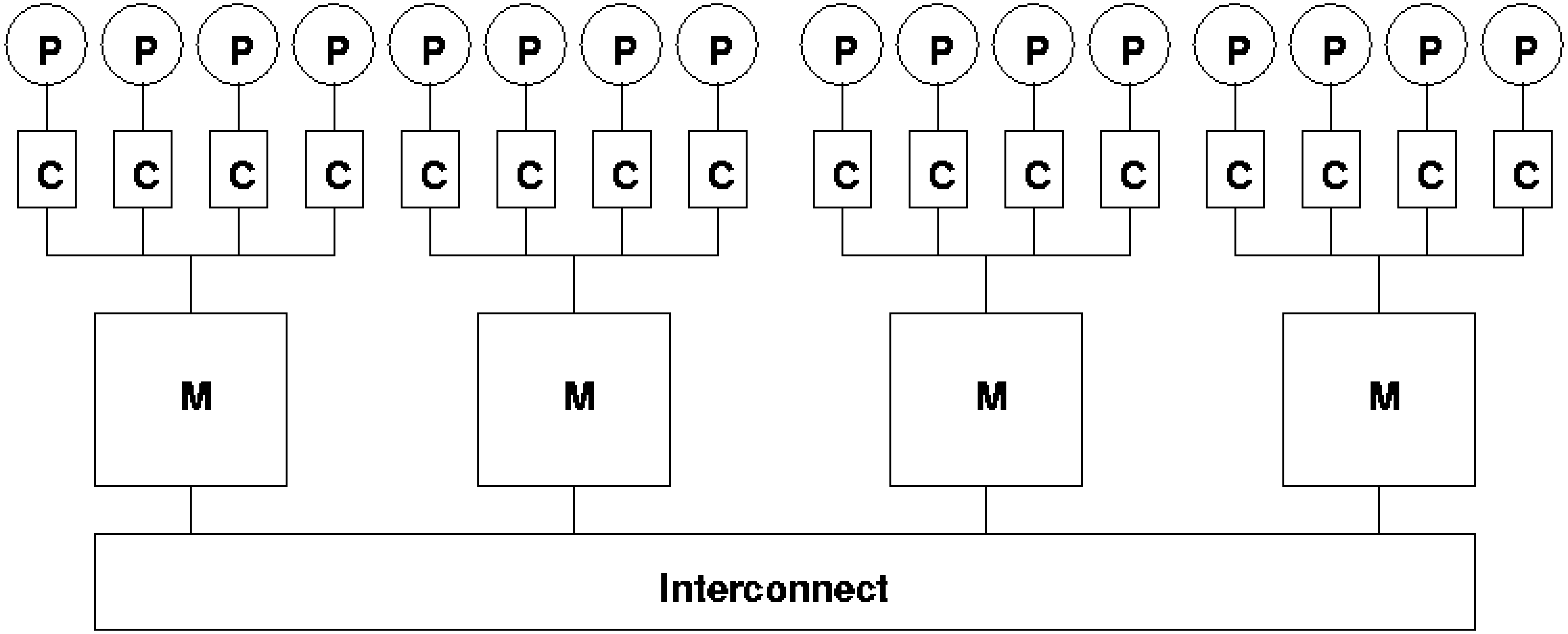
Advanced OpenMP

Lecture 4: OpenMP and MPI

Motivation

- 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



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?

Issues

We need to consider:

- Development / maintenance costs
- Portability
- Performance

Development / maintenance

- 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

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?)

Thread Safety

- 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

Performance

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

Replicated data

- 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%

Poorly scaling MPI codes

- 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

- 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

Limited MPI process numbers

- 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.

MPI implementation not tuned for SMP clusters

- 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

Styles of mixed-mode programming

- 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
}
```

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.
}
```

Pitfalls

- 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

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
```

Implicit barrier added here

```
     CALL MPI_BSEND(A(N*nthreads),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

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

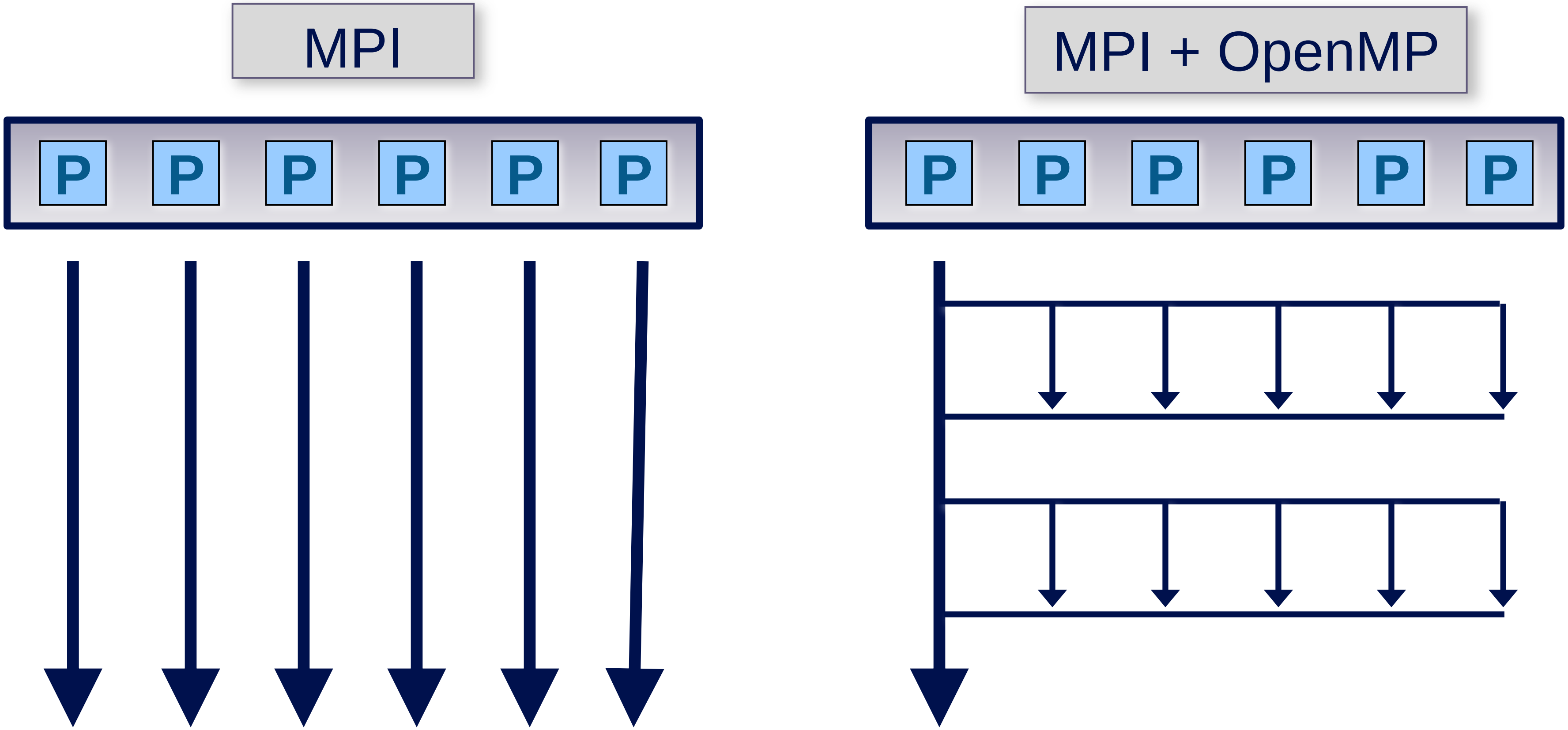
- Advantages
  - Messages from different threads can (in theory) overlap
    - many MPI implementations serialise them internally.
  - Natural for threads to communicate only their “own” data
  - Fewer concerns about synchronising threads (responsibility passed to the MPI library)
- Disdavantages
  - 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.

End points

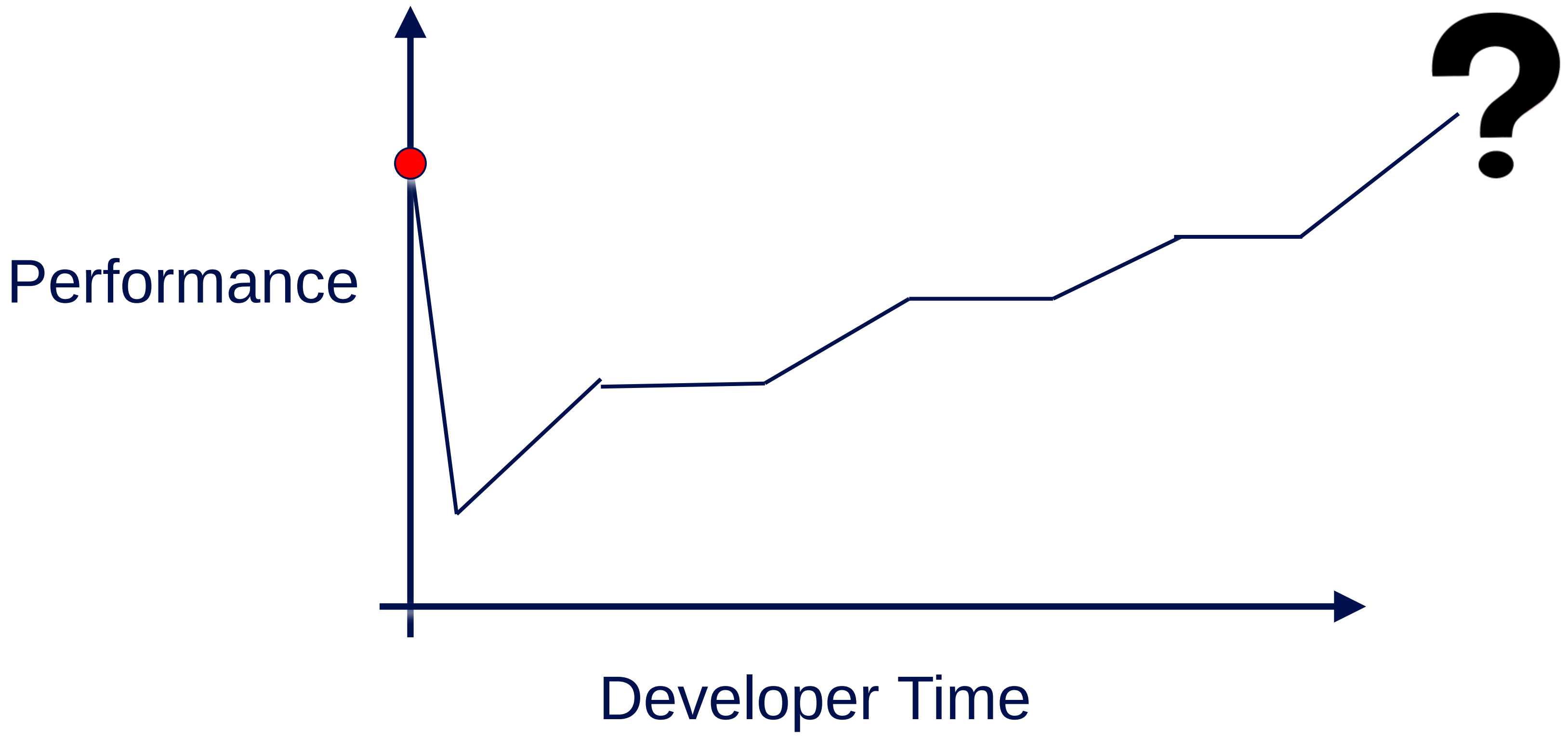
- A possible solution to permit more easier use and efficient implementations of Multiple is to extend MPI so that an MPI rank may have multiple source and destination identifiers (end points)
- e.g. if we want 4 threads per MPI process we could create an MPI communicator with 4 end points per rank
  - 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?

Performance

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



Consequences



Summary

- 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