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Message Passing Interface (MPI)

Summer School 2017 – Effective High Performance Computing

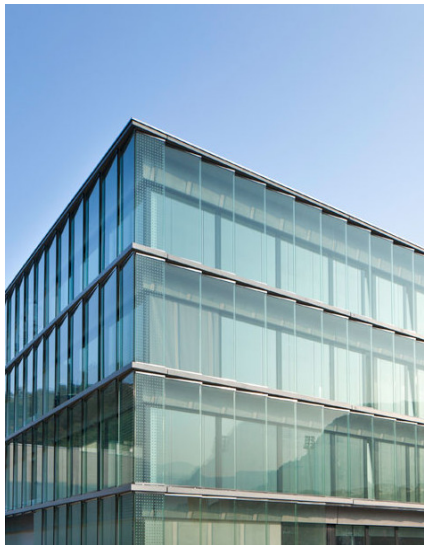
Tim Robinson, CSCS

July 19–20, 2017

Course Objectives

- Hybrid OpenMP/MPI, preparing MPI for OpenMP

General Course Structure



- An introduction to MPI
- Point-to-point communications
- Collective communications
- Topology
- Datatypes
- Other topics

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 - Hybrid OpenMP/MPI



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Configure MPI to enable OpenMP

Why OpenMP with MPI

There are two main motivations:

- To reduce the memory footprint (both in application and in communication buffers)
- To increase scalability (but you might not be faster than with MPI alone)

Reducing memory requirements

- Memory per core is generally decreasing
- MPI applications require some data to be replicated between MPI processes
 - Read-only lookup table where every process has a copy
 - Halo regions of neighbours
 - MPI internal data structures, e.g. communication buffers

Local domain size	halos	% data in halos
$100^3 = 1,000,000$	$102^3 - 100^3 = 61,208$	6%
$50^3 = 125,000$	$52^3 - 50^3 = 15,608$	11%
$20^3 = 8,000$	$22^3 - 20^3 = 2,648$	25%

Improving performance

- In the regime where MPI is scaling well, OpenMP will introduce overhead
- OpenMP can be used to exploit lower levels of parallelism
 - Might be hard to load balance with MPI
 - Might have irregular communication pattern
- In some cases collective communication overheads might be reduced
- OpenMP has in-built load balancing capabilities (loop schedules, tasks)

Preparing MPI for OpenMP

MPI requires to be setup with threads enabled:

- `MPI_Init` should be replaced by `MPI_Init_thread`

Pseudo-code

```
MPI_Init_thread(required, provided, ierror)
```

`required` specifies the requested level of thread support, and the actual level of support is then returned into `provided`.

You should check the value of `provided` after the call

MPI Thread level

- `MPI_THREAD_SINGLE`: Only one thread will execute (MPI-only application)
- `MPI_THREAD_FUNNELED`: Only master thread will make MPI calls (master = the thread calling `MPI_Init_thread`)
- `MPI_THREAD_SERIALIZED`: Only one thread at a time will make MPI calls (user responsibility)
- `MPI_THREAD_MULTIPLE`: Any thread may call MPI at any time, however that leads to slower performance (lock mechanism in MPI)

Checking the level of thread support provided

- The four classes of support are guaranteed to be monotonically increasing $\text{MPI_THREAD_SINGLE} < \text{MPI_THREAD_FUNNELED} < \text{MPI_THREAD_SERIALIZED} < \text{MPI_THREAD_MULTIPLE}$
- Therefore you can test to make sure at least the level you require is provided and exit if not:

Pseudo-code

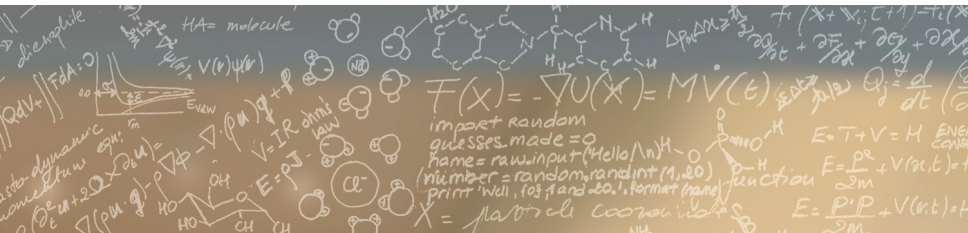
```
if (provided < requested) {  
    printf("Not high enough level of thread support.\n");  
    MPI_Abort(MPI_COMM_WORLD, 1);  
}
```



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Thank you for your attention.