MPI Optimisation

Advanced Message-Passing Programming











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Overview

Can divide overheads up into four main categories:

- Lack of parallelism
- Load imbalance
- Synchronisation
- Communication





Lack of parallelism

- Tasks may be idle because only a subset of tasks are computing
- Could be one task only working, or several.
 - work done on task 0 only
 - with split communicators, work done only on task 0 of each communicator
- Usually, the only cure is to redesign the algorithm to exploit more parallelism.





Extreme scalability

- Note that sequential sections of a program which scale as O(p) or worse can severely limit the scaling of codes to very large numbers of processors.
- Let us assume a code is perfectly parallel except for a small part which scales as O(p)
 - e.g. a naïve global sum as implemented for the MPP pi example!
- Time taken for parallel code can be written as

$$T_p = T_s \left(\frac{\left(1 - a \right)}{p} + ap \right)$$

where T_s is the time for the sequential code and a is the fraction of the sequential time in the part which is O(p).



Compare with Amdahl's Law

$$T_p = T_s \left(\frac{\left(1 - a \right)}{p} + a \right)$$

For example, take a = 0.0001

For 1000 processors, Amdahl's Law gives a speedup of \sim 900 For an O(p) term, the maximum speedup is \sim 50 (at p =100).

 Note: this assumes strong scaling, but even for weak scaling this will become a problem for 10,000+ processors





WolframAlpha

- O(1) term in scaling with a=0.0001 assuming strong-scaling (Amdahl's law):
 - http://www.wolframalpha.com/input/?i=maximum+1%2F%28%281-0.0001%29%2Fp%2B0.0001%29+with+p+from+1+to+100000
- O(p) term in scaling with a=0.0001 assuming strong-scaling:
 - http://www.wolframalpha.com/input/?i=maximum+1%2F%28%281-0.0001%29%2Fp%2B0.0001+*+p%29+with+p+from+1+to+1000
- O(p) term in scaling with a=0.0001 assuming weak-scaling:
 - http://www.wolframalpha.com/input/?i=maximum+1%2F%28%281-0.0001%29%2B0.0001+*+p%29+with+p+from+1+to+10000
- O(log2(p)) term in scaling with a=0.0001 assuming strong-scaling:
 - http://www.wolframalpha.com/input/?i=maximum+1%2F%28%281-0.0001%29%2Fp%2B0.0001+*+log2%28p%2B1%29%29+with+p+from+1+to+100000
- O(log2(p)) term in scaling with a=0.0001 assuming weak-scaling:
 - http://www.wolframalpha.com/input/?i=maximum+1%2F%28%281-0.0001%29%2B0.0001+*+log2%28p%2B1%29%29+with+p+from+1+to+100000
- O(log2(p)/p) term in scaling with a=0.0001 assuming strong-scaling:
 - http://www.wolframalpha.com/input/?i=maximum+1%2F%28%281-
 0.0001%29%2Fp%2B0.0001+*+log2%28p%2B1%29%2Fp%29+with+p+from+1+to+100000





Load imbalance

- All tasks have some work to do, but some more than others....
- In general a much harder problem to solve than in shared variables model
 - need to move data explicitly to where tasks will execute
- May require significant algorithmic changes to get right
- Again scaling to large processor counts may be hard
 - the load balancing algorithms may themselves scale as O(p) or worse.





- MPI profiling tools report the amount of time spent in each MPI routine
- For blocking routines (e.g. Recv, Wait, collectives) this time may be a result of load imbalance.
- The task is blocked waiting for another task to enter the corresponding MPI call
 - the other tasks may be late because it has more work to do
- Tracing tools often show up load imbalance very clearly
 - but may be impractical for large codes, large task counts, long runtimes





Synchronisation

- In MPI most synchronisation is coupled to communication
 - Blocking sends/receives
 - Waits for non-blocking sends/receives
 - Collective comms are (mostly) synchronising
- MPI_Barrier is almost never required for correctness
 - can be useful for timing
 - can be useful to prevent buffer overflows if one task is sending a lot of messages and the receiving task(s) cannot keep up.
 - think carefully why you are using it!
- Use of blocking point-to-point comms can result in unnecessary synchronisation.
 - Can amplify "random noise" effects (e.g. OS interrupts)





Communication

- Point-to-point communications
- Collective communications





Small messages

- Point to point communications typically incur a start-up cost
 - sending a 0 byte message takes a finite time
- Time taken for a message to transit can often be well modeled as $T_n = T_I + N_h T_h$

where T_l is start-up cost or *latency*, N_b is the number of bytes sent and T_b is the time per byte. In terms of *bandwidth B*:

$$T_p = T_l + \frac{N_b}{B}$$

- Faster to send one large message vs many small ones
 - e.g. one allreduce of two doubles vs two allreduces of one double
 - derived data-types can be used to send messages with a mix of types





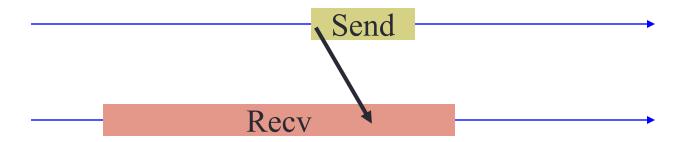
Communication patterns

- Can be helpful, especially when using trace analysis tools, to think about communication patterns
 - Note: nothing to do with OO design!
- We can identify a number of patterns which can be the cause of poor performance.
- Can be identified by eye, or potentially discovered automatically
 - e.g. the SCALASCA tool highlights common issues





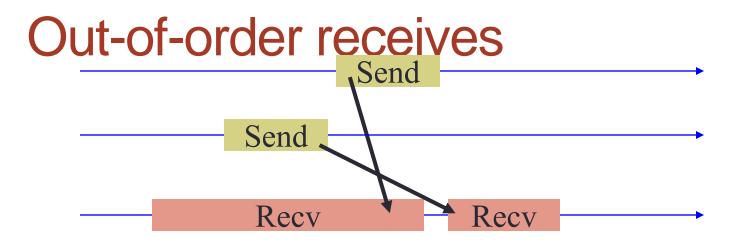
Late Sender



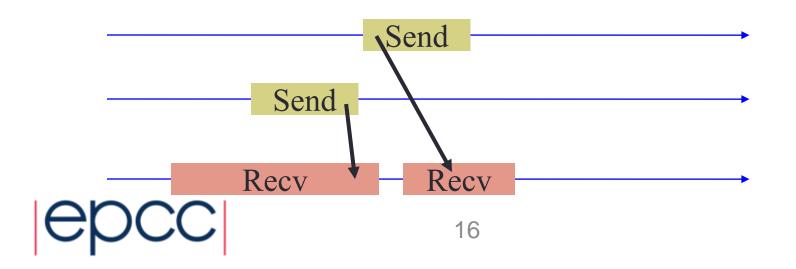
• If blocking receive is posted before matching send, then the receiving task must wait until the data is sent.





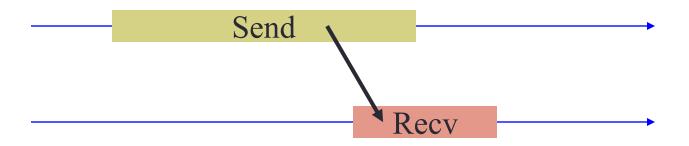


 Late senders may be the result of having blocking receives in the wrong order.





Late Receiver



- If send is synchronous, data cannot be sent until receive is posted
 - either explicitly programmed, or chosen by the implementation because message is large
 - sending task is delayed



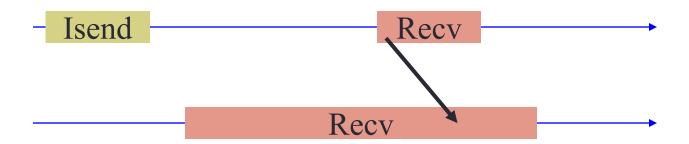


MPI Progression

- You probably think of MPI as running continuously
 - e.g. asynchronous / non-blocking comms happen "in the background"
 - communications and calculation overlap in time
- This is not generally true
 - MPI library is single-threaded by default, i.e. communications can only be processed when your program calls an MPI function
 - MPI treats calls as manual interrupts and will try to "progress" communications by matching outstanding sends and receives before actually doing what you have asked it to!
- If you issue a non-blocking send
 - it may be sent immediately if there is an existing receive
 - if not, it cannot be sent until the next explicit MPI call (which may be unrelated to the outstanding communication itself)



Late Progress



- Non-blocking send returns, but implementation has not yet sent the data.
 - A copy has been made in an internal buffer
- Send is delayed until the MPI library is re-entered by the sender.
 - receiving task waits until this occurs





Non-blocking comms

- Both late senders and late receivers may be avoidable by more careful ordering of computation and communication
- However, these patterns can also occur because of "random noise" effects in the system (e.g. network congestion, OS interrupts)
 - not all tasks take the same time to do the same computation
 - not all messages of the same length take the same time to arrive
- Can be beneficial to avoid delays by using all non-blocking comms entirely (Isend, Irecv, WaitAll)
 - post all the Irecv's as early as possible





Halo swapping

```
loop many times:
   irecv up; irecv down
   isend down; isend up
   update the core of the array
   wait for all 4 communications
   do all calculations involving halos
end loop
```

- Receives not necessarily ready in advance
 - remember your recv's match someone else's sends!





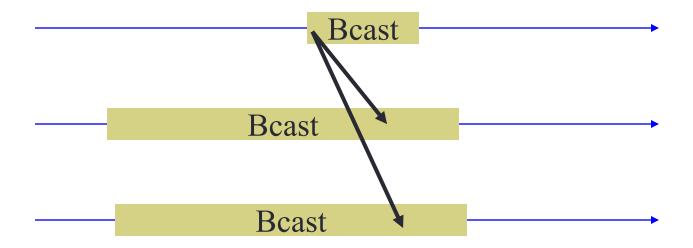
Collective communications

 Can identify similar synchronisation patterns for collective comms as for point-to-point...





Late Broadcaster

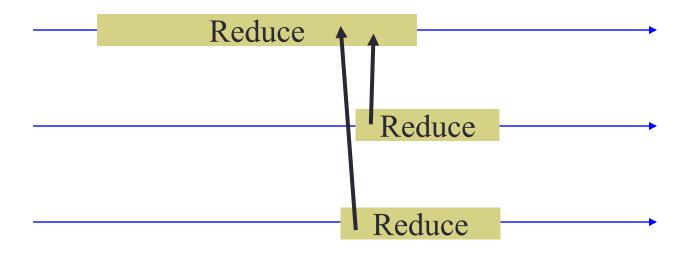


- If broadcast root is late, all other tasks have to wait
- Also applies to Scatter, Scattery





Early Reduce

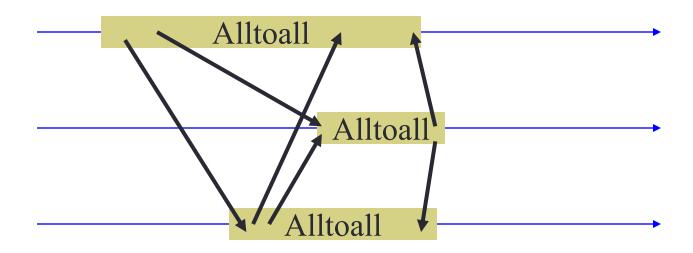


- If root task of Reduce is early, it has to wait for all other tasks to enter reduce
- Also applies to Gather, GatherV





Wait at NxN



- Other collectives require all tasks to arrive before any can leave.
 - all tasks wait for last one
- Applies to Allreduce, Reduce_Scatter, Allgather, Allgatherv, Alltoall, Alltoallv





Collectives

- Collective comms are (hopefully) well optimised for the architecture
 - Rarely useful to implement them your self using point-to-point
- However, they are expensive and force synchronisation of tasks
 - helpful to reduce their use as far as possible
 - e.g. in many iterative methods, a reduce operation is often needed to check for convergence
 - may be beneficial to reduce the frequency of doing this, compared to the sequential algorithm
- Non-blocking collectives added in MPI-3
 - may not be that useful in practice ...





Summary

Can divide overheads up into four main categories:

- Lack of parallelism
 - Cannot split work up into enough pieces
- Load imbalance
 - Pieces for each processor are not identical amount of work
- Synchronisation
 - Processors waiting for each other
- Communication
 - Inefficient patterns of communication



