Programming with MPI

Miscellaneous Guidelines

Nick Maclaren

nmm1@cam.ac.uk

March 2010

Summary

This is a miscellaneous set of practical points
Over–simplifies some topics in extra lectures
Mostly not about MPI, but languages and systems

Done this way, because course has become too long

- Remember that everything here is a half truth

Good as a guideline, but no more than that

- Remember extra lectures if any weird problems

Or you use a facility in a non–trivial way

Composite Types

So far, mainly contiguous arrays of basic types
n–D arrays stored in array element order
Fortran 77 and C are similar

Advanced collectives allow one level of separation

- Fortran 90 arrays not always contiguous
  An N–D array may have N levels of separation
- C and C++ have structures and pointers
  And "objects" are often built using them
- Fortran 90 and C++ have "classes"

Shortcuts (Hacks)

In a simple case, you can put the code inline
Or pack multiple transfers into one function

- Do whichever is simplest and cleanest

1: Pack up your data for export
2: Do the actual data transfer
3: Unpack the data you have imported

OR

1: Transfer the first simple array
2: Transfer the second simple array

. . .

n: Rebuild them into a consistent structure

C++ PODs and C structs

C++ PODs and similar C structs are easy
Use as array of sizeof bytes (type MPI_BYTE)

But you must follow these rules:

- Do it only when using the same executable
- Do it only between identical types
- Don't do it if they contain pointers
- Don't do it if have any environment data

And watch out for variable sized structs

C, C++ and POSIX

Some C, C++ and POSIX features are toxic
Often cause chaos to almost all other interfaces
Can be used safely, but only by real experts

<signal.h>, <setjmp.h>, <fenv.h>
POSIX threading, signal handling, scheduling
timer control, alarm, sleep, ...

It's easy to break MPI's rules using C++ exceptions
E.g. releasing an in–use non–blocking buffer

Fortran Assumed Shape Arrays

Good Fortran 90 uses assumed shape arrays
MPI 3 supports them properly, but not covered here

- MPI 2 uses assumed size arrays (i.e. Fortran 77)

Generally requires a copy, on call and return
Ignore this if not a performance problem
See Fortran course for some more details

- Only real problem is with non–blocking transfers

Convert to Fortran 77 (e.g. explicit shape)
In a common parent of both send/receive and wait

Fortran Type Checking

A routine must use compatible arguments everywhere
MPI buffers can be of any supported type
So the compiler may object to your use of them

- This is also fixed in MPI 3

If compiler objects to buffer argument type:

- Keep all calls in one module the same

Fortran compilers rarely check over all program

- Or write trivial wrappers in external procedures

E.g. My_Send_Integer and My_Send_Double

Fortran Derived Types

Fortran 2003 supports BIND(C) for interoperability
BIND(C) derived types are like C++ PODs

In general, don't treat them like PODs
And never do if they contain allocatable arrays

- No option but to transfer them as components

Tedious, messy, but not difficult

- Don't assume SEQUENCE means C–compatible

Has its uses for MPI, but too complicated to describe

Debugging vs Tuning

In practice, these overlap to a large extent

- Tuning MPI is more like tuning I/O than code

Many performance problems are logic errors
E.g. everything is waiting for one process

Many logic errors show up as poor performance

- So don't consider these as completely separate

Partial Solution

- Design primarily for debuggability

KISS – Keep It Simple and Stupid

This course has covered many MPI-specific points

See also How to Help Programs Debug Themselves

- Do that, and you rarely need a debugger

Diagnostic output is usually good enough

- Only then worry about performance

MPI Memory Optimisation

The examples waste most of their memory
Here are some guidelines for real programs:

- Don't worry about small arrays etc.

If they total less than 10%, so what?

- For big ones, allocate only what you need

For example, for gather and scatter

- Reuse large buffers or free them after use

Be careful about overlapping use, of course

MPI Performance

- Ultimately only elapsed time matters

The real time of program, start to finish

- All other measurements are just tuning tools

This actually simplifies things considerably

- You may want to analyse this by CPU count

Will tell you the scalability of the code

Design For Performance (1)

Here is the way to do this

- Localise all major communication actions

In a module, or whatever is appropriate for you
Keep its code very clean and simple

- Don't assume any particular implementation

This applies primarily to the module interface
Keep it generic, clean and simple

- Keep the module interfaces fairly high level

E.g. a distributed matrix transpose

Design For Performance (2)

Use the highest level appropriate MPI facility

- E.g. use its collectives where possible

Collectives are easier to tune, surprisingly

Most MPI libraries have had extensive tuning

- It is a rare programmer who will do as well

mpi_timer implements MPI_Alltoall many ways

Usually, 1–2 are faster than built–in MPI_Alltoall

Not often the same ones, and often by under 2%

Design For Performance (3)

- Put enough timing calls into your module

Summarise time spent in MPI and in computation

- Check for other processes or threads

Only for ones active during MPI transfers

Now look at the timing to see if you have a problem

- If it isn't (most likely), do nothing

- Try using only some of the cores for MPI

It's an easy change, but may not help

High-Level Approach (1)

Try to minimise inter–process communication
There are three main aspects to this:

- Amount of data transferred between processes

Inter–process bandwidth is a limited resource

- Number of transactions involved in transfer

The message–passing latency is significant

- One process needs data from another

May require it to wait, wasting time

High-Level Approach (2)

Partitioning is critical to efficiency
That will be described in the next lecture

You can bundle multiple messages together
Sending one message has a lower overhead

You can minimise the amount of data you transfer
Only worthwhile if your messages are large

You can arrange all processes communicate at once
Can help a lot because of progress issues

Bundling

On a typical cluster or multi–core system:
Packets of less than 1 KB are inefficient
Packets of more than 10 KB are no problem

Avoid transferring a lot of small packets
$\Rightarrow$ Packing up multiple small transfers helps
But only if significant time spent in them

- Remember integers can be stored in doubles

Timer Synchronisation (1)

This means synchronisation across processes
I.e. are all results from MPI_Wtime consistent?

Almost always the case on SMP systems
Will often be the case even on clusters

- Generally, try to avoid assuming or needing it

Rarely compare timestamps across processes

- If you use only local intervals, you are OK

Time passes at the same rate on all processes

Timer Synchronisation (2)

Beyond that is a job for real experts only

Parallel time is like relativistic time
Event ordering depends on the observer

There is a solution in directory Posixtime
Functions to return globally consistent time

I wrote this for a system with inconsistent clocks
Please ask about synchronisation if you need to

MPI and Normal I/O (1)

This means language, POSIX and Microsoft I/O

There are serious problems – not because of MPI
Caused by the system environment it runs under

- Will cover most common configuration only

If it doesn't apply, look at the extra lecture
Or ask your administrator to help you

MPI and Normal I/O (2)

There are two, very different, classes of file

- Normal named and scratch files
- stdin, stdout and stderr

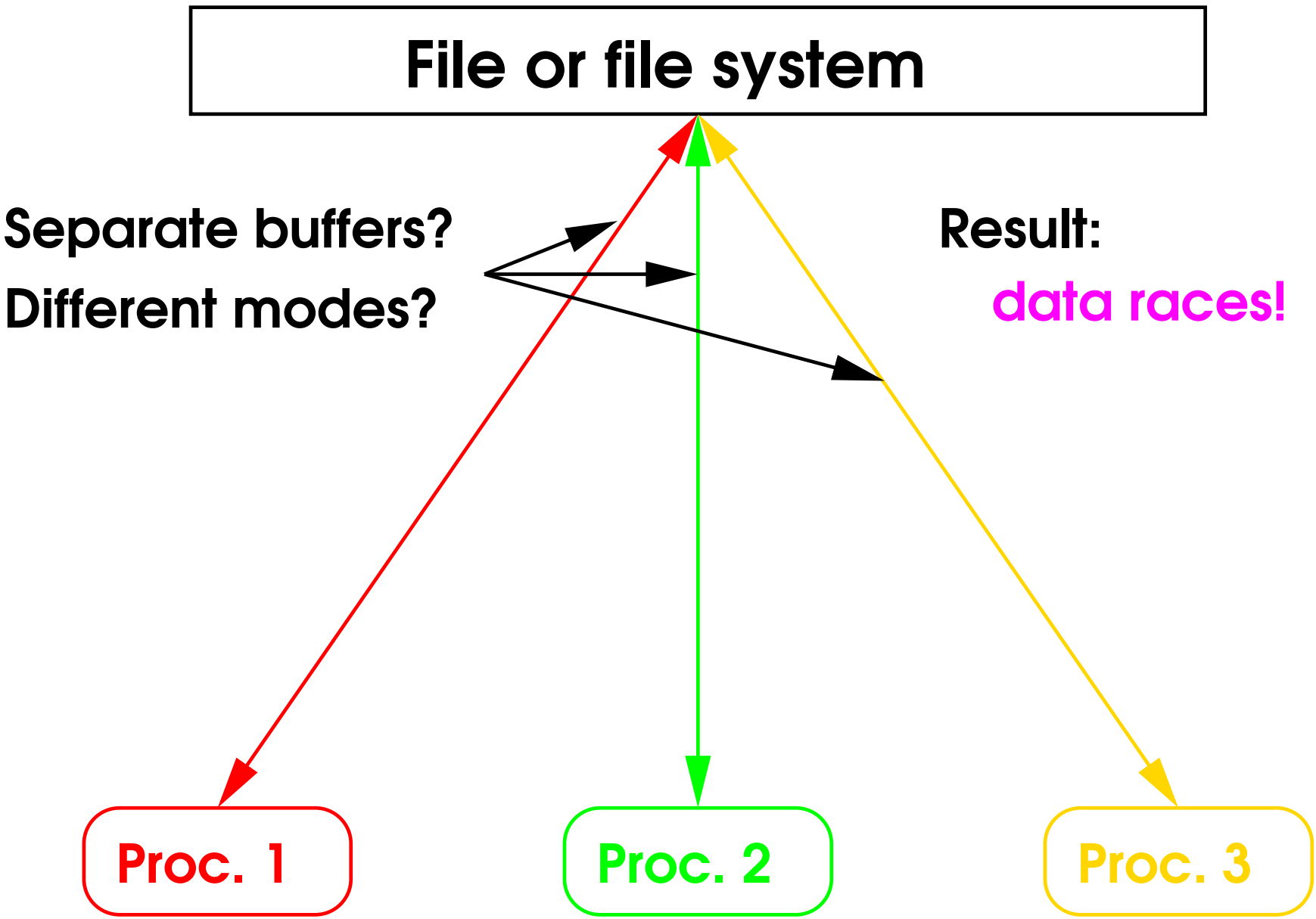
Former local to process – latter global to program

Problems are caused by the system environment
E.g. clusters of distributed memory systems
Or shared file descriptors on SMP systems

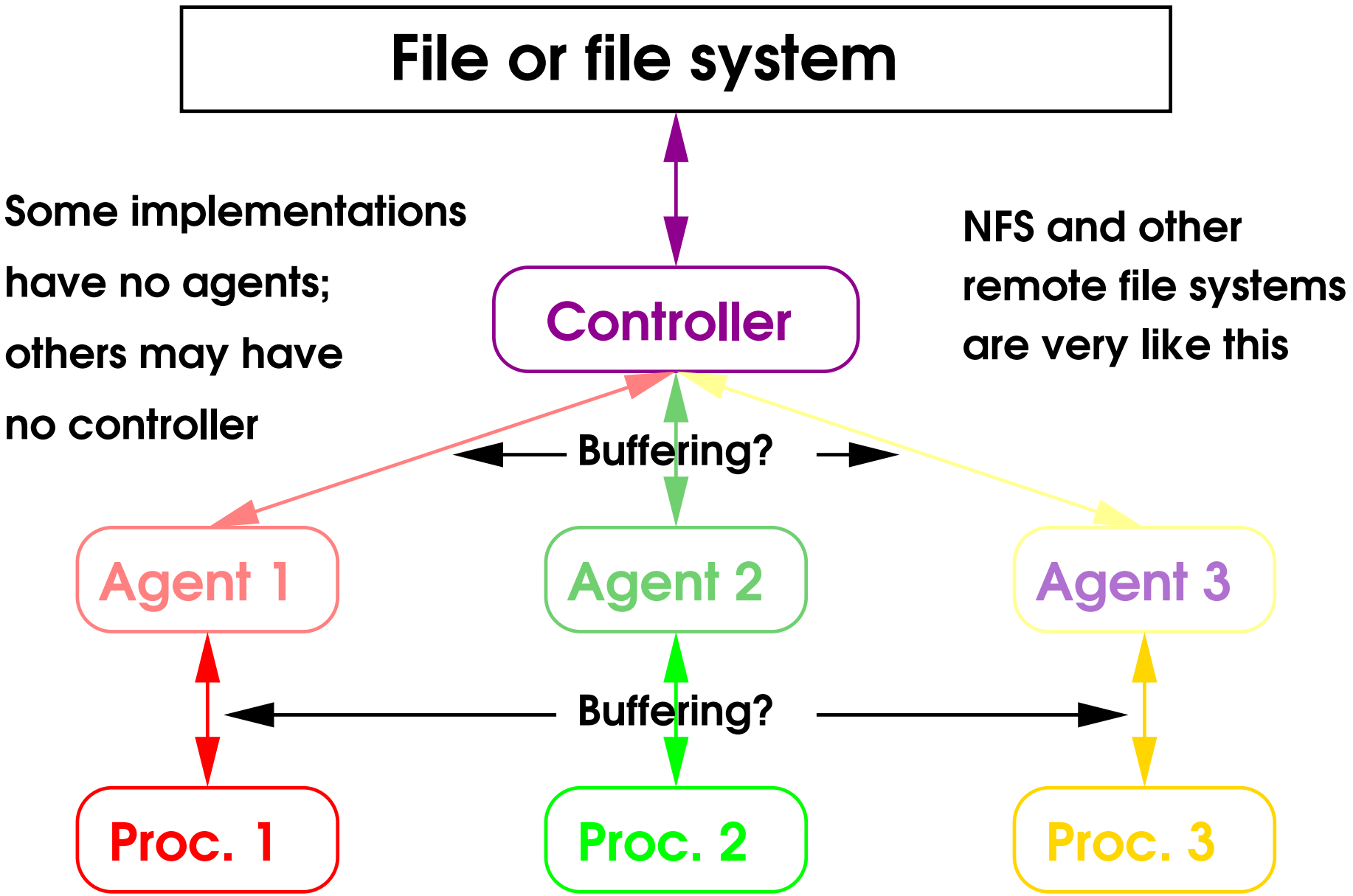
- These issues are NOT specific to MPI

Other parallel interfaces have the same problems

Shared I/O Descriptors



Agent−based I/O Handling



Shared File Access (1)

- Assume all processes share a filing system

Directly, using POSIX, or indirectly, using NFS
Or with the Microsoft and other equivalents

- And that all processes share a working directory

With luck, that's controllable or your home directory
The details are very system–dependent, as usual

- Here are some rules on how to use files safely

Shared File Access (2)

- Always use write–once or read–many

That applies to the whole duration of the run

- All updates and accesses must be considered

Including any that are done outside MPI

I.e. if a file is updated at any time in the run
only one process opens it in the whole run

Any number of processes may read a file
provided that no process updates it

Directories

- Regard a directory as a single file (it is)

If you change it in any way in any process

- Don't access it from any other process

Creating a file in it counts as a change, of course

If you do, a parallel directory listing may fall over!
Listing a read–only directory is safe

- Can create and delete separate files fairly safely

[But not under Microsoft DFS, I am afraid]
Create and delete any single file in one process

Scratch Files

Don't assume where scratch files go
That statement applies even on serial systems
It is even more complicated on parallel ones

It's common to have shared working directories
But separate, distributed scratch directories

- Just a warning – clean code rarely has trouble

Standard Units

Issues arise from implementation details

- Almost always show up with output

Probably just because almost all programs use it!

- It is an almost unbelievable can of worms

Don't even try to program round the problems
Only solution is to bypass the issue entirely

- These issues are NOT specific to MPI

Other parallel interfaces have the same problems

Avoiding the Mess

The "right" solution is also the simplest
Only root process does stdin/stdout I/O
See the extra I/O lecture for the full details on this

It does all the reading from stdin
It broadcasts or scatters it to the others

It gathers all of the output from the others
And then it writes it to stdout

This can also be done for file I/O

Handling Standard I/O

You have learnt all of the techniques you need
Or look at the extra I/O lecture for details
It has quite a lot of worked examples

If root process both handles I/O and computation
I do not recommend doing it asynchronously
It's extremely hard to make such code reliable

- Code the I/O transfers as a collective

That's not too difficult to debug and tune

Error Messages etc.

- Just write to stderr or equivalent

Fortran users may need to use FLUSH

It may well get mangled (reasons given above)
It may get lost on a crash or MPI_Abort
But it's simple, and errors are rare, right?

Same applies to stdout, with some programs

- Beyond that, use a dedicated I/O process

Just as we described for stdout above

Practicals

There's a trivial one on transferring structures

There are some practicals on I/O handling
Mainly spooling it through the root process

You have already learnt all of the techniques needed

- You are likely to need to be able to do this

Handling I/O is a bit tricky for the time available

But do look at the handouts and extra lectures

- You are likely to need to be able to do this

Appendix: Progress

MPI has an arcane concept called "progress"
Good news: needn't understand it in detail

MPI does not specify how it is implemented
Progress can be achieved in many ways

Bad news: do need to understand these issues

Will describe a few of the most common methods

Behind The Scenes (1)

MPI does not specify synchronous behaviour
All transfers can occur asynchronously
And, in theory, so can almost all other actions

Transfers can overlap computation, right?
Unfortunately, it isn't as simple as that

Many I/O mechanisms are often CPU bound
TCP/IP over Ethernet is often like that

Will come back to this in a moment

Behind The Scenes (2)

MPI transfers also include data management
E.g. scatter/gather in MPI derived datatypes

InfiniBand has such functionality in hardware
Does your implementation use it, or software?

Does your implementation use asynchronous I/O?
POSIX's spec. (and .NET's?) is catastrophic

May implement transfers entirely synchronously
Or may use a separate thread for transfers

Eager Execution

This is one of the mainly synchronous methods
Easiest to understand, not usually most efficient

All MPI calls complete the operation they perform
Or as much of it as they can, at the time of call

- MPI_Wtime gives the obvious results

Slow calls look slow, and fast ones look fast

- Often little point in non–blocking transfers

But see later for more on this one

Lazy Execution

This is one of the mainly synchronous methods
Just not in the way most people expect

Most MPI calls put the operation onto a queue
All calls complete queued ops that are "ready"

- MPI_Wtime gives fairly strange results

One MPI call often does all of the work for another
The total time is fairly reliable, though

Possibly the most common implementation type

Asynchronous Execution

MPI calls put the operation onto a queue
Another process or thread does the work

- MPI_Wtime gives very strange results

Need to check the time used by the other thread

- Start by not using all CPUs for MPI

Further tuning is tricky – ask for help

Fairly rare – I have seen it only on AIX
May become more common on multi–core systems

Asynchronous Transfers

Actual data transfer is often asynchronous
E.g. TCP/IP+Ethernet uses a kernel thread

- One critical question is if it needs a CPU

If so, using only some CPUs may well help (a lot)

- Sometimes, non–blocking transfers work better

Even on implementations with eager execution

- And sometimes, blocking transfers do

Even with asynchronous execution