

Message Passing Programming

Designing MPI Applications



Reusing this material



This work is licensed under a Creative Commons Attribution-NonCommercial-ShareAlike 4.0 International License.

http://creativecommons.org/licenses/by-nc-sa/4.0/deed.en_US

This means you are free to copy and redistribute the material and adapt and build on the material under the following terms: You must give appropriate credit, provide a link to the license and indicate if changes were made. If you adapt or build on the material you must distribute your work under the same license as the original.

Acknowledge EPCC as follows: “© EPCC, The University of Edinburgh, www.epcc.ed.ac.uk”

Note that this presentation contains images owned by others. Please seek their permission before reusing these images.

Overview

- Lecture will cover
 - MPI portability
 - maintenance of serial code
 - general design
 - debugging
 - verification

MPI Portability

- Potential deadlock
 - you may be assuming that **MPI_Send** is asynchronous
 - it often is buffered for small messages
 - but threshold can vary with implementation
 - a correct code should run if you replace all **MPI_Send** calls with **MPI_Ssend**
- Buffer space
 - cannot assume that there will be space for **MPI_Bsend**
 - default buffer space is zero!
 - be sure to use **MPI_Buffer_Attach**
 - some advice in MPI standard regarding required size

Data Sizes

- Be careful of data sizes or layout
 - use runtime enquiry functions for Fortran types
 - be careful of compiler-dependent padding for structures
- Changing precision
 - when changing from, say, `float` to `double`, must change all the MPI types from `MPI_FLOAT` to `MPI_DOUBLE` as well
- Easiest to achieve with an include file
 - e.g. every routine includes `precision.h`

Changing Precision: C

- Define a header file called, e.g. `precision.h`
 - `typedef float RealNumber`
 - `#define MPI_REALNUMBER MPI_FLOAT`
- Include in every function
 - `#include "precision.h"`
 - `...`
 - `RealNumber x;`
 - `MPI_Routine(&x, MPI_REALNUMBER, ...);`
- Global change of precision now easy
 - edit 2 lines in one file: `float`->`double`, `MPI_FLOAT`->`MPI_DOUBLE`

Changing Precision: Fortran

- Define a module called, e.g., `precision`
 - `integer, parameter :: REALNUMBER=kind(1.0e0)`
 - `integer, parameter :: MPI_REALNUMBER = MPI_REAL`
- Use in every subroutine
 - `use precision`
 - `...`
 - `REAL(kind=REALNUMBER) :: x`
 - `call MPI_ROUTINE(x, MPI_REALNUMBER, ...)`
- Global change of precision now easy
 - change `1.0e0` -> `1.0d0`, `MPI_REAL`-> `MPI_DOUBLE_PRECISION`

Testing Portability

- Run on more than one machine
 - assuming the implementations are different
 - many parallel clusters will use the same open-source MPI
 - e.g. OpenMPI or MPICH2
 - running on two different mid-sized machines may not be a good test
- More than one implementation on same machine
 - e.g. run using both MPICH2 **and** OpenMPI on your laptop
 - very useful test, and can give interesting performance numbers
- More than one compiler
 - `user@cluster$ module switch mpich2-gcc mpich2-intel`

Serial Code

- Adding MPI can destroy a code
 - would like to maintain a serial version
 - i.e. can compile and run identical code without an MPI library
 - not simply running MPI code with $P=1$!
- Need to separate off communications routines
 - put them all in a separate file
 - provide a dummy library for the serial code
 - no explicit reference to MPI in main code

Example: Initialisation

```
! parallel routine
subroutine par_begin(size, procid)
  implicit none
  integer :: size, procid
  include "mpif.h"
  call mpi_init(ierr)
  call mpi_comm_size(MPI_COMM_WORLD, size, ierr)
  call mpi_comm_rank(MPI_COMM_WORLD, procid, ierr)
  procid = procid + 1
end subroutine par_begin

! dummy routine for serial machine
subroutine par_begin(size, procid)
  implicit none
  integer :: size, procid
  size = 1
  procid = 1
end subroutine par_begin
```

Example: Global Sum

```
! parallel routine
subroutine par_dsum(dval)
  implicit none
  include "mpif.h"
  double precision :: dval, dtmp
  call mpi_allreduce(dval, dtmp, 1, MPI_DOUBLE_PRECISION, &
                    MPI_SUM, comm, ierr)

  dval = dtmp
end subroutine par_dsum

! dummy routine for serial machine
subroutine par_dsum(dval)
  implicit none
  double precision dval
end subroutine par_dsum
```

Example Makefile

```
SEQSRC= \  
    demparams.f90 demrand.f90 demcoord.f90 demhalo.f90 \  
    demforce.f90 demlink.f90 demcell.f90 dempos.f90 \  
    demons.f90
```

```
MPISRC= \  
    demparallel.f90 \  
    demcomms.f90
```

```
FAKESRC= \  
    demfakepar.f90 \  
    demfakecomms.f90
```

```
#PARSRC=$(FAKESRC)  
PARSRC=$(MPISRC)
```

Advantages of Comms Library

- Can compile serial program from same source
 - makes parallel code more readable
- Enables code to be ported to other libraries
 - more efficient but less versatile routines may exist
 - e.g. Cray-specific SHMEM library
 - can even choose to only port a subset of the routines
- Library can be optimised for different MPIs
 - e.g. choose the fastest send (**S**send, **S**end, **B**send?)

Design

- Separate the communications into a library
- Make parallel code similar as possible to serial
 - e.g. use of halos in case study
 - could use the same update routine in serial and parallel

```
serial:    update(new, old, M,  N );
parallel: update(new, old, MP, NP);
```
 - may have a large impact on the design of your serial code
- Don't try and be too clever
 - don't agonise whether one more halo swap is really necessary
 - just do it for the sake of robustness

General Considerations

- Compute everything everywhere
 - e.g. use routines such as **Allreduce**
 - perhaps the value only really needs to be known on the master
 - but using **Allreduce** makes things simpler
 - no serious performance implications
- Often easiest to make P a compile-time constant
 - may not seem elegant but can make coding much easier
 - e.g. definition of array bounds
 - put definition in an include file
 - a clever **Makefile** can reduce the need for recompilation
 - only recompile routines that define arrays rather than just use them
 - pass array bounds as arguments to all other routines

Debugging

- Parallel debugging can be hard
- Don't assume it's a parallel bug!
 - run the serial code first
 - then the parallel code with $P=1$
 - then on a small number of processes ...
- Writing output to separate files can be useful
 - e.g. log.00, log.01, log.02, for ranks 0, 1, 2, ...
 - need some way easily to switch this on and off
- Some parallel debuggers exist
 - Totalview is the leader across all largest platforms
 - Allinea DDT is becoming more common across the board

General Debugging

- People seem to write programs DELIBERATELY to make them impossible to debug!
 - my favourite: the silent program
 - “my program doesn’t work”
 - \$ `mprun -np 6 ./program.exe`
 - \$ `SEGV core dumped`
 - where did this crash?
 - did it run for 1 second? 1 hour? in a batch job this may not be obvious
 - did it even start at all?

Why don’t people write to the screen!!!

Program should output like this

```
$ mprun -np 6 ./program.exe
Program running on 6 processes
Reading input file input.dat ...
... done
Broadcasting data ...
... done
rank 0: x = 3
rank 1: x = 5
etc etc
Starting iterative loop
iteration 100
iteration 200
finished after 236 iterations
writing output file output.dat ...
... done
rank 0: finished
rank 1: finished
...
Program finished
```

Typical mistakes

- Don't write raw numbers to the screen!

- what does this mean?

```
$ mprun -np 6 ./program.exe
```

```
1 3 5.6
```

```
3 9 8.37
```

- programmer has written

```
$ printf("%d %d %f\n", rank, j, x);
```

```
$ write(*,*) rank, j, x
```

- Takes an extra 5 seconds to type:

```
$ printf("rank, j, x: %d %d %f\n", rank, j, x);
```

```
$ write(*,*) `rank, j, x: `, rank, j, x
```

- and will save you HOURS of debugging time

- Why oh why do people write raw numbers?!?!?

Debugging walkthrough

- My case study code gives the wrong answer
- Stages:
 - initialise data
 - distribute to processes
 - update for many steps
 - requiring halo swaps
 - collect data back
 - write data out
- Final stage shows the error
 - but where did it first go wrong?

Where is it going wrong?

- On initialisation?
 - On distribute (i.e. scatter) ?
 - On update?
 - on halo swaps?
 - on left/right swaps?
 - on up/down swaps?
 - On collection (i.e gather) ?
 - On output?
- All these can be checked individually with simple tests

Common mistake

- There was a bug, but I changed something ...
 - and it now works (but I don't know why)
- All is OK!
- No!
 - there is a bug
 - you **MUST** find it
 - if not, it will come back later to bite you **HARD**
- Debugging is an experimental science

Verification: Is My Code Working?

- Should the output be identical for any P ?
 - very hard to accomplish in practice due to rounding errors
 - may have to look hard to see differences in the last few digits
 - typically, results vary slightly with number of processes
 - need some way of quantifying the differences from serial code
 - and some definition of “acceptable”
- What about the same code for fixed P ?
 - identical output for two runs on same number of processes?
 - should be achievable with some care
 - not in specific cases like dynamic task farms
 - possible problems with global sums
 - MPI doesn't require reproducibility, but most implementations are
 - without this, debugging is almost impossible

Parallelisation

- Some parallel approaches may be simple
 - but not necessarily optimal for performance
 - case study example is very simple due to 1D decomposition
 - but not particularly efficient for large P
 - often need to consider what is the realistic range of P
- Some people write incredibly complicated code
 - step back and ask: what do I actually want to do?
 - is there an existing MPI routine or collective communication?
 - should I reconsider my approach if it prohibits me from using existing routines, even if it is not quite so efficient?

Optimisation

- Keep running your code
 - on a number of input data sets
 - with a range of MPI processes
- If scaling is poor
 - find out what parallel routines are the bottlenecks
 - again, much easier with a separate comms library
- If performance is poor
 - work on the serial code
 - return to parallel issues later on

Conclusions

- Run on a variety of machines
- Keep it simple
- Maintain a serial version
- Don't assume all bugs are parallel bugs
- Find a debugger you like (good luck to you)