Message Passing Programming

Designing MPI Applications

Reusing this material

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 often 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-pgi mpich2-gcc`**

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 (`Ssend`, `Send`, `Bsend`?)

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 know 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:
  - read data in
  - distribute to processes
  - update many times
    - 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 input?
- On distribute?
- On update?
  - on halo swaps?
  - on left/right swaps?
  - on up/down swaps?
- On collection?
- On output?

- All these can be checked with simple tests

Common mistake

- 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)