

Message Passing Programming

Tips and tricks

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Aims

- To write correct MPI programs
 - that are portable to many systems
 - that are efficient
 - that are easy to maintain

Common problems in MPI

- Assuming MPI_Send is asynchronous
- Data sizes
- Non-portability
- Programs with specific process counts
- Not calling collectives collectively
- Incorrect use of non-blocking
- Sending lots of small messages
- Array allocation issues in C
- Array syntax issues in Fortran
- Code readability
- Debugging problems

Assuming MPI_Send is asynchronous

- Potential deadlock
 - you may be assuming that **MPI_Send** is asynchronous
 - it often *is* buffered for small messages
 - but threshold will vary with implementation
 - your code may run on one machine and deadlock on another
 - correct code will run with all **MPI_Send** calls replaced by **MPI_Ssend**
- Buffer space
 - cannot assume that there will be space for **MPI_Bsend**
 - default buffer space may be zero!
 - be sure to use **MPI_Buffer_attach**
 - some advice in MPI standard regarding required size
 - allow for space for message headers: **MPI_BSEND_OVERHEAD**

Data Sizes

- Be careful of data sizes or layout
 - use runtime enquiry functions for Fortran types
 - be careful of compiler-dependent padding for structures
- Do not use magic compiler flags to change precision!
`cc -convert-floats-to-doubles *.c`
- 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`

Non-portability

- Correct C code should compile correctly with *any* C compiler
- Correct MPI code should also run correctly with *any* MPI library
- Run on more than one machine
 - assuming the MPI libraries are different
 - many parallel clusters will use the same open-source MPI
 - e.g. OpenMPI or MPICH2
 - running on two different HPC systems 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`

Code Readability

- 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?)

Not calling collectives correctly

- Collectives must be called by all processes in communicator
 - this will not work correctly on more than a single process

```
if (rank == 0) MPI_Bcast(x, 10, MPI_INT, 0, MPI_COMM_WORLD);
```

- an **Allreduce** called like this would deadlock
- Compute everything everywhere
 - e.g. use routines such as **Allreduce** in preference to **Reduce**
 - perhaps the value only really needs to be known on the master
 - but using **Allreduce** makes things simpler
 - no serious performance implications

Error checking and reductions

```
// Check for valid results
MPI_Reduce(&partial, &sum,
           1, MPI_FLOAT, MPI_SUM, 0, MPI_COMM_WORLD);
MPI_Bcast(&sum, 1, MPI_FLOAT, 0, MPI_COMM_WORLD);
if (sum < 0)
{
    if (rank == 0) printf("Error: sum = %f\n", sum)
    MPI_Finalize();
}
```

- Do not use reduce + broadcast!
 - use allreduce

Sending lots of small messages

```
for (j=0; j < N; j++)  
{  
    MPI_Send(&x[0][j], 1, MPI_INT, dest, 0, comm);  
}
```

- Send a single message of size N

```
MPI_Send(&x[0][0], N, MPI_INT, dest, 0, comm);
```

- Use a derived type, e.g. a vector, for equivalent loop over i

```
MPI_Send(&x[0][0], 1, my_mpi_vector, dest, 0, comm);
```

Programs with specific process counts

- Do not write code like:

```
if (rank == 0) {  
    for (i=1; i <= N/4; i++)  
        pi = pi + 1.0/(1.0 + pow((((double)i)-0.5)/((double) N),2.0));  
} else if (rank == 1)  
    for (i=N/4+1; i <= N/2; i++)  
        pi = pi + 1.0/(1.0 + pow((((double)i)-0.5)/((double) N),2.0));  
} else ...
```

- 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 and *check at runtime* that size = P !!
 - a clever Makefile can reduce the need for recompilation
 - only recompile routines that define arrays rather than use them

Incorrect use of non-blocking

```
if (rank == 0) {  
    for (i=1; i < size; i++) {  
        MPI_Issend(x, 10, MPI_INT, i, 0, comm, &request);  
    }  
} else MPI_Irecv(x, 10, MPI_INT, 0, 0, comm, &request);  
  
// now start computation
```

- Need multiple requests on rank 0
 - and they *must* be waited on at some later point
- Why use non-blocking here at all?
 - avoid complication unless this is performance critical

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
 - Allinea DDT is becoming more common across the board
 - a commercial product
 - debuggers can powerful tools but also very complicated

General Debugging

- People seem to write programs DELIBERATELY to make them impossible to debug!
 - my favourite: the silent program
 - “my program doesn’t work”
 - \$ `mpirun -n 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?!?!

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
 - start with the serial code
 - then $P = 1$
 - then a small process count ...

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

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

Fortran array syntax

- MPI derived types enable strided data to be sent/received
 - no explicit copy in/out required
- For Fortran
 - why not use Fortran array syntax?
- Some subtleties for non-blocking operations

Non-blocking operations

- What is wrong with this code?

```
allocate(buf(n))  
call MPI_Issend(buf, n, ....)  
deallocate(buf)
```

- Non-blocking send may still be ongoing at deallocation
 - code could crash or give unpredictable behaviour
 - only safe to deallocate the memory after the matching wait
- Identical issues in C using malloc and free
 - however, the problem arises in a more subtle way in Fortran
 - due to its more sophisticated array handling

Fortran array syntax

```
real, dimension(m,n) :: array  
call MPI_Issend(array(1,1:n), n, MPI_REAL, ...)  
...
```

- Looks ok but compiler will probably do:

```
allocate buf(n)  
buf(1:n) = array(1,1:n)  
call MPI_Issend(buf, n, MPI_REAL, ...)  
array(1,1:n) = buf(1:n)  
deallocate(buf)
```

- so buf may not exist when message is sent
- issue even more severe for non-blocking receive

Solutions

- Note this *only an issue for non-blocking operations*
 - e.g. can do normal blocking send and receive using array syntax
- Advice
 - avoid array syntax, even for contiguous sections (e.g. columns)
`call MPI_Issend(array(1,1), m, ...)`
 - rather than
`call MPI_Issend(array(1:m,1), m, ...)`
- Derived datatypes (e.g. vectors) for non-contiguous rows

`call MPI_Issend(array(1,1), 1, rowtype, ...)`

Array allocation issues with C

C: **x[16]**

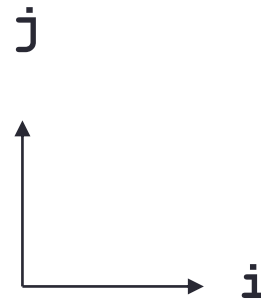
F: **x(16)**

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
---	---	---	---	---	---	---	---	---	----	----	----	----	----	----	----

C: **x[4][4]**

F: **x(4,4)**

4	8	12	16
3	7	11	15
2	6	10	14
1	5	9	13



13	14	15	16
9	10	11	12
5	6	7	8
1	2	3	4

- Data is contiguous in memory
 - different conventions in C and Fortran
 - for statically allocated C arrays **x == &x[0][0]**

Aside: Dynamic Arrays in C

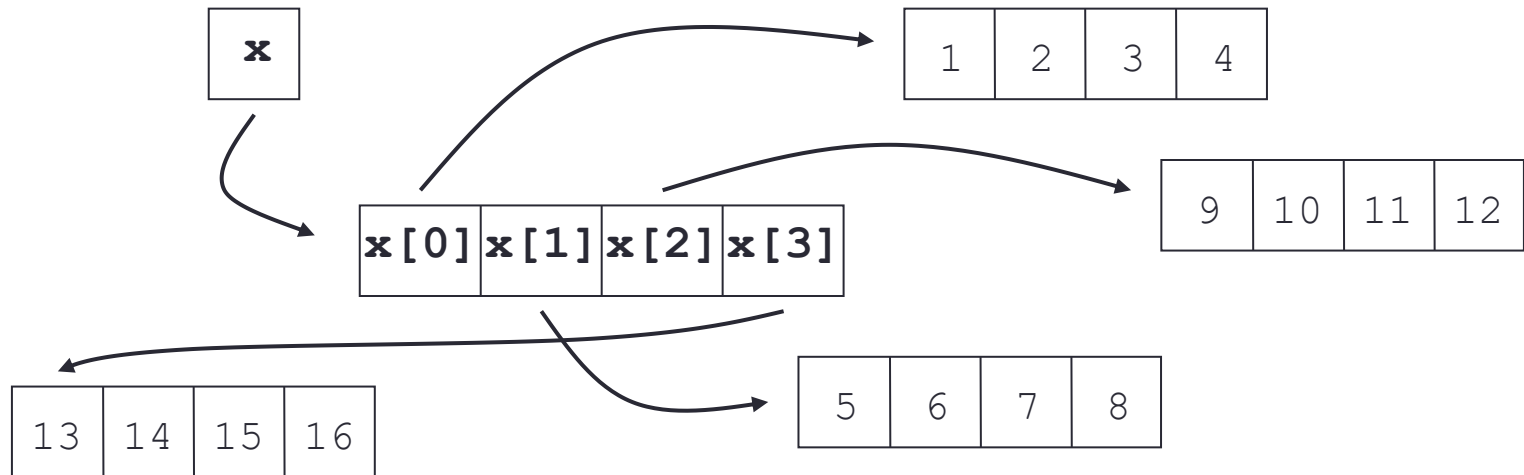
```
float **x = (float **) malloc(4, sizeof(float *));
```

```
for (i=0; i < 4; i++)
```

```
{
```

```
    x[i] = (float *) malloc(4, sizeof(float));
```

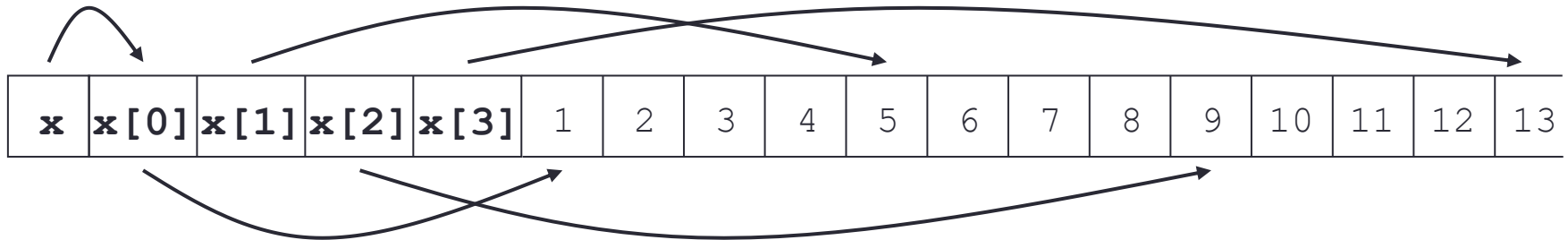
```
}
```



- Data non-contiguous, and `x != &x[0][0]`
 - cannot use regular templates such as vector datatypes
 - cannot pass `x` to any MPI routine

Arralloc

```
float **x = (float **) arralloc(sizeof(float), 2, 4, 4);  
/* do some work */  
free((void *) x);
```



- Data is now contiguous, but still **x** **!=** **&x[0][0]**
 - can now use regular template such as vector datatype
 - must pass **&x[0][0]** (start of contiguous data) to MPI routines
 - see **MPP-arralloc.tar** for example of use in practice
- Clearest to use always use **&x[i][j]** syntax
 - correct for both static and (contiguously allocated) dynamic arrays

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)