MPI version of the Serial Code With One-Dimensional Decomposition

Timothy H. Kaiser, Ph.D.
tkaiser@mines.edu

Overview

We will choose one of the two dimensions and subdivide the domain to allow the distribution of the work across a group of distributed memory processors

We will focus on the principles and techniques used to do the MPI work in the model

Examples:

http://geco.mines.edu/workshop

STEP1: introduce the MPI environment

- Need to include “mpif.h” to define MPI constants
- Need to define our own constants
  - numnodes - how many processors are running
  - myid - Which processor am I
  - mpi_err - error code returned by most calls
  - mpi_master - the id for the master node
- Suggestion - add the following module to your source and “use” it in the program stommel

```
module mpi
    include "mpif.h"
    integer numnodes,myid,mpi_err
    integer, parameter::mpi_master=0
end module
```

STEP1: Start the MPI environment

- Add the following to your program

```
call MPI_INIT( mpi_err )
call MPI_COMM_SIZE(MPI_COMM_WORLD,numnodes,
mpi_err)
call MPI_COMM_RANK(MPI_COMM_WORLD, myid, mpi_err)
write(*,*)’from ‘, myid,’numnodes=‘,numnodes
```

- To stop, add the following next

```
call MPI_Finalize(mpi_err)
stop
```

Input

We read the data on processor 0 and send to the others

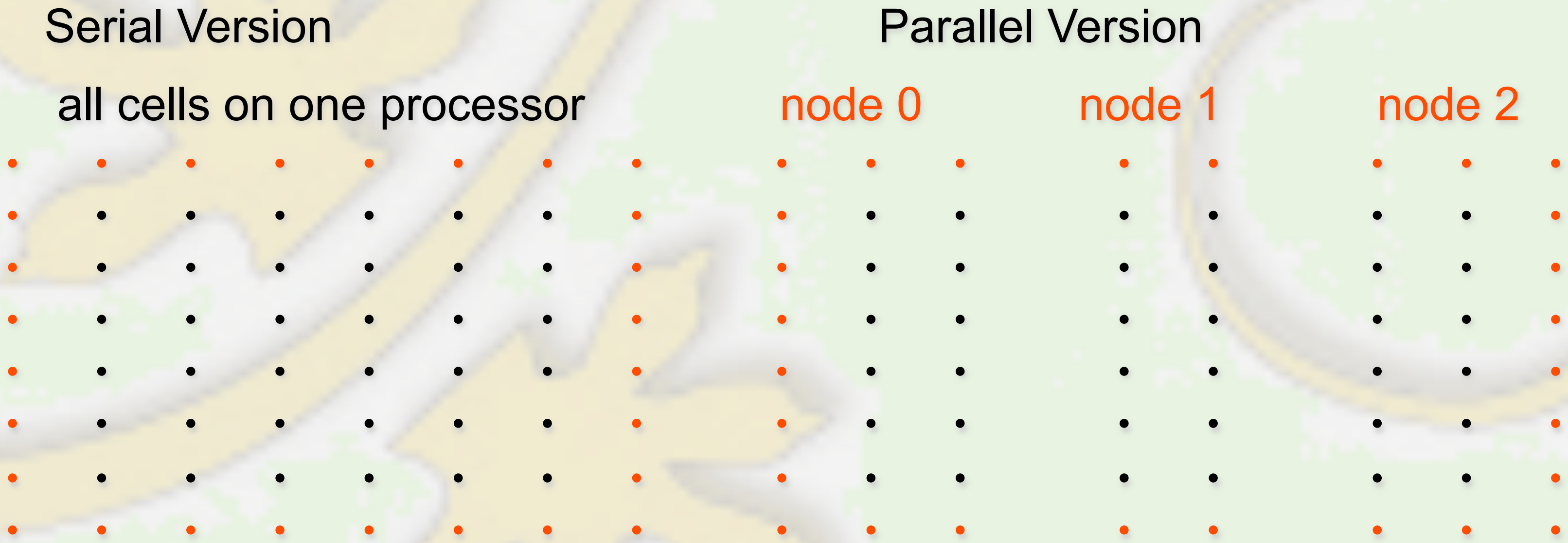
```
if(myid .eq. mpi_master)then
     read(*,*)nx,ny
     read(*,*)lx,ly
     read(*,*)alpha,beta,gamma
     read(*,*)steps
 endif
```

We use MPI_BCAST to send the data to the other processors

- We use 8 calls
- Can you do it in 2?
- How about 1?

Domain Decomposition (1d)

Physical domain is sliced into sets of columns so that computation in each set of columns will be handled by different processors. Why do columns and not rows?



Serial Version

all cells on one processor

Parallel Version

node 0

node 1

node 2

Domain Decomposition (1d)

We set our array bounds differently on each processor so that:

- We take our original grid and break it into numnodes subsections of size nx/numnodes
- Each processor calculates for a different subsection of the grid
- No two processors calculate psi for the same (I,J)

We add special boundary cells for each subsection of the grid called ghost cells

The values for the ghost cells are calculated on neighboring processors and sent using MPI calls.

Domain Decomposition (1d)

With ghost cells our decomposition becomes...

Serial Version

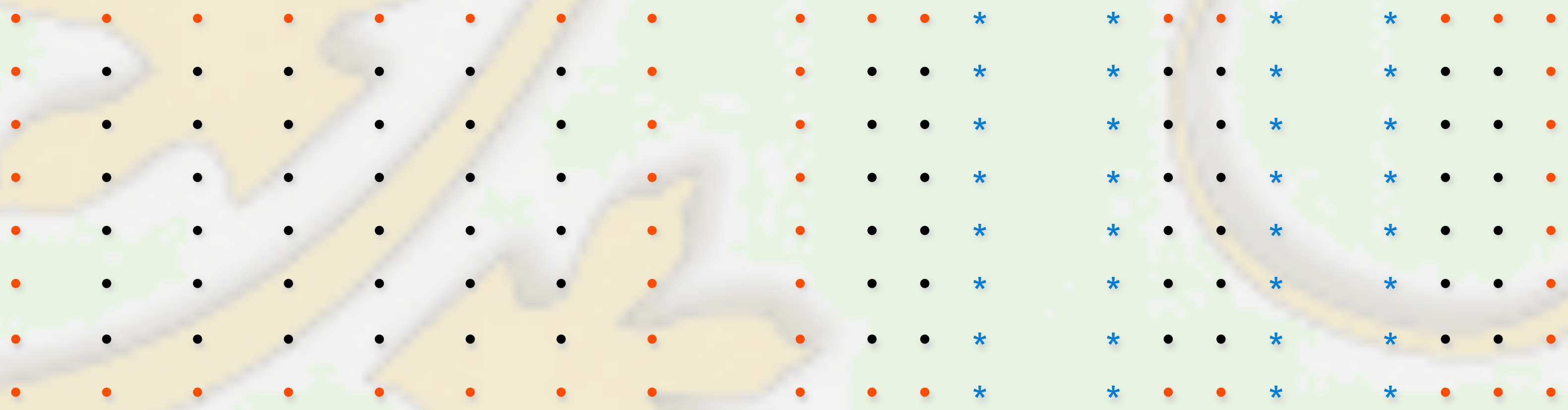
all cells on one processor

Parallel Version

node 0

node 1

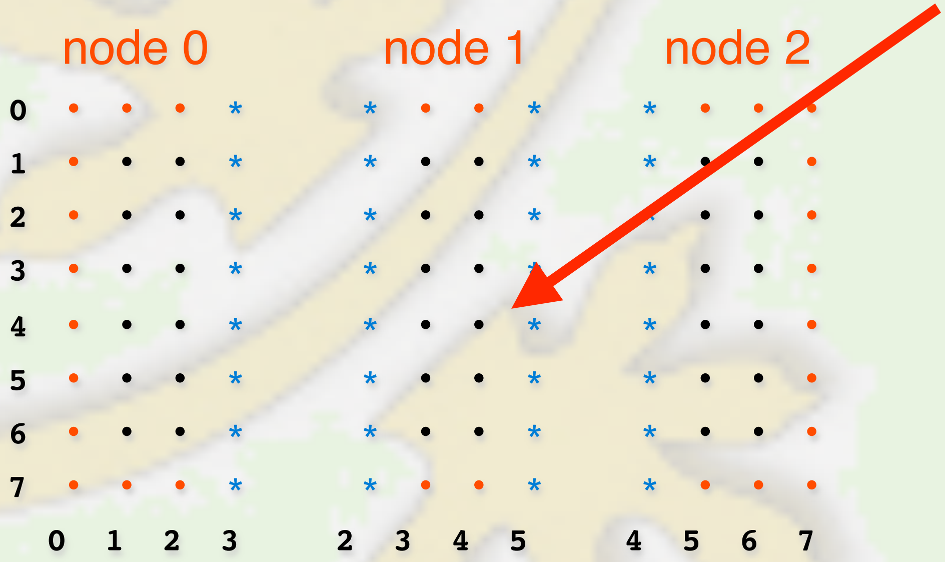
node 2



Domain Decomposition (1d)

How and why are ghost cells used?

Node 0 allocates space for psi(0:7,0:3) but calculates psi(1:6,1,2)
Node 1 allocates space for psi(0:7,2:5) but calculates psi(1:6,3,4)
Node 2 allocates space for psi(0:7,4:7) but calculates psi(1:6,5,6)



To calculate the value for psi(4,4) node1 requires the value from psi (4,3),psi(5,4),psi(3,4),psi(4,5)

Where does it get the value for psi (4,5)? From node2, and it holds the value in a ghost cell

Domain Decomposition (1d)

Source code for setting up the distributed grid with ghost cells

```
! we stripe the grid across the processors
    i1=1
    i2=ny
    dj=real(nx,b8)/real(numnodes,b8)
    j1=nint(1.0_b8+myid*dj)
    j2=nint(1.0_b8+(myid+1)*dj)-1
    write(*,101)myid,i1,i2,j1,j2
101 format("myid= ",i3,3x,                            &
           " (",i3," <= i <= ",i3,") , ", &
           " (",i3," <= j <= ",i3,")")
! allocate the grid to (i1-1:i2+1,j1-1:j2+1) this includes boundary
  cells
    allocate(psi(i1-1:i2+1,j1-1:j2+1))
```

Try adding this to your program. What do you get?

Ghost cell updates

When do we update ghost cells?

Each trip through our main loop we call do_transfer to update the ghost cells

Our main loop becomes...

```
do i=1,steps
    call do_jacobi(psi,new_psi,mydiff,i1,i2,j1,j2)
    call do_transfer(psi,i1,i2,j1,j2)
    write(*,*)i,diff
enddo
```

How do we update ghost cells?

Processors send and receive values to and from neighbors
Need to exchange with left and right neighbors except processors on far left and right only transfer in 1 direction

Trick 1 to avoid deadlock

Even # processors	Odd # processors
send left	receive from right
receive from left	send to right
send right	receive for left
receive from right	send to left

Trick 2 to handle the end processors

Send to MPI_PROC_NULL instead of a real processor

How do we update ghost cells?

```
! How many cells are we sending
    num_x=i2-i1+3


! Where are we sending them
    myleft=myid-1
    myright=myid+1
    if(myleft .le. -1)myleft=MPI_PROC_NULL
    if(myright .ge. numnodes)myright=MPI_PROC_NULL
```

How do we update ghost cells?

For even-numbered processors...

```
if(even(myid))then
! send to left
  call MPI_SEND(psi(:,j1),  num_x,MPI_DOUBLE_PRECISION,myleft, &
            100,MPI_COMM_WORLD,mpi_err)
! rec from left
  call MPI_RECV(psi(:,j1-1),num_x,MPI_DOUBLE_PRECISION,myleft, &
            100,MPI_COMM_WORLD,status,mpi_err)
! rec from right
  call MPI_RECV(psi(:,j2+1),num_x,MPI_DOUBLE_PRECISION,myright, &
            100,MPI_COMM_WORLD,status,mpi_err)
! send to right
  call MPI_SEND(psi(:,j2),  num_x,MPI_DOUBLE_PRECISION,myright, &
            100,MPI_COMM_WORLD,mpi_err)
else
```

How do we update ghost cells?
For odd-numbered processors...

```
Else ! we are on an odd column processor
! rec from right
  call MPI_RECV(psi(:,j2+1),num_x,MPI_DOUBLE_PRECISION,myright, &
               100,MPI_COMM_WORLD,status,mpi_err)
! send to right
  call MPI_SEND(psi(:,j2),  num_x,MPI_DOUBLE_PRECISION,myright, &
               100,MPI_COMM_WORLD,mpi_err)
! send to left
  call MPI_SEND(psi(:,j1),  num_x,MPI_DOUBLE_PRECISION,myleft, &
               100,MPI_COMM_WORLD,mpi_err)
! rec from left
  call MPI_RECV(psi(:,j1-1),num_x,MPI_DOUBLE_PRECISION,myleft, &
               100,MPI_COMM_WORLD,status,mpi_err)
endif
```

How do we update ghost cells?
It’s a 4-stage operation
Example with 4 nodes:

	Proc 0	Proc 1	Proc 2	Proc 3
Stage 1	Send left to MPI_PROC_NULL	Receive right from Proc 2	Send left to Proc 1	Receive right from MPI_PROC_NULL
Stage 2	Receive left from MPI_PROC_NULL	Send right to Proc 2	Receive left from Proc 1	Send right to MPI_PROC_NULL
Stage 3	Receive right from Proc 1	Send right to Proc 0	Receive right from Proc 3	Send right to Proc 2
Stage 4	Send right to Proc 1	Receive right from Proc 0	Send right to Proc 3	Receive right from Proc 2

Only a few other modifications

Force and do_jacobi are not modified

We modify the boundary condition routine only to set value for true boundaries and ignore ghost cells

```
subroutine bc(psi,i1,i2,j1,j2)
! sets the boundary conditions
! input is the grid and the indices for the interior cells
    use numz
    use mpi
    use input, only : nx,ny
    implicit none
    real(b8),dimension(i1-1:i2+1,j1-1:j2+1):: psi
    integer,intent(in):: i1,i2,j1,j2
! do the top edges
    if(i1 .eq.  1) psi(i1-1,:)=0.0_b8
! do the bottom edges
    if(i2 .eq. ny) psi(i2+1,:)=0.0_b8
! do left edges
    if(j1 .eq.  1) psi(:,j1-1)=0.0_b8
! do right edges
    if(j2 .eq. nx) psi(:,j2+1)=0.0_b8
end subroutine bc
```

Residual

- In our serial program, the routine do_jacobi calculates a residual for each iteration
- The residual is the sum of changes to the grid for a jacobi iteration
- Now the calculation is spread across all processors
- To get the global residual, we can use the MPI_Reduce function

```
call MPI_REDUCE(mydiff,diff,1,MPI_DOUBLE_PRECISION, &
        MPI_SUM,mpi_master,MPI_COMM_WORLD,mpi_err)
if(myid .eq. mpi_master)write(*,*)i,diff
```

Our main loop is now…

Call the do_jacobi subroutine
Update the ghost cells
Calculate the global residual

```
do i=1,steps
    call do_jacobi(psi,new_psi,mydiff,i1,i2,j1,j2)
    call do_transfer(psi,i1,i2,j1,j2)
    call MPI_REDUCE(mydiff,diff,1,MPI_DOUBLE_PRECISION, &
             MPI_SUM,mpi_master,MPI_COMM_WORLD,mpi_err)
    if(myid .eq. mpi_master)write(*,*)i,diff
enddo
```

Final change

We change the write_grid subroutine so that each node writes its part of the grid to a different file.

Function unique returns a file name based on a input string and the node number

We change the open statement in write_grid to:

```
open(18,file=unique("out1d_"),recl=max(80,15*((jend-jstart)+3)+2))
```

Unique

We add an interface to unique in the module face

Unique is the function:

```
function unique(name)
    use numz
    use mpi
    character (len=*) name
    character (len=20) unique
    character (len=80) temp
    if(myid .gt. 99)then
      write(temp,"(a,i3)")trim(name),myid
    else
        if(myid .gt. 9)then
            write(temp,"(a,'0',i2)")trim(name),myid
        else
            write(temp,"(a,'00',i1)")trim(name),myid
        endif
    endif
    unique=temp
    return
end function unique
```

Try it!

- Compile
  - `make`
- Run (something like this)
  - `stf_00 < stommel.in`
  - `mpirun -np 4 stf_01 < stommel.in`
-

Suggested exercises

Study, compile, and run the program st_01 on various numbers of processors

Change it to use 2 or 1 MPI_bcast calls instead of 8
Hint: (The "correct" way to do it with 1 call is to use F90- and MPI-derived data types)

Do the decomposition in rows

Do periodic boundary conditions

Modify the write_grid routine to output the whole grid from node 0

2d decomposition

- The program is almost identical
- We now have our grid distributed in a block fashion across the processors instead of striped
- We can have ghost cells on 1, 2, 3 or 4 sides of the grid held on a particular processor

Example 2d Decomposition
50 x 50 grid on 4 processors

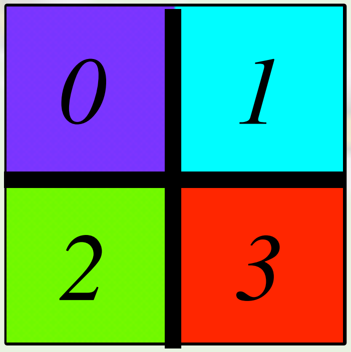
Grid on each processor is allocated to:

pid= 0 (0 <= i <= 26) , (0 <= j <= 26)
pid= 1 (0 <= i <= 26) , (25 <= j <= 51)
pid= 2 (25 <= i <= 51) , (0 <= j <= 26)
pid= 3 (25 <= i <= 51) , (25 <= j <= 51)

But each processor calculates only for:

pid= 0 (1 <= i <= 25) , (1 <= j <= 25)
pid= 1 (1 <= i <= 25) , (26 <= j <= 50)
pid= 2 (26 <= i <= 50) , (1 <= j <= 25)
pid= 3 (26 <= i <= 50) , (26 <= j <= 50)

Extra cells are ghost cells



Grid Distributed across 4 processors

Only three changes need to be made to our program

- Given an arbitrary number of processors, find a good topology (number of rows and columns of processors)
- Make new communicators to allow for easy exchange of ghost cells
  - Set up communicators so that every processor in the same row is in a given communicator
  - Set up communicators so that every processor in the same column is in a given communicator
- Add the up/down communication

Given an arbitrary number of processors, find a good topology (number of rows and columns of processors)

```
 nrow=nint(sqrt(float(numnodes)))
 ncol=numnodes/nrow
 do while (nrow*ncol .ne. numnodes)
     nrow=nrow+1
     ncol=numnodes/nrow
 enddo
 if(nrow .gt. ncol)then
     i=ncol
     ncol=nrow
     nrow=i
 endif
myrow=myid/ncol+1
 mycol=myid - (myrow-1)*ncol + 1
```

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

Make new communicators to allow for easy exchange of ghost cells

```
! make the row and col communicators
! all processors with the same row will be in the same ROW_COMM
call MPI_COMM_SPLIT(MPI_COMM_WORLD,myrow,mycol,ROW_COMM,mpi_err)
call MPI_COMM_RANK( ROW_COMM, myid_row, mpi_err )
call MPI_COMM_SIZE( ROW_COMM, nodes_row, mpi_err )

! all processors with the same col will be in the same COL_COMM
call MPI_COMM_SPLIT(MPI_COMM_WORLD,mycol,myrow,COL_COMM,mpi_err)
call MPI_COMM_RANK( COL_COMM, myid_col, mpi_err )
call MPI_COMM_SIZE( COL_COMM, nodes_col, mpi_err )

! find id of neighbors using the communicators created above
mytop  =myid_col-1;if( mytop    .lt. 0        )mytop  =MPI_PROC_NULL
mybot  =myid_col+1;if( mybot    .eq. nodes_col)mybot  =MPI_PROC_NULL
myleft =myid_row-1;if( myleft   .lt. 0        )myleft =MPI_PROC_NULL
myright=myid_row+1;if( myright  .eq. nodes_row)myright=MPI_PROC_NULL
```

Communication up/down

```
 if(even(myid_row))then
! send to top
        call MPI_SEND(psi(i1,:),num_y,MPI_DOUBLE_PRECISION,mytop,      &
                      10, COL_COMM,mpi_err)
! rec from top
        call MPI_RECV(psi(i1-1,:),num_y,MPI_DOUBLE_PRECISION,mytop,   &
                      10,COL_COMM,status,mpi_err)
! rec from bot
        call MPI_RECV(psi(i2+1,:),num_y,MPI_DOUBLE_PRECISION,mybot,   &
                      10,COL_COMM,status,mpi_err)
! send to bot
        call MPI_SEND(psi(i2,:),num_y,MPI_DOUBLE_PRECISION,mybot,      &
                      10, COL_COMM,mpi_err)
    else
```

Communication up/down (continued)

```
! rec from bot
        call MPI_RECV(psi(i2+1,:),num_y,MPI_DOUBLE_PRECISION,mybot,    &
                      10,COL_COMM,status,mpi_err)
! send to bot
        call MPI_SEND(psi(i2,:),num_y,MPI_DOUBLE_PRECISION,mybot,      &
                      10,COL_COMM,mpi_err)
! send to top
        call MPI_SEND(psi(i1,:),num_y,MPI_DOUBLE_PRECISION,mytop,      &
                      10,COL_COMM,mpi_err)
! rec from top
        call MPI_RECV(psi(i1-1,:),num_y,MPI_DOUBLE_PRECISION,mytop,    &
                      10,COL_COMM,status,mpi_err)
    endif
```

The rest of the examples:

http://geco.mines.edu/workshop