MPI Version of the Stommel Code with One and Two Dimensional Decomposition

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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

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

Suggestion - 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
```

STEP2: Try it!

Compile

```
f90 -ffree stommel.f -o st_1d
```

Run

```
mpprun -n 3 st_1d
```

Try running again. Do you get the same output?

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

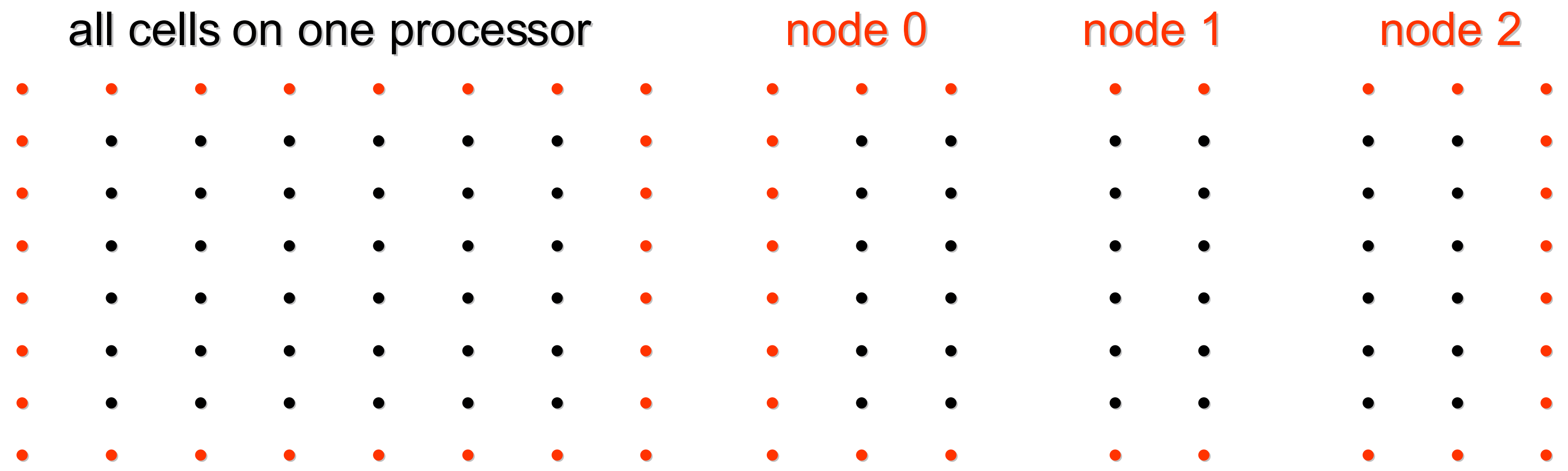
- We use 8 calls
- Can you do it in 2?
- How about 1?

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

Parallel Version

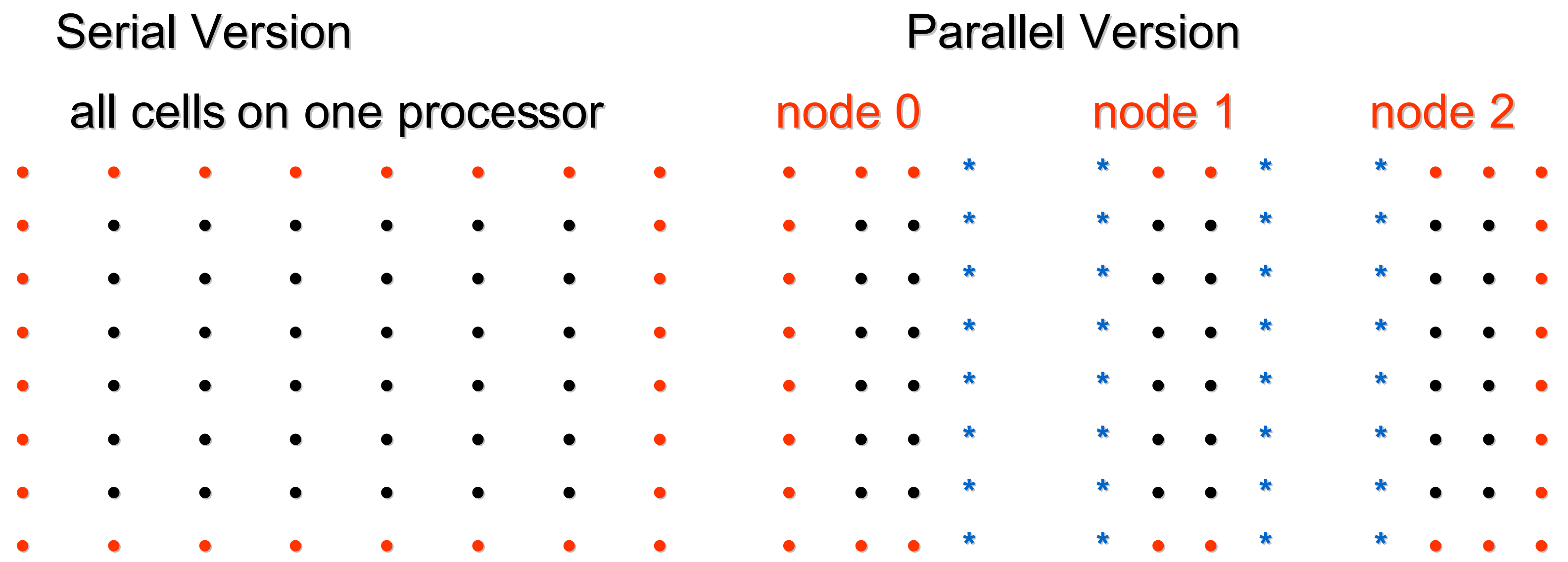


Domain Decomposition (1d)

- Fortran 90 allows us to set arbitrary bounds on arrays
- 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)
  - For whichever processor hold Psi(I,J) it corresponds exactly to Psi(I,J) in the serial program
- 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)

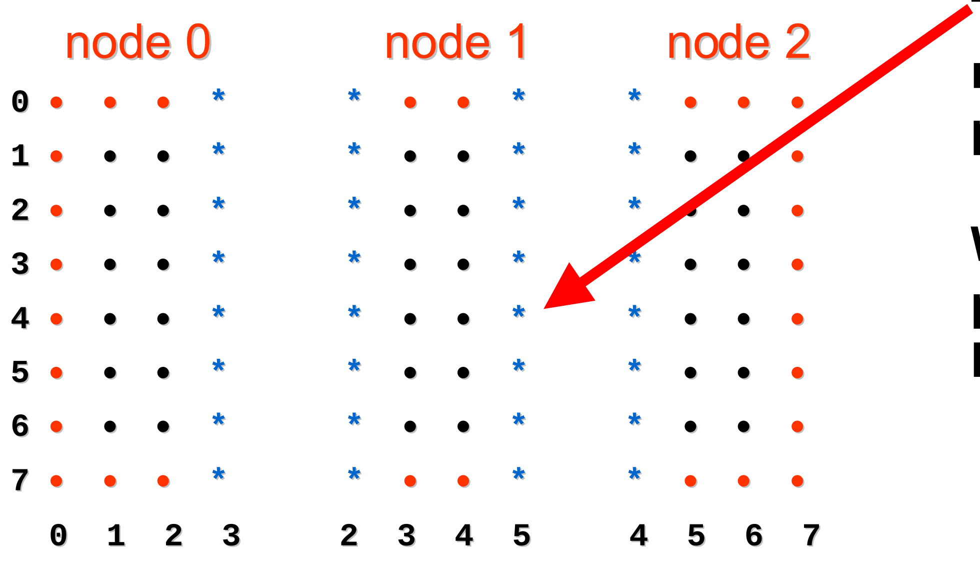
With ghost cells out decomposition becomes...



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 up date 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:

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

Only a few other modifications

Force and do_jacobi are not modified

We modify the boundary condition routine to only 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 an 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
```

Suggested exercises

Study, compile and run the program st_1d.f 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

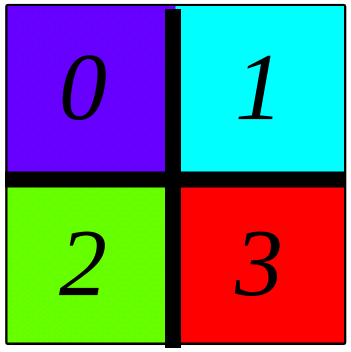
Grid on each processor is allocated to:

```
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
```

We may want the master to do all output

Each processor holds a section of the grid

If each node writes we end up with a lot of pieces

If we have good communication it may be faster for 1 processor to write the file

We want a scalable solution

Write the grid from the master

Write a line (row) at a time

```
Do I=i0,i3   (A four step process)
    (1) Processors find how much of the line they
        hold
    (2) Processors tell master how much of the line
        they have (MPI_GATHER)
    (3) Processors send the data to the master
        (MPI_GATHERV)
    (4) Master prints the line
Enddo
```

Processors find how much of the line they hold

```
! Check to see if the present line is within
! the section that I hold
if(i .ge. istart .and. i .le. iend)then
    dj=jend-jstart+1
    mystart=jstart
    myend=jend
    icol=i
else ! I don't send anything
    dj=0
    mystart=jstart
    myend=jstart
    icol=istart
endif
```

Processors tell master how much of the line they have (MPI_GATHER)

```
call MPI_GATHER(dj    , 1,  MPI_INTEGER, &
               counts, 1,  MPI_INTEGER, &
              mpi_master,MPI_COMM_WORLD,mpi_err)
```

Each processor sends its "number to be sent" value in dj, type MPI_INTEGER

Mpi_master gets a "number to be sent" from each processor in the array counts

Processors send the data to the master (MPI_GATHERV)

```
if(myid .eq. mpi_master)then
    do k=1,numnodes-1
        offsets(k)=counts(k-1)+offsets(k-1)
    enddo
endif
call MPI_GATHERV(psi(icol,mystart:myend),dj,&
                 MPI_DOUBLE_PRECISION,      &
                 arow,counts,offsets,    &
                 MPI_DOUBLE_PRECISION,      &
                 mpi_master,MPI_COMM_WORLD, &
                 mpi_err)
```

Processors send the data to the master (MPI_GATHERV)

`Psi(icol,mystart:myend)` : data being sent

`Dj` : number of values being sent

`Arow` : data ends up here

`Counts` : array that holds the number of values being sent from each processor

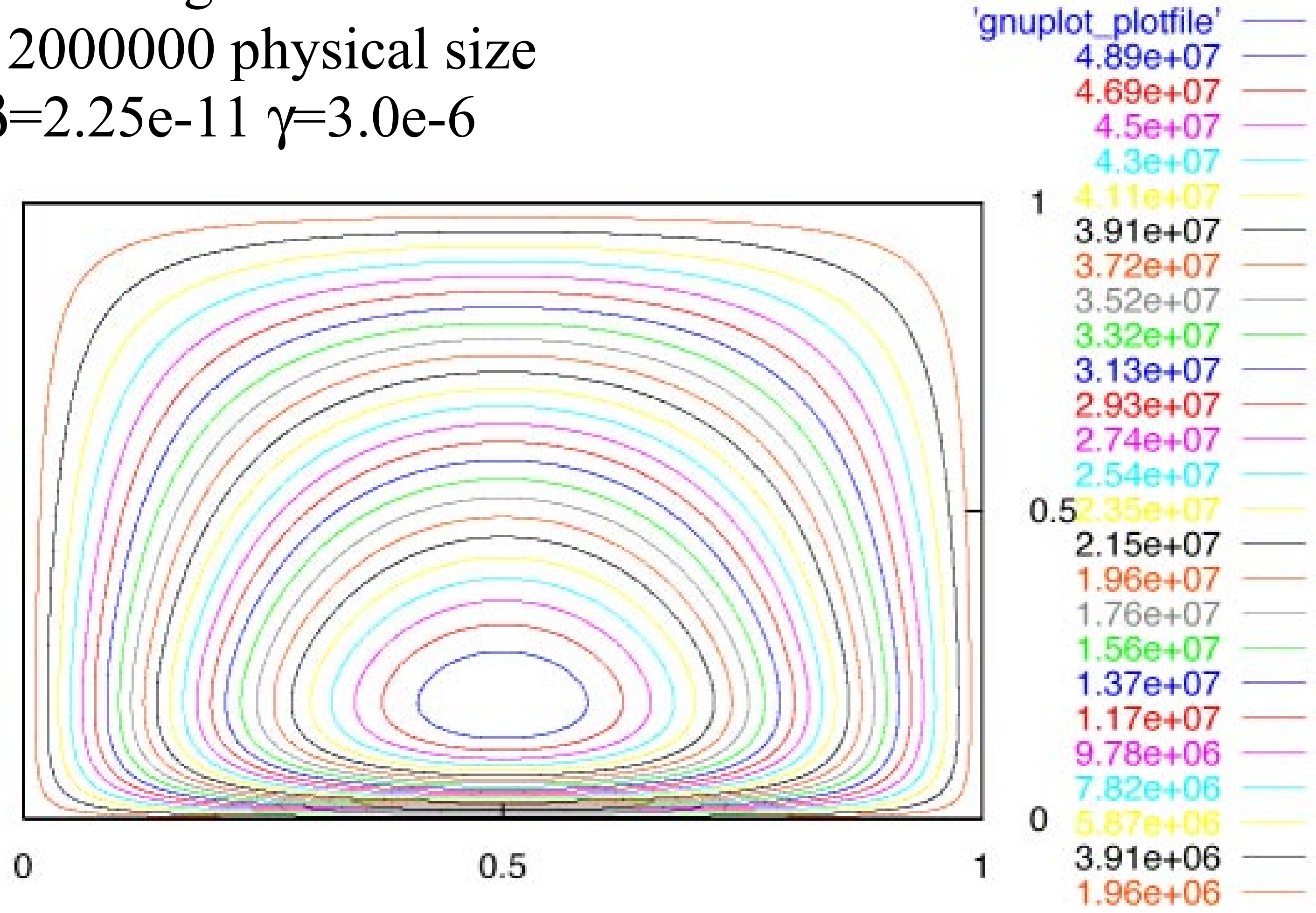
`Offsets` : array that holds a pointer to the beginning of values received from each processor, calculated form counts

Master writes the data

```
if(myid .eq. mpi_master)then
  do j=j0,j3
    write(18,'(g14.7)',advance="no")arow(j)
  enddo
  write(18,*)
endif
```

The answer is: (after 75,000 iterations)

200 x 200 interior grid size
2000000 x 2000000 physical size
α=1.0e-9 β=2.25e-11 γ=3.0e-6


'gnuplot_plotfile'
4.89e+07
4.69e+07
4.5e+07
4.3e+07
4.11e+07
3.91e+07
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3.32e+07
3.13e+07
2.93e+07
2.74e+07
2.54e+07
2.35e+07
2.15e+07
1.96e+07
1.76e+07
1.56e+07
1.37e+07
1.17e+07
9.78e+06
7.82e+06
5.87e+06
3.91e+06
1.96e+06