Foundations of High Performance Computing

Lecture 7: Domain Decomposition by means of MPI

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“Foundation of HPC” course

DATA SCIENCE & SCIENTIFIC COMPUTING

Agenda

- Domain Decomposition approach
- A Real example

Domain Decomposition

- A fundamental technique in both parallel programming and MPI programming
- The way to solve very large problems in memory on distributed memory architecture
- Useful to know some trick of the trade to deal with that using MPI

What is domain decomposition?

- Perform a numerical simulation (e.g. solve an equation) on a domain of given shape
- Discretize the domain using a mesh or particles
- Split the work (and memory!) among N processors
- Can be done “geographically” or purely on the data, irrespective of their spatial location
- Domains can have complex shapes

Goals to achive..

- All processors having equal (in terms of wall- clock time) amounts of work

  ==> “Load balancing”

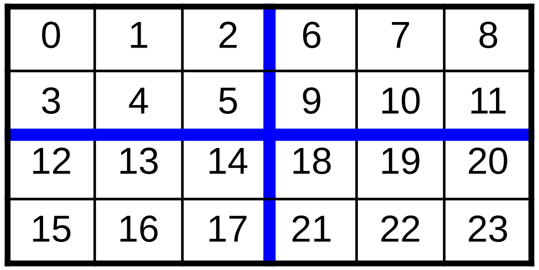
- Minimum number of communication steps between the processors

  ==> “Communication scheduling”

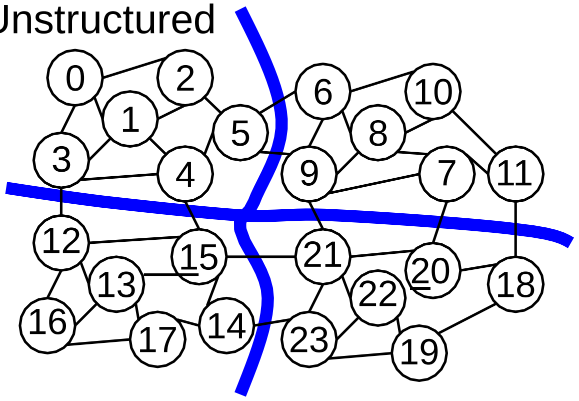
- Minimum amount of data that needs to be communicated. No deadlocks.

Domain Decomposition

Cartesian



Unstructured



Examples with 4 sub-domains

Non geographical approaches

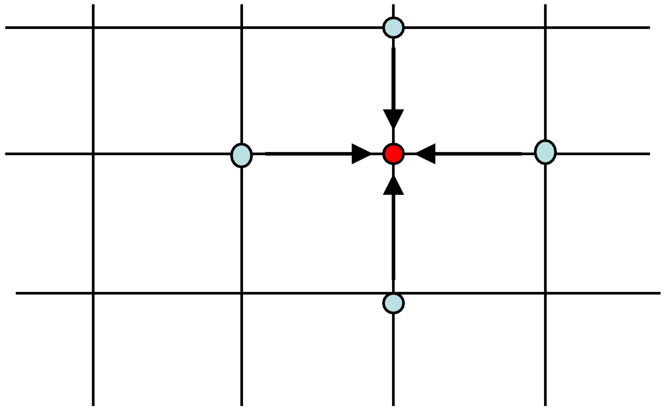
- Partition the data irrespective of their physical location in the computational domain
- Example: long range MD
  - having N interacting particles, each processor receives N/P particles. Since all of them have to communicate to all anyway, neighborhood relations are not important
  - Best load balance due to finest granularity
  - Easy to compute
  - No re-balancing needed if particles move

Cartesian coordinates = regular meshes

Operations on meshes

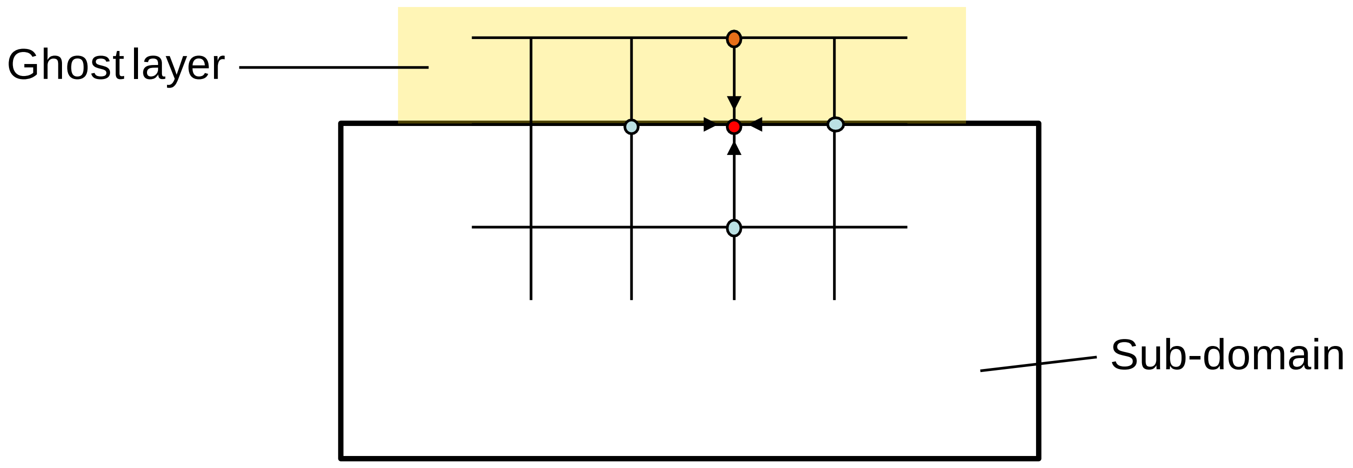
The values at mesh nodes are updated such as to numerically solve a given equation:

- **Finite differences** (Stencil methods)
  Values of mesh nodes are updated using the values of (any set of) nearby nodes.
- Ex: a 5-point stencil (diffusion equation)



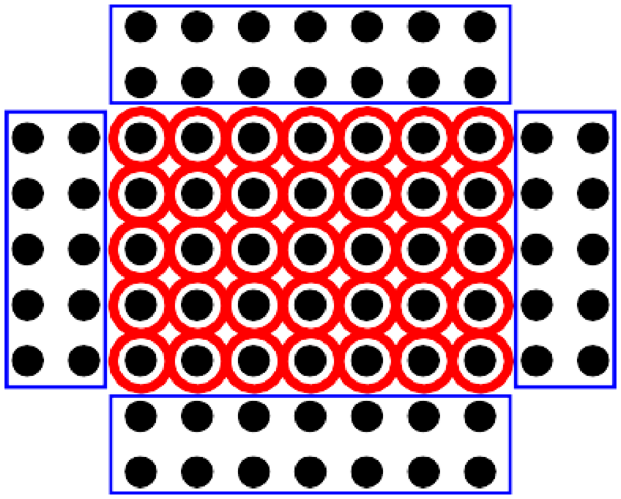
Operations on meshes

- Ghost layers around each sub-domain provide the needed values at the sub-domain boundaries



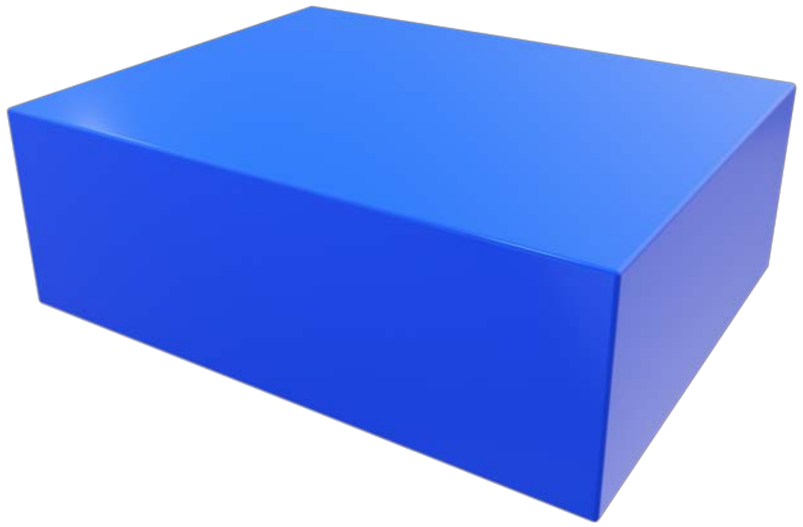
Ghost cells or halo area

- To calculate the new grid points of a sub-domain, additional grid points from other sub-domains are needed.
- They are stored in halos (ghost cells, shadows)
- Halo depends on form of stencil



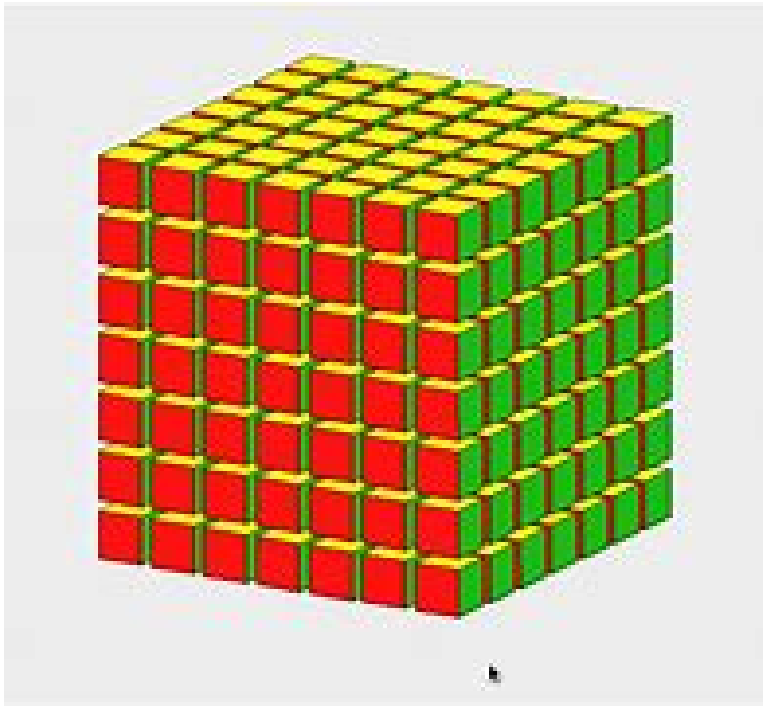
1. Splitting the domain..

- Consider a 3D box
- We can split along 1/2/3 dimensions
- Which is the best choice in term of performance (i.e scalability) ?



Example:a cube

- Let us consider the following parameters:
    - N^3 size of the cubic matrix
    - P processor
    - Cyclic/Periodic boundary condition:
        - two neighbors in each direction
    - W: width of the " ghost cells" or halo
- Define in term of these parameters the cost of the communication message

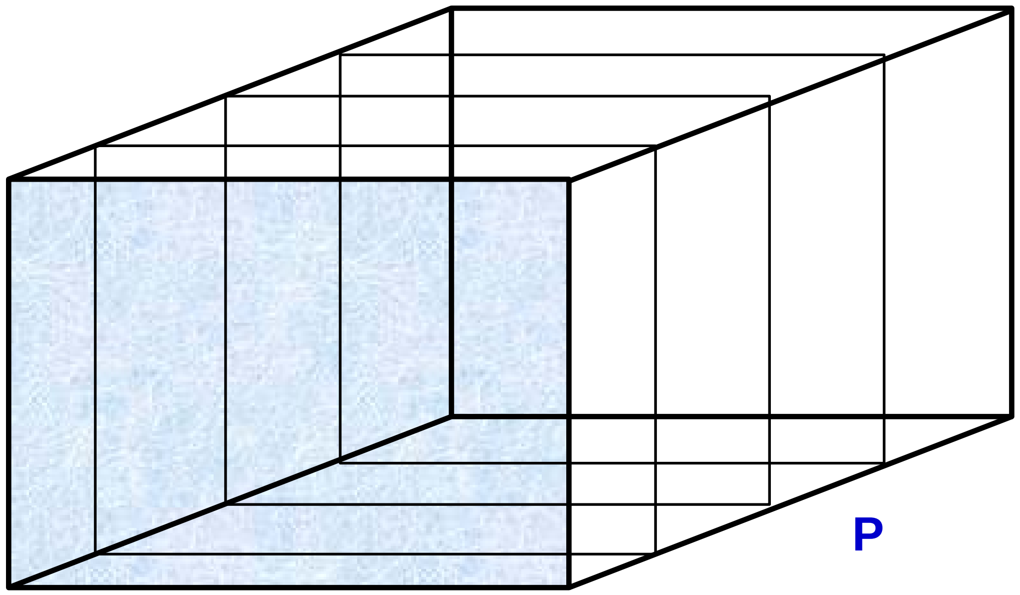


Domain decomposition: 1D

- Splitting along 1 dimension:

1D communication

$= n^{\mathbf{2}} * \mathbf{2} * w * \mathbf{1}$

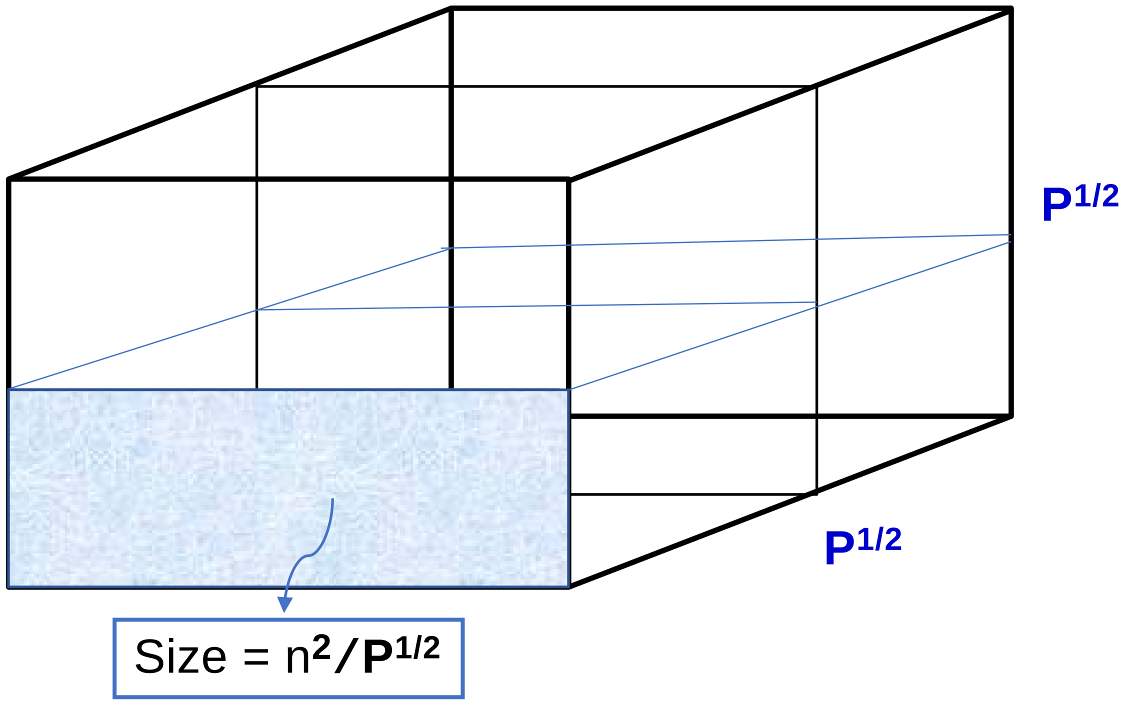


Domain decomposition: 2D

- Splitting along 2 dimension:

2D communication

$= n^{2} * 2 * w * 2/P^{1/2}$

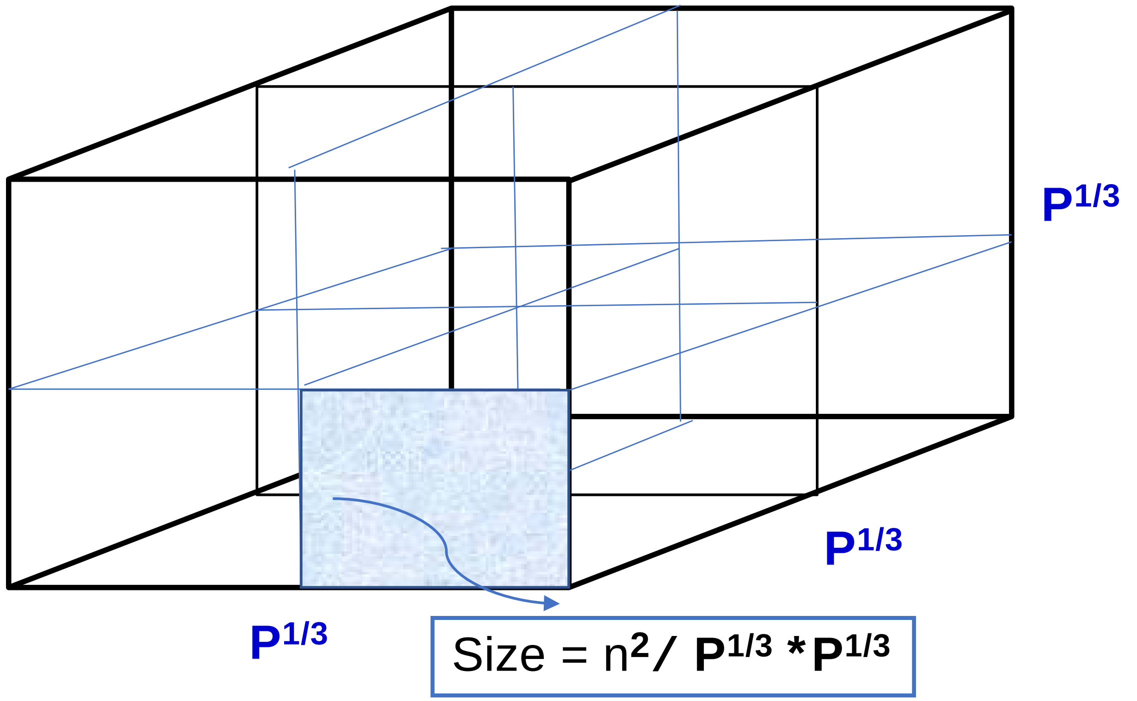


Domain decomposition: 3D

- Splitting along 3 dimension:

3D communication

$= n^2 * 2 * w * 3/P^{2/3}$



What about scalability of communication ?

Process	1D	2D	3D
[redacted]	[redacted]	[redacted]	[redacted]
2,00	2,00	2,83	3,78
4,00	2,00	2,00	2,38
8,00	2,00	1,41	1,50
16,00	2,00	1,00	0,94
32,00	2,00	0,71	0,60
64,00	2,00	0,50	0,38

Domain Decomposition 101

1. Split the domain into blocks.
2. Assign blocks to MPI-processes one-to-one.
3. Provide a "map" of neighbors to each process.
4. Write or modify your code so it only updates a single block.
5. Insert communication subroutine calls where needed.
6. Adjust the boundary conditions code.
7. Use "ghost cells/halo".

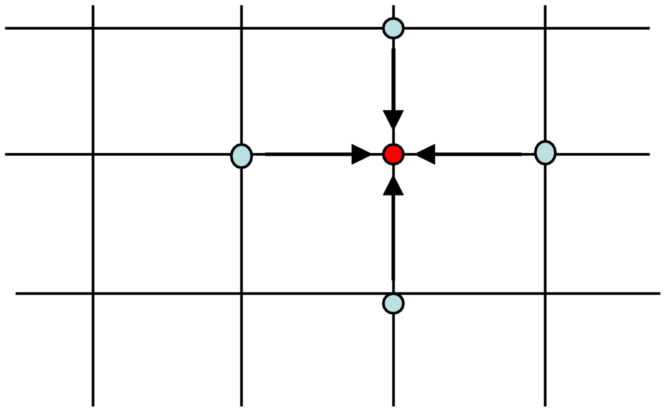
Real example: Jacobi solver..

- prototype for many stencil-based iterative methods in numerical analysis and simulation
- Basic form: solve the diffusion equation for a scalar function: $\Phi(\boldsymbol{r}, t)$

$$\frac{\partial \Phi}{\partial t} = \Delta \Phi \,,$$

Straightforward 2D serial implementation: the stencil

```
do k = 1,kmax
 do i = 1,imax
   phi(i,k,t1) = 0.25 * phi(i+1,k,t0) + 0.25 * phi(i-1,k,t0)
               + 0.25 * phi(i,k+1,t0) + 0.25 * phi(i,k-1,t0)
   enddo
  enddo
```



All taken from reference 4

The full serial algorithm..

- Ensure that the code produces a converged result.

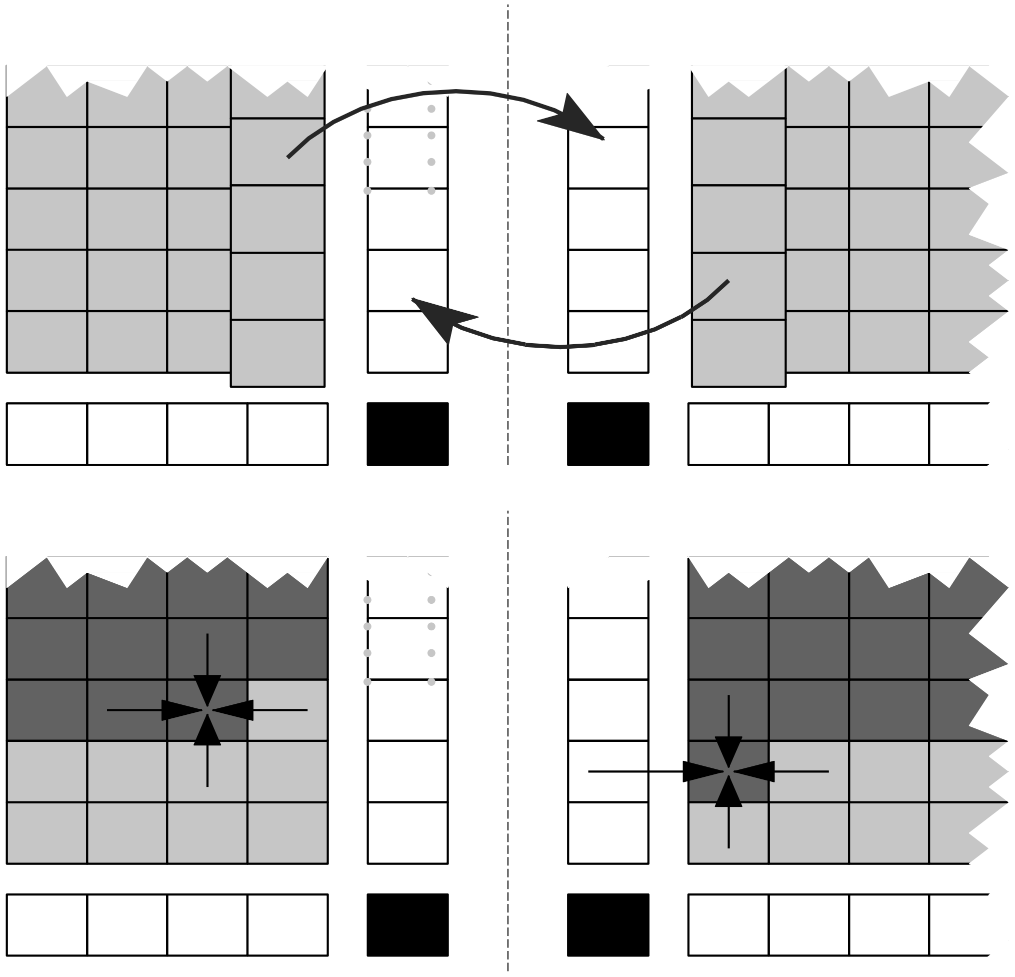
```
double precision, dimension(0:imax+1,0:kmax+1,0:1) :: phi
double precision :: maxdelta,eps
 integer :: t0,t1
 eps = 1.d-14 ! convergence threshold
 t0 = 0 ; t1 = 1
 maxdelta = 2.d0*eps
 do while(maxdelta.gt.eps)
 maxdelta = 0.d0
do k = 1,kmax
   do i = 1,imax
          phi(i,k,t1) = 0.25 * phi(i+1,k,t0) + 0.25 * phi(i-1,k,t0)
                      + 0.25 * phi(i,k+1,t0) + 0.25 * phi(i,k-1,t0)
          maxdelta = max(maxdelta,abs(phi(i,k,t1)-phi(i,k,t0)))

  enddo
      enddo
! swap arrays
i = t0 ; t0=t1 ; t1=i
 enddo
```

What happens in the parallel implementation ?

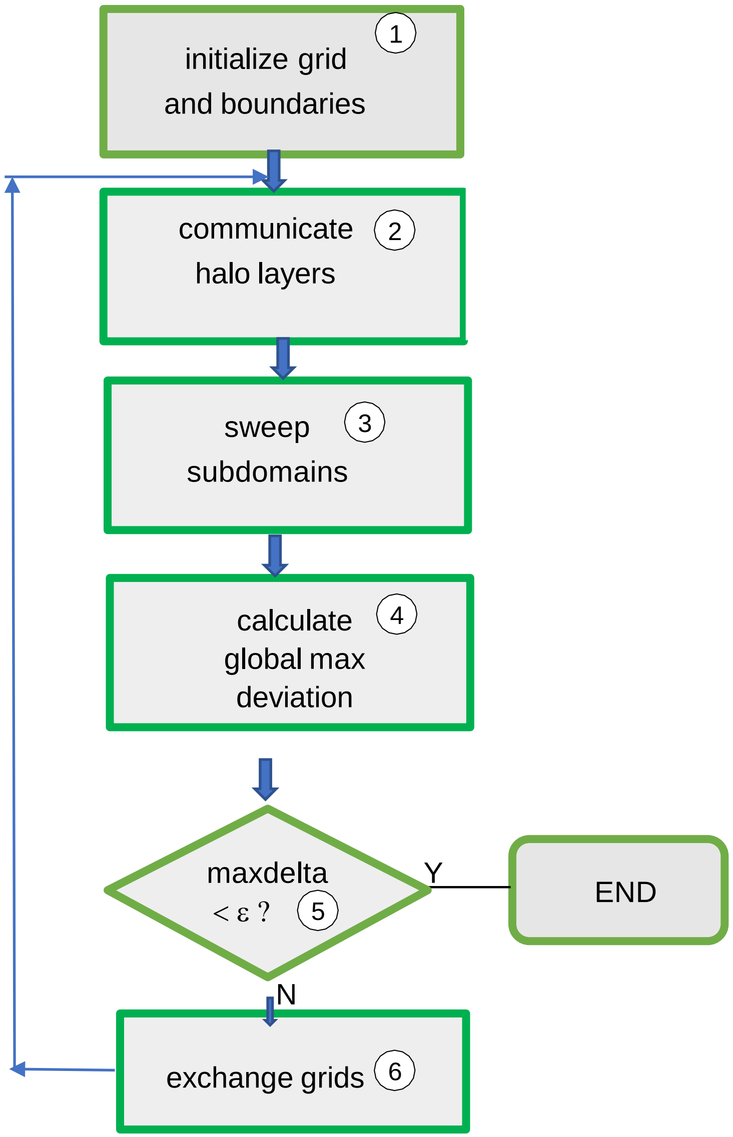
- The computational core works the same but:
  - Convergence criterion is no longer enough on subdomains but need to be computed globally

  ➔ requires a reduce operation among all processors
  - We need to take care of boundary conditions : Cell close to border require special care and require halo layers

The parallel data distribution..



The parallel algorithm



A few remarks

- Initialization is done with virtual topology

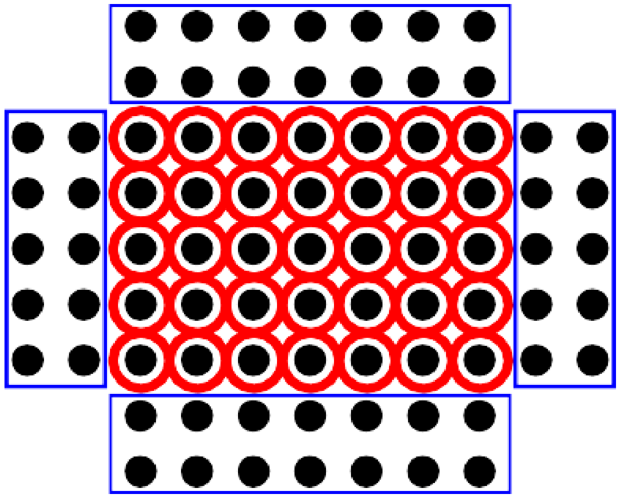
```
call MPI_Dims_create(numprocs, 3, proc_dim, ierr)

if(myid.eq.0) write(*,'(a,3(i3,x))') 'Grid: ', &
     (proc_dim(i),i=1,3)

l_reorder = .true.
call MPI_Cart_create(MPI_COMM_WORLD, 3, proc_dim, pbc_check, &
     l_reorder, GRID_COMM_WORLD, ierr)

if(GRID_COMM_WORLD .eq. MPI_COMM_NULL) goto 999

call MPI_Comm_rank(GRID_COMM_WORLD, myid_grid, ierr)
call MPI_Comm_size(GRID_COMM_WORLD, nump_grid, ierr)
```

Halo communication

- We use point to point communication to exchange halo layer.
- Point-to-point communication requires consecutive message buffers.
- Do we have contiguous location in memory for the halo ?

Not at all…

- only those boundary cells that are consecutive in the inner (i) dimension are also consecutive in memory (fortran column-major order..)
- Whole layers in the i-j, i-k, and j-k planes are never consecutive

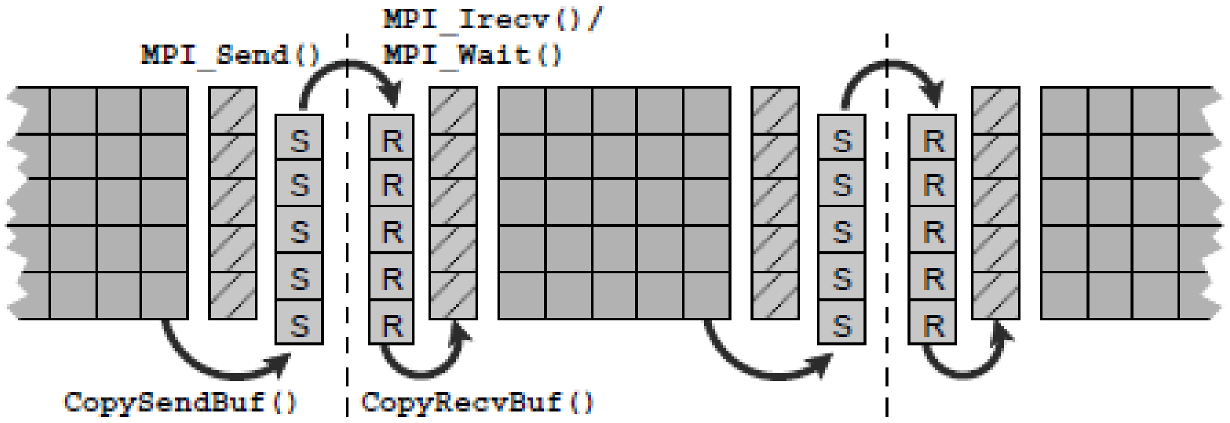


How to deal with this issue ?

- Send each chunk in a separate message discouraged:
  - This approach would flood the network with short messages, and latency has to be paid for every request
- BEST SOLUTION
  - intermediate buffer must be used to gather boundary data to be communicated to a neighbor’s ghost layer.

Halo exchange in one direction..

- We use two intermediate buffers per process, one for sending and one for receiving.



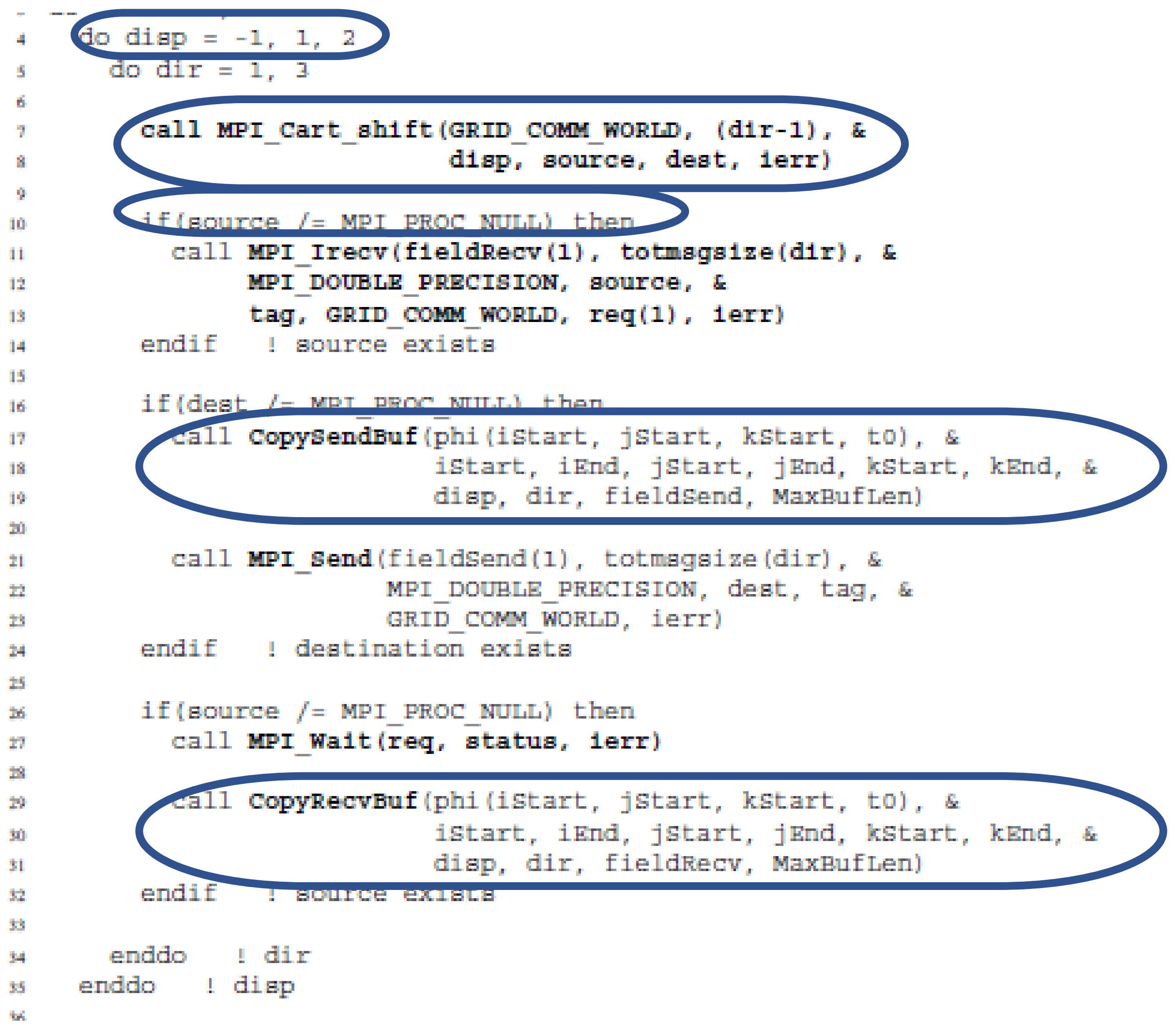
Dimension of the buffer…

- halo data can be different along different Cartesian directions

➔ the size of the intermediate buffer must be chosen to accommodate the largest possible halo

```fortran
integer, dimension(1:3) :: totmsgsize

! j-k plane
totmsgsize(3) = loca_dim(1)*loca_dim(2)
MaxBufLen=max(MaxBufLen,totmsgsize(3))
! i-k plane
totmsgsize(2) = loca_dim(1)*loca_dim(3)
MaxBufLen=max(MaxBufLen,totmsgsize(2))
! i-j plane
totmsgsize(1) = loca_dim(2)*loca_dim(3)
MaxBufLen=max(MaxBufLen,totmsgsize(1))

allocate(fieldSend(1:MaxBufLen))
allocate(fieldRecv(1:MaxBufLen))
```

Halo exchange.



```
do disp = -1, 1, 2
  do dir = 1, 3

    call MPI_Cart_shift(GRID_COMM_WORLD, (dir-1), &
                        disp, source, dest, ierr)

    if(source /= MPI_PROC_NULL) then
      call MPI_Irecv(fieldRecv(1), totmsgsize(dir), &
           MPI_DOUBLE_PRECISION, source, &
           tag, GRID_COMM_WORLD, req(1), ierr)
    endif   ! source exists

    if(dest /= MPI_PROC_NULL) then
      call CopySendBuf(phi(iStart, jStart, kStart, t0), &
                       iStart, iEnd, jStart, jEnd, kStart, kEnd, &
                       disp, dir, fieldSend, MaxBufLen)

      call MPI_Send(fieldSend(1), totmsgsize(dir), &
                    MPI_DOUBLE_PRECISION, dest, tag, &
                    GRID_COMM_WORLD, ierr)
    endif   ! destination exists

    if(source /= MPI_PROC_NULL) then
      call MPI_Wait(req, status, ierr)

      call CopyRecvBuf(phi(iStart, jStart, kStart, t0), &
                       iStart, iEnd, jStart, jEnd, kStart, kEnd, &
                       disp, dir, fieldRecv, MaxBufLen)
    endif   ! source exists

  enddo   ! dir
enddo   ! disp
```

For full 3D implementation

- See github repo…

Exercise

- Familiarize with the program and start running it on different number of processors and different sizes.
- Tomorrow we discuss performance model and scalability behavior