Using coarrays to solve a domain-decomposition problem

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1 Introduction

Coarrays have been part of the Fortran standard since the 2008 standard, but their use does not seem to be ubiquitous. See [1] for a description of this feature. This note tries to demonstrate that designing a parallel algorithm that uses coarrays can be straightforward, although, as usual with parallel programs, it is not always easy. The algorithm in question concerns the solution of a diffusion equation on a rectangular grid. To enhance the performance, the grid is split up into smaller rectangular areas, subgrids or domains, each of which is assigned to a single image.¹ The complication is that each subgrid needs to communicate with its neighbours and that is where the coarray feature comes in.

The methodology is demonstrated with a small program. The numerical method used is the simplest possible, so that all emphasis is on the coarray aspects. The concentration in grid cell (i,j) is calculated via the following explicit formula:

$$C_{i,j}^{t+\Delta t} = C_{i,j}^t + \frac{D\Delta t}{\Delta x^2} \left(C_{i-1,j}^t + C_{i+1,j}^t + C_{i,j-1}^t + C_{i,j+1}^t - 4C_{i,j}^t \right)$$
(1)

where the combination $D\Delta t/\Delta x^2$ can be abbreviated to a single factor, as the explicit factors do not play an independent role (see the description of the input).

 $^{^{1}}$ The program described here is based on a regular two-dimensional rectangular grid, but that is for the sake of simplicity only. We want to focus on the coarray aspects in a non-trivial situation.

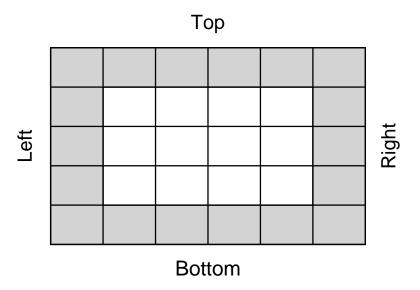


Figure 1: Sketch of the subgrid. The grid cells in gray are the boundary cells. The grid dimensions are 3 rows and 4 columns – the boundary cells are added to this.

2 The grid layout

A sketch of a subgrid, with some terminology, is shown in Figure 1. The four sides of the grids are represented by an extra row or column of grid cells, so that the boundary conditions can be taken care of. There are three types of boundary condition in the program:

- The concentration on the boundary can have a fixed value constant in time and along the boundary. This is implemented by setting the concentration in the extra grid cells to that value at the start of the calculation.
- The diffusive flux over the boundary is zero mathematically speaking, $\partial C/\partial \underline{n} = 0$ This can be implemented effectively by copying the concentration in the row or column of grid cells next to the boundary cells into these boundary cells at each time step. The discretised flux is then zero.
- The side is adjacent to that of another subgrid. Then the concentrations on the inside of both subgrids will have to be copied to the adjacent subgrid see picture 2. Again, this has to happen at each time step, or at least frequently enough.

Thus, the boundary conditions are simple enough to allow the *same* formula to be used for all internal cells:

```
\begin{array}{lll} dconc &= 0.0 \\ dconc \, (2 : length + 1, 2 : width + 1) &= \& \\ & diff\_factor \ * \ ( \ conc \, (1 : length \, , 2 : width + 1) \, \& \\ & + \ conc \, (3 : length + 2, 2 : width + 1) \, \& \\ & + \ conc \, (2 : length + 1, 1 : width) \, \& \\ & + \ conc \, (2 : length + 1, 3 : width + 2) \, \& \\ & - \ 4.0 \ * \ conc \, (2 : length + 1, 2 : width + 1) \, ) \\ conc &= conc \, + \, dconc \end{array}
```

This can be made slightly more compact by calculating the new concentration directly, instead of via an array for the derivative. However, the derivative can easily be used in a further refinement of the program to determine if convergence has been reached yet.

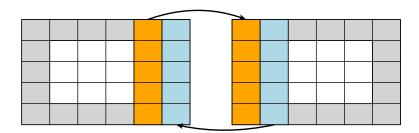


Figure 2: Boundary condition for two adjacent subgrids. The concentration in the orange cells on the left is copied to the boundary cells on the right. Similarly for the lightblue cells, but then from right to left.

3 The demonstration program

To make the demonstration a bit more interesting, the program uses a fairly flexible method to construct the complete grid:²

- Each subgrid is defined in an input file of its own. The definition should include the dimensions (number of rows and columns, without the extra rows and columns for the boundaries), the types of boundaries and either the value to be applied or the subgrid to which it is adjacent.
- The first subgrid may contain the number of time steps to calculate and the diffusion parameter, a combination of the actual time step, the diffusion coefficient and the grid cell size (assumed to be the same in both x and y directions).

For example:

²The program is listed in the appendix for easy reference.

```
# Corner: lower-left
#
grid 20 20
left-boundary open 1.0
right-boundary image 2
top-boundary closed
bottom-boundary closed
initial 1.0

timespan 1000
diff-factor 0.1
```

The demonstration program uses three subgrids that are arranged as shown in Figure 4.

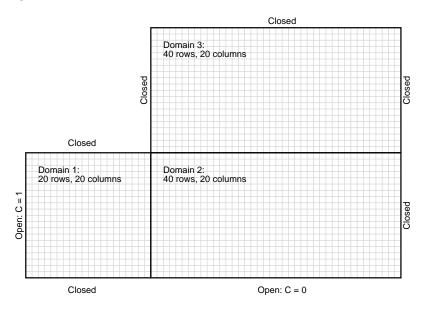


Figure 3: Domains in the sample calculation.

The input is read by a separate subroutine, read_input, which fills a data structure domain with the information that is specific for the subgrid. Since the variable is a *local* variable, each image has its own variable, independent of the other images.

Two complications occur:

• As we define the complete grid via fixed subgrids, we may have more images than there are subgrids. That means a number of subgrids will be idle. In the program we deal with this situation by distinguishing two so-called *teams*, images that act as a separate group and can be synchronised independently of the other groups:

```
write( filename, '(a,i0,a)') 'corner_', this_image(), '.inp'

open( 10, file = filename, status = 'old', iostat = ierr )

if ( ierr == 0 ) then
    running_image = this_image()
    call read_input( domain )

    write(*,*) 'Image-', this_image(), domain, '-->-', running_image
    this_team = 1

else
    this_team = 2
    write(*,*) 'Image-', this_image(), '-inactive'
endif

! We need to make sure all images have finished the initialisation
! form team ( this_team, active_inactive )
```

Almost the whole program is now split into two parts via the change team construct:

• We need to give the arrays that are used to exchange the boundary values, left_concentration etc., a size that is first of all equal on each image (a requirement for coarrays) and that is large enough to fit all sides in the whole grid that are shared by two subgrids. In the figure domain 1 is adjacent to domain 2, and domain 2 is also adjacent to domain 3. The longest shared side in the horizontal direction therefore covers 40 (plus 2) grid cells and the longest shared side in the vertical direction covers 20 (plus 2) grid cells.

The collective coarray routine co_max comes in very handy. The *local* variables xmax and ymax are first set to the domain size in each image and then set via this routine to the maximum over all images:

```
!
! Prepare the calculation
!
xmax = domain%nx
ymax = domain%ny
call co_max( xmax )
call co_max( ymax )
```

The maximum value is broadcast to all images, so that they can allocate the coarrays for the boundaries:

```
\begin{array}{ll} \textbf{allocate}(& \texttt{left\_concentration}(\texttt{ymax}+2)[*] & \texttt{)} \\ \textbf{allocate}(& \texttt{right\_concentration}(\texttt{ymax}+2)[*] & \texttt{)} \\ \textbf{allocate}(& \texttt{top\_concentration}(\texttt{xmax}+2)[*] & \texttt{)} \\ \textbf{allocate}(& \texttt{bottom\_concentration}(\texttt{xmax}+2)[*] & \texttt{)} \end{array}
```

We can use the codimension [*], because the subgrids have no particular ordering. In more complex situations you may want to arrange the images in some grid of their own and then a multi-dimensional codimension is useful [2].

The concentration array and the array with the time derivative are local arrays that should be allocated to the size of the subgrid that is associated with the image, very classically:

```
allocate( conc(domain%nx+2,domain%ny+2) )
allocate( dconc(domain%nx+2,domain%ny+2) )
```

Note: the concentration array might be made a coarray too, for easier collecting the information over the whole grid for output. In this program the end result per subgrid is written to a separate file instead. A post-processing program could then stitch the results together for presentation purposes.

3.1 Computational core

The heart of the program is the loop over time where the new concentration is calculated and the boundary conditions are exchanged. An excerpt is shown below:

```
!
! Do the calculation
!
do i = 1,timespan
```

```
dconc = 0.0
    dconc(2:length+1,2:width+1) = diff_factor * ( ... )
    conc = conc + dconc
    left_concentration (1: width+2)
                                       = \operatorname{conc}(2,:)
    right\_concentration (1: width+2) = conc (length+1,:)
    top\_concentration (1: length + 2) = conc (:, width + 1)
    bottom\_concentration(1:length+2) = conc(:,2)
    ! Wait for all the images before copying the boundaries
    ! (note: sync all works on the current team, which is not the initial team
    sync all
    ! Left
    if ( domain%boundary_type(1) == 2 ) then
        conc (1,:) = right_concentration (1:width+2)[domain%connecting_domain (1
    elseif ( domain%boundary_type(1) = 0 ) then
        conc(1,:) = conc(2,:)
    endif
    ! Similarly the other sides
    . . .
    ! And when everything has been copied, continue
    sync all
enddo
```

There are two instances of the sync all statement: the first to make sure all images within the team are ready with the current time step and also have filled the array to exchange the boundary data and the second to actually exchange the boundary data and make sure all are ready for the next step.³ The fragment in between the two statements uses the coarrays to do the exchange.

4 Summary

A summary of the demonstration program may be useful:

³The sync all statement only synchronises the images in the current team, not all images.

- The first step is to read the input files that define the domains (subgrids). Each domain is associated with one image.
- To manage the images that are *not* associated with a domain, two teams are formed. The second team simply waits for the calculation to finish.
- The first team, however, does the integration over time and exchanges the boundary data at each time step. For this synchronisation is required, otherwise we cannot be sure that the data that are copied from one domain to the other are consistent.
- When the calculation has finished, the resulting concentrations are written to separate files, so that they can be visualised (see Figure 4). This is simply an easy solution, probably not the best possible.

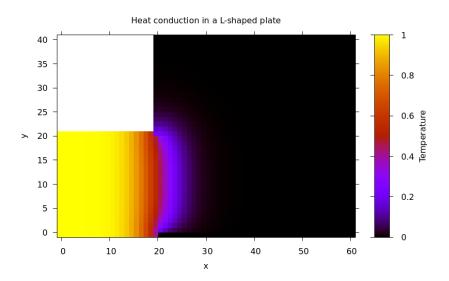


Figure 4: Solution of the diffusion problem on three domains in an L-shape. (Courtesy Ivan Pribec.)

5 Caveats

The program was written in several stages – the description above is the end result. The earlier stages are, however, also of interest and they are described in some detail in this section.

Some emphasis has been put on the management of the inactive images. This is, because they are waited upon by the sync all statements. If they are

stopped early in the program's execution, such as after noticing that they are not associated to a domain:

```
open( 10, file = filename, status = 'old', iostat = ierr )
if ( ierr == 0 ) then
    running_image = this_image()
    call read_input( domain )

    write(*,*) 'Image-', this_image(), domain, '--->-', running_image
else
    write(*,*) 'Image-', this_image(), '-stopped'
    stop
endif
```

the sync all statements will wait forever.

Attempts to use the sync images statement instead and only wait for the active images failed for unknown reasons. The program would simply lock up in the same way as with sync all.

The alternative was to detect that some images were inactive and then stop the program: the user would have to set the environment variable that controls the number of images, FOR_COARRAY_NUM_IMAGES for the Intel Fortran compiler, or specify the default number of images at compile time. As this is a somewhat unfriendly method, the final version uses teams. And as can be seen in the code, that is rather easy to accomplish in this case.

6 An MPI-based equivalent

With this coarrays-based version completed, it became obvious that an MPI-based version should follow. The demonstration program does not require much complicated interaction, so it should be easy to transform it to use MPI instead. Just as with the coarrays, each process, the MPI equivalent of "image", takes care of one subgrid. But there were some tricky parts:

- While in the coarrays version an image addresses the arrays on the neighbouring images directly, this is not possible with MPI: there you send a message to the receiving process which is the neighbour in the multidomain set-up, and this should actively pick it up. So there is more explicit cooperation required.
- Each process needs to know which subgrids are adjacent. One solution would be for each process to send messages to each other process to relay this information, but with N subgrids, this would mean 4(N-1) messages per subgrid, or roughly $4N^2$ in total. If N is small, this is not a real problem, but suppose you have 100 or 1000 subgrids, then this might become a serious matter. In a two-dimensional geometry, you would expect only in the order of 4N interfaces.

You need to make sure that the processes have received the messages and
have processed the information. There is probably a clear construction to
achieve this, but it seemed cumbersome. Instead, the solution chosen here
was to have the main process gather the information from each subgrid
on its neighbours and then send that entire piece of information to each
process, so that it could determine what subgrids are adjacent.

All in all, the following fragment implements this information exchange:

Now each process has all the information necessary: it knows which of its sides are adjacent to which subgrid (or whether it is simply an external boundary).

Sending the results of time T to the correct neighbour requires a message for this neighbour:

```
\operatorname{conc}\left(\operatorname{length}+2\,,:\right) = \operatorname{conc}\left(\operatorname{length}+1\,,:\right) endif
```

The program that resulted probably contains too much "juggling" of the IDs of the various subgrids. This is partly due to the fact that with MPI the process IDs start with zero instead of one, as with coarrays, and I wanted the code to stay as close to the coarrays version as possible. Another reason is that the left-hand side in one subgrid is the right-hand side in the adjacent subgrid. This may have confused the coding more than necessary. But whatever the merits and shortcomings of this second demo program, it does work and gives exactly the same results as the coarrays version.

A Source code of the coarrays version

The source of the demonstration program is shown here in full. It contains traces of its development, such as extra output to see what is happening. It could also be useful to characterise the sides by integer parameters instead of the literal numbers 1, 2, 3 and 4.

Also note: There is no guarantee that the program is flawless. (The listing is shown in a fixed-size font, because of the page width.)

```
! corner.f90 --
      Solve a diffusion problem defined on several connected domains
      Stopping the images that have no role in the calculation means
      that a "sync all" statement causes a deadlock. It will wait for
      all original images.
      Hm, keeping a list of running images does not solve the problem
      At least not with this version of Ifort (2021.9.0)
      Use teams to split off the inactive images
program corner
    use iso_fortran_env
    implicit none
    type(team_type) :: active_inactive
    type domain_type
        integer
                              :: nx, ny
        integer, dimension(4) :: boundary_type
        integer, dimension(4) :: connecting_domain
        real, dimension(4)
                              :: boundary_value
                                                        = -999.0
        real
                              :: initial_concentration = -999.0
    end type domain_type
```

```
type(domain_type) :: domain
real, allocatable :: left_concentration(:)[:]
real, allocatable :: right_concentration(:)[:]
real, allocatable :: top_concentration(:)[:]
real, allocatable :: bottom_concentration(:)[:]
real, allocatable :: conc(:,:)
real, allocatable :: dconc(:,:)
integer, allocatable :: running_image[:]
integer, allocatable :: list_running_images(:)
character(len=80) :: filename
                :: i, ierr
integer
integer
                 :: xmax, ymax, length, width
integer
                 :: this_team
integer
                 :: timespan
real
                  :: diff_factor
allocate( running_image[*] )
running_image = 0
write( filename, '(a,i0,a)' ) 'corner_', this_image(), '.inp'
open( 10, file = filename, status = 'old', iostat = ierr )
if ( ierr == 0 ) then
    running_image = this_image()
    call read_input( domain )
    write(*,*) 'Image ', this_image(), domain, ' --> ', running_image
    this_team = 1
else
    this_team = 2
    write(*,*) 'Image ', this_image(), ' inactive'
endif
! We need to make sure all images have finished the initialisation
form team ( this_team, active_inactive )
! Select the team and enter the team construct
change team ( active_inactive )
    if ( team_number() == 1 ) then
```

```
! Prepare the calculation
xmax = domain%nx
ymax = domain%ny
call co_max( xmax )
call co_max( ymax )
call co_broadcast( timespan, 1 )
call co_broadcast( diff_factor, 1 )
if ( this_image() == 1 ) then
    write(*,*) 'Overall grid sizes: ', xmax, ymax
endif
allocate( left_concentration(ymax+2)[*]
allocate( right_concentration(ymax+2)[*] )
allocate( top_concentration(xmax+2)[*]
allocate( bottom_concentration(xmax+2)[*] )
allocate( conc(domain%nx+2,domain%ny+2) )
allocate( dconc(domain%nx+2,domain%ny+2) )
! Set up the concentrations
length = domain%nx
width = domain%ny
if (domain%initial_concentration /= -999.0) then
    conc = domain%initial_concentration
    conc = 0.0
endif
if ( domain%boundary_type(1) == 1 ) then
    conc(1,:) = domain%boundary_value(1)
endif
! Right
if ( domain%boundary_type(2) == 1 ) then
    conc(length+2,:) = domain%boundary_value(2)
\verb"endif"
! Top
if ( domain%boundary_type(3) == 1 ) then
    conc(:,width+2) = domain%boundary_value(3)
endif
! Bottom
if ( domain%boundary_type(4) == 1 ) then
```

```
conc(:,1) = domain%boundary_value(4)
endif
! Do the calculation
do i = 1, timespan
   if ( mod(i,100) == 0 ) then
       write(*,*) this_image(), i
   endif
   dconc = 0.0
   dconc(2:length+1,2:width+1) = &
       diff_factor * ( conc(1:length,2:width+1) + conc(3:length+2,2:width+1) &
                        + conc(2:length+1,1:width) + conc(2:length+1,3:width+2) &
                        - 4.0 * conc(2:length+1,2:width+1) )
    ! Or use an explicit loop ...
    !do k = 2,length+1
        do l = 2, width+1
            dconc(k,1) = &
                 diff_factor * (conc(k-1,1) + conc(k+1,1) + conc(k,l-1) + conc(k,l+1)
                                 -4.0 * conc(k,1))
         enddo
    !enddo
   conc = conc + dconc
   left_concentration(1:width+2)
                                     = conc(2,:)
   right_concentration(1:width+2) = conc(length+1,:)
   top_concentration(1:length+2)
                                     = conc(:,width+1)
   bottom_concentration(1:length+2) = conc(:,2)
    ! Wait for all the images before copying the boundaries
    ! (note: sync all works on the current team, which is not the initial team at this po
   sync all
    ! Left
   if ( domain%boundary_type(1) == 2 ) then
       conc(1,:) = right_concentration(1:width+2)[domain%connecting_domain(1)]
   elseif ( domain%boundary_type(1) == 0 ) then
       conc(1,:) = conc(2,:)
   endif
    ! Right
   if ( domain%boundary_type(2) == 2 ) then
        conc(length+2,:) = left_concentration(1:width+2)[domain%connecting_domain(2)]
   elseif ( domain\%boundary\_type(2) == 0 ) then
        conc(length+2,:) = conc(length+1,:)
```

```
! Top
                if ( domain\%boundary\_type(3) == 2 ) then
                    conc(:,width+2) = bottom_concentration(1:length+2)[domain%connecting_domain(3)]
                elseif ( domain\%boundary\_type(3) == 0 ) then
                    conc(:,width+2) = conc(:,width+1)
                endif
                ! Bottom
                if ( domain\%boundary\_type(4) == 2 ) then
                    conc(:,1) = top_concentration(1:length+2)[domain%connecting_domain(4)]
                elseif ( domain\%boundary\_type(4) == 0 ) then
                    conc(:,1) = conc(:,2)
                endif
                ! And when everything has been copied, continue
                sync all
            enddo
            write(*,*) 'Image ', this_image(), ' has reached the end'
            write( filename, '(a,i0,a)' ) 'report_corner_', this_image(), '.out'
            open( 20, file = filename )
            do i = 1,width
                write( 20, '(*(g10.3))' ) conc(:,i)
            enddo
        else
            ! The second team has no task ...
            write(*,*) 'Image ', this_image(), ' is idle'
        endif
    end team
    ! Wait for all images
    sync all
contains
subroutine read_input( domain )
    type(domain_type), intent(inout) :: domain
    character(len=80) :: line
    character(len=20) :: keyword, type
```

endif

```
integer
          :: ierr, k
do
     read( 10, '(a)', iostat = ierr ) line
     if ( ierr /= 0 ) then
         exit
     endif
     read( line, *, iostat = ierr ) keyword
     select case ( keyword )
         case( '#' )
             ! Simply skip
         case( 'timespan' )
             read( line, *, iostat = ierr ) keyword, timespan
         case( 'diff-factor' )
             read( line, *, iostat = ierr ) keyword, diff_factor
         case( 'grid' )
             read( line, *, iostat = ierr ) keyword, domain%nx, domain%ny
         case( 'initial' )
             read( line, *, iostat = ierr ) keyword, domain%initial_concentration
         case( 'left-boundary', 'right-boundary', 'top-boundary', 'bottom-boundary' )
             select case ( keyword )
                 case( 'left-boundary' )
                     k = 1
                 case( 'right-boundary' )
                    k = 2
                 case( 'top-boundary' )
                    k = 3
                 case( 'bottom-boundary' )
                    k = 4
             end select
             read( line, *, iostat = ierr ) keyword, type
             select case ( type )
                 case( 'closed' )
                     domain%boundary_type(k) = 0
                     read( line, *, iostat = ierr ) keyword, type
                 case( 'open' )
                     domain%boundary_type(k) = 1
                     read( line, *, iostat = ierr ) keyword, type, domain%boundary_value(k)
```

B Source code of the MPI-based version

Below is an excerpt of the MPI-based demo program. The parts that are almost the same as in the coarrays version have been left out. The program may be simplified further, but that is a possible next step.

The domain_type derived type has an extra component: destination to keep track of both sides.

```
!
! Initialise the MPI environment
call MPI_INIT(ierror)
call MPI_COMM_SIZE(MPI_COMM_WORLD, size_Of_Cluster, ierror)
call MPI_COMM_RANK(MPI_COMM_WORLD, process_Rank, ierror)
root = 0
! Read the input and check the number of processes
write( filename, '(a,i0,a)' ) 'corner_', process_Rank+1, '.inp'
! Prepare the calculation
call MPI_ALLREDUCE( domain%nx, xmax, 1, MPI_INTEGER, MPI_MAX, MPI_COMM_WORLD, ierror )
call MPI_ALLREDUCE( domain%ny, ymax, 1, MPI_INTEGER, MPI_MAX, MPI_COMM_WORLD, ierror )
call MPI_BCAST( timespan,
                             1, MPI_INTEGER, root, MPI_COMM_WORLD, ierror)
call MPI_BCAST( diff_factor, 1, MPI_REAL,
                                           root, MPI_COMM_WORLD, ierror )
! Exchange the connectivity information:
```

```
! Gather the information on the root process and then send it off to each
! process. In turn, each process examines the array connection to fill
! the destination field.
allocate( connection(4,size_Of_Cluster) )
call MPI_GATHER( domain%connecting_domain, size(domain%connecting_domain), MPI_INTEGER, &
                 connection, size(connection,1), MPI_INTEGER, root, MPI_COMM_WORLD, ierror )
call MPI_Barrier( MPI_COMM_WORLD, ierror )
call MPI_BCAST( connection, size(connection), MPI_INTEGER, root, MPI_COMM_WORLD, ierror )
call MPI_Barrier( MPI_COMM_WORLD, ierror )
do j = 1,size(connection,2)
    do i = 1,size(connection,1)
        if ( connection(i,j) == process_Rank+1 ) then
            domain%destination(side(i)) = j - 1    ! Shift by 1 required
        endif
    enddo
enddo
! Do the calculation
do i = 1, timespan
    ! We can send these arrays without having to wait. Use the tag to identify
    ! the boundary.
    ! For now: use blocking send and receive
    if ( domain%destination(1) /= -1 ) then
        call MPI_SEND( left_concentration, width+2, MPI_REAL, domain%destination(1), 2, &
                       MPI_COMM_WORLD, ierror )
    endif
    ... similarly the other three sides
    ! Wait for all the processes before copying the boundaries
    ! We need to know which domains want our information!
    call MPI_Barrier( MPI_COMM_WORLD, ierror )
```

```
! Left
    if ( domain\%boundary\_type(1) == 2 ) then
        call MPI_REGV( right_concentration, width+2, MPI_REAL, domain%connecting_domain(1)-1, 1, 8
                       MPI_COMM_WORLD, status, ierror )
        conc(1,:) = right_concentration(1:width+2)
    elseif ( domain%boundary_type(1) == 0 ) then
        conc(1,:) = conc(2,:)
    endif
    ... similarly the other three sides
    ! And when everything has been copied, continue
    call MPI_Barrier( MPI_COMM_WORLD, ierror )
enddo
write(*,*) 'Process ', process_Rank, ' has reached the end'
... write out the result per subgrid
! Wait for all images
call MPI_Barrier( MPI_COMM_WORLD, ierror )
call MPI_FINALIZE(ierror)
```

References

- [1] Michael Metcalf, John Reid, Malcolm Cohen, and Reinhold Bader. *Modern Fortran explained*. Oxford University Press.
- [2] Anton Shterenlikht and Luis Cebamanos. Cellular automata beyond 100k cores: MPI vs Fortran coarrays.