Code Parallelization

a guided walk-through

f.salvadore@cineca.it

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Code Parallelization

two **stages** to write a parallel code

- **problem domain**
  - algorithm
- **program domain**
  - implementation

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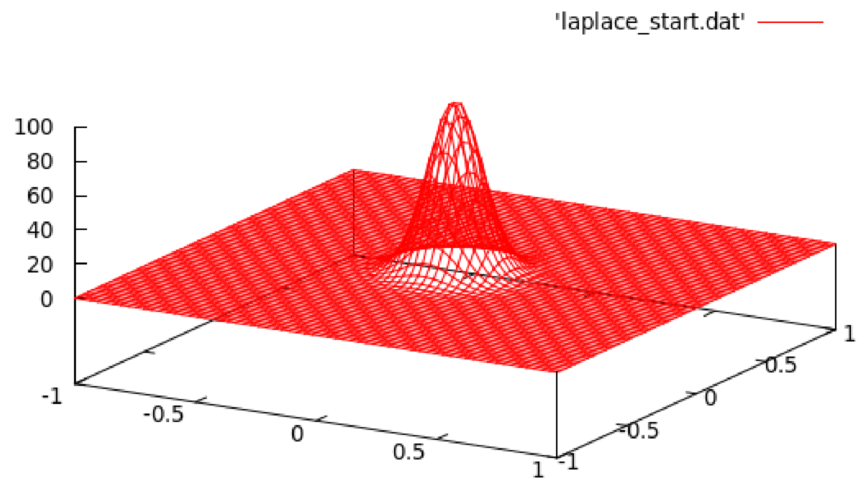
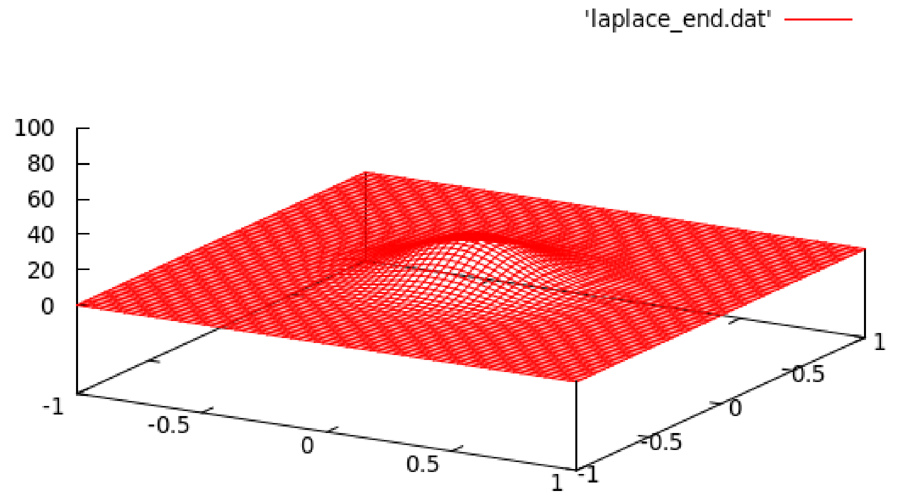
Problem domain

- Naive iterative solver of Laplace equation for a variable T
  - Start with a Gaussian field
  - Iterate replacing each value with the mean value of the four neighboring points
  - Stop when either the maximum amount of iterations or the convergence is reached





Problem domain

- Analyze the algorithm (trivial for the Laplace example):
  - Is the serial algorithm suitable for a a distribute parallel MPI implementation?
  - Is the serial algorithm still the best wrt performances for an MPI version of the code?

- Identify the most **computationally demanding** parts of the problem
  - But remember that an MPI parallelization is difficult to develop incrementally

Concurrency

Find concurrency:

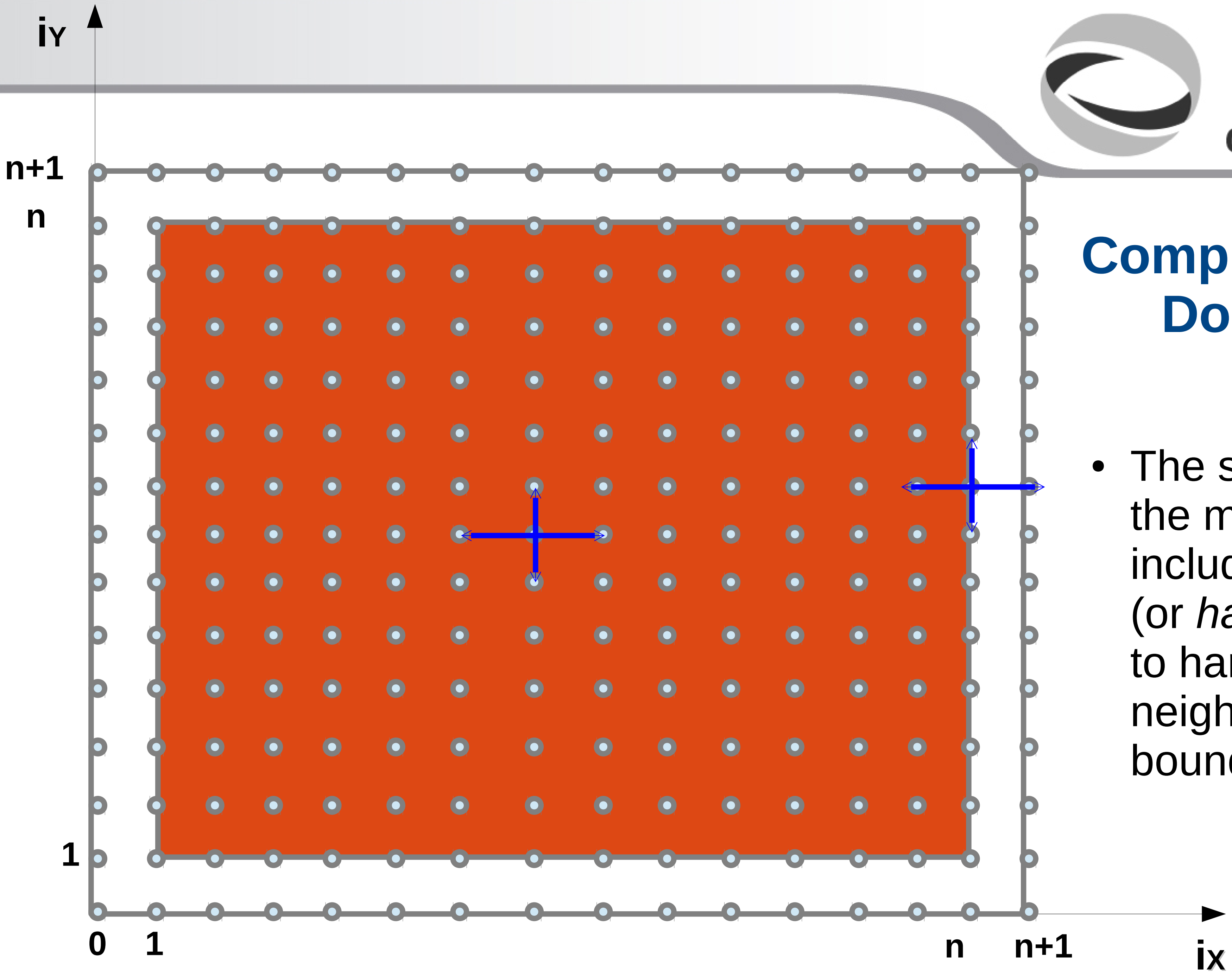
- **similar** operations that can be applied to **different parts** of the data structure

- domain **decomposition**: divide data into chunks that can be operated concurrently
  - a task works only **its chunk** of data
  - map **local** to **global** variables

Dependencies

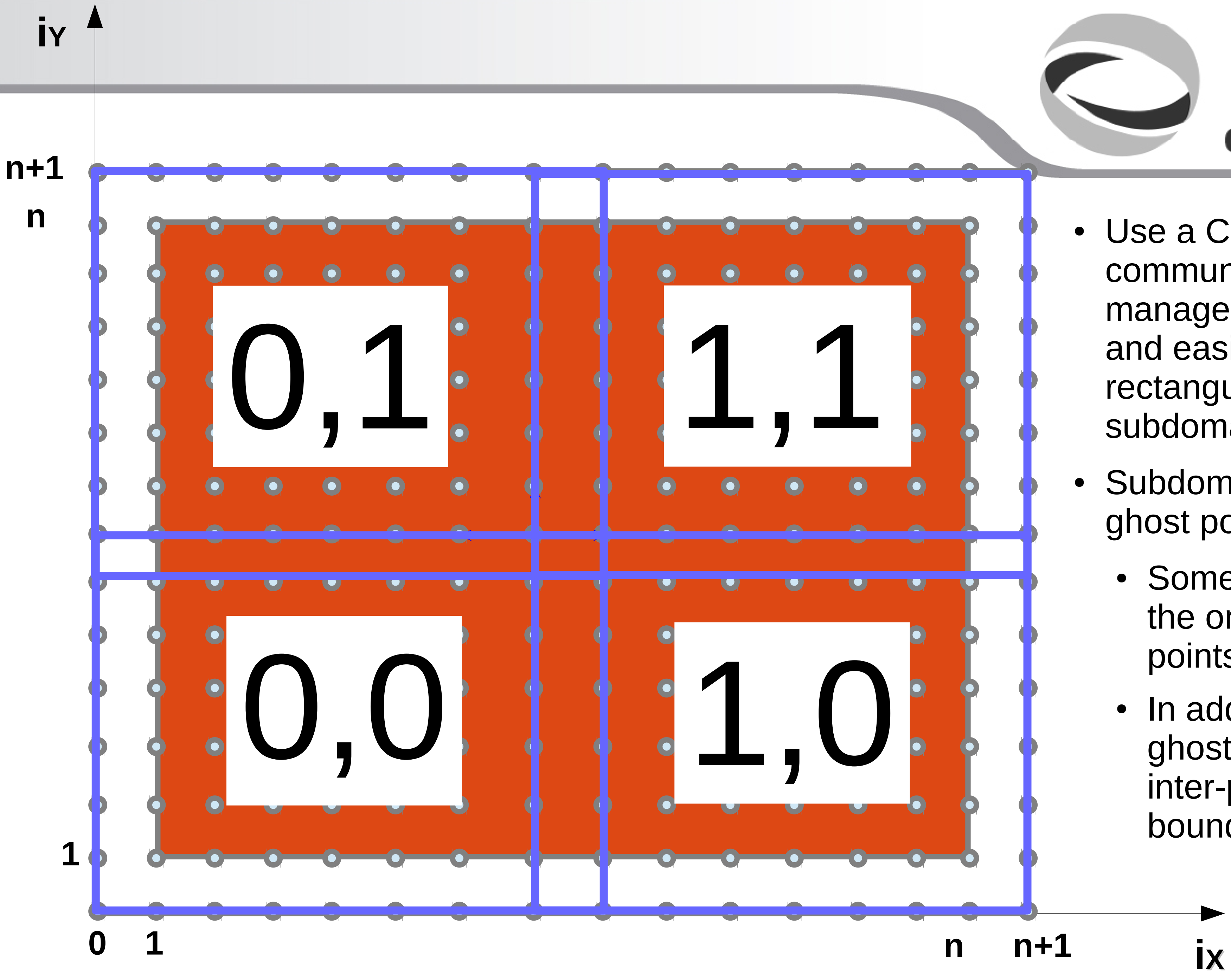
Handle dependencies among tasks:

- Tasks needs access to some portion of another task local data (**data sharing**)
- Understand the kind and the amount of communications among processes required to make anything consistent

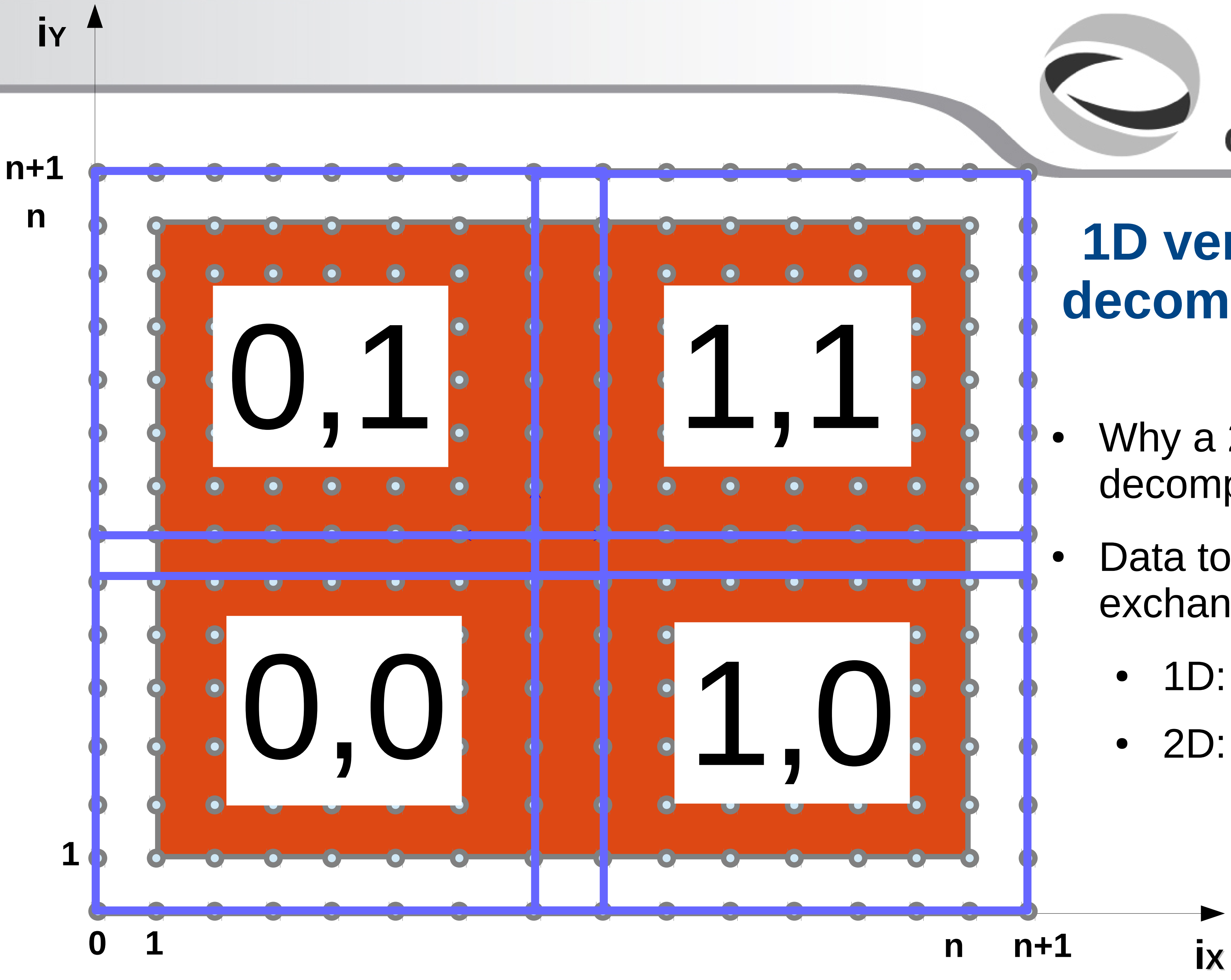


Computational Domain

- The shape of the matrixes include ghost (or *halo*) points to handle (the neighbour of) boundary points



- Use a Cartesian communicator to manage the processes and easily map them to rectangular subdomains
- Subdomains need ghost points too
  - Some of them are the original ghost points
  - In addition there are ghost points among inter-process boundaries



1D versus 2D decomposition

- Why a 2D decomposition?
- Data to be exchanged:
  - 1D: 2N
  - 2D: $4N/\sqrt{N\_proc}$

Program domain

2 different **stages** to parallelize a serial code

- **problem domain**
  - algorithm
- **program domain**
  - Implementation **(the fun part)**

The serial code: Laplace equation

```
program laplace
   [ … variable declarations … ]
   [ … input parameters ... ]
   [ … allocate variables … ]
   [ … initialize field … ]
   [ … print initial output … ]


  [ … computational core … ]


  [ … print final output … ]
  [ … deallocate variables … ]
end program laplace
```

```
do while (var > tol .and. iter <= maxIter)
     iter = iter + 1
     var = 0.d0
     do j = 1, n
       do i = 1, n
         Tnew(i,j) = 0.25d0 * (T(i-1,j)+T(i+1,j)+T(i,j-1)+T(i,j+1))
         var = max(var, abs( Tnew(i,j) - T(i,j) ))
       end do
     end do

     Tmp =>T; T =>Tnew; Tnew => Tmp;

     if( mod(iter,100) == 0 ) &
         write(*,"(a,i8,e12.4)") ' iter, variation:', iter, var

  end do
```

The tasks

- (1) Develop an MPI parallel version of the laplace.f90/laplace.c serial codes (init and save functions are in init_save.f90/c files)
    - (a) Start with a basic MPI implementation using a Cartesian topology and blocking communications
    - (b) Try to enhance the solution using advanced features
- (2) Add the OMP parallelization to the blocking MPI version to finally develop an hybrid MPI-OMP implementation of the code
    - Explore the different thread support levels

MPI Basic - Hints / 1

- First create the Cartesian communicator
  - And find the ranks of the neighboring processes
- Define the sizes of the domain for each rank
  - Also define the offsets of the sub-domains with respect to the global domain
  - If possible try to handle the remainders, otherwise force a constraint
- After that, **init_field** is easy to parallelize: **ind2pos** (the function which maps the index to the position in the grid) remains unchanged provided that the global indexes are passed to it
- The print function (**save_gnuplot**) parallelization
  - might be postponed: check the error at each time step to know if the results are correct
  - to parallelize it, let the rank=0 collect all the fields and print (just for didactic purposes) but the right way is using MPI I/O
- At each iteration update the ghost points with the boundary points of the neighboring processes
  - MPI_Sendrecv may be a good choice
  - Declare, allocate and use buffers to perform the communications

MPI Basic - Hints / 2

- Initialize MPI:
  - MPI_Init / MPI_Comm_rank / MPI_Comm_size
- Input
  - Make only rank=0 read from input
  - MPI_Bcast the 3 input numbers to all the processes
- Cartesian topology for processes
  - MPI_Dims_create – decompose the number of processes in a rectangular way cart_dims(:)
  - MPI_Cart_create – create the Cartesian communicator
  - MPI_Comm_rank on the Cartesian communicator
  - MPI_Cart_coords – find the coordinates of my process cart_coord(:)
  - MPI_Cart_shift (in x and y) – find the ranks of neighboring processes
- Associate the cartesian topology to the computational grid
  - Find for each process the sub-domain size and the start indexes wrt to the global domain (in x and y): mymsize_x, mymsize_y, mystart_x, mystart_y
    - mymsize_x = n/cart_dims(1)
    - mystart_x = mymsize_x *cart_coord(1)
  - Handle the remainders or force to be multiple (...)
- Allocate T, Tnew, and the buffers (4 send and 4 receive buffers), including the ghost points (size=mymsize_x+2). Ghosts not needed for buffers.
- Declare everything you need!

MPI Basic - Hints / 3

- Parallelize **init_fields**
  - Pass mystart_x,mystart_y,mymsize_x,mymsize_y as arguments
  - Modify the loop bounds from 0 to mymsize_x/y+1
  - Modify the call to ind2pos (pass ix+mystart_x instead of ix)
- Parallelize print function (**save_gnuplot**) parallelization
  - to parallelize it, let the rank=0 collect all the fields and print ASCII (just for didactic purposes)
  - the right way would be MPI I/O
- **To focus on MPI advanced features, parallel versions of init_fields and save_gnuplot are already provided**

MPI Basic - Hints / 4

- Main compute loop:
  - Modify the loops bounds (from 1 to mymsize_x/y)
  - MPI_Allreduce to the error variable (max among all the processes)
  - You are ready to check the first results, just print the error variable after one step: serial and parallel codes must give the same results
- **To focus on MPI advanced features, the parallel versions (except for communications) are already provided**
- Now you can start adding the communications
  - Inside the main compute loop
  - Usually just before the updates

MPI Basic - Hints / 5

- Communications
  - 4 MPI_Sendrecv are enough: send to left + recv from right, send to right + recv from left, send to top + recv from bottom, send to bottom + recv from top
- Send to left + recv from right
- Copy left boundary to a buffer
  - buffer_s_rl(1:mymsize_y) = T(1,1:mymsize_y)
- Send to left and receive from right
  - MPI_Sendrecv(buffer_s_rl, mymsize_y, MPI_DOUBLE_PRECISION, dest_rl, tag,
    buffer_r_rl, mymsize_y, MPI_DOUBLE_PRECISION, source_rl, tag,
    cartesianComm, status, ierr)
- Copy back the received buffer
  - if(source_rl >= 0) T(mymsize_x+1,1:mymsize_y) = buffer_r_rl(1:mymsize_y)
  - Why is the if required? Because MPI_Cart_shift return MPI_PROC_NULL when a neighboring process does not exist
  - MPI_Sendrecv can correctly handle it (no send or receive is performed in that case)
  - But the copy back from buffer to T must be avoided (otherwise T would be filled with unexpected values)

MPI Basic - Hints / 6

- Now probably you will face problems
  - Errors when compiling: check the arguments of MPI calls, the MPI types, and for Fortran the kinds
  - Start verifying that the MPI code still works using 1 processor (mpirun -np 1 …)
  - Then try to add the decomposition only on one dimension (mpirun -np 2 …)
  - You can check the residuals or you can also check the field to understand the origin of the error
- **Do not discourage! Parallelizing a code –even simple – is not straightforward**

MPI Advanced - Improvements

- So far we have a basic MPI parallelization of the original serial code
- Actually many improvements are possible
  - which may be possibly mixed

Use **non-blocking Communications** and **overlap** them with computations

Derived datatypes
Avoid copies on buffers even for not contiguous memory regions

Group communications using just one MPI **neighbour alltoall** call

Use **Remote Memory Access** to avoid explicit send-recv match (not very useful for this example)

MPI Advanced - (1) Overlap communications with computations

- In spite of MPI_Sendrecv, non blocking MPI calls can be employed
  - MPI_Isend, MPI_Irecv, …
- But, how to make them useful to enhance the scalability?
  - Since the MPI communications are needed only for ghost nodes some operations can be performed simultaneously
  - Which operations? The operations which do not involve the ghost points...
- As always, man (and the web, of course) is your friend:

```
man MPI_Init
```

(2) Using derived datatypes

- Restart from basic MPI version
- So far we have been using buffers as temporary storage for non-contiguous memory regions to send/recv (rows for Fortran and columns for C)
- But this can be avoided making the code more readable and possibly improving the performances
- Create two derived datatypes (actually just one is really mandatory)
  - A type for a matrix row (contiguous in C and vector in Fortran)
  - A type for a matrix column (contiguous in Fortran and vector in C)
- Then send/recv only 1 element of this type
  - No buffer is needed!
  - Just pass to MPI_Sendrecv the first element of the submatrix to pass and specify one element of the contiguous/vector type to pass
  - Hint: do not forget to commit the type after creation!

(3) Using Neighbor collective call

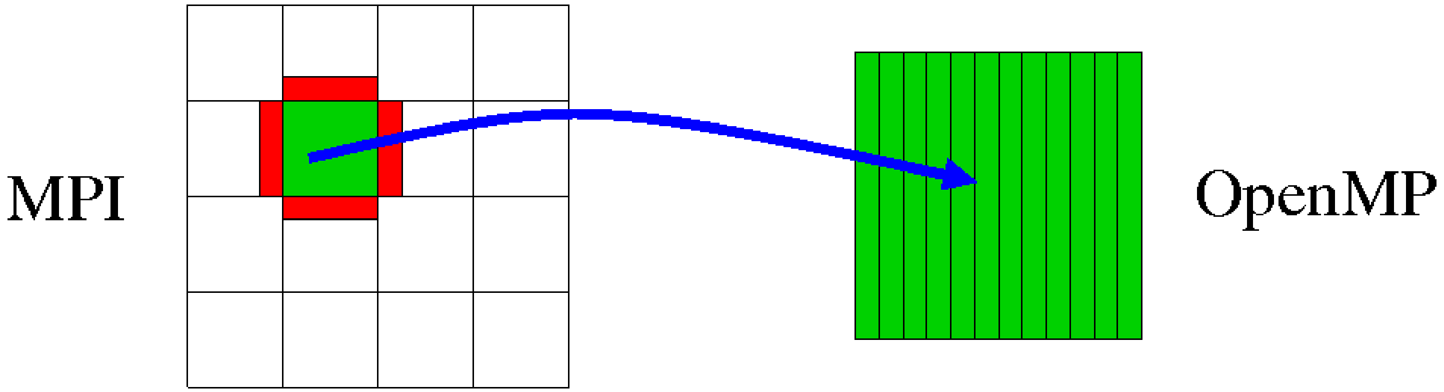
- Restart from basic MPI version
- Instead of 4 Sendrecv we can exploit the neighbour communication functions from MPI 3
  - Prepare a single send buffer with all the 4 buffers to send
  - Remember: for a Cartesian topology *the sequence of neighbors in the send and receive buffers at each process is defined by order of the dimensions, first the neighbor in the negative direction and then in the positive direction with displacement 1*
  - Use MPI_Ineighbor_alltoallv and then MPI_Wait
  - Copy back the received buffers (the same order apply)

(4) Using RMA

- Start from the derived datatype version
  - It makes much more sense
- First create two windows win_1 and win_2: one corresponding to T and one corresponding to Tnew
  - To get the win_size be standard and use MPI_Type_size
- Instead of the sendrecv:
  - MPI_Win_fence
  - MPI_Put for each edge: the starting address is the same as send of sendrecv and the displacement can be extracted from the recv of sendrecv
  - MPI_Win_fence again
- Beware:
  - the pointers of T and Tnew are switched during the computations but the windows do not switch at least in our basic version
  - therefore the fence/put previous block have to be duplicated for even and odd iterations: for odd iterations use win_1, for even iterations use win_2. Guess why?

(1) MPI + OpenMP – Hints

- To mix MPI and OpenMP the simplest way is to open the OMP parallel region just around the main computing loop (the update iteration loop from T to Tnew)
  - No direct interaction between MPI and OpenMP
  - But MPI_THREAD_FUNNELED should be required according to the standard
  - Actually MPI_THREAD_SINGLE (i.e., MPI_Init) also usually works (at least for OpenMPI)
  - 5 minutes should be enough to complete the hybridization
- Remember to add the *openmp* compilation option



(2) MPI + OpenMP – Hints

- But the parallel region may be enlarged to include the MPI communications
  - If the communications are performed by the master threads, MPI_THREAD_FUNNELED is enough
  - The communications may overlap with the computations: *master threads* performs the communications and then update the boundaries
  - At the same time, the other threads start doing bulk updating
  - Probably master threads collaborate after a while in doing that
  - The OMP schedule should be modified accordingly
- Remember
  - OMP master forces the code to be executed only by master thread
  - And the other threads go on

(3) MPI + OpenMP – Hints

- The parallel region may be further enlarged including the entire while loop
  - MPI_THREAD_SINGLE must be employed
  - Now we can overlap pointer exchange and the MPI reduction for the error
- Some OMP barriers are needed: where and why?
- Use OMP single
  - to do tasks which must be executed only by one thread: e.g. “iter=iter+1”
  - Or for the MPI_Allreduce

(4) MPI + OpenMP – Hints

- What about “each thread executing an MPI communication”?
  - You need MPI_THREAD_MULTIPLE support
  - Each thread performs a send/recv: how to implement in OpenMP?
  - The other threads immediately start the core updating loop...
  - Then wait for the other threads to finish (how?) and update the boundaries

Evaluating performances

- The different versions can lead to different results in term of performances
  - But the actual improvements depend on several factors
  - And are probably limited for such a didactic example
  - Testing in **realistic scenarios** is mandatory
  - For our case let us consider a 5000x5000 grid

	1	2	...	32768
MPI basic				
Overlap				
DDT				
Neighbour				
RMA				

Evaluating performances / 2

- To evaluate the improvement given by the hybrid programming the scaling evaluation can be more complex
  - No improvement expected for such a simple case

N_MPI / N_OpenMP	1	2	...	4096
1				
2				
4				
8				
16				

(1) MPI_THREAD_FUNNELED/1

```
do while (var > tol .and. iter <= maxIter)
   <...>
!$omp parallel do reduction(max:myvar)
   do j = 1, mymsize_y
     do i = 1, mymsize_x
        Tnew(i,j) = 0.25d0 * ( T(i-1,j) + T(i+1,j) +  &
                               T(i,j-1) + T(i,j+1) )
        myvar = max(myvar, abs( Tnew(i,j) - T(i,j) ))
     end do
   end do
!$omp end parallel do
   <...>
enddo
```

(1) MPI_THREAD_FUNNELED / 2

```
do while (var > tol .and. iter <= maxIter)
   <...>
!$omp parallel
!$omp master
   <MPI SEND_RECV>
   <BOUNDARY UPDATE>
!$omp end master
!$omp do reduction(max:myvar) schedule(dynamic,125)
   <CORE UPDATE>
!$omp end do
!$omp master
   myvar = max(myvar,mastervar)
!$omp end master
!$omp end parallel
   <...>
enddo
```

(2) MPI_THREAD_SERIALIZED

```
!$omp parallel
   do while (var > tol .and. iter <= maxIter)
!$omp barrier
!$omp single
      iter = iter + 1 ; var = 0.d0 ;  myvar = 0.d0 ;  mastervar = 0.d0
!$omp end single
!$omp master
      <MPI SEND_RECV>
      <BOUNDARY UPDATE>
!$omp end master
!$omp do reduction(max:myvar) schedule(dynamic,125)
      <CORE UPDATE>
!$omp end do
!$omp single
      Tmp =>T; T =>Tnew; Tnew => Tmp;
!$omp end single nowait
!$omp single
      myvar = max(myvar,mastervar)
      call MPI_Allreduce(myvar, var, 1, MPI_DOUBLE_PRECISION, &
                         MPI_MAX, MPI_COMM_WORLD, ierr)
!$omp end single
   end do
!$omp end parallel
```

(3) MPI_THREAD_MULTIPLE

```
!$omp parallel
   do while (var > tol .and. iter <= maxIter)
!$omp barrier
!$omp single
      iter = iter + 1 ; var = 0.d0 ;
      myvar = 0.d0 ;  mastervar = 0.d0
!$omp end single
!$omp single
      <1 MPI SEND_RECV>
!$omp single nowait
!$omp single
      <2 MPI SEND_RECV>
!$omp single nowait
!$omp single
      <3 MPI SEND_RECV>
!$omp single nowait
!$omp single
      <4 MPI SEND_RECV>
!$omp single nowait
```

```
!$omp do reduction(max:myvar) schedule(dynamic,125)
      <CORE UPDATE>
!$omp end do
!$omp do reduction(max:myvar)
      <BOUNDARY UPDATE>
!$omp end do
!$omp single
      Tmp =>T; T =>Tnew; Tnew => Tmp;
!$omp end single nowait
!$omp single
  call MPI_Allreduce(myvar, var, 1, &
  MPI_DOUBLE_PRECISION,MPI_MAX,MPI_COMM_WORLD, ierr)
!$omp end single
   end do
!$omp end parallel
```