Code Parallelization

a guided walk-through

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Code Parallelization

two **stages** to write a parallel code

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

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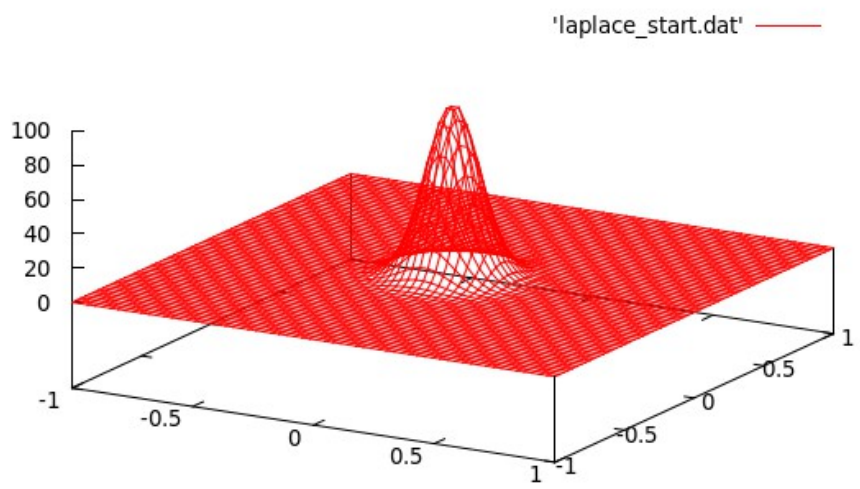
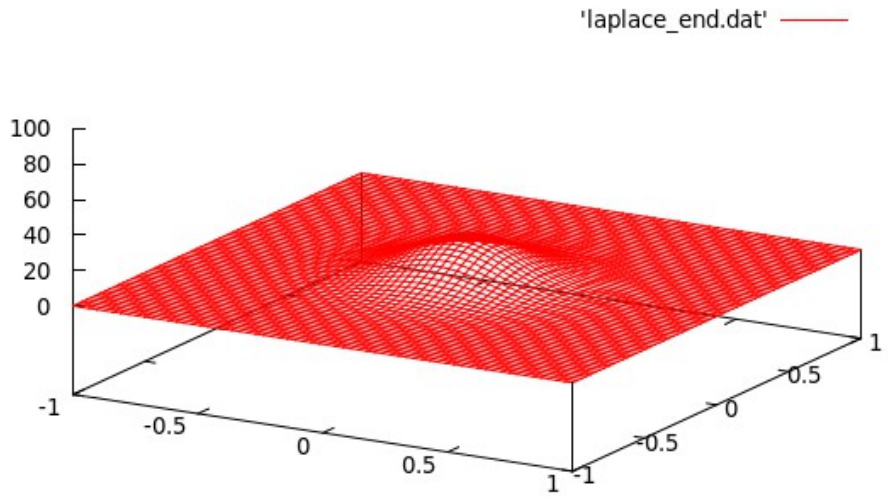
Problem domain

- 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:

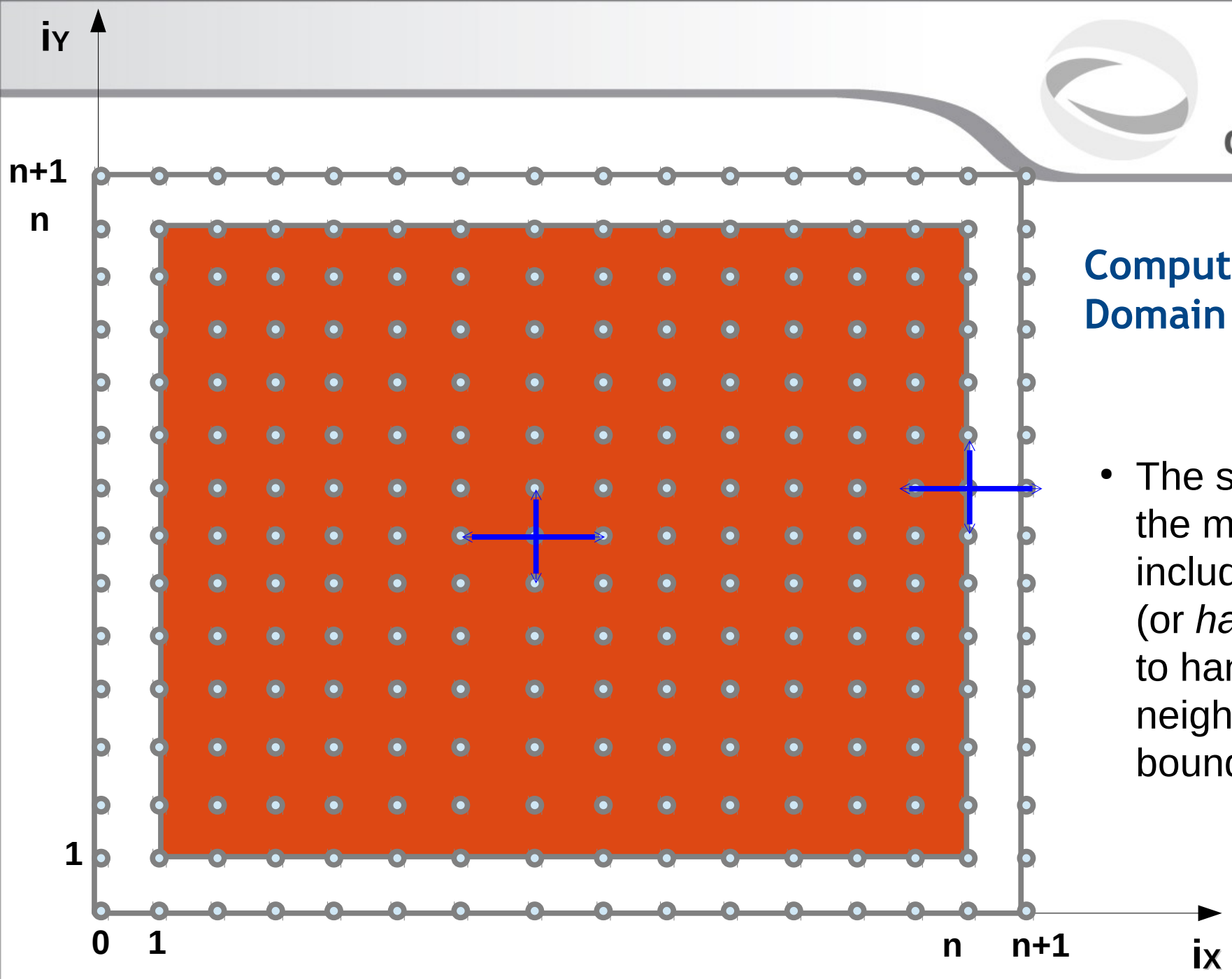
- **similar** operations that can be applied to **different parts** of the data structure

- 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

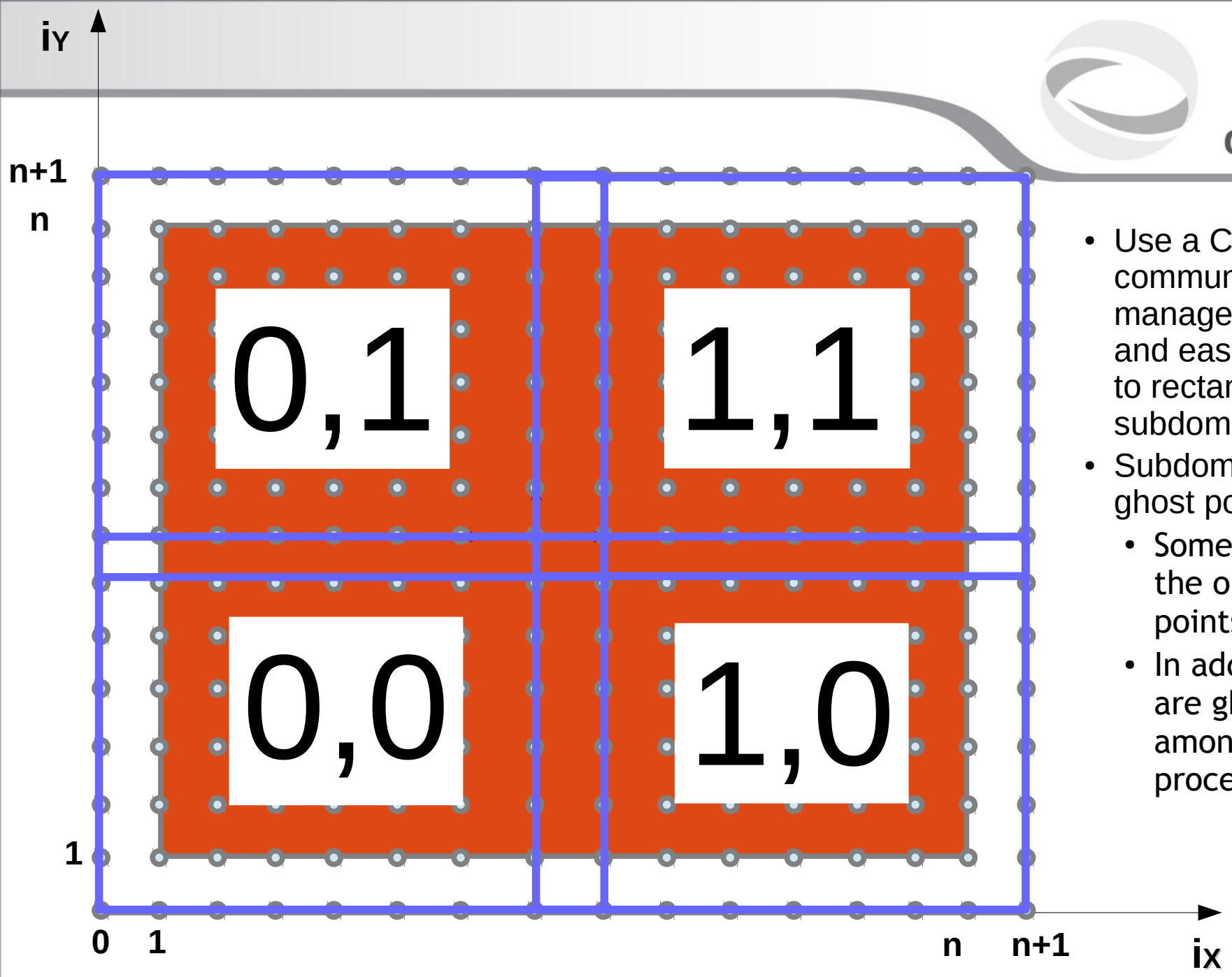
Handle dependencies among tasks:

- 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

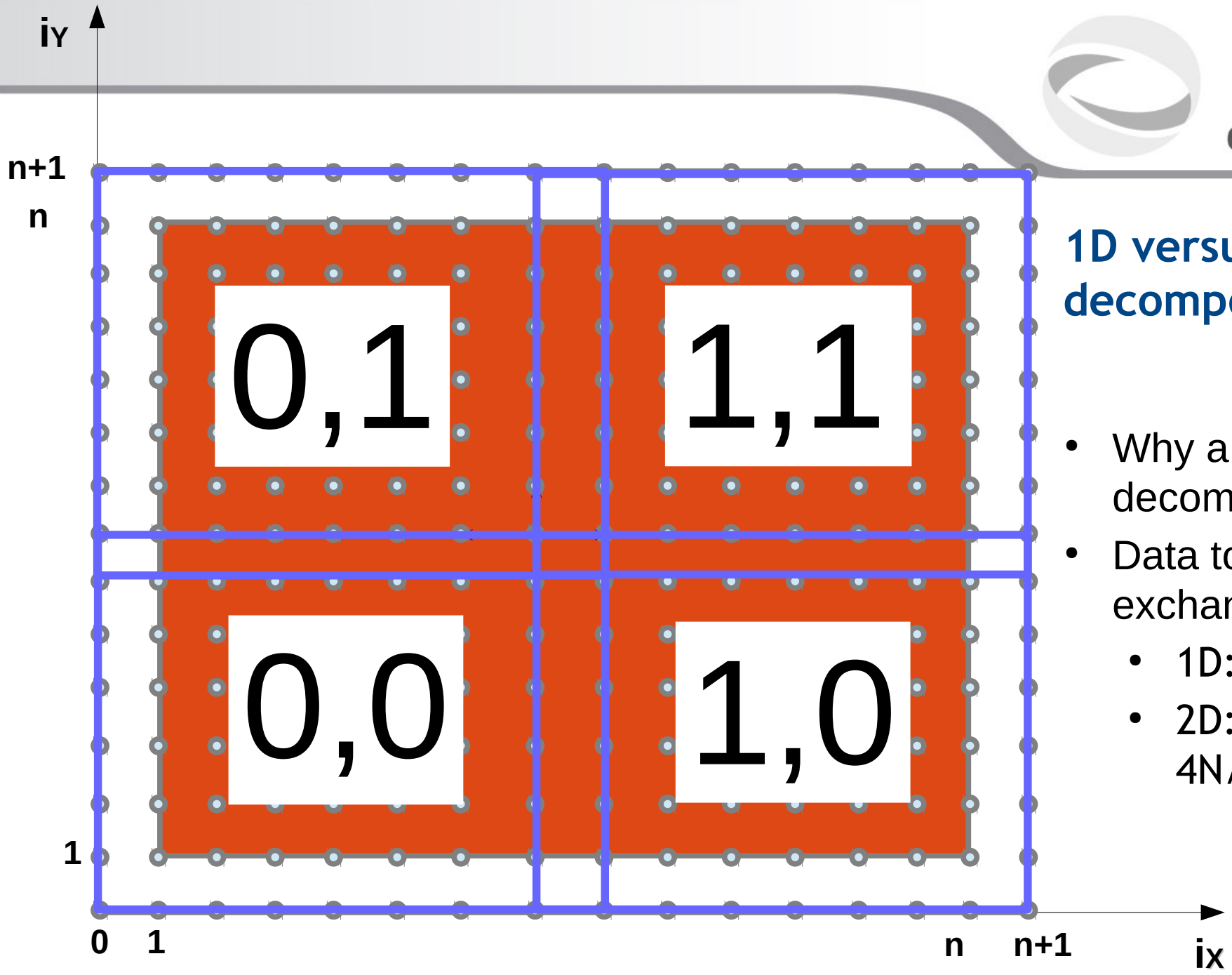


Computational Domain

- 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)**

Program domain

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

- problem domain
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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 derived data types
  - (c) Try to enhance the solution using non-blocking communications and overlapping computations with communications
- (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 skeletons of parallel versions are already provided
- You have to add:

  (1) **Broadcasting of input parameters**

  (2) Cartesian topology setup

  (3) SendRecv communications

  (4) AllReduce communication

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
- E.g., send to left + recv from right
  - Copy left boundary to a buffer
  - Send to left and receive from right
- Copy back the received buffer
  - A conditional statement is required: where and why?

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
  - two common possibilities

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

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

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:

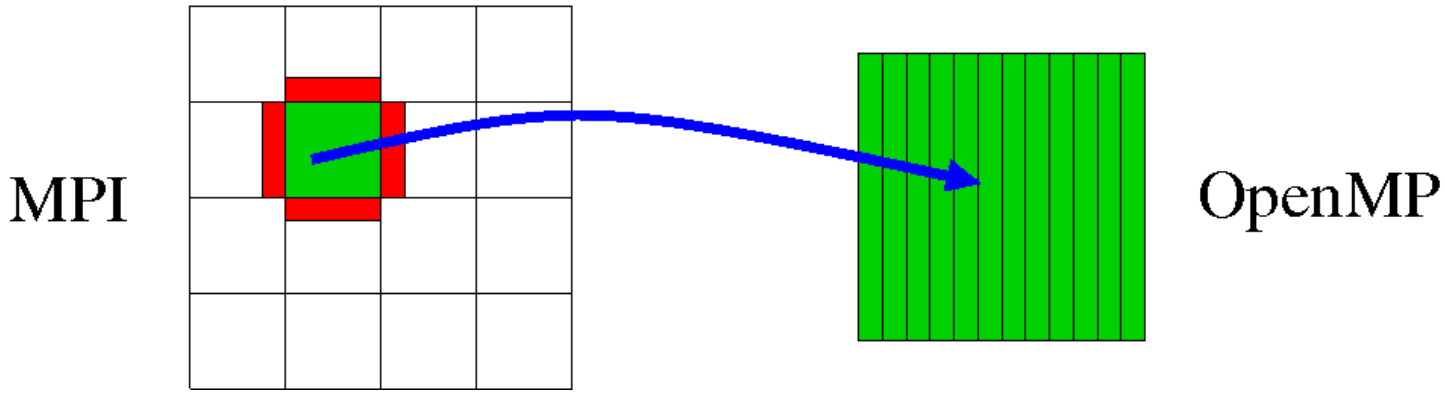
  man MPI_Init

(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 MPI derived datatypes (actually just one is really mandatory)
  - A type for a matrix row: which type is needed in Fortran? And in C?
  - A type for a matrix column: which type is needed in Fortran? And 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 derived types to pass
  - Hint: do not forget to commit the type after creation!

(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_SERIALIZED 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	...	256
MPI basic				
Overlap				
DDT				

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	...	256
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
```