MAX-PLANCK-INSTITUT
FÜR PLASMAPHYSIK

Multi Regions-of-Interest
in REFMUL3

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EUROfusion

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TÉCNICO LISBOA

Model and numerics

Solve for Maxwell's curl equations + constitutive relation (current density)

$$\nabla \times \mathbf{H} = \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} + \sigma \mathbf{E} + \mathbf{J}$$

$$\nabla \times \mathbf{E} = -\mu_0 \frac{\partial \mathbf{H}}{\partial t} - \sigma^\star \mathbf{H}$$

$$\frac{\partial \mathbf{J}}{\partial t} = \varepsilon_0 \omega_p^2 \mathbf{E} + \vec{\omega}_c \times \mathbf{J}$$

using the Finite Difference Time Domain (FDTD) method in Cartesian meshes

`REFMUL3` code

3D full-wave C code: hybrid OpenMP/MPI (3D) + OpenMP target offload (GPU)

K.S. Yee, *IEEE Trans Antennas Propag* **14** (1966) 302
L. Xu and N. Yuan *IEEE Antennas Wirel Propag Lett* **5** (2006) 335

F. Silva, S. Heuraux and T. Ribeiro *Proc. IRW13* (2017)
F. Silva, S. Heuraux, T. Ribeiro et al. *Fus Eng Des* **202** (2024) 114354

Motivation

What are regions-of-interest (ROI)?

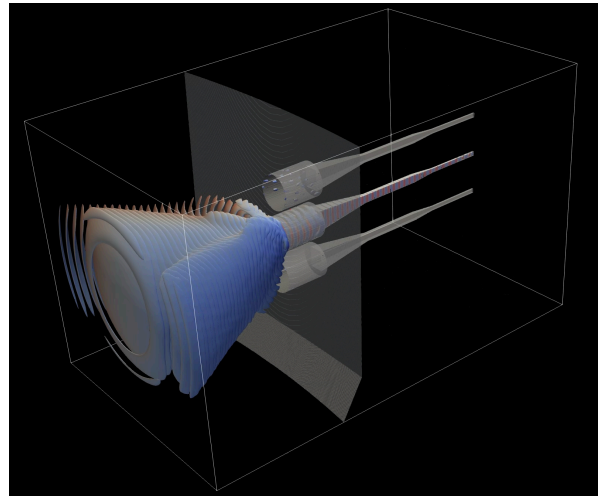
- wherever waves propagate!

Why do we need to consider them?

- wave-free volumes are currently computed
  - outside the vessel
  - inside metalic structures

Avoid:

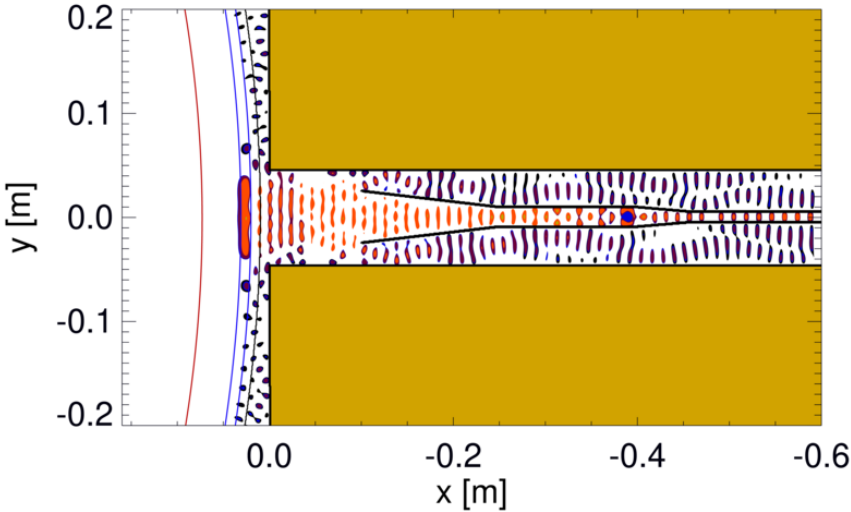
Waste of resources!



Outline

Outline

Example in 2D (simpler to illustrate)



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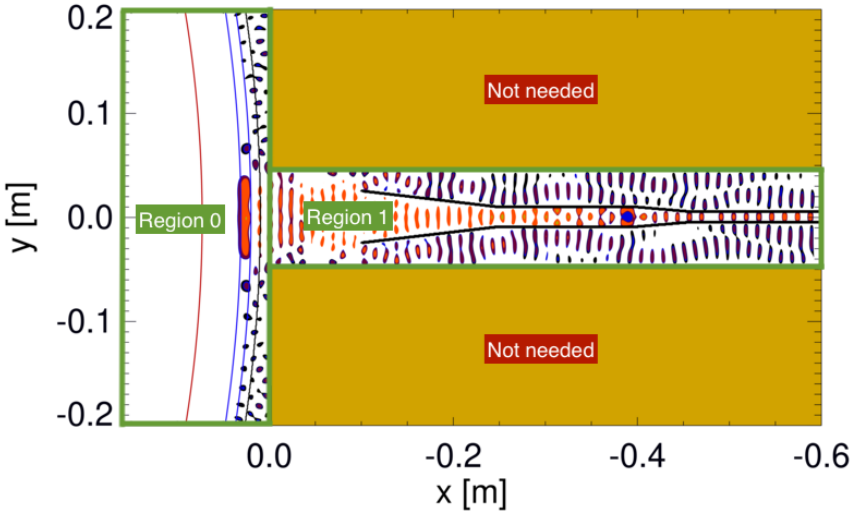

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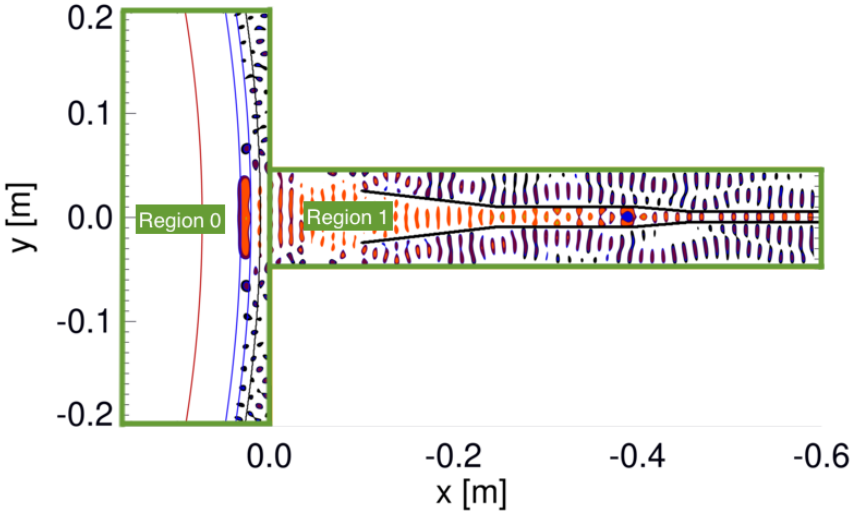
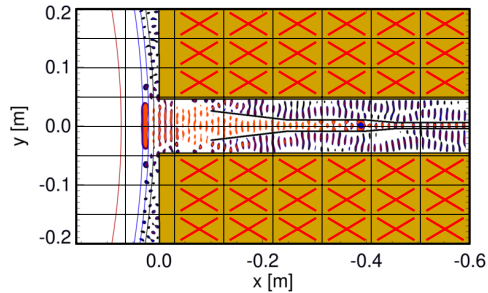


How to proceed?

A) Remove void subdomains

- Preprocess the decomposition
- Find/remove empty subdomains
- Caution: MPI Cartesian topology
- Issue: low granularities (e.g. GPUs)



B) Define regions-of-interest (ROI)

- Global virtual space
- More effective
- Same grid-resolution for all ROIs
- Challenge: non-matching subdomains

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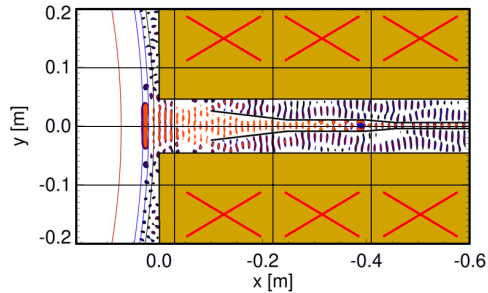

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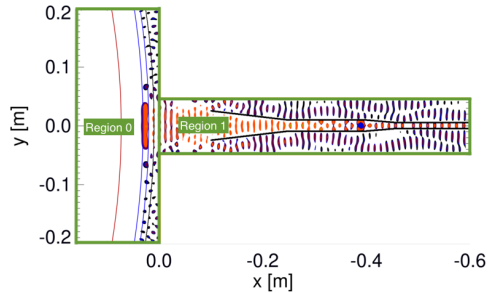

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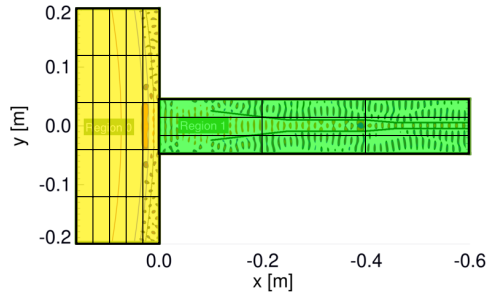
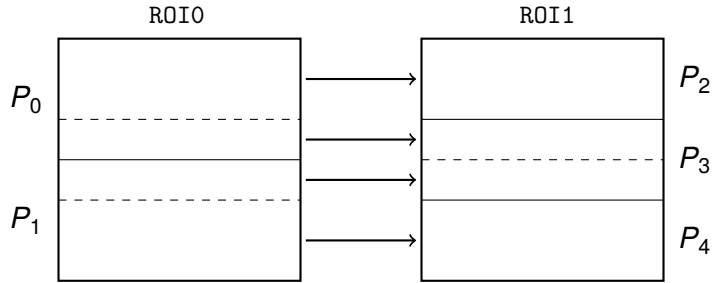


Outline

Starting point: non-matching subdomains

2D data sent from left to right, 1D domain decomposition (inspired in [1])



Beyond simple point-to-point communication

Each MPI task sends different messages to multiple MPI tasks

[1] *Using Advanced MPI: Modern Features of the Message-Passing* (2014) by W. Gropp, T. Hoefler, R. Thakur and E. Lusk

MPI collective communication function: `MPI_Alltoallv()`

```
1 int MPI_Alltoallv(
2   void *sendbuf, int *sendcnts, int *sendispls, MPI_Datatype sendtype,
3   void *recvbuf, int *recvcnts, int *recvdispls, MPI_Datatype recvtype,
4   MPI_Comm comm);
```

Parameters

- `sendbuf`: pointer to the send buffer containing the data to be sent.
- `sendcnts`: integer array (of length group size) specifying the number of elements to send to each task.
- `sendispls`: integer array (of length group size) specifying the displacement of first element relative to `sendbuf`.
- `sendtype`: data type of send buffer elements (handle).
- `recvbuf`: address of receive buffer (choice).
- `recvcnts`: integer array (of length group size) specifying the number of elements to receive from each task.
- `recvdispls`: integer array (of length group size) specifying the displacement of first relative to `recvbuf`.
- `recvtype`: data type of receive buffer elements (handle).
- `comm`: communicator (handle).

MPI collective communication function: `MPI_Alltoallv()`

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Parameters

- `sendbuf`: pointer to the send buffer containing the data to be sent.
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- `recvcnts`: integer array (of length group size) specifying the number of elements to receive from each task.
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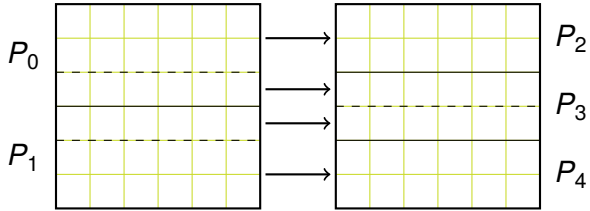
- `recvtype`: data type of receive buffer elements (handle).
- `comm`: communicator (handle).

Communication send patterns: 6x6 grid



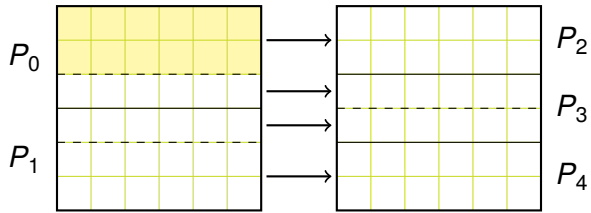
`sendcnts[ntasks]`

task	0	1	2	3	4
0					
1					
2					
3					
4					

`sendispls[ntasks]`

task	0	1	2	3	4
0					
1					
2					
3					
4					

Communication send patterns: 6x6 grid



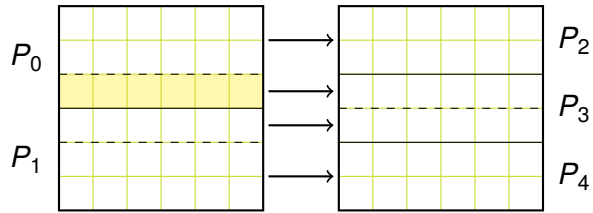
`sendcnts[ntasks]`

task	0	1	2	3	4
0	0	0	12		
1					
2					
3					
4					

`sendispls[ntasks]`

task	0	1	2	3	4
0	0	0	0		
1					
2					
3					
4					

Communication send patterns: 6x6 grid



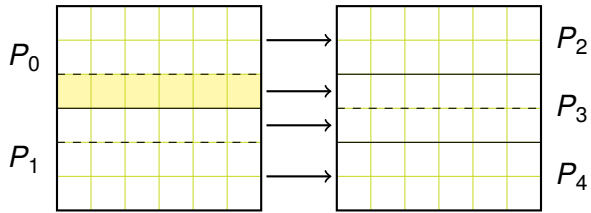
`sendcnts[ntasks]`

task	0	1	2	3	4
0	0	0	12	6	
1					
2					
3					
4					

`sendispls[ntasks]`

task	0	1	2	3	4
0	0	0	0	12	
1					
2					
3					
4					

Communication send patterns: 6x6 grid



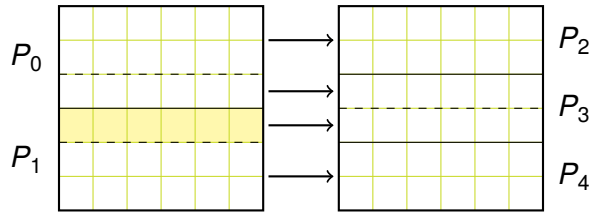
`sendcnts[ntasks]`

task	0	1	2	3	4
0	0	0	12	6	0
1					
2					
3					
4					

`sendispls[ntasks]`

task	0	1	2	3	4
0	0	0	0	12	0
1					
2					
3					
4					

Communication send patterns: 6x6 grid



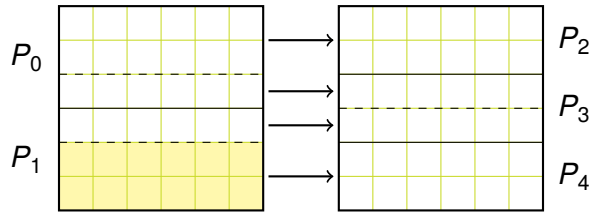
`sendcnts[ntasks]`

task	0	1	2	3	4
0	0	0	12	6	0
1	0	0	0	6	
2					
3					
4					

`sendispls[ntasks]`

task	0	1	2	3	4
0	0	0	0	12	0
1	0	0	0	0	
2					
3					
4					

Communication send patterns: 6x6 grid



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task	0	1	2	3	4
0	0	0	12	6	0
1	0	0	0	6	12
2					
3					
4					

`sendispls[ntasks]`

task	0	1	2	3	4
0	0	0	0	12	0
1	0	0	0	0	6
2					
3					
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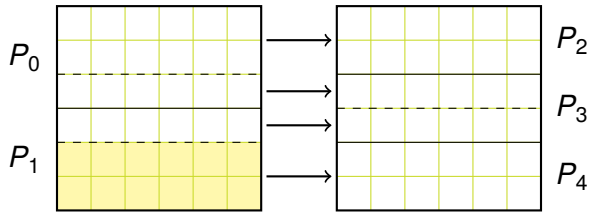


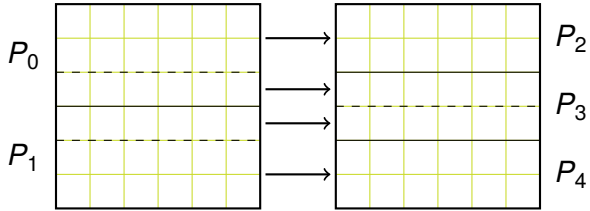
`sendcnts[ntasks]`

task	0	1	2	3	4
0	0	0	12	6	0
1	0	0	0	6	12
2	0	0	0	0	0
3	0	0	0	0	0
4	0	0	0	0	0

`sendispls[ntasks]`

task	0	1	2	3	4
0	0	0	0	12	0
1	0	0	0	0	6
2	0	0	0	0	0
3	0	0	0	0	0
4	0	0	0	0	0

Communication receive patterns: 6x6 grid



`recvcnts[ntasks]`

task	0	1	2	3	4
0					
1					
2					
3					
4					

`recvispls[ntasks]`

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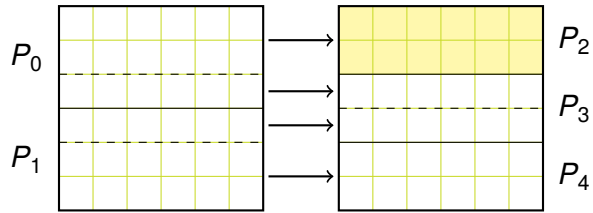
0					
1					
2					
3					
4					

Communication receive patterns: 6x6 grid



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0	0	0	0	0	0
1	0	0	0	0	0
2	12				
3					
4					

`recvispls[ntasks]`

task	0	1	2	3	4
0	0	0	0	0	0
1	0	0	0	0	0
2	0				
3					
4					

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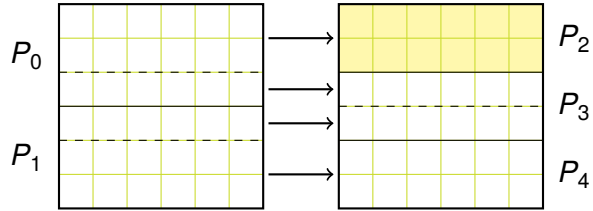

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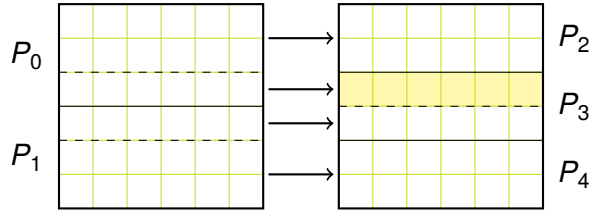
task	0	1	2	3	4
0	0	0	0	0	0
1	0	0	0	0	0
2	12	0	0	0	0
3					
4					

`recvispls[ntasks]`

task	0	1	2	3	4
0	0	0	0	0	0
1	0	0	0	0	0
2	0	0	0	0	0
3					
4					

Communication receive patterns: 6x6 grid



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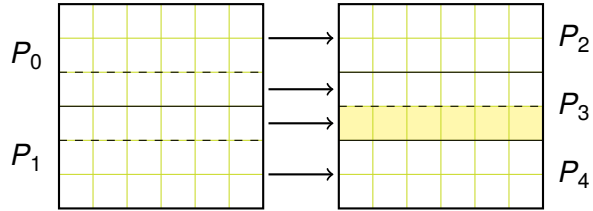
task	0	1	2	3	4
0	0	0	0	0	0
1	0	0	0	0	0
2	12	0	0	0	0
3	6				
4					

`recvispls[ntasks]`

task	0	1	2	3	4
0	0	0	0	0	0
1	0	0	0	0	0
2	0	0	0	0	0
3	0				
4					

Communication receive patterns: 6x6 grid



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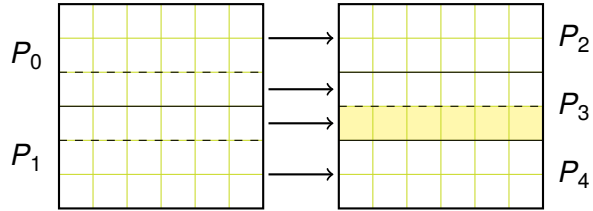
task	0	1	2	3	4
0	0	0	0	0	0
1	0	0	0	0	0
2	12	0	0	0	0
3	6	6			
4					

`recvispls[ntasks]`

task	0	1	2	3	4
0	0	0	0	0	0
1	0	0	0	0	0
2	0	0	0	0	0
3	0	6			
4					

Communication receive patterns: 6x6 grid



`recvcnts[ntasks]`

task	0	1	2	3	4
0	0	0	0	0	0
1	0	0	0	0	0
2	12	0	0	0	0
3	6	6	0	0	0
4					

`recvispls[ntasks]`

task	0	1	2	3	4
0	0	0	0	0	0
1	0	0	0	0	0
2	0	0	0	0	0
3	0	6	0	0	0
4					

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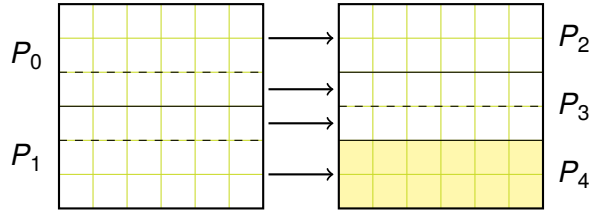

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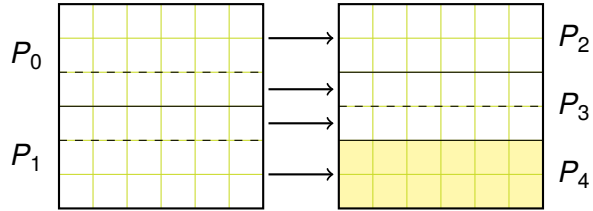
task	0	1	2	3	4
0	0	0	0	0	0
1	0	0	0	0	0
2	12	0	0	0	0
3	6	6	0	0	0
4	0	12			

`recvispls[ntasks]`

task	0	1	2	3	4
0	0	0	0	0	0
1	0	0	0	0	0
2	0	0	0	0	0
3	0	6	0	0	0
4	0	0			

Communication receive patterns: 6x6 grid



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0	0	0	0	0	0
1	0	0	0	0	0
2	12	0	0	0	0
3	6	6	0	0	0
4	0	12	0	0	0

`recvispls[ntasks]`

task	0	1	2	3	4
0	0	0	0	0	0
1	0	0	0	0	0
2	0	0	0	0	0
3	0	6	0	0	0
4	0	0	0	0	0

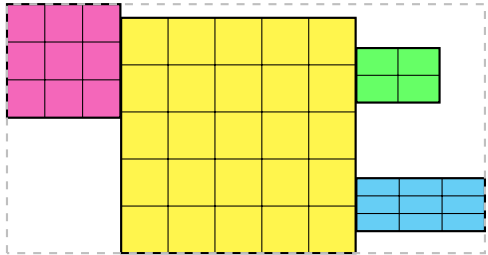
Compute arguments for `MPI_Alltoallv()`

```
1  /* loop ranks in remote ROI only, since there are no local ROI exchanges */
2  for (int iRank = myRankF[color_rm]; iRank < myRankL[color_rm]; iRank++) {
3    if (color == color_here) {
4      jF_rm = calc_jF(iRank - myRankF[color_rm], nRanks_ROI[color_rm], Ni, Nj);
5      jL_rm = calc_jL(iRank - myRankF[color_rm], nRanks_ROI[color_rm], Ni, Nj);
6      if (jF <= jL_rm && jL >= jF_rm) {
7        commcounts[iRank] = ( min(jL, jL_rm) - max(jF, jF_rm) + 1) * Ni;
8        commispls[iRank] = displs;
9        displs += commcounts[iRank];}
10     else {
11       commcounts[iRank] = 0;
12       commdispls[iRank] = 0;}
13   } else {  /* color == color_rm */
14     commcounts[iRank] = 0;
15     commdispls[iRank] = 0;}
16 }
```

Computing `*counts` & `*displs` is easier than using point-to-point communication

Outline

Generalizations in 2D

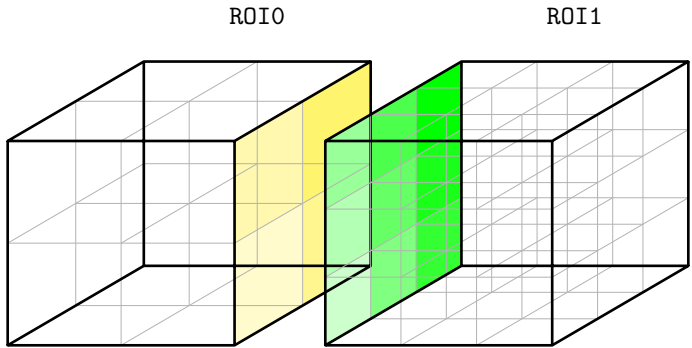


- 2D domain decomposition: adjust computation of `counts` & `displs`
- Exchange of ghost-layers: communication buffers become 1D
- MPI communicators & groups: subset of MPI tasks in each ROI interface
- $>$ 2 ROIs: global virtual space (not allocated) as reference frame

General 2D domain decomposed multi-ROI configurations: implemented and tested

Outline

Towards 3D

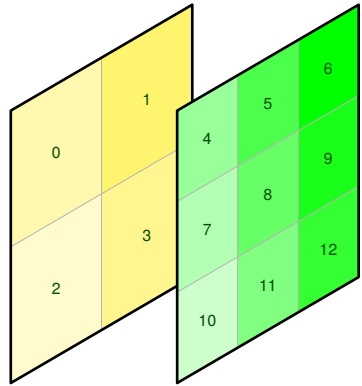


Important difference:

Communication buffers between 3D ROIs are 2D faces decomposed in 2D

Interface communication

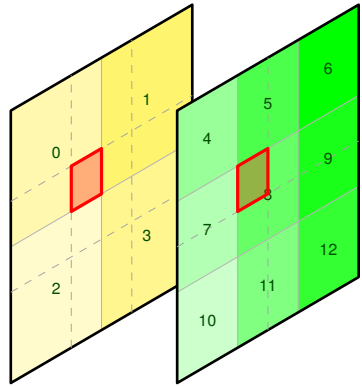
2D communication buffers



Interface communication

2D communication buffers

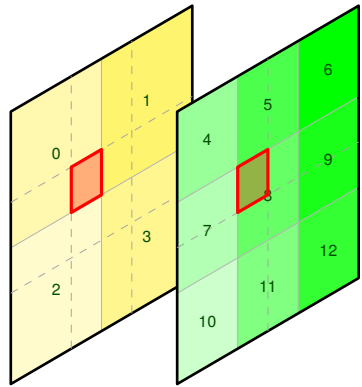
- Exchanged data: subsets of 2D data
- Memory access pattern is non-contiguous!



Interface communication

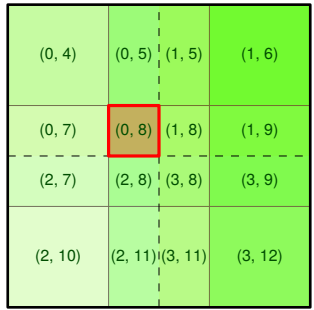
2D communication buffers

- Exchanged data: subsets of 2D data
- Memory access pattern is non-contiguous!
- Arrays of `counts` and `displs` + `MPI_Alltoallv()`: not enough
- Further concepts required, e.g. `blocksize` and `stride`



Non-contiguous memory access

How can we generalize our algorithm?



superposition of interface communication buffers and data layout

Solution:

Use most general `MPI_Alltoallw()` call together with MPI derived data types

MPI derived data types + `MPI_Alltoallw()` (ongoing)

```
1 int MPI_Alltoallw(
2   void *sendbuf, int *sendcnts, int *sendispls, MPI_Datatype *sendtype,
3   void *recvbuf, int *recvcnts, int *recvdispls, MPI_Datatype *recvtype,
4   MPI_Comm comm);
```

Strategy

- Compute `counts` and `displs` as before (using Cartesian topology)
- Use this information to create array of MPI derived data types (DDT)
- Each DDT describes memory access pattern to communication buffers
- Call `MPI_Alltoallw()` (not `v`!) using array of DDTs as argument

Note:

Already implemented for 2D multi-ROI case, extension to 3D ongoing...

Outline

Summary & outlook

Multi regions-of-interest

- Same grid-resolution for all ROIs
- Non-matching interface subdomains
- Communication algorithm devised
- Tailored all-to-all communication + memory access patterns
- General multi-ROI 2D configuration: implemented
- Extension to 3D ongoing: should be finished soon...

Outlook

- Deployment to `REFMUL3`: left for future work