MPI derived datatypes & Cartesian grids

CPS343

Parallel and High Performance Computing

Spring 2020

Outline

1. MPI Datatypes
   - Datatypes in MPI
   - Derived Datatypes in MPI
2. Extended example of vector type
   - Cartesian Grids
   - Cartesian communicator example

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Built-in Datatypes

- The MPI standard defines many built in datatypes, mostly mirroring standard C/C++ or FORTRAN datatypes
- These are sufficient when sending single instances of each type
- They are also usually sufficient when sending contiguous blocks of a single type
- Sometimes, however, we want to send non-contiguous data or data that is comprised of multiple types
- MPI provides a mechanism to create **derived datatypes** that are built from simple datatypes

Typemaps

- Derived datatypes in MPI are described by a **typemap**
- Typemaps consist of an order pair or sequence of ordered pairs each containing
  - a basic datatype
  - a displacement (integer offset)
- For example, a typemap might consist of {(double,0),(char,8)} indicating the type has two elements:
  - a double precision floating point value starting at displacement 0, and
  - a single character starting at displacement 8.

Typemaps

- Types also have **extent**, which indicates how much space is required for the type
- The extent of a type may be more than the sum of the bytes required for each component
- For example, on a machine that requires double-precision numbers to start on an 16-byte boundary the type $\{(\text{double},0),(\text{char},8)\}$ will have an extent of 16 even though it only requires 9 bytes

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Derived Datatypes

MPI provides for user-constructed datatypes to handle a wide variety of situations. Constructors exist for the following types of derived datatypes:

- Contiguous
- Vector
- Hvector
- Indexed
- Hindexed
- Indexed_block
- Struct

The "H" routines are the same as the similarly named types except that strides and block displacements are specified in bytes.

Creating and using a new datatype

Two steps are necessary to create and use a new datatype in MPI:

1. *Create* the type using one of MPI's type construction routines (explained next),
2. *Commit* the type using `MPI_Type_commit()`.

Once a type has been committed it may be used in send, receive, and other buffer operations.

A committed type can be released with `MPI_Type_free()`.

Contiguous type

The contiguous datatype allows for a single type to refer to multiple contiguous elements of an existing datatype.

```
int MPI_Type_contiguous(
  int count,                // replication count
  MPI_Datatype oldtype,     // old datatype
  MPI_Datatype* newtype)    // new datatype
```

Contiguous type

The contiguous datatype allows for a single type to refer to multiple contiguous elements of an existing datatype.

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  int count,                // replication count
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  MPI_Datatype* newtype)    // new datatype
```

The new datatype is essentially an array of `count` elements having type `oldtype`. For example, the following two code fragments are equivalent:

```
  MPI_Send(a, n, MPI_DOUBLE, dest, tag, MPI_COMM_WORLD);
```

and

```
  MPI_Datatype rowtype;
  MPI_Type_contiguous(n, MPI_DOUBLE, &rowtype);
  MPI_Type_commit(&rowtype);
  MPI_Send(a, 1, rowtype, dest, tag, MPI_COMM_WORLD);
```

Vector type

The vector datatype is similar to the contiguous datatype but allows for a constant non-unit *stride* between elements.

```
int MPI_Type_vector(
  int count,            // number of blocks
  int blocklength,      // number of elements in each block
  int stride,           // number of elements between each block
  MPI_Datatype oldtype,  // old datatype
  MPI_Datatype* newtype) // new datatype
```

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  int stride,           // number of elements between each block
  MPI_Datatype oldtype,  // old datatype
  MPI_Datatype* newtype) // new datatype
```
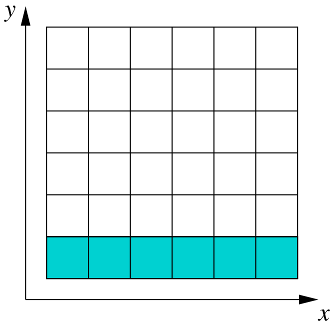

For example, suppose an nx × ny Cartesian grid is stored so data in rows (constant y) is contiguous. The following two types can be used to communicate a single row and a single column of the grid:

```
  MPI_Datatype xSlice, ySlice;
  MPI_Type_vector(nx, 1, ny, MPI_DOUBLE, &xSlice);
  MPI_Type_vector(ny, 1, 1, MPI_DOUBLE, &ySlice);
  MPI_Type_commit(&xSlice);
  MPI_Type_commit(&ySlice);
```

Vector type

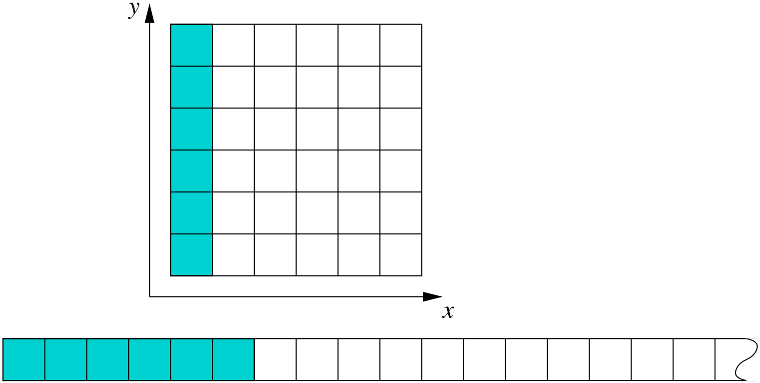
```
MPI_Type_vector(nx, 1, ny, MPI_DOUBLE, &xSlice);
```



Note: In contrast to how we view matrices, in C/C++ elements in a row of a Cartesian grid have non-unit stride: `u[0][0]` and `u[1][0]` are not contiguous.

Vector type

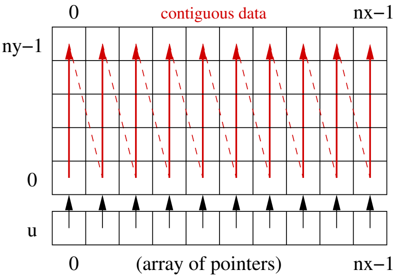
```
MPI_Type_vector(ny, 1, 1, MPI_DOUBLE, &ySlice);
```



In general, the last index corresponds to the dimension with unit stride and the first index corresponds to the dimension with greatest stride.

Vector type

```
double** u = new double* [nx];
u[0] = new double [nx * ny];

for ( i = 1; i < nx; i++ )
    u[i] = &u[0][i * ny];
```



- Note that by this construction `u` is a pointer to a pointer.
- `u[0]` is a pointer to the start of the first grid *column*.
- Consecutive locations in memory correspond to consecutive values of the last array index; in this case that is along the *y* axis.
- If the grid was 3-dimensional, consecutive memory locations would be along *z*, consecutive *z*-columns would be adjacent on the *y* axis, and finally *yz*-slices would be adjacent along the *x* axis.

Indexed type

The indexed datatype provides for varying strides between elements.

```
int MPI_Type_indexed(
  int count,                  // number of blocks
  int* blocklengths,          // number of elements per block
  int* displacements,         // displacement for each block
  MPI_Datatype oldtype,       // old datatype
  MPI_Datatype* newtype)      // new datatype
```

Indexed type

The indexed datatype provides for varying strides between elements.

```
int MPI_Type_indexed(
  int count,                // number of blocks
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  int* displacements,       // displacement for each block
  MPI_Datatype oldtype,     // old datatype
  MPI_Datatype* newtype)    // new datatype
```
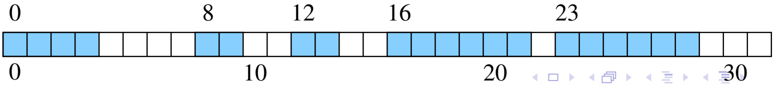

This generalizes the vector type; instead of a constant stride, blocks can be of varying length and displacements. For example, the code fragment

```
  int blocklen[] = {4, 2, 2, 6, 6};
  int disp[] = {0, 8, 12, 16, 23};
  MPI_Datatype mytype;
  MPI_Type_indexed(5, blocklen, disp, MPI_DOUBLE, &mytype);
  MPI_Type_commit(&mytype);
```

defines a type that corresponds to the shaded cells:



Struct type

The most general constructor allows for the creation of types representing general C/C++ structs/classes.

```
int MPI_Type_create_struct(
  int count,                    // number of blocks
  int* blocklengths,            // number of elements per block
  MPI_Aint* displacements,      // byte displacement of each block
  MPI_Datatype* datatypes,      // type of elements in each block
  MPI_Datatype* newtype)        // new datatype
```

The type `MPI_Aint` is an *address* type; variables of this type can hold valid addresses (byte offsets from the start of memory).

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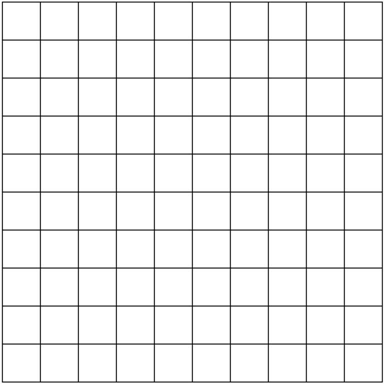
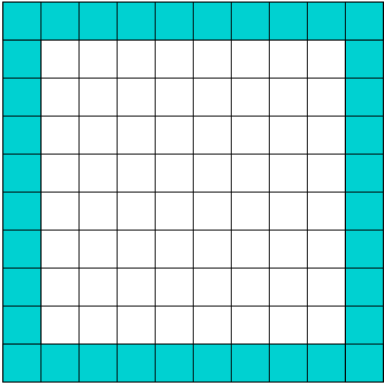
A sample grid



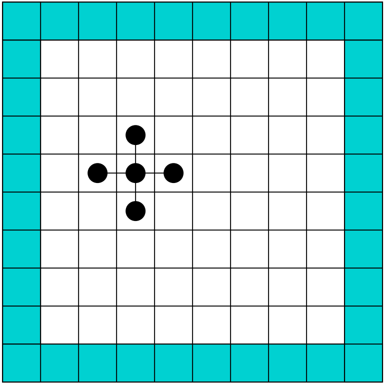
- Typical 10×10 grid
- Lines separate grid elements

Grid boundary



- Grid boundary in cyan
- Typically contains constant data
- Grid points on interior change

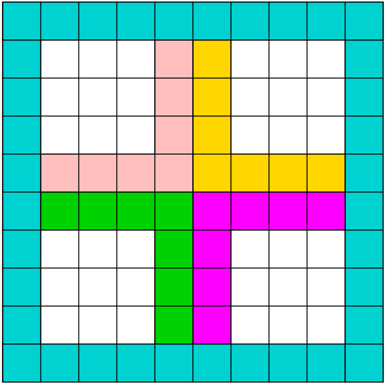
Grid boundary



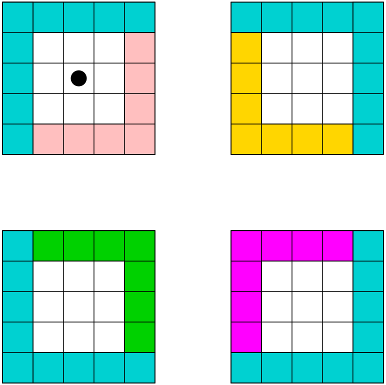
- Grid boundary in cyan
- Typically contains constant data
- Grid points on interior change
- We will assume grid elements are updated using a 5-point finite-difference stencil

Partitioning the grid

- Suppose we want to partition the domain into four subdomains
- Could be done vertically or horizontally
- In this case, we'll partition in both directions

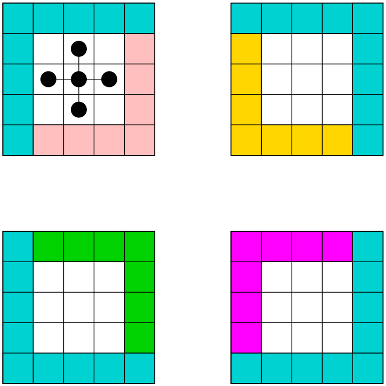


Partitioning the grid



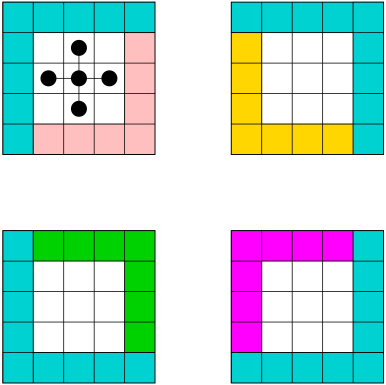
- To update the grid point marked with the black dot information is needed from its four neighbors

Partitioning the grid



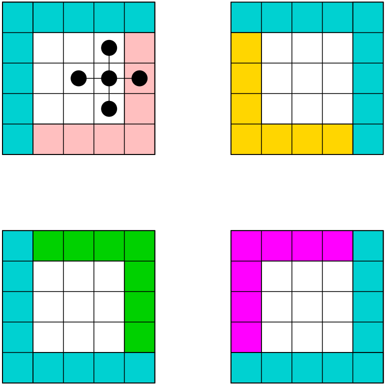
- To update the grid point marked with the black dot information is needed from its four neighbors
- The stencil shows the grid points needed for the update

Partitioning the grid



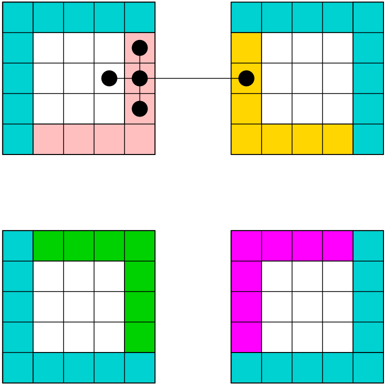
- To update the grid point marked with the black dot information is needed from its four neighbors
- The stencil shows the grid points needed for the update
- All accessed grid points are inside the local subdomain

Partitioning the grid



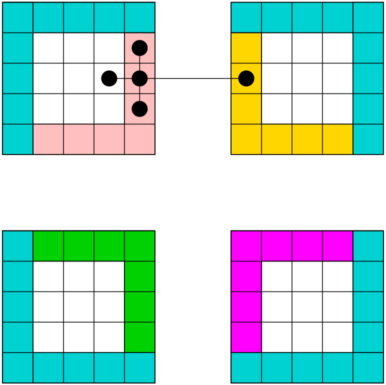
- To update the grid point marked with the black dot information is needed from its four neighbors
- The stencil shows the grid points needed for the update
- All accessed grid points are inside the local subdomain
- To update an adjacent grid point we still only need to access points inside the subdomain

Partitioning the grid



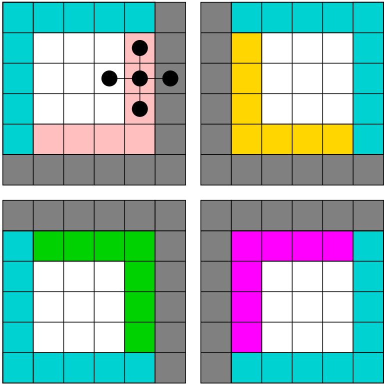
- To update the grid point marked with the black dot information is needed from its four neighbors
- The stencil shows the grid points needed for the update
- All accessed grid points are inside the local subdomain
- To update an adjacent grid point we still only need to access points inside the subdomain
- But moving over one more, we now need information from an adjacent subdomain

Adding interior boundaries



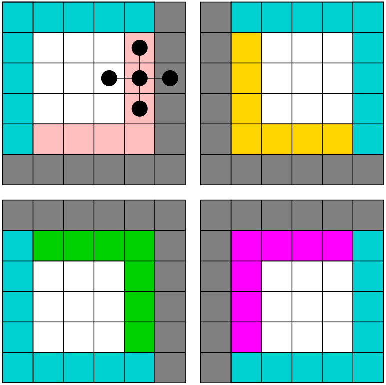
- Assuming a message passing environment, we want to minimize communication

Adding interior boundaries



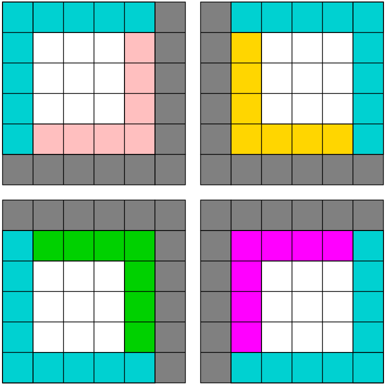
- Assuming a message passing environment, we want to minimize communication
- To facilitate this, we create additional grid locations to hold copies of data from adjacent subdomains; these are often called *ghost points* or the *halo region*

Adding interior boundaries



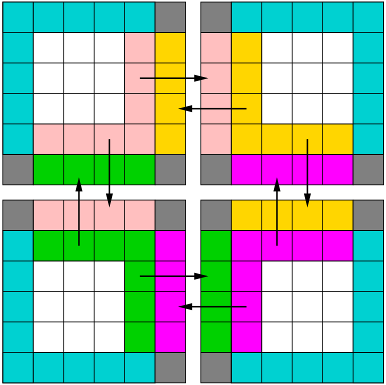
- Assuming a message passing environment, we want to minimize communication
- To facilitate this, we create additional grid locations to hold copies of data from adjacent subdomains; these are often called *ghost points* or the *halo region*
- Still need to transfer, but now blocks can be transferred

Adding interior boundaries



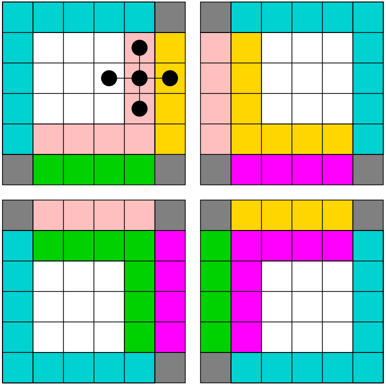
- Before each new set of updates...

Adding interior boundaries



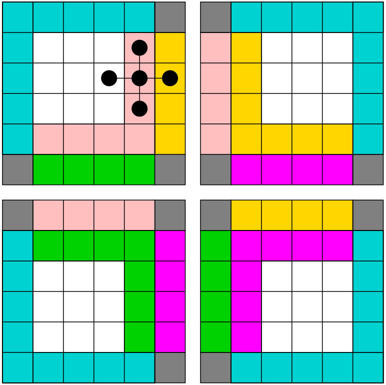
- Before each new set of updates...
- Interior boundary data is sent to processes working on adjacent subdomains

Adding interior boundaries



- Before each new set of updates...
- Interior boundary data is sent to processes working on adjacent subdomains
- Now accesses are once again limited to local subdomain

Adding interior boundaries



- Before each new set of updates...
- Interior boundary data is sent to processes working on adjacent subdomains
- Now accesses are once again limited to local subdomain
- True boundary data can be copied, but will not be used

Typical application

- An important application that uses this pattern of data access is the numerical solution of boundary value problems involving partial differential equations
- Programs are iterative, and repeatedly updates grid points with various "sweeps" through the domain.
- Between each sweep interior boundary data must be communicated
- Need to avoid deadlock situations; suppose both processes exchanging data send before receiving? This may or may not be a problem, depending on how `MPI_Send()` is implemented.
- We can avoid any problems, however, by using the `MPI_Sendrecv()` function.

MPI_Sendrecv()

The calling sequence for MPI_Sendrecv() is

```
int MPI_Sendrecv(
  void* sendbuf,           // address of send buffer
  int sendcount,           // number of elements to send
  MPI_Datatype sendtype,   // type of elements to send
  int dest,                // rank of destination
  int sendtag,             // send tag
  void* recvbuf,           // address of receive buffer
  int recvcount,           // number of elements to receive
  MPI_Datatype recvtype,   // type of elements to receive
  int source,              // rank of source
  int recvtag,             // receive tag
  MPI_Comm comm,           // communicator
  MPI_Status* status)      // status object
```

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MPI Cartesian communicator

Steps necessary to set up a Cartesian communicator:

1. Construct new communicator to use rather than `MPI_COMM_WORLD`
2. Determine my portion of grid
3. Determine my neighbors
4. Adjust boundaries as needed
5. Create necessary MPI data types
6. Communicate!

MPI Cartesian communicator code block 1

```
// Create Cartesian communicator
MPI_Dims_create( numProcesses, 2, dims );
MPI_Cart_create( MPI_COMM_WORLD, 2, dims, periodic,
                 reorder, &comm2d );
MPI_Comm_rank( comm2d, &myRank );
```

- `dims[]` is a two-dimensional array that contains the number of blocks in the x and y dimensions we want the grid to have. If these values are 0 then MPI chooses them for us.
- Entries in `periodic[]` are non-zero to indicate the grid is periodic in the corresponding dimension. Zero entries (as in this example) mean grid is non-periodic.
- If `reorder` is nonzero then processes can be be reassigned ranks, possibility different than those they received during MPI initialization.
- Rank will be determined relative to `comm2d` communicator, not `MPI_COMM_WORLD`.

MPI Cartesian communicator code block 2

```
// Figure out the size of my portion of the grid.
// x0, y0, x1 and y1 are the starting and ending
// indices of both dimensions of our portion of
// the grid.

MPI_Cart_get( comm2d, 2, dims, periodic, coords );
decompose1d( NX, dims[0], coords[0], &x0, &x1 );
decompose1d( NY, dims[1], coords[1], &y0, &y1 );
```

- `periodic[]` gets filled with 0s or 1s to indicate if the grid is periodic along the corresponding dimension.
- `coords[]` gets filled with coordinates (indexed from 0) of the block associated with the this process.
- `decompose1d()` returns the start and ending values of subinterval for this process. (See *Using MPI* by Gropp et al.)

MPI Cartesian communicator code block 3

```
// Figure out who my neighbors are.  left, right,
// down, and up will be set to the rank of the
// process responsible for the corresponding block
// relative to the position of the block we are
// responsible for.  If there is no neighbor in a
// particular direction the returned rank will be
// MPI_PROC_NULL which will be ignored by subsequent
// MPI_sendrecv() calls.

MPI_Cart_shift( comm2d, 0, 1, &left, &right );
MPI_Cart_shift( comm2d, 1, 1, &down, &up );
```

- Second argument is shift axis: 0, 1, 2... for x, y, z...
- Third argument for displacement to neighboring block:
  > 0 for "up" shift,
  < 0 for "down" shift.

MPI Cartesian communicator code block 4

```
// Adjust domain bounds to account for internal
// domain boundary data.  If we have a neighbor
// in a given direction (rank of neighbor is non-
// negative) then we need to adjust the starting
// or ending index.

if ( left  >= 0 ) x0--;
if ( right >= 0 ) x1++;
if ( down  >= 0 ) y0--;
if ( up    >= 0 ) y1++;
nx = x1 - x0 + 1;  // actual x size of our grid
ny = y1 - y0 + 1;  // actual y size of our grid
```

MPI Cartesian communicator code block 5

```
// Create my portion of the grid.  For the exchange
// to work properly we must have a constant stride
// in each dimension.  This is accomplished by
// allocating an array of pointers then allocating
// the full data array to the first pointer.  The
// remaining pointers are set to point to the start
// of each "row" of contiguous data in the single
// linear array.

double** u = new double* [nx];
u[0] = new double [nx * ny];
for ( i = 1; i < nx; i++ ) u[i] = &u[0][i * ny];
```

MPI Cartesian communicator code block 6

```
// Create datatypes for exchanging x and y slices
MPI_Type_vector( nx, 1, ny, MPI_DOUBLE, &xSlice );
MPI_Type_commit( &xSlice );

MPI_Type_vector( ny, 1, 1, MPI_DOUBLE, &ySlice );
MPI_Type_commit( &ySlice );
```

Recall that

- first argument is number of data blocks
- second argument is number of data elements in a block
- third argument is the *stride*
- last argument is pointer to variable for new type

MPI Cartesian communicator code block 7

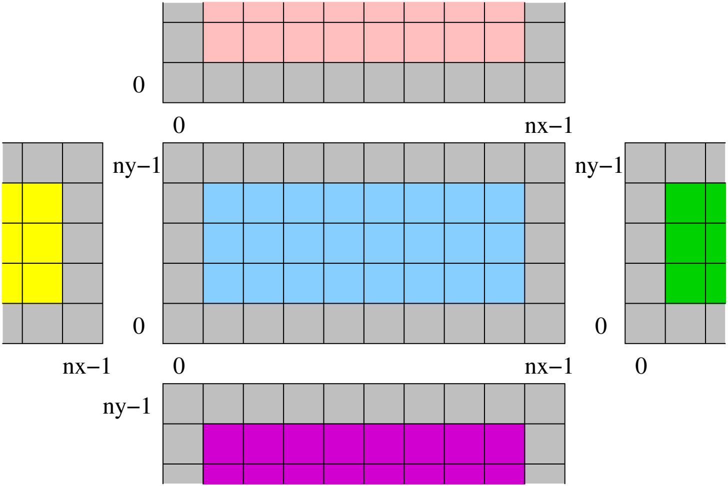
```
// Exchange x-slices with top and bottom neighbors
MPI_Sendrecv( &u[0][ny-2], 1, xSlice, up,   TAG,
              &u[0][0],    1, xSlice, down, TAG,
              comm2d, MPI_STATUS_IGNORE );
MPI_Sendrecv( &u[0][1],    1, xSlice, down, TAG,
              &u[0][ny-1], 1, xSlice, up,   TAG,
              comm2d, MPI_STATUS_IGNORE );

// Exchange y-slices with left and right neighbors
MPI_Sendrecv( &u[nx-2][0], 1, ySlice, right, TAG,
              &u[0][0],    1, ySlice, left,  TAG,
              comm2d, MPI_STATUS_IGNORE );
MPI_Sendrecv( &u[1][0],    1, ySlice, left,  TAG,
              &u[nx-1][0], 1, ySlice, right, TAG,
              comm2d, MPI_STATUS_IGNORE );
```

Note the format of the first argument to each send-receive call. Doing this ensures that the correct address is passed regardless of how the array `u` is allocated.

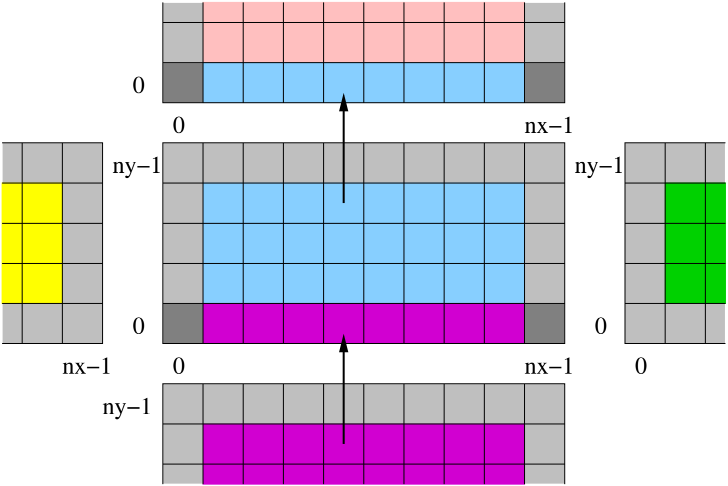
Exchange example

Grid subdomain and its four neighbors



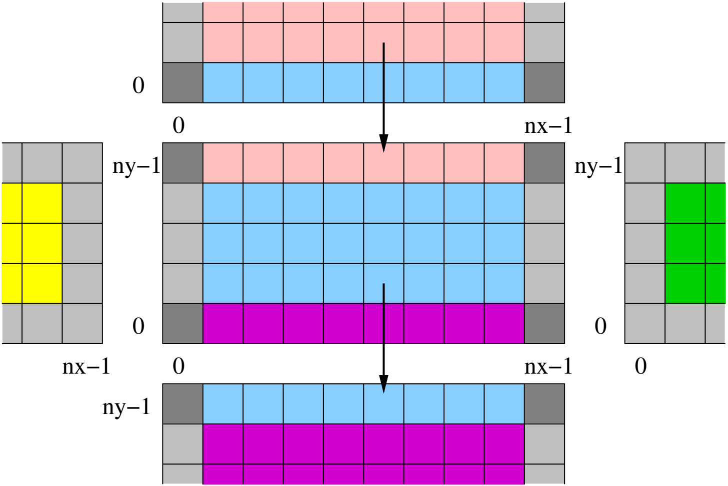
Exchange example

Send x-slice starting at `u[0][ny-2]`; receive into x-slice starting at `u[0][0]`



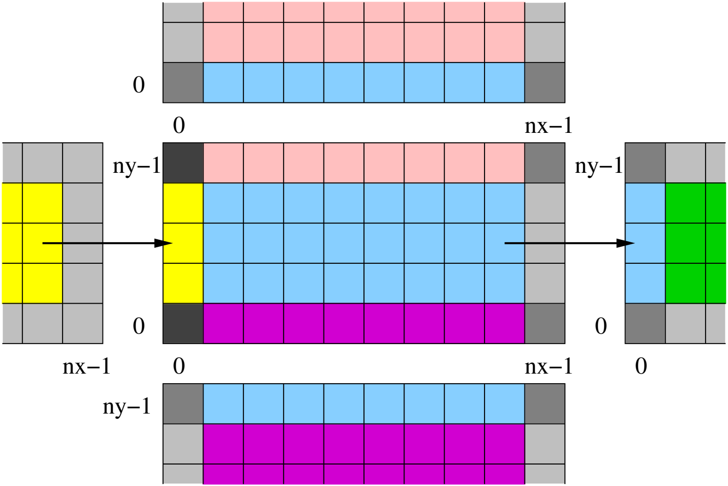
Exchange example

Send x-slice starting at `u[0][1]`; receive into x-slice starting at `u[0][ny-1]`



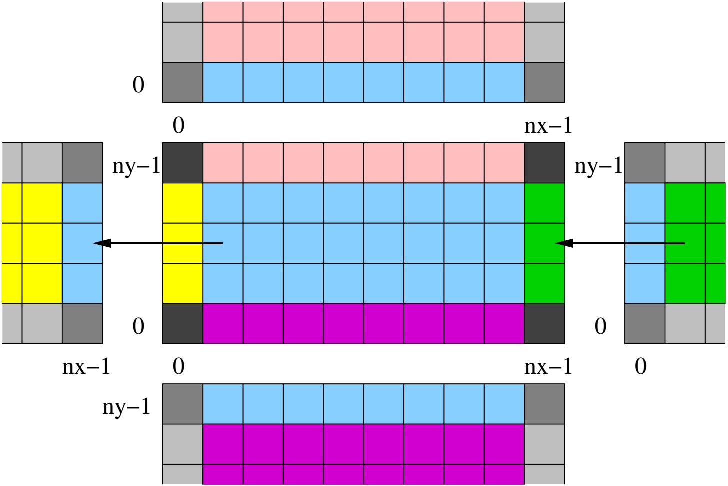
Exchange example

Send y-slice starting at `u[nx-2][0]`; receive into y-slice starting at `u[0][0]`



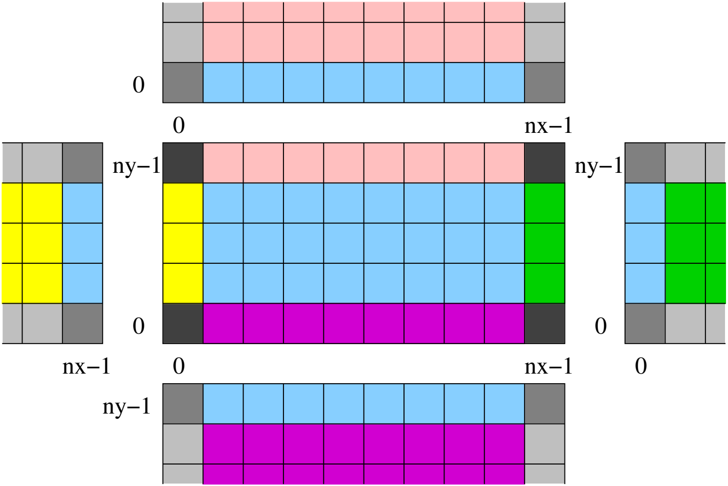
Exchange example

Send y-slice starting at `u[1][0]`; receive into y-slice starting at `u[nx-1][0]`



Exchange example

Interior nodes on subdomain can now be updated; dark gray nodes not referenced.



Exchanges at domain boundary

- You may wonder what happens with a process responsible for a subdomain at the top (or bottom) of the grid executes the command

```
MPI_Sendrecv( &u[0][ny-2], 1, xSlice, up,   TAG,
              &u[0][0],    1, xSlice, down, TAG,
              comm2d, MPI_STATUS_IGNORE );
```

- There is no neighboring subdomain above (or below)...
- Recall that `up`, `down`, `left`, and `right` were rank values returned by `MPI_Cart_shift()`. In the case of a subdomain at the top, `up` will be `MPI_PROC_NULL`. Any send or receive operations to or from a process with this rank will be ignored.
- If, however, we'd indicated the grid was periodic, then `up` would be assigned the rank of the process responsible for the bottom subdomain in the same subdomain column; in other words it wraps around.