Advanced Parallel Programming

Derived Datatypes

ARCHER Training Courses

Sponsors

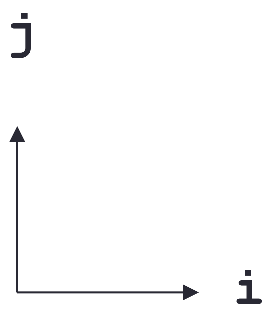
Reusing this material

Overview

- Lecture will cover
  - derived datatypes
  - memory layouts
  - vector datatypes
  - floating vs fixed datatypes
  - subarray datatypes

My Coordinate System (how I draw arrays)

x[i][j]



x[0][3]	x[1][3]	x[2][3]	x[3][3]
x[0][2]	x[1][2]	x[2][2]	x[3][2]
x[0][1]	x[1][1]	x[2][1]	x[3][1]
x[0][0]	x[1][0]	x[2][0]	x[3][0]

x(i,j)

x(1,4)	x(2,4)	x(3,4)	x(4,4)
x(1,3)	x(2,3)	x(3,3)	x(4,3)
x(1,2)	x(2,2)	x(3,2)	x(4,2)
x(1,1)	x(2,1)	x(3,1)	x(4,1)

Basic Datatypes

- MPI has a number of pre-defined datatypes
  - eg **MPI_INT / MPI_INTEGER, MPI_FLOAT / MPI_REAL**
  - user passes them to send and receive operations

- For example, to send 4 integers from an array x

C: `int[10];`

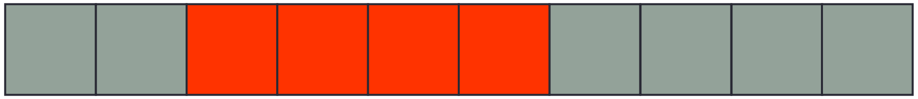
F: `INTEGER x(10)`

```
MPI_Send(x, 4, MPI_INT, ...);
MPI_SEND(x, 4, MPI_INTEGER, ...)
```

Derived Datatypes

- Can send different data by specifying different buffer

```
MPI_Send(&x[2], 4, MPI_INT, ...);
MPI_SEND(x(3),  4, MPI_INTEGER, ...)
```



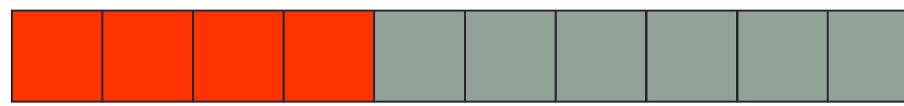
  – but can only send a single block of contiguous data

- Can define new datatypes called *derived types*
  – various different options in MPI
  – we will use them to send data with gaps in it: a **vector type**
  – other MPI derived types correspond to, for example, C structs

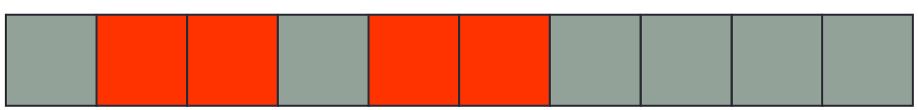
Simple Example

- Contiguous type

```
MPI Datatype my_new_type;
MPI_Type_contiguous(count=4, oldtype=MPI_INT, newtype=&my_new_type);
MPI_Type_commit(&my_new_type);

INTEGER MY_NEW_TYPE
CALL MPI_TYPE_CONTIGUOUS(4, MPI_INTEGER, MY_NEW_TYPE, IERROR)
CALL MPI_TYPE_COMMIT(MY_NEW_TYPE, IERROR)


MPI_Send(x, 1, my_new_type, ...);

MPI_SEND(x, 1, MY_NEW_TYPE, ...)
```



- Vector types correspond to patterns such as



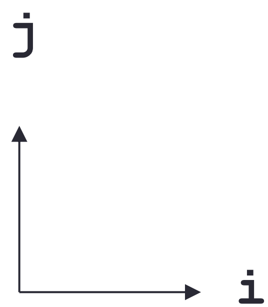
Array Layout in Memory

C: `x[16]` F: `x(16)`

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16

C: `x[4][4]` F: `x(4,4)`

4	8	12	16
3	7	11	15
2	6	10	14
1	5	9	13

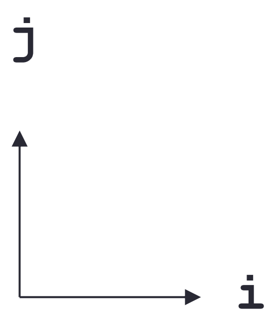


13	14	15	16
9	10	11	12
5	6	7	8
1	2	3	4

- Data is contiguous in memory
  - different conventions in C and Fortran
  - for statically allocated C arrays `x == &x[0][0]`

Process Grid

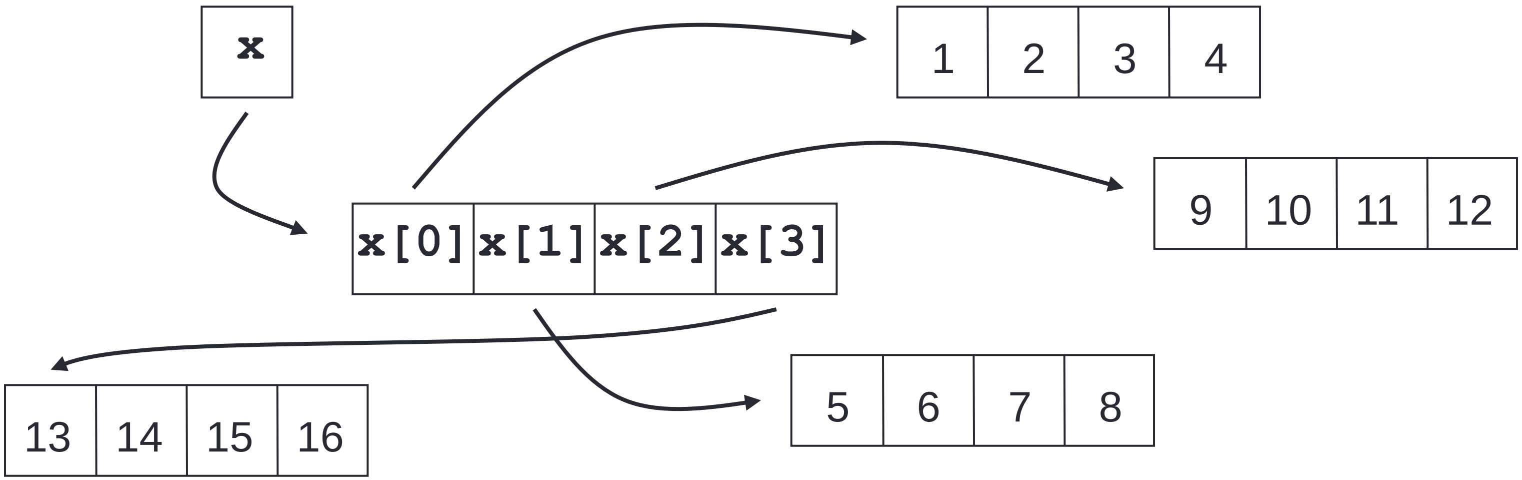
- I use C convention for *process* coordinates, even in Fortran
  - ie processes always ordered as for C arrays
    - and array indices also start from 0
- Why?
  - this is what is returned by MPI for cartesian topologies
  - turns out to be convenient for future exercises
- Example: *process* rank layout on a 4x4 *process* grid
  - rank 6 is at position (1,2), ie i = 1 and j = 2, for C and Fortran



3	7	11	15
2	6	10	14
1	5	9	13
0	4	8	12

Aside: Dynamic Arrays in C

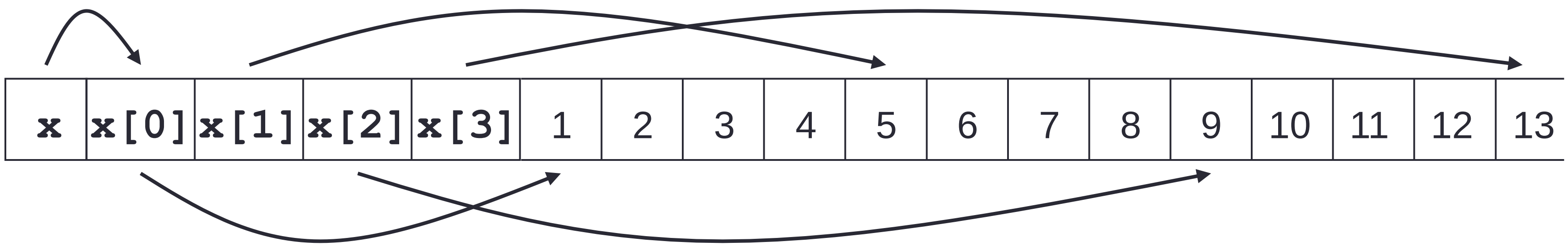
```
float **x = (float **) malloc(4, sizeof(float *));

for (i=0; i < 4; i++)
{
  x[i] = (float *) malloc(4, sizeof(float));
}
```



- Data non-contiguous, and `x != &x[0][0]`
  - cannot use regular templates such as vector datatypes
  - cannot pass `x` to any MPI routine

Arralloc

```
float **x = (float **) arralloc(sizeof(float), 2, 4, 4);
/* do some work */
free((void *) x);
```

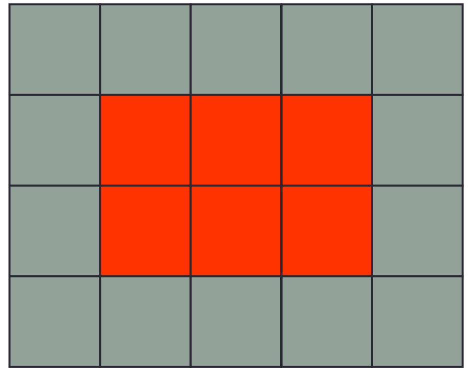


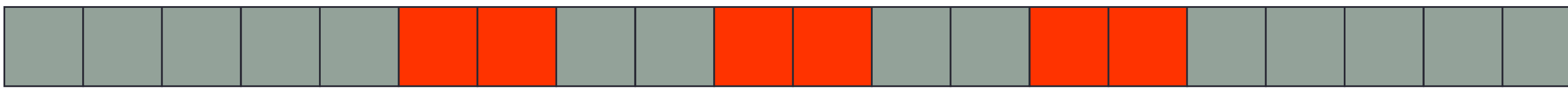
- Data is now contiguous, but still **`x != &x[0][0]`**
  - can now use regular template such as vector datatype
  - must pass **`&x[0][0]`** (start of contiguous data) to MPI routines
  - see **`PSMA-arralloc.tar`** for example of use in practice

- Will illustrate all calls using **`&x[i][j]`** syntax
  - correct for both static and (contiguously allocated) dynamic arrays

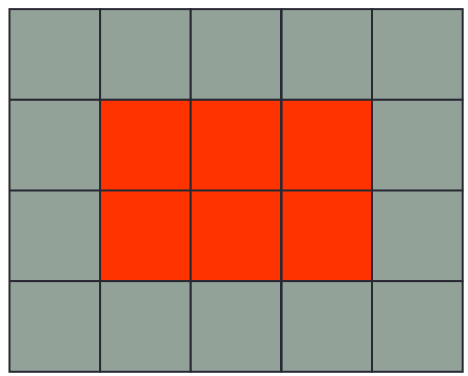
Array Subsections in Memory

C: **`x[5][4]`**

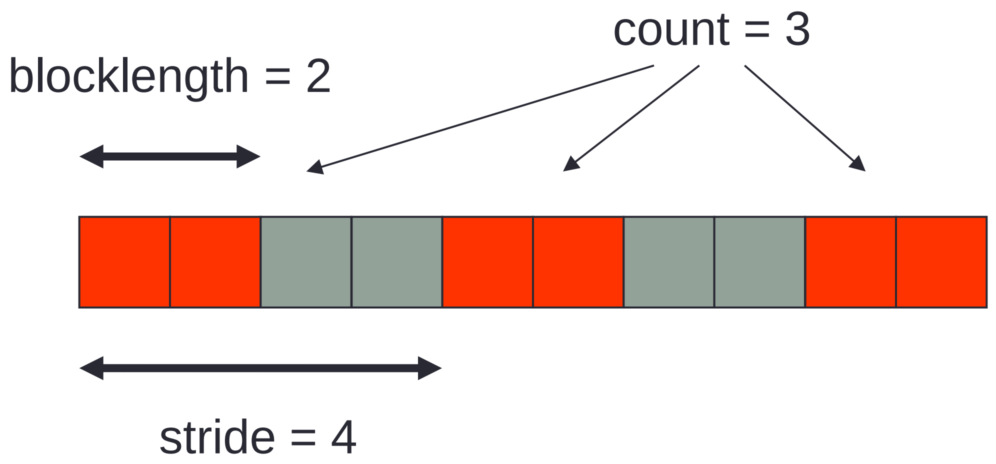


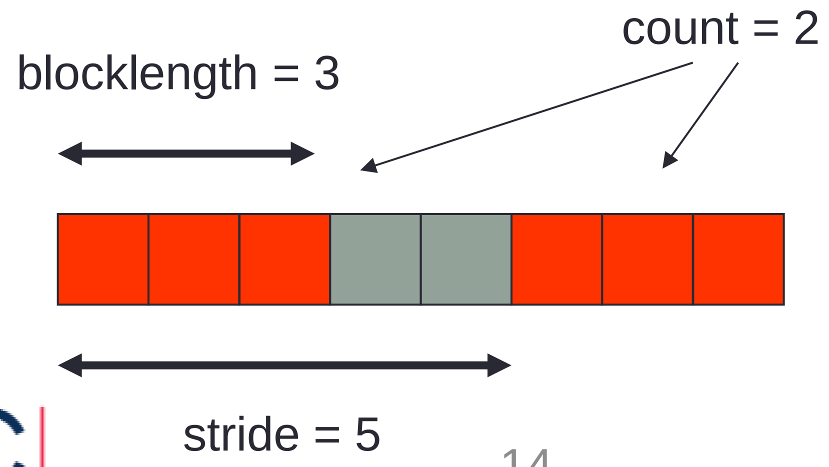


F: **`x(5,4)`**



Equivalent Vector Datatypes





Definition in MPI

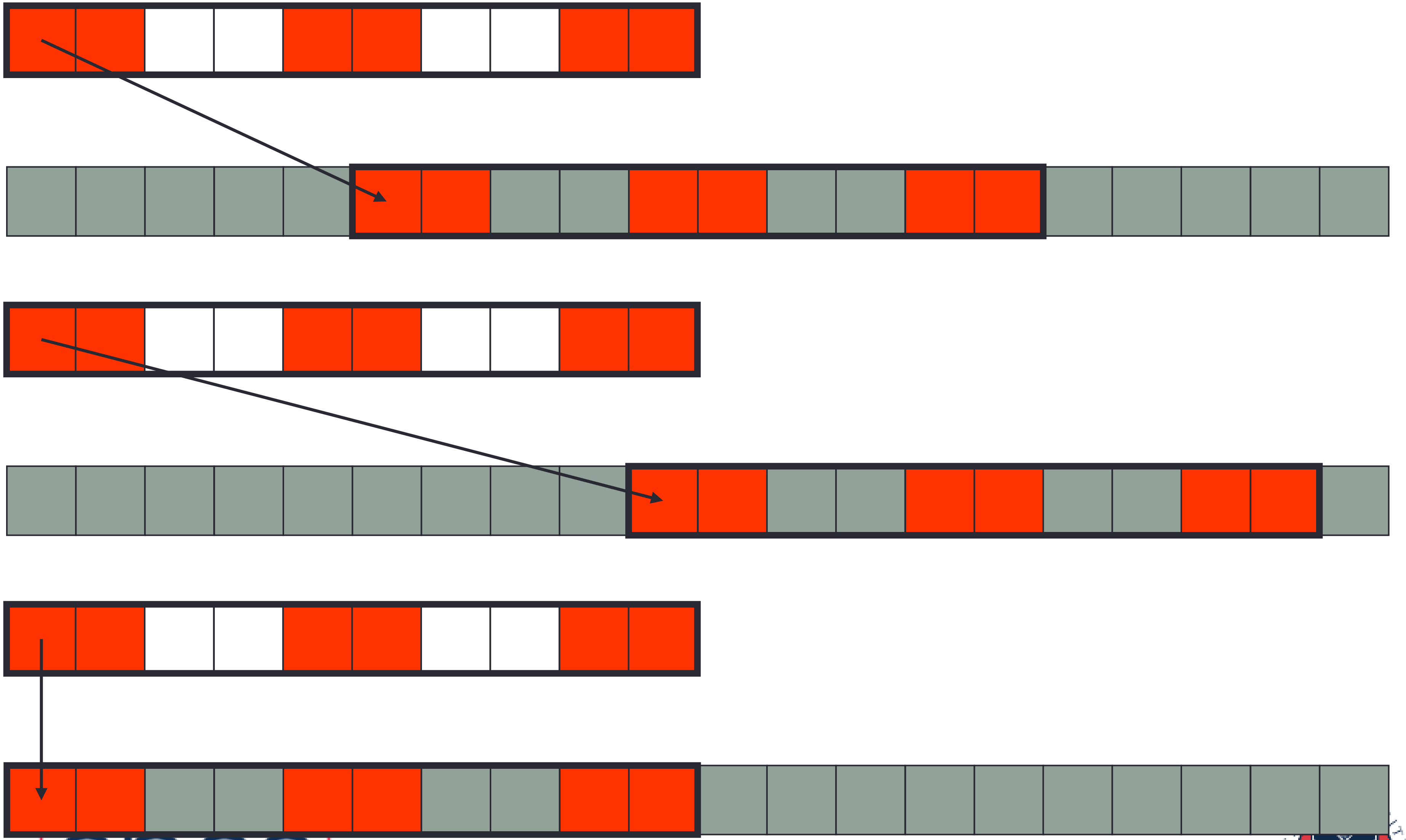
```
MPI_Type_vector(int count, int blocklength, int stride,
            MPI_Datatype oldtype, MPI_Datatype *newtype);
```

```
MPI_TYPE_VECTOR(COUNT, BLOCKLENGTH, STRIDE,
                 OLDTYPE, NEWTYPE, IERR)
INTEGER COUNT, BLOCKLENGTH, STRIDE, OLDTYPE
INTEGER NEWTYPE, IERR
```

```
MPI_Datatype vector3x2;
MPI_Type_vector(3, 2, 4, MPI_FLOAT, &vector3x2)
MPI_Type_commit(&vector3x2)
```

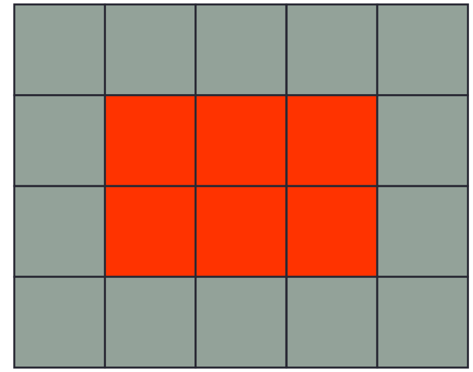
```
integer vector3x2
call MPI_TYPE_VECTOR(2, 3, 5, MPI_REAL, vector3x2, ierr)
call MPI_TYPE_COMMIT(vector3x2, ierr)
```

Datatypes as Floating Templates

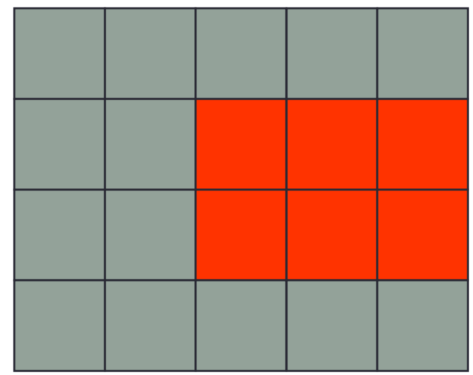


Choosing the Subarray Location

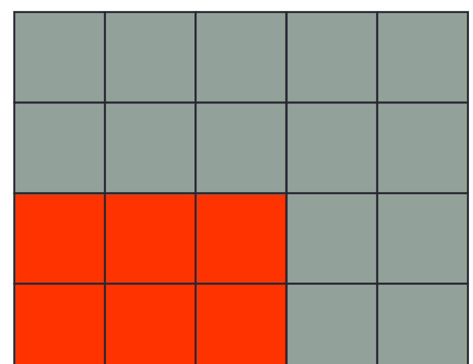
```
MPI_Send(&x[1][1], 1, vector3x2, ...);
MPI_SEND(x(2,2)  , 1, vector3x2, ...)
```



```
MPI_Send(&x[2][1], 1, vector3x2, ...);
MPI_SEND(x(3,2)  , 1, vector3x2, ...)
```

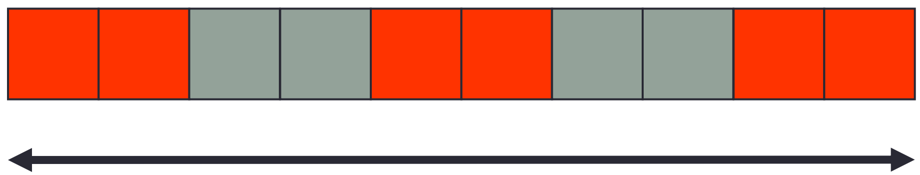


```
MPI_Send(&x[0][0], 1, vector3x2, ...);
MPI_SEND(x(1,1)  , 1, vector3x2, ...)
```



Datatype Extents

- When sending multiple datatypes
  - datatypes are read from memory separated by their extent
  - for basic datatypes, extent is the size of the object
  - for vector datatypes, extent is distance from first to last data



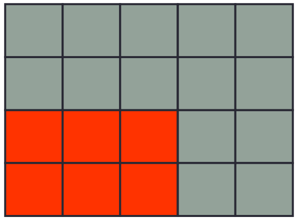
extent = 10*extent(basic type)

extent = 8*extent(basic type)

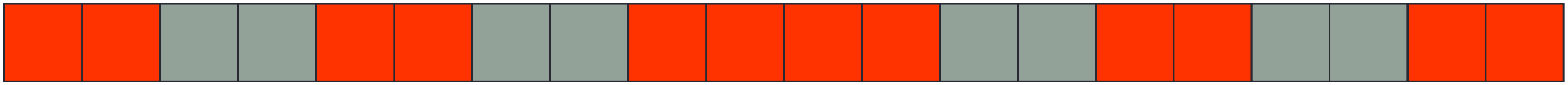
- Extent *does not* include trailing spaces

Sending Multiple Vectors

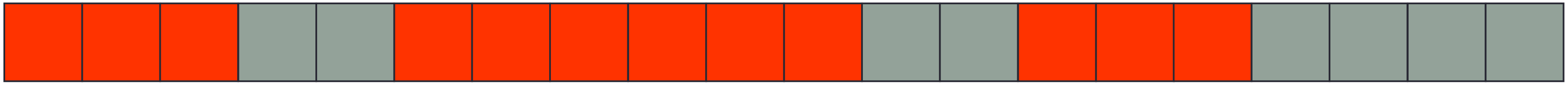
```
MPI_Send(&x[0][0], 1, vector3x2, ...);

MPI_SEND(x(1,1)   , 1, vector3x2, ...)
```



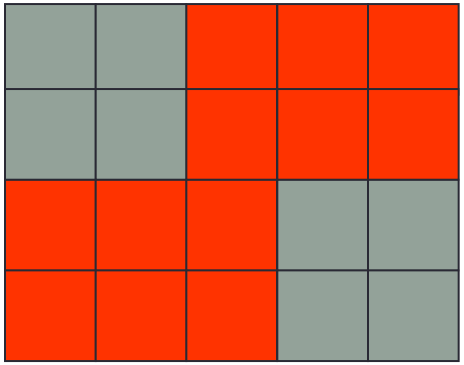
```
MPI_Send(&x[0][0], 2, vector3x2, ...);
```



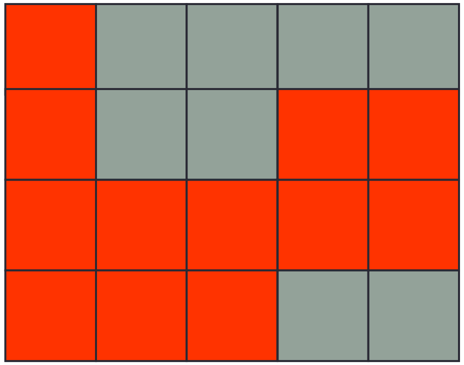
```
MPI_SEND(x(1,1)   , 2, vector3x2, ...)
```



C



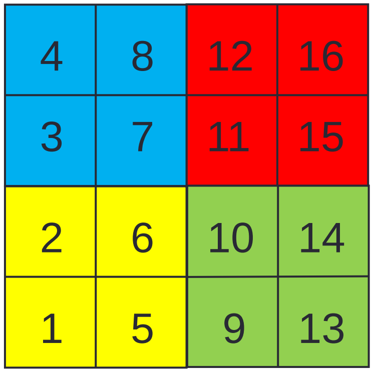
F



Issues with Vectors

- Sending multiple vectors is not often useful
  - extents are not defined as you might expect for 2D arrays
- A 3D array subsection is not a vector
  - but cannot easily use 2D vectors as building blocks due to extents
  - becomes even harder for higher-dimensional arrays
- It is possible to set the extent manually
  - routine is called **`MPI_Type_create_resized`**
  - this is not a very elegant solution
- For example, difficult to use vectors with **`MPI_Scatter`** to scatter 2D datasets

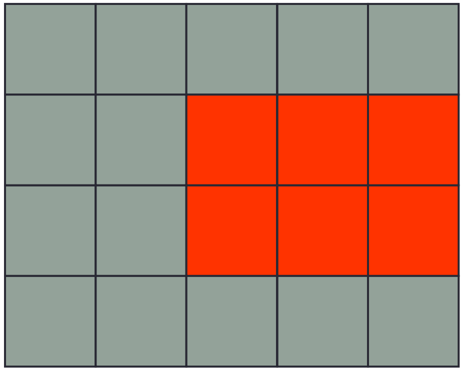
Aside: `MPI_Scatter` for master IO



- Problem (i): displacements are not constant
  - here, offsets from origin are 0, 2, 8 and 10 (floats)
- Solution
  - use **`MPI_Scatterv`** which takes separate displacement for each rank
- Problem (ii): displacements multiplied by extent = 6 floats
  - required offsets are not an integer multiple of the extent!
- Solution
  - use **`MPI_Type_create_resized`** to reset extent to, e.g., one float

Floating vs Fixed Datatypes

- Vectors are “floating” datatypes
  - this may have some advantages, eg define a single halo datatype and use for both up and down halos
  - actual location is selected by passing address of appropriate element
  - equivalent in MPI-IO is specifying a displacement into the file
    - this will turn out to be rather clumsy
- “Fixed” datatype
  - always pass starting address of array
  - datatype encodes both the shape and position of the subarray



- How do we define a fixed datatype?
  - requires a datatype with leading spaces
  - difficult to do with vectors
  - using **`MPI_Type_create_resized`** very ugly

Subarray Datatype

- A single call that defines multi-dimensional subsections
  - much easier than vector types for 3D arrays
  - datatypes are fixed
  - pass the starting address of the array to all MPI calls

```
MPI_Type_create_subarray(int ndims, int array_of_sizes[],
 int array_of_subsizes[], int array_of_starts[],
 int order, MPI_Datatype oldtype, MPI_Datatype *newtype)
```

```
MPI_TYPE_CREATE_SUBARRAY(NDIMS, ARRAY_OF_SIZES,
 ARRAY_OF_SUBSIZES, ARRAY_OF_STARTS, ORDER,
 OLDTYPE, NEWTYPE, IERR)
```

```
INTEGER NDIMS, ARRAY_OF_SIZES(*), ARRAY_OF_SUBSIZES(*),
  ARRAY_OF_STARTS(*), ORDER, OLDTYPE, NEWTYPE, IERR
```

C Definition

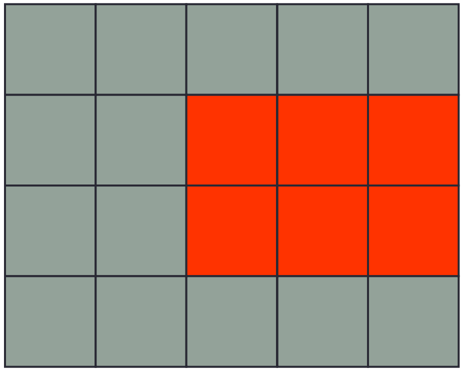
```
#define NDIMS 2
MPI_Datatype subarray3x2;
int array_of_sizes[NDIMS], array_of_subsizes[NDIMS],
    arrays_of_starts[NDIMS];

array_of_sizes[0]    = 5; array_of_sizes[1]    = 4;
array_of_subsizes[0] = 3; array_of_subsizes[1] = 2;
array_of_starts[0]   = 2; array_of_starts[1]   = 1;

order = MPI_ORDER_C;

MPI_type_create_subarray(NDIMS, array_of_sizes,
 array_of_subsizes, array_of_starts, order,
 MPI_FLOAT, &subarray3x2);
MPI_TYPE_COMMIT(&subarray3x2);
```

Fortran Definition

```
integer, parameter :: ndims = 2
integer subarray3x2
integer, dimension(ndims) :: array_of_sizes,
 array_of_subsizes,
                             arrays_of_starts
! Indices start at 0 as in C !

array_of_sizes(1)    = 5; array_of_sizes(2)    = 4
array_of_subsizes(1) = 3; array_of_subsizes(2) = 2
array_of_starts(1)   = 2; array_of_starts(2)   = 1

order = MPI_ORDER_FORTRAN
call MPI_TYPE_CREATE_SUBARRAY(ndims, array_of_sizes,
 array_of_subsizes, array_of_starts, order,
 MPI_REAL, subarray3x2, ierr)
```

Usage

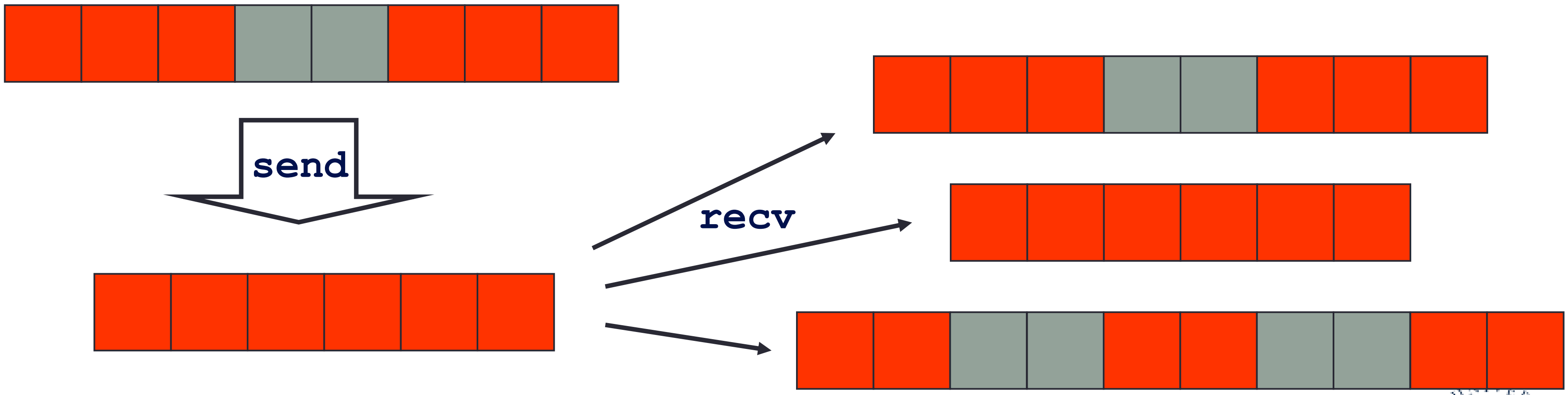
```
MPI_Send(&x[0][0], 1, subarray3x2, ...);
MPI_SEND(x       , 1, subarray3x2, ...)
MPI_SEND(x(1,1)  , 1, subarray3x2, ...)
```



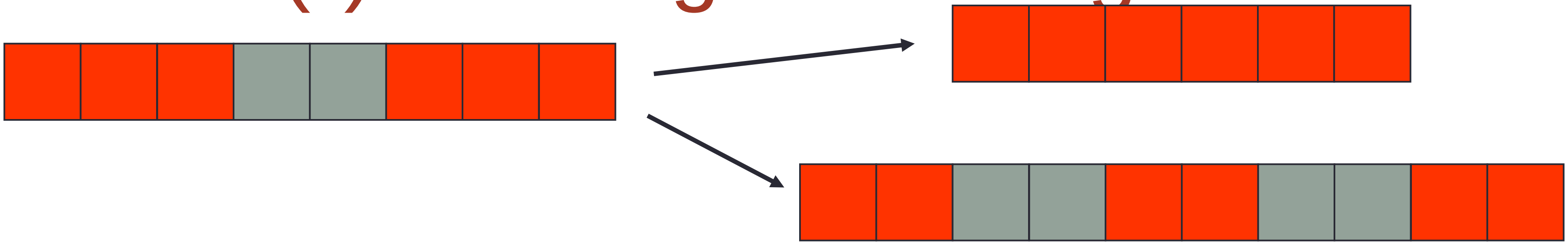
- Generalisation to IO
  - each process counts from the start of the file
  - each process has a different subarray datatype
  - actual displacements from file origin depend on the position of the process in the process array
  - this is all already encoded in the datatype

Notes (i): Matching messages

- A datatype is defined by two attributes:
  - type signature: a list of the basic datatypes in order
  - type map: the locations (displacements) of each basic datatype
- For a receive to match a send only signatures need to match
  - type map is defined by the receiving datatype
- Think of messages being packed for transmission by sender
  - and independently unpacked by the receiver



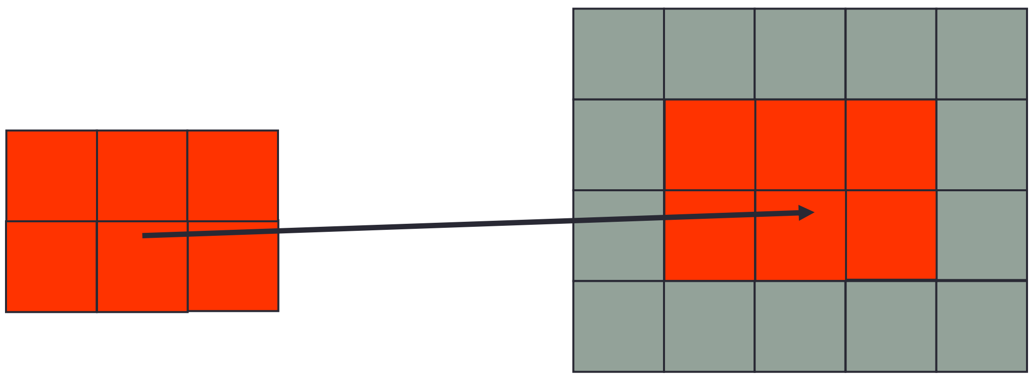
Notes(ii): Message Matching



`Send(1, subarray3x2)` matches `Recv(6, MPI_FLOAT)`

`Send(1, subarray3x2)` matches `Recv(1, subarray2x3)`

- Can be useful when scattering data directly to array with halos



Notes (iii)

- There is an overhead to defining a derived type
  - a real code may have many calls to the IO routines
  - no need to re-define the data types every time
  - array sizes unlikely to change: define types once at start of program
- If you do create lots of derived types in a program ...
  - they take up memory!
  - clear up the memory using MPI_Type_free whenever possible
- But try and avoid:
  - do loop = 1, 1000000
    - do stuff
    - define type
    - use type
    - free type
  - end do