Parallel Computing

Ekkapot Charoenwanit

Software Systems Engineering
TGGS
KMUTNB

Lecture 12:

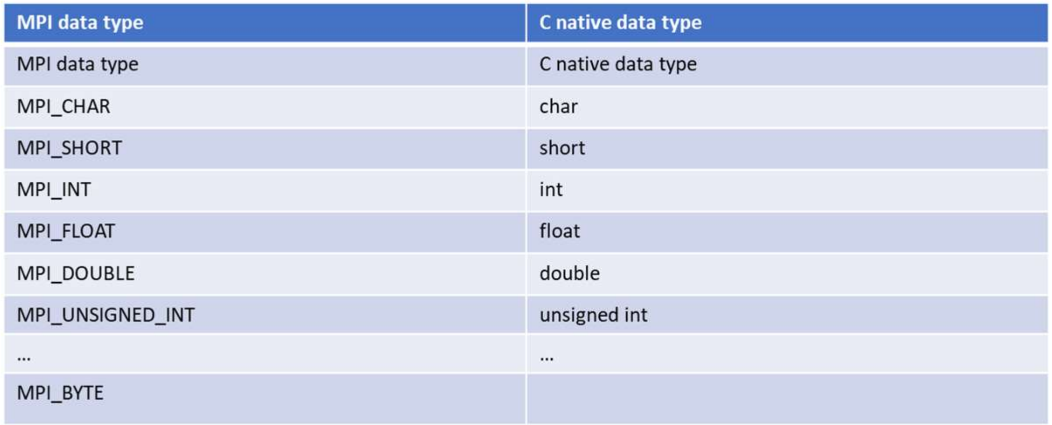
- ❑ Distributed-Memory Programming with MPI
  - Derived Datatypes

MPI: Datatype

MPI Datatypes are opaque objects called **handles**.

- Used to interpret and access the contents of a memory buffer

MPI defines **primitive datatypes** that describe **a single data element**.



MPI data type	C native data type
MPI data type	C native data type
MPI_CHAR	char
MPI_SHORT	short
MPI_INT	int
MPI_FLOAT	float
MPI_DOUBLE	double
MPI_UNSIGNED_INT	unsigned int
…	…
MPI_BYTE	

More complex datatypes can be **derived** from these primitive datatypes.

MPI: Datatype

- We often want to exchange messages that
  - contain values with different datatypes such as a **C struct**
  - are non-contiguous such as a block of matrix elements
- One naïve solution to sending non-contiguous data is by packing the non-contiguous data into a contiguous memory buffer at the sender and unpacking at the receiver.
  - This might require additional memory-to-memory copy operations at both sides.
- Rather, MPI allows specifying **more general, mixed-typed and non-continuous** memory buffers.
  - It is up to the given MPI implementation to decide whether data should be first packed into a contiguous buffer before being transmitted or whether it can be collected directly from where the data is kept.

MPI: Type Signature and Type Map

A **general datatype** is a general object that describe two things as follows:

- A sequence of basic datatypes
- A sequence of byte displacements

The **type signature** of a datatype is a sequence of datatypes described by a given type and count:

- e.g., {MPI_INT, MPI_INT, MPI_DOUBLE}, which describes the datatype as a sequence of two integers followed by one double.

The **type map of a datatype** is a sequence of basic datatypes and their displacements

- e.g., {(MPI_INT,0),(MPI_INT,4),(MPI_DOUBLE,8)}

Datatypes are local objects:

- They may differ across MPI processes
- Each process performs the marshalling and unmarshaling of messages in a transparent manner.

MPI: Terminology

Lower and Upper Bound

- $lb(datatype) = \min(disp_i)$
- $ub(datatype) = \max\left(disp_i + sizeof(type_i)\right) + padding$

Extent

- $extent(datatype) = ub(datatype) - lb(datatype)$
- The extent of a datatype is the step size in bytes when accessing consecutive elements of that datatype

Size

- $size(datatype) = \sum_i sizeof(type_i))$
- The size of a datatype is the amount in bytes taken by the datatype, **excluding any gaps in it**.

MPI: Basic Datatype

Example: MPI_DOUBLE

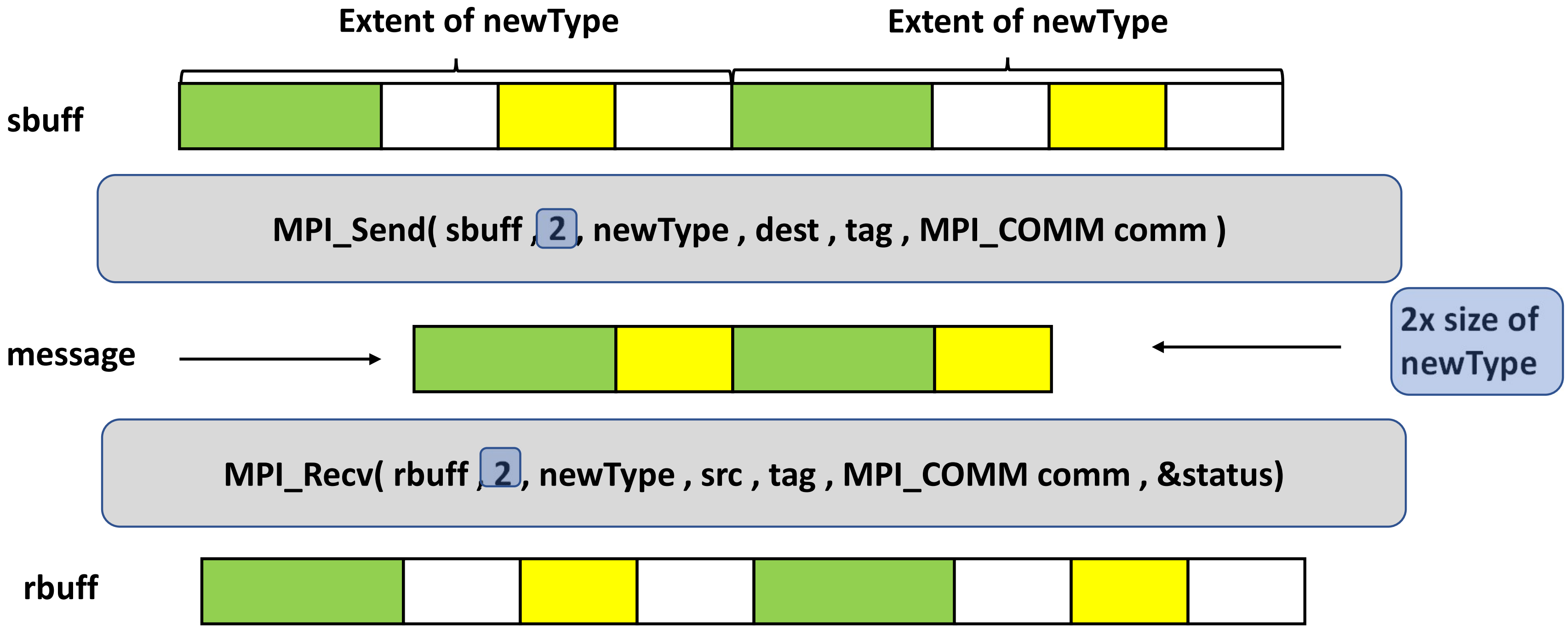
Type map = {(MPI_DOUBLE,0)}

- ○ $lb(MPI\_DOUBLE) = 0$
- ○ $ub(MPI\_DOUBLE) = sizeof(double) = 8$
- ○ $extent(MPI\_DOUBLE) = ub - lb = 8$
- ○ $size(MPI\_DOUBLE) = 8$

All primitive MPI datatypes have a lower bound of 0

The upper bound may be adjusted appropriately, depending on alignment constraints on the programming language and the machine.

MPI: What it looks like in action



Extent of newType

Extent of newType

sbuff

```
MPI_Send( sbuff , 2 , newType , dest , tag , MPI_COMM comm )
```

message

2x size of newType

```
MPI_Recv( rbuff , 2 , newType , src , tag , MPI_COMM comm , &status)
```

rbuff

MPI: Contiguous Datatypes

Create a sequence of elements of an existing datatype

C

```
MPI_ Type_contiguous( int count , MPI_Datatype oldType , MPI_DataType * newType)
```

- The new datatype ***newType*** represents a contiguous sequence of ***count*** elements of ***oldType***.
- The elements (of ***newType***) are separated from each other by the **extent** of ***oldType.***
- Useful for sending entire rows (C/C++) or columns (Fortran) of matrices

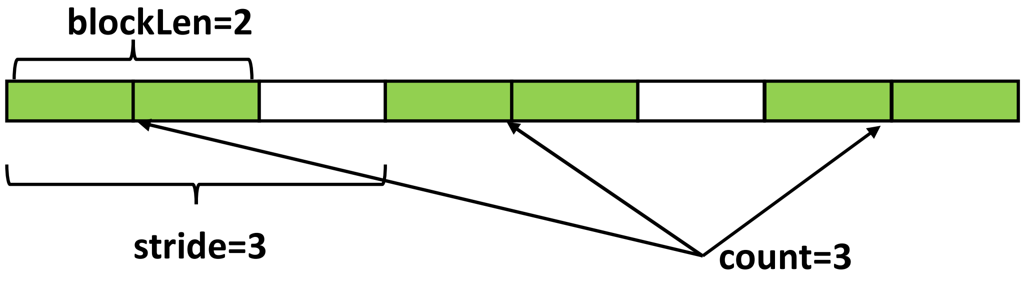
MPI: Vector Datatypes

Create a sequence of equally spaced blocks of elements of an existing datatype

C

```
MPI_ Type_vector( int count , int blockLen , int stride , MPI_DataType oldType , MPI_Datatype * newType)
```

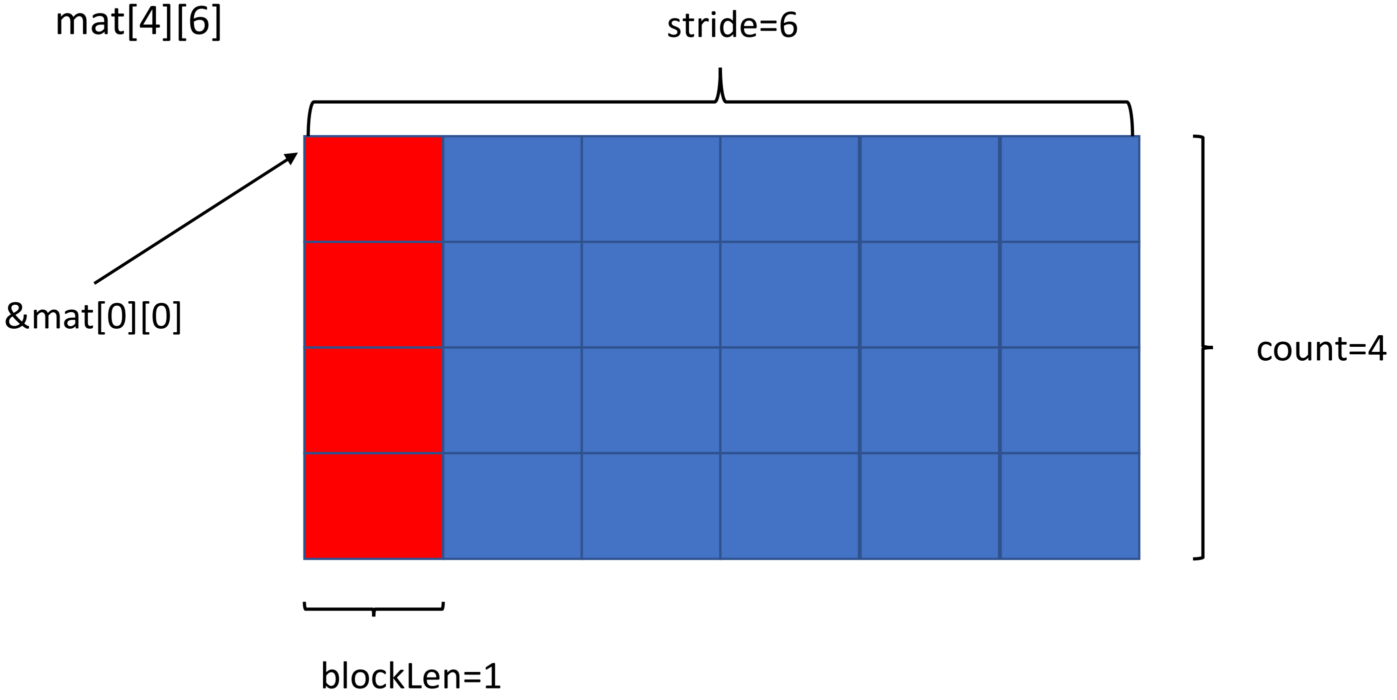
- The new datatype ***newType*** represents a sequence of ***count*** blocks, each of which contains ***blockLen*** elements of ***oldType***.
- Every two consecutive blocks are separated by ***stride*** elements of ***oldType***.



MPI: Vector Datatypes

Example: one column of a C/C++ matrix with 4 rows and 6 columns

mat[4][6]

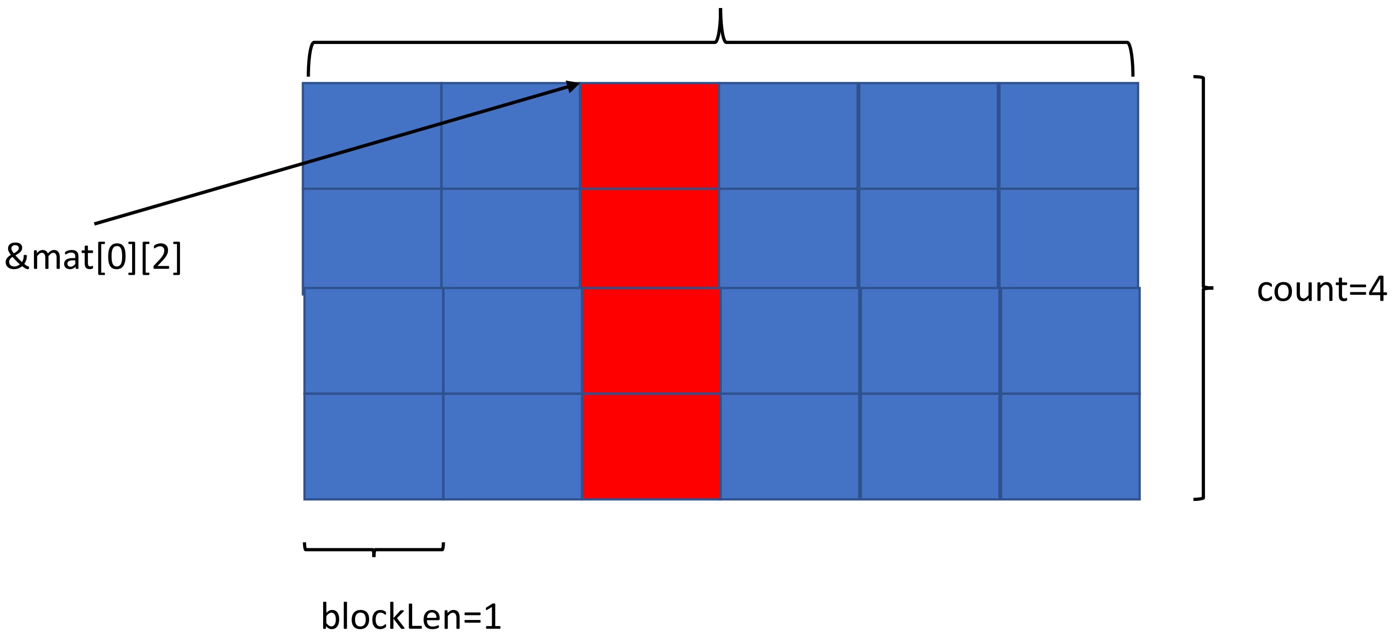


MPI: Vector Datatypes

Example: one column of a C/C++ matrix with 4 rows and 6 columns

mat[4][6]

stride=6



&mat[0][2]

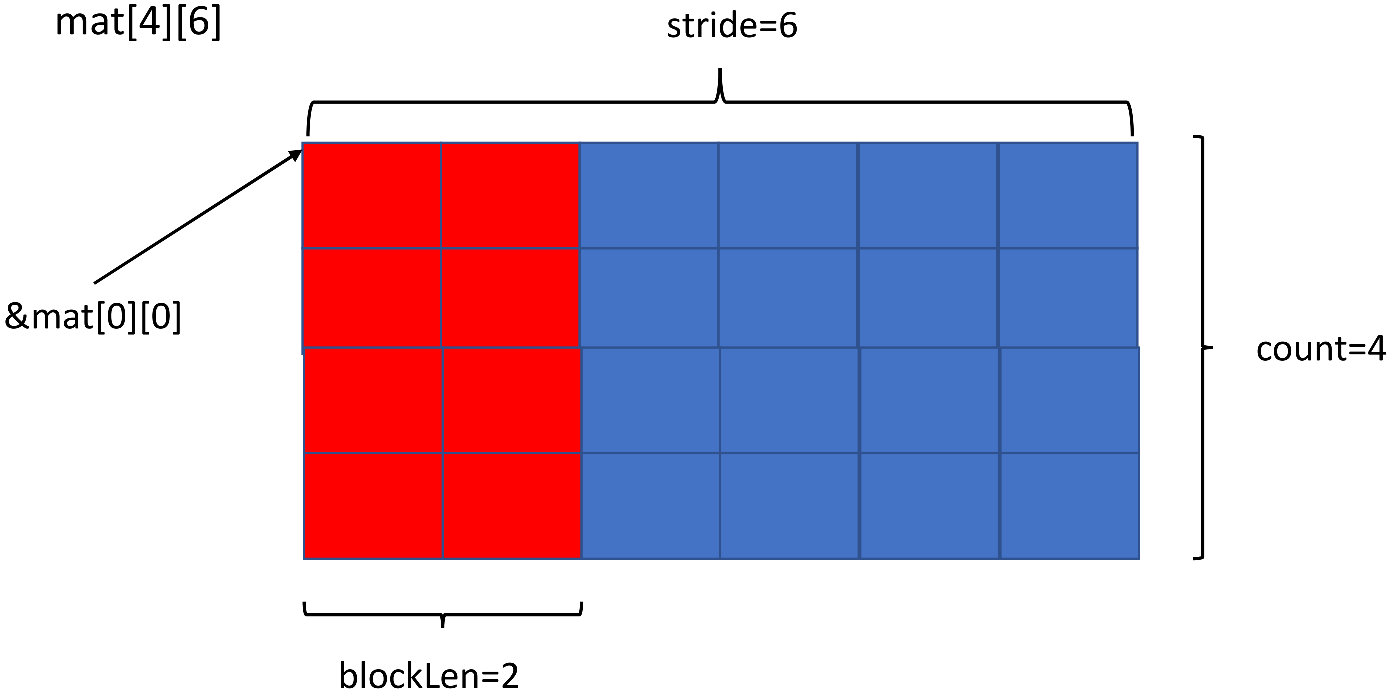
count=4

blockLen=1

MPI: Vector Datatypes

Example: two columns of a C/C++ matrix with 4 rows and 6 columns

mat[4][6]



MPI: Indexed Datatypes

Create an indexed list of arbitrary-sized blocks within a matrix

C

```
MPI_ Type_indexed( int count , const int array_of_blocklengths [] , const int array_of_displacements [] ,
                MPI_DataType oldType , MPI_Datatype * newType)
```

The new datatype ***newType*** represents a sequence of ***count*** blocks, where the i^{th} block

- contains an ***array_of_blocklengths[i]*** elements of the old datatype ***oldType*** and
- Every two consecutive blocks are separated by ***stride*** elements each.

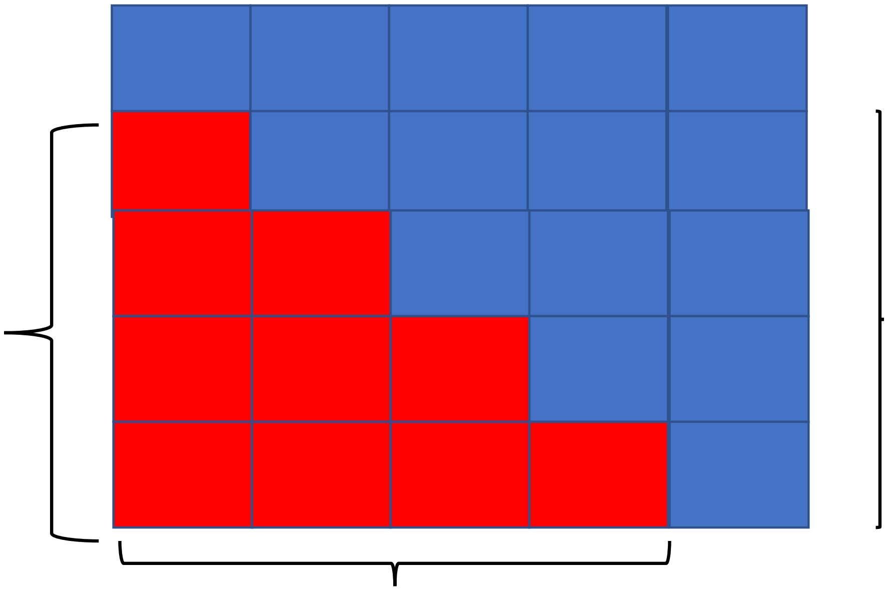
Useful for custom-shaped data of matrices with a fixed dimension

- Lower or upper triangular matrices

MPI: Indexed Datatypes

Example: lower triangle of a matrix of dimension 5 x 5

mat[4][6]



array_of_ displacements=[5,10,15,20]

count=4

array_of_blocklengths = [0,1,2,3,4]

MPI: Structure Datatypes

The most generic datatype constructor

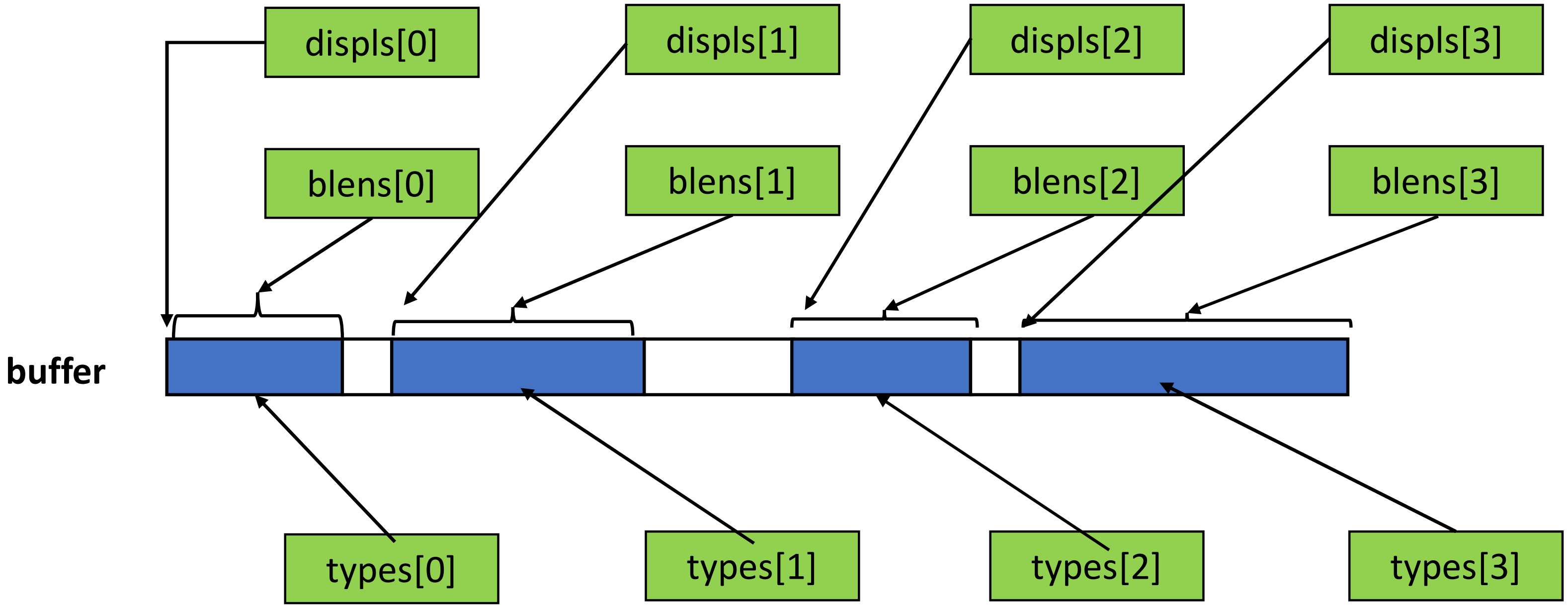
- Useful for C/C++ structures

C

```
MPI_ Type_create_struct( int count , const int array_of_blocklengths [] ,
                         const int array_of_displacements [] ,
                         const int array_of_types [],
                         MPI_Datatype * newType
                   )
```

- ***count***: the number of blocks in the datatype
- ***array_of_blocklengths***: the number of elements in each block
- ***array_of_displacements***: the displacement in bytes from the start of each block
- ***array_of_types***: the datatype of the elements in each block
- ***newType***: handle of the new datatype

MPI: Structure Datatypes



MPI: Structure Datatypes

```
typedef struct{
        float mass;
        double pos[3];
        char sym;
}Particle;

int blens = { 1 , 3 , 1 } ;

MPI_Aint displs [3] = { offsetof(Particle,mass} , offsetof(Particle,pos) , offsetof(Particle,sym)};

MPI_Datatype types[3] = { MPI_FLOAT , MPI_DOUBLE , MPI_CHAR };

MPI_Datatype particleType;

MPI_Type_create_struct( 3 , blens , displs , types , &particleType );
```

MPI: Registering Derived Datatypes

Register a derived datatype for using with communication operations

C

```
MPI_ Type_ commit( MPI_Datatype * newType)
```

- Datatypes need to be committed before they can be used in communication operations.
- All primitive datatypes, e.g., MPI_INT, MPI_FLOAT etc., are already committed.
- Intermediate datatypes defined by the user that are used to implement more complex datatypes but are not used in communication operations **can be left uncommitted**.

MPI: Registering Derived Datatypes

Deregister and free up a derived datatype

C

```
MPI_ Type_ free( MPI_Datatype * datatype)
```

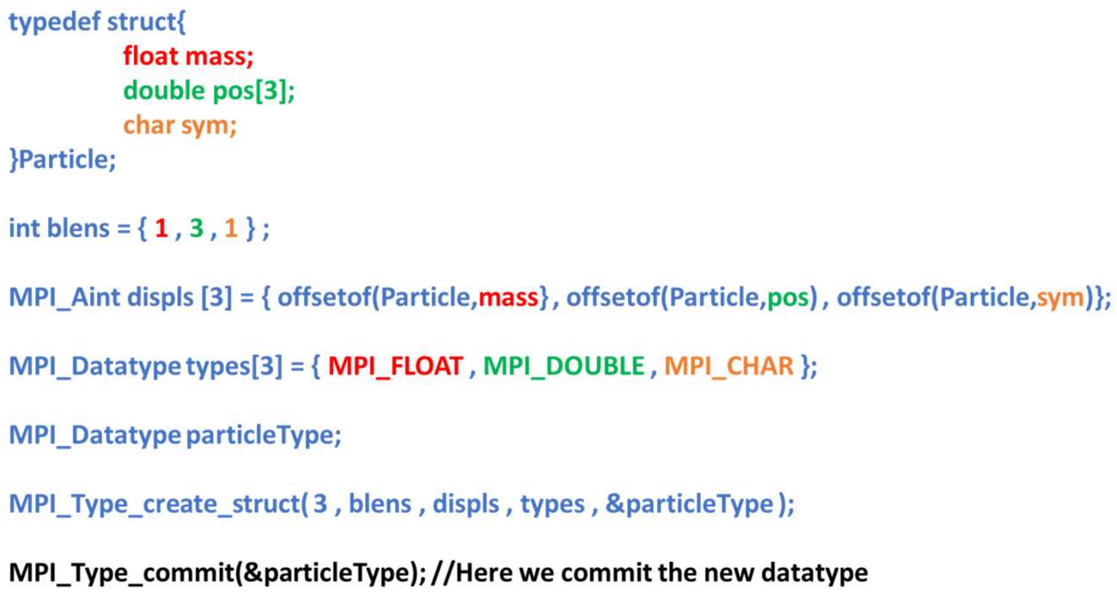
- Derived datatypes that were previously derived from the freed datatype are unaffected.
- Upon a successful return, ***datatype*** is set to **MPI_TYPE_NULL**.

MPI: Structure Datatypes

```
typedef struct{
            float mass;
            double pos[3];
            char sym;
}Particle;

int blens = { 1 , 3 , 1 } ;

MPI_Aint displs [3] = { offsetof(Particle,mass} , offsetof(Particle,pos) , offsetof(Particle,sym)};

MPI_Datatype types[3] = { MPI_FLOAT , MPI_DOUBLE , MPI_CHAR };
MPI_Datatype particleType;
MPI_Type_create_struct( 3 , blens , displs , types , &particleType );
MPI_Type_commit(&particleType); //Here we commit the new datatype
```

MPI: Structure Datatypes

The handle ***particleType*** can now be used to send and receive **ONE** element of ***Particle***.



```
typedef struct{
            float mass;
            double pos[3];
            char sym;
}Particle;

int blens = { 1 , 3 , 1 } ;

MPI_Aint displs [3] = { offsetof(Particle,mass} , offsetof(Particle,pos) , offsetof(Particle,sym)};

MPI_Datatype types[3] = { MPI_FLOAT , MPI_DOUBLE , MPI_CHAR };

MPI_Datatype particleType;

MPI_Type_create_struct( 3 , blens , displs , types , &particleType );

MPI_Type_commit(&particleType); //Here we commit the new datatype
```

MPI: Structure Datatypes

We need to resize to the actual size of the structure.

```
typedef struct{
                float mass;
                double pos[3];
                char sym;
}Particle;

int blens = { 1 , 3 , 1 } ;

MPI_Aint displs [3] = { offsetof(Particle,mass} , offsetof(Particle,pos) ,
offsetof(Particle,sym)};

MPI_Datatype types[3] = { MPI_FLOAT , MPI_DOUBLE , MPI_CHAR };
MPI_Datatype intermediateType;
MPI_Type_create_struct( 3 , blens , displs , types , &intermediateType );

MPI_Aint true_extent = sizeof(Particle);
MPI_Type_create_resized(intermediateType,0,true_extent,&particleType);
MPI_Type_commit(&particleType);
```

Note that there is no need to commit the intermediate type unless it will be used in communication operations.

References

[1] *William Gropp, Ewing Lusk, and Anthony Skjellum. 2014. Using MPI: Portable Parallel Programming with the Message-Passing Interface. The MIT Press.*

[2] *Marc-Andre Hermanns. 2021. MPI in Small Bites. PPCES 2021.*