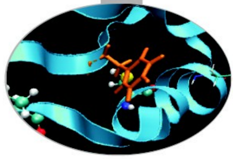
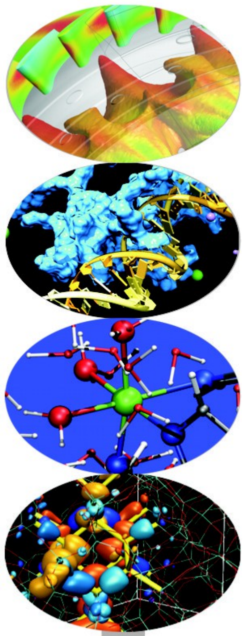
SuperComputing Applications and Innovation



INTRODUCTION TO MPI – MPI DATATYPES



Introduction to Parallel Computing with MPI and OpenMP

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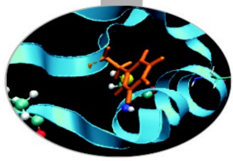
DERIVED DATATYPE



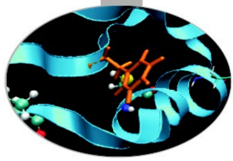
What are?

Derived datatypes are datatypes that are built from the basic MPI datatypes (e.g. MPI_INT, MPI_REAL, …)

Why datatypes?

- Since all data is labeled by type, an MPI implementation can support communication between processes on machines with very different memory representations and lenghts of elementary datatypes (heterogeneous communication)
- Specifying application-oriented layout of data in memory
  - can reduce memory-to memory copies in the implementaion
  - allows the use of special hardware (scatter/gather) when available
- Specifying application-oriented layout of data on a file can reduce systems calls and physical disk I/O

DERIVED DATATYPE



You may need to send messages that contain:

1. non-contiguous data of a single type (e.g. a sub-block of a matrix)
2. contiguous data of mixed types (e.g., an integer count, followed by a sequence of real numbers)
3. non-contiguous data of mixed types

Possible solutions:

1. make multiple MPI calls to send and receive each data element
   → If advantegeous, copy data to a buffer before sending it
2. use MPI_pack/MPI_Unpack to pack data and send packed data (datatype MPI_PACKED)
3. use MPI_BYTE to get around the datatype-matching rules. Like MPI_PACKED, MPI_BYTE can be used to match any byte of storage (on a byte-addressable machine), irrespective of the datatype of the variable that contains this byte.

Additional latency costs due to multiple calls

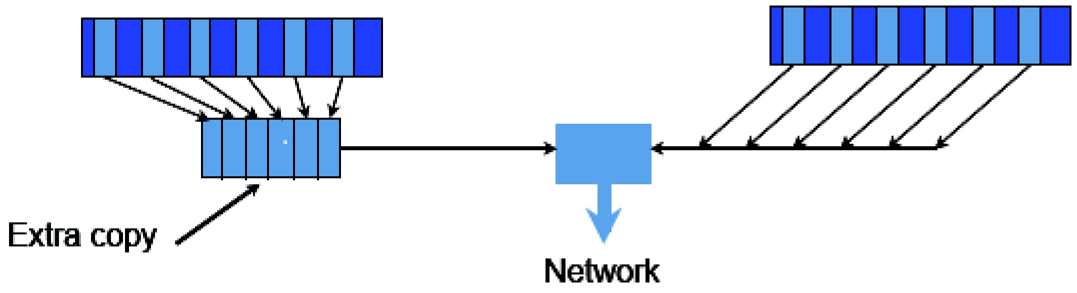
Additional latency costs due to memory copy

Not portable to a heterogeneous system using MPI_BYTE or

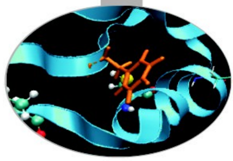
DERIVED DATATYPE

Datatype solution:

1. The idea of MPI derived datatypes is to provide a simple, portable, elegant and efficient way of communicating non-contiguous or mixed types in a message.
   - During the communication, the datatype tells MPI system where to take the data when sending or where to put data when receiving.
1. The actual performances depend on the MPI implementation
2. **Derived datatypes are also needed for getting the most out of MPI-I/O.**



DEFINITION



A **general datatype** is an **opaque object** able to describe a buffer layout in memory by specifing:

- A sequence of basic datatypes
- A sequence of integer (byte) displacements.

Typemap = {(type 0, displ 0), … (type n-1, displ n-1)}

– pairs of basic types and displacements (in byte)

Type signature = {type 0, type 1, … type n-1}

– list of types in the typemap

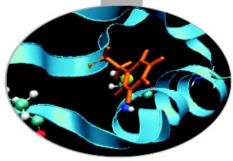
– gives size of each elements

– tells MPI how to interpret the bits it sends and received

Displacement:

– tells MPI where to get (when sending) or put (when receiving)

TYPEMAP

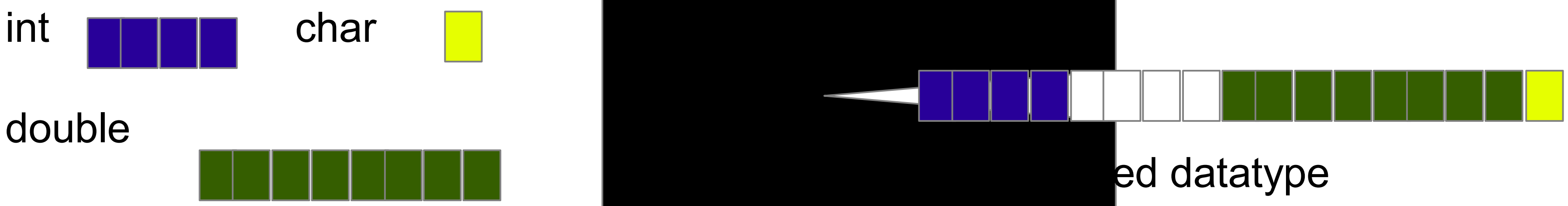


Example:
Basic datatype are particular cases of a general datatype, and are predefined:

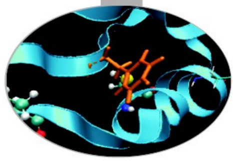
MPI_INT = {(int, 0)}

General datatype with typemap

Typemap = {(int,0) [redacted] }



HOW TO USE

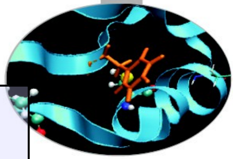


General datatypes (differently from C or Fortran) are created (and destroyed) at run-time through calls to MPI library routines.

Implementation steps are:

1. Creation of the datatype from existing ones with a **datatype constructor**.
2. Allocation (**committing**) of the datatype before using it.
3. **Usage of the derived datatype** for MPI communications and/or for MPI-I/O
4. Deallocation (**freeing**) of the datatype after that it is no longer needed.

COMMITTING AND FREEING



MPI_TYPE_COMMIT (datatype)

INOUT datatype: datatype that is committed (handle)

- Before it can be used in a communication or I/O call, each derived datatype has to be committed

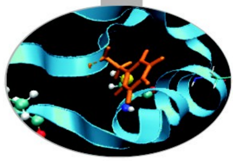
MPI_TYPE_FREE (datatype)

INOUT datatype: datatype that is freed (handle)

Mark a datatype for deallocation

Datatype will be deallocated when all pending operations are finished

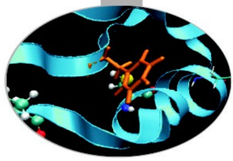
MPI TYPE CONTIGUOUS



MPI_TYPE_CONTIGUOUS (count, oldtype, newtype)

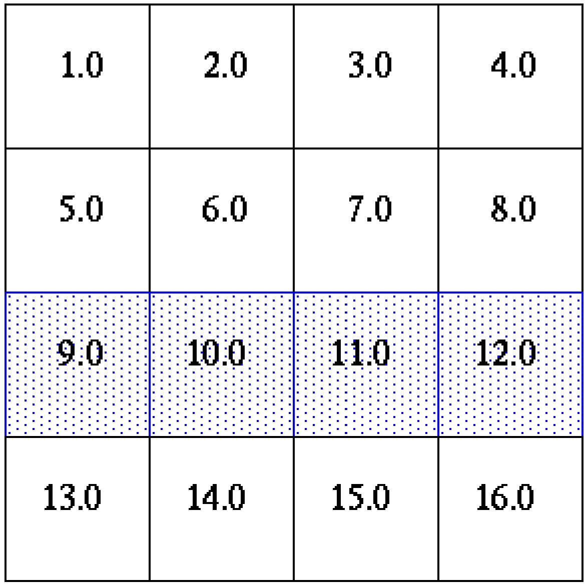
IN count: replication count (non-negative integer)
IN oldtype: old datatype (handle)
OUT newtype: new datatype (handle)

- MPI_TYPE_CONTIGOUS constructs a typemap consisting of the **replication** of a **datatype** into contiguous locations.
- newtype is the datatype obtained by concatenating count copies of oldtype.



MPI TYPE CONTIGUOUS

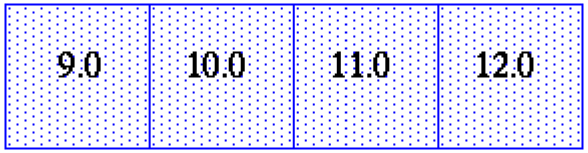
```
count = 4;
MPI_Type_contiguous(count, MPI_FLOAT, &rowtype);
```



1.0	2.0	3.0	4.0
5.0	6.0	7.0	8.0
▨ 9.0	▨ 10.0	▨ 11.0	▨ 12.0
13.0	14.0	15.0	16.0

a[4][4]

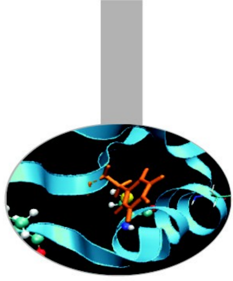
```
MPI_Send(&a[2][0], 1, rowtype, dest, tag, comm);
```



▨ 9.0	▨ 10.0	▨ 11.0	▨ 12.0

1 element of rowtype

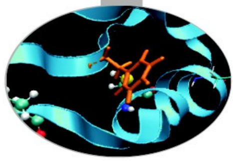
MPI TYPE VECTOR



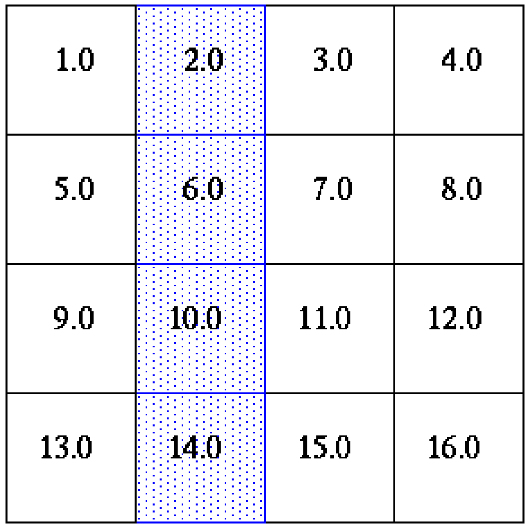
MPI_TYPE_VECTOR (count, blocklength, stride, oldtype, newtype)

IN count: Number of blocks (non-negative integer)
IN blocklen: Number of elements in each block (non-negative integer)
IN stride: Number of elements (NOT bytes) between start of each block (integer)
IN oldtype: Old datatype (handle)
OUT newtype: New datatype (handle)

- Consists of a number of elements of the same datatype repeated with a certain stride

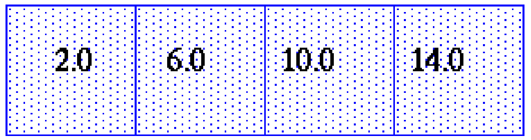


```
count = 4;   blocklength = 1;   stride = 4;
MPI_Type_vector(count, blocklength, stride, MPI_FLOAT,
&columntype);
```



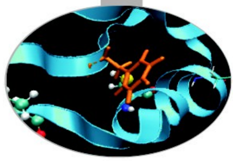
a[4][4]

```
MPI_Send(&a[0][1], 1, columntype, dest, tag, comm);
```



1 element of columntype

MPI TYPE HVECTOR



MPI_TYPE_CREATE_HVECTOR (count, blocklength, stride, oldtype, newtype)

IN count: Number of blocks (non-negative integer)
IN blocklen: Number of elements in each block (non-negative integer)
IN stride: Number of bytes between start of each block (integer)
IN oldtype: Old datatype (handle)
OUT newtype: New datatype (handle)

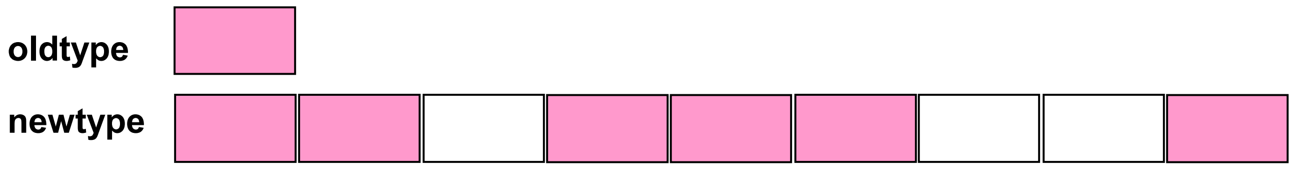
- It’s identical to MPI_TYPE_VECTOR, except that stride is given in bytes, rather than in elements
- “H” stands for heterogeneous

MPI TYPE INDEXED

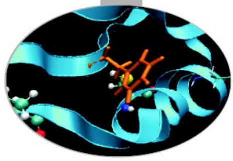
MPI_TYPE_INDEXED (count, array_of_blocklengths, array_of_displacements, oldtype, newtype)

IN count: number of blocks – also number of entries in array_of_blocklenghts and array_of_displacements (non-negative integer)
IN array_of_blocklengths: number of elements per block (array of non-negative integers)
IN array_of_displacements: displacement for each block, in multiples of oldtype extent (array of integer)
IN oldtype: old datatype (handle)
OUT newtype: new datatype (handle)

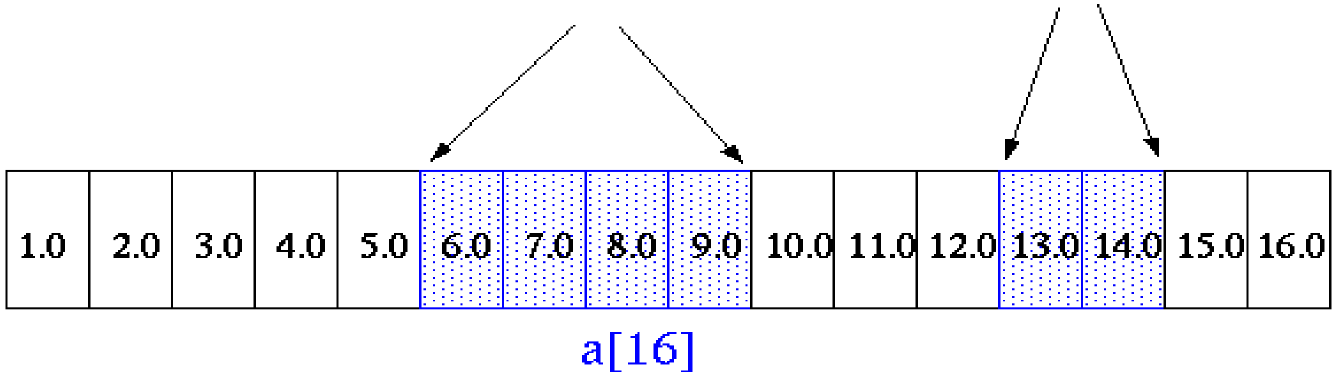
- Creates a new type from blocks comprising identical elements
- The size and displacements of the blocks can vary



count=3, array_of_blocklenghths=(/2,3,1/), array_of_displacements=(/0,3,8/)

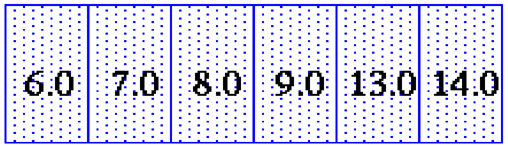


```
count = 2;      blocklengths[0] = 4;        blocklengths[1] = 2;
                displacements[0] = 5;       displacements[1] = 12;
```



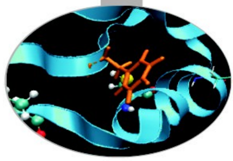
```
MPI_Type_indexed(count, blocklengths, displacements, MPI_FLOAT, &indextype);
```

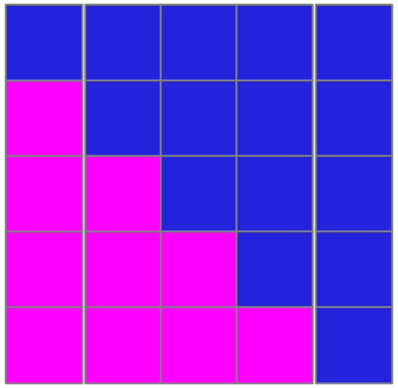
```
MPI_Send(&a, 1, indextype, dest, tag, comm);
```



1 element of indextype

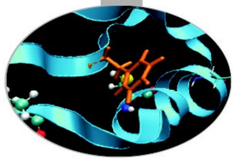
MPI TYPE INDEXED EXAMPLE (FORTRAN)





```
! upper triangular matrix
real, dimension(100,100) ::  a
integer, dimension(100) :: displ, blocklen
integer :: i, upper, ierr

! compute start and size of the rows
do i=1,100
    displ(i) = 100*i+i

    blocklen(i) = 100-i

end do

! create and commit a datatype for upper triangular matrix
CALL MPI_TYPE_INDEXED (100, blocklen, disp, MPI_DOUBLE, upper,ierr)
CALL MPI_TYPE_COMMIT (upper,ierr)
! … send it …
CALL MPI_SEND (a, 1, upper, dest, tag, MPI_COMM_WORLD, ierr)
MPI_Type_free (upper, ierr)
```

MPI TYPE HINDEXED

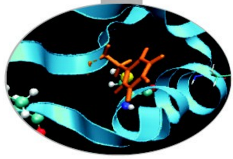


MPI_TYPE_CREATE_HINDEXED (count, array_of_blocklengths,
array_of_displacements, oldtype, newtype)

IN count: number of blocks – also number of entries in array_of_blocklengths and array_of_displacements (non-negative integer)
IN array_of_blocklengths: number of elements in each block (array of non-negative integers)
IN array_of_displacements: byte displacement of each block (array of integer)
IN oldtype: old datatype (handle)
OUT newtype: new datatype (handle)

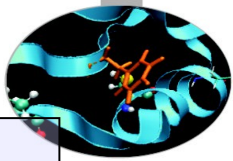
- This function is identical to MPI_TYPE_INDEXED, except that block displacements in array_of_displacements are specified in bytes, rather that in multiples of the oldtype extent

MPI TYPE INDEXED BLOCK



```
MPI_TYPE_CREATE_INDEXED_BLOCK (count, blocklengths,
                               array_of_displacements, oldtype, newtype)

        IN count: length of array of displacements (non-negative integer)
        IN blocklengths: size of block   (non-negative integer)
        IN array_of_displacements: array of displacements (array of integer)
        IN oldtype: old datatype (handle)
        OUT newtype: new datatype (handle)
```

- Similar to MPI_TYPE_INDEXED, except that the block-length is the same for all blocks.
- There are many codes using indirect addressing arising from unstructured grids where the blocksize is always 1 (gather/scatter). This function allows for constant blocksize and arbitrary displacements.



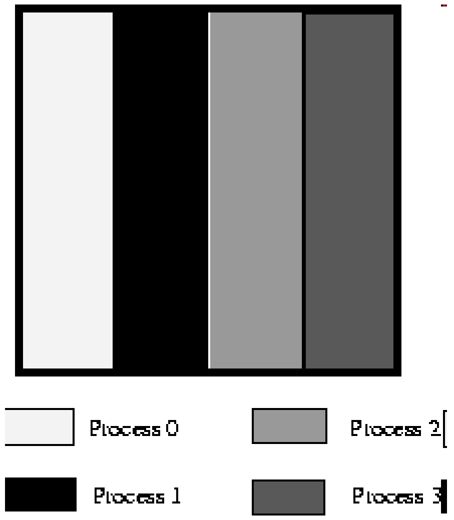
MPI TYPE SUBARRAY

MPI_TYPE_CREATE_SUBARRAY (ndims, array_of_sizes, array_of_subsizes, array_of_starts, order, oldtype, newtype)

IN ndims: number of array dimensions (positive integer)
IN array_of_sizes: number of elements of type oldtype in each dimension of the full array (array of positive integers)
IN array_of_subsizes: number of elements of type oldtype in each dimension of the subarray (array of positive integers)
IN array_of_starts: starting coordinates of the subarray in each dimension (array of non-negative integers)
IN order: array storage order flag (state: MPI_ORDER_C or MPI_ORDER_FORTRAN)
IN oldtype: array element datatype (handle)
OUT newtype: new datatype (handle)

The subarray type constructor creates an MPI datatype describing an n dimensional subarray of an n-dimensional array. The subarray may be situated anywhere within the full array, and may be of any nonzero size up to the size of the larger array as long as it is confined within this array.

MPI TYPE SUBARRAY EXAMPLE (C)



MPI_TYPE_CREATE_SUBARRAY (ndims, array_of_sizes, array_of_subsizes, array_of_starts, order, oldtype, newtype)

```
double subarray[100][25];
MPI_Datatype filetype;
int sizes[2], subsizes[2], starts[2];
int rank;

MPI_Comm_rank(MPI_COMM_WORLD, &rank);

sizes[0]=100; sizes[1]=100;
subsizes[0]=100; subsizes[1]=25;
starts[0]=0; starts[1]=rank*subsizes[1];

MPI_Type_create_subarray(2, sizes, subsizes, starts,
MPI_ORDER_C, MPI_DOUBLE, &filetype);

MPI_Type_commit(&filetype);
```

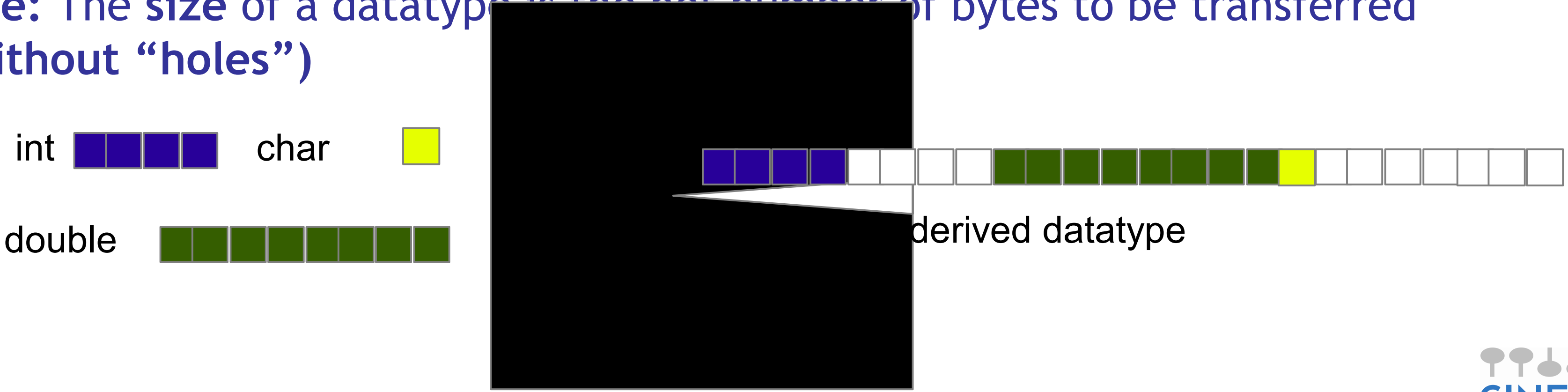
SIZE AND EXTENT

The MPI datatype for structures – MPI_TYPE_CREATE_STRUCT – requires dealing with memory addresses and further concepts:

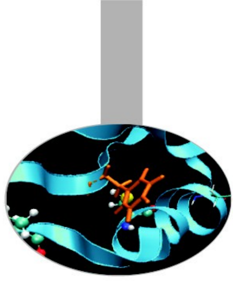
Typemap: pairs of basic types and displacements

Extent: The **extent** of a datatype is the span from the lower to the upper bound **(including “holes”)**

Size: The **size** of a datatype is the net number of bytes to be transferred **(without “holes”)**



SIZE AND EXTENT

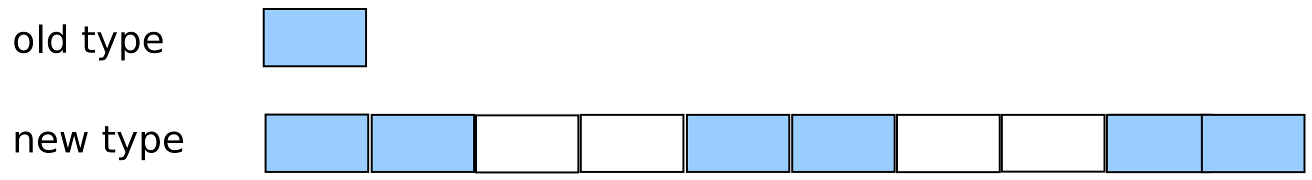


Basic datatypes:

- size = extent = number of bytes used by the compiler

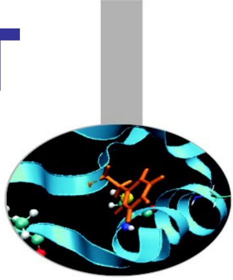
Derived datatypes:

- **extent include holes but...**
- **beware of the type vector: final holes are a figment of our imagination**



- size = 6 x size of “old type”
- extent = 10 x extent of “old type”

QUERY SIZE AND EXTENT OF DATATYPE



- Returns the total number of bytes of the entry datatype

MPI_TYPE_SIZE (datatype, size)

IN datatype: datatype (handle)

OUT size: datatype size (integer)

- Returns the lower bound and the extent of the entry datatype

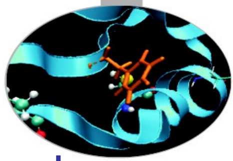
MPI_TYPE_GET_EXTENT (datatype, lb, extent)

IN datatype: datatype to get information on(handle)

OUT lb: lower bound of datatype (integer)

OUT extent: extent of datatype (integer)

EXTENT



- Extent controls how a datatype is used with the count field in a send and similar MPI operations
- Consider

```
call MPI_Send(buf,count,datatype,...)
```

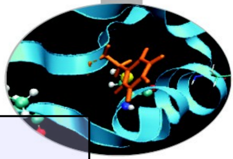
- What actually gets sent?

```
do i=0,count-1
     call MPI_Send(bufb(1+i*extent(datatype)),1,datatype,...)
enddo
```

where *bufb* is a byte type like *integer*1*

- *extent* is used to decide where to send from (or where to receive to in MPI_Recv) for count>1
  - Normally, this is right after the last byte used for (i-1)

MPI TYPE STRUCT

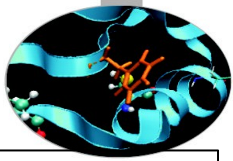


```
MPI_TYPE_CREATE_STRUCT (count, array_of_blocklengths,
                    array_of_displacements, array_of_oldtypes, newtype )

IN count: number of blocks (non-negative integer) -- also number of entries the following arrays
IN array_of_blocklenghts: number of elements in each block
                                   (array of non-negative integer)
IN array_of_displacements: byte displacement of each block
                               (array of integer)
IN array_of_oldtypes: type of elements in each block
                         (array of handles to datatype objects)
OUT newtype: new datatype (handle)
```

This subroutine returns a new datatype that represents count blocks. Each block is defined by an entry in array_of_blocklengths, array_of_displacements and array_of_types.

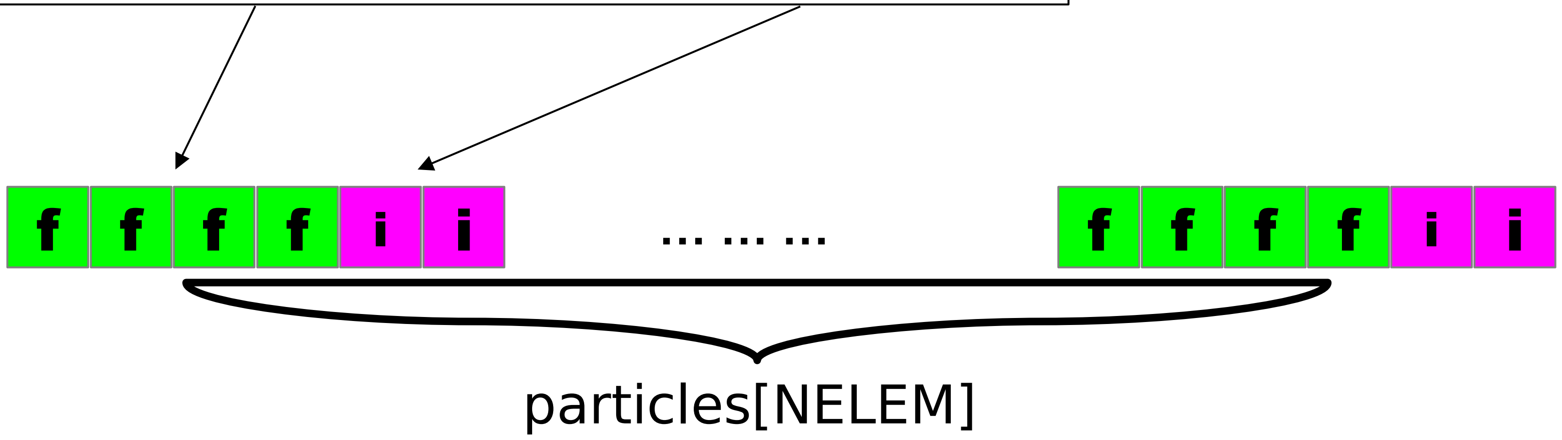
- Displacements are expressed in bytes (since the type can change!)
- To gather a mix of different datatypes scattered at many locations in space into one datatype that can be used for the communication.

USING EXTENT (NOT SAFE)



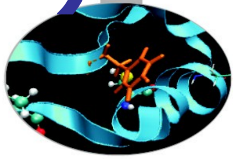
```
struct {
   float x, y, z, velocity;
   int n, type;
} Particle;

Particle particles[NELEM];
```

```
MPI_Type_extent(MPI_FLOAT, &extent);

count = 2;
blockcounts[0] = 4;          blockcount[1] = 2;
oldtypes[0]= MPI_FLOAT;        oldtypes[1] = MPI_INT;
displ[0] = 0;                displ[1] = 4*extent;
```



```
MPI_Type_struct (count, blockcounts, displ, oldtypes, &particletype);
MPI_Type_commit(&particletype);
```

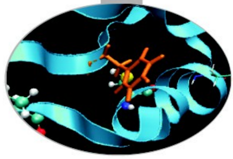
USING EXTENT (NOT SAFE)



```
struct {
   float x, y, z, velocity;
   int n, type;
} Particle;

Particle particles[NELEM];
```

```
int count, blockcounts[2];
MPI_Aint displ[2];
MPI_Datatype particletype, oldtypes[2];

count = 2;
blockcounts[0] = 4; blockcount[1] = 2;
oldtypes[0]= MPI_FLOAT; oldtypes[1] = MPI_INT;

MPI_Type_extent(MPI_FLOAT, &extent);
displ[0] = 0; displ[1] = 4*extent;

MPI_Type_create_struct (count, blockcounts, displ,
oldtypes,
&particletype);

MPI_Type_commit(&particletype);

MPI_Send (particles, NELEM, particletype, dest, tag,

                MPI_COMM_WORLD);

MPI_Free(&particletype);
```

USING EXTENT (NOT SAFE)



- C struct may be automatically padded by the compiler, e.g.

```
struct mystruct {
    char a;
    int b;
    char c;
} x
```

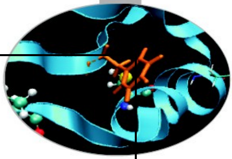
```
struct mystruct {
    char a;
    char gap_0[3];
    int b;
    char c;
    char gap_1[3];
} x
```

- **Using extents to handle structs is not safe! Get the addresses**

MPI_GET_ADDRESS (location, address)
IN location: location in caller memory (choice)
OUT address: address of location (integer)

- The address of the variable is returned, which can then be used to determine the correct relative dispacements
- Using this function helps with portability

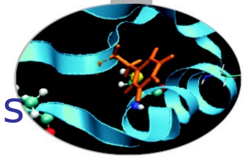
USING DISPLACEMENTS



```
struct PartStruct {
          char class;
   double d[6];
          int b[7];
} particle[100];
```

```
MPI_Datatype ParticleType;
int count = 3;
MPI_Datatype type[3] = {MPI_CHAR, MPI_DOUBLE,
MPI_INT};
int blocklen[3] = {1, 6, 7};
MPI_Aint disp[3];

MPI_Get_address(&particle[0].class, &disp[0]);
MPI_Get_address(&particle[0].d, &disp[1]);
MPI_Get_address(&particle[0].b, &disp[2]);
/* Make displacements relative */
disp[2] -= disp[0]; disp[1] -= disp[0]; disp[0] = 0;

MPI_Type_create_struct (count, blocklen, disp, type,
&ParticleType);
MPI_Type_commit (&ParticleType);

MPI_Send(particle,100,ParticleType,dest,tag,comm);
MPI_Type_free (&ParticleType);
```

FORTRAN TYPES



- According to the standard the memory layout of Fortran derived data is much

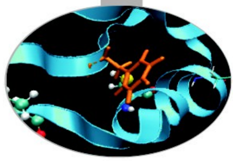
  more liberal
- An array of types, may be implemented as 5 arrays of scalars!

```
type particle
   real :: x,y,z,velocity
   integer :: n
end type particle
type(particle) ::
particles(Np)
```

```
type particle
   sequence
   real :: x,y,z,velocity
   integer :: n
end type particle
type(particle) ::
particles(Np)
```

- The memory layout is guaranteed using sequence or bind(C) type attributes
  - Or by using the (old style) commons...
- With Fortran 2003, MPI_Type_create_struct may be applied to common blocks, sequence and bind(C) derived types
  - it is implementation dependent how the MPI implementation computes the alignments (sequence, bind(C) or other)
- The possibility of passing **particles** as a type depends on MPI implementation: try **particle%x** and/or study the MPI standard and Fortran 2008 constructs

PERFORMANCE



Performance depends on the datatype – more general datatypes are often slower

- some MPI implementations can handle important special cases: e.g., constant stride, contiguous structures

- Overhead is potentially reduced by:
  - Sending one long message instead of many small messages
  - Avoiding the need to pack data in temporary buffers
- Some implementations are slow