HPC.nrw

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MPI in Small Bites

PPCES 2026

HPC.NRW Competence Network

Derived Datatypes

HPC.NRW Competence Network

MPI in Small Bites

MPI Datatypes

- MPI datatypes are opaque handles
  - Instructions for accessing the binary content of a memory buffer
- MPI predefines basic datatypes for each language binding
  - Distinct handles for C/C++ and Fortran (e.g., MPI_INT vs. MPI_INTEGER)
  - Describe a single data element
- More complex MPI datatypes can be constructed (derived)
  - Matrix rows & columns, diagonal matrices, structures

Terminology

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- Type signature
  - A sequence of basic datatypes described by a given type and count
  - Example: {MPI_INT, MPI_INT, MPI_DOUBLE}

- Type map
  - A sequence of basic datatypes and their displacements
  - Example: {(MPI_INT, 0), (MPI_INT, 4), (MPI_DOUBLE, 8)}

- Datatypes are local objects
  - May differ across processes
  - Enable transparent type marshalling (encoding & decoding of data)

Terminology II

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- Lower and upper bound:
  - *lb*(datatype) = min $disp_j$
  - *ub*(datatype) = max ($disp_j$ + sizeof($type_j$)) + padding
- Extent
  - *extent*(datatype) = *ub*(datatype) – *lb*(datatype)
  - The size of the step when accessing consecutive elements of that type
- Size
  - *size*(datatype) =
  - The total amount of bytes taken by the datatype, not counting any gaps in it

Basic datatype example

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- Example: MPI_INT
  - *type map* = { (*MPI_INT*, 0) }
  - *lb* = 0
  - *ub* = 4
  - *extent* = 4 bytes
  - *size* = 4 bytes
- All predefined basic MPI datatypes have lower bound 0, i.e. data is flush with the buffer start
- Platform-specific alignment rules are taken into account
  - The upper bound is therefore adjusted if necessary

Using Datatypes

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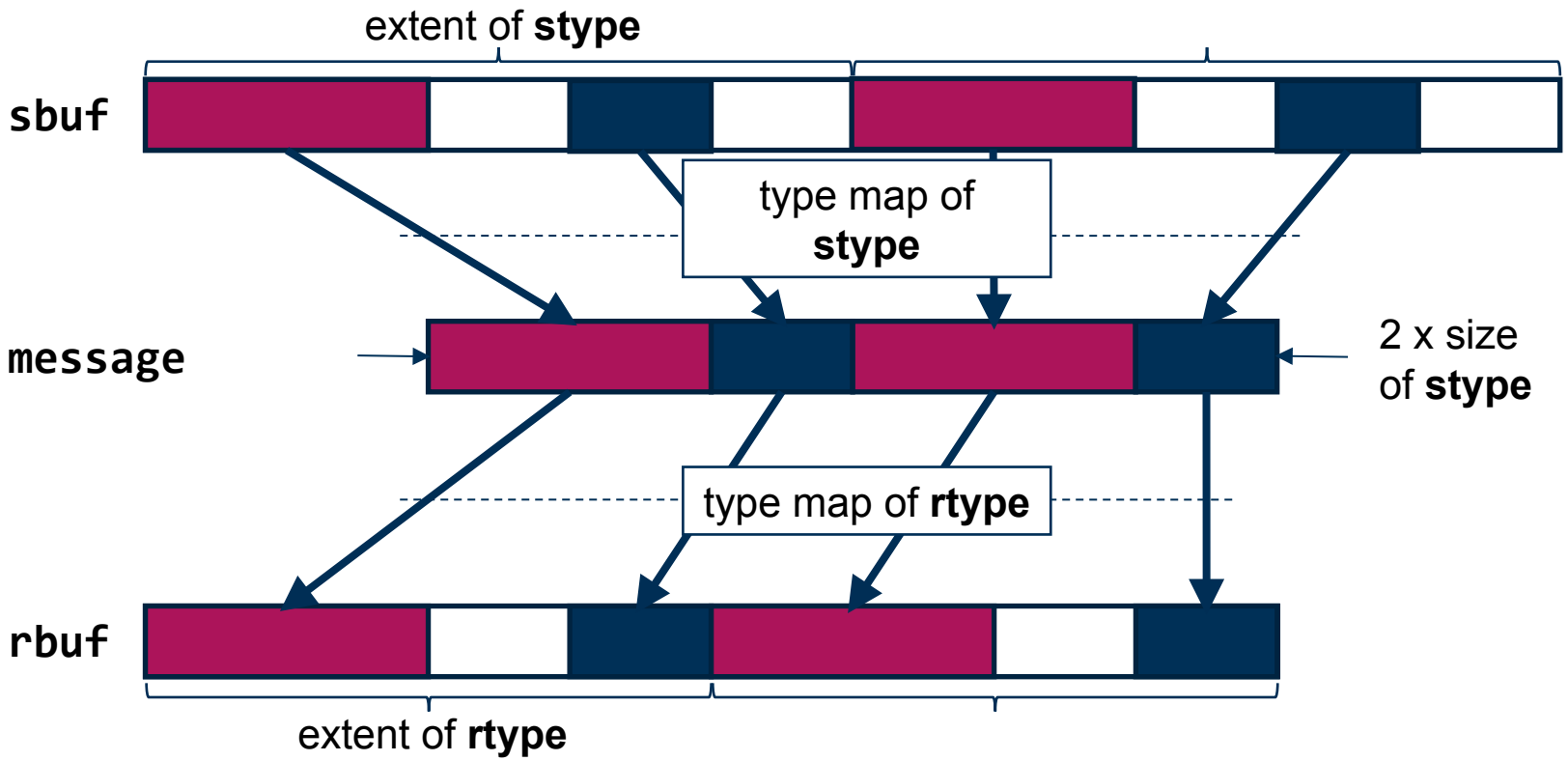
```
MPI_Send(sbuf, 2, stype, dest, 0, MPI_COMM_WORLD);
```




```
MPI_Recv(rbuf, 2, rtype, src, 0, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
```

Contiguous Datatypes

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- Create a sequence of elements of an existing datatype

```
MPI_Type_contiguous (int count, MPI_Datatype oldtype, MPI_Datatype *newtype)
```

  - The new datatype represents a contiguous sequence of **count** elements of **oldtype**
  - The elements are separated from each other by the extent of **oldtype**
  - A send/receive of one element of **newtype** is congruent with a receive/send of **count** elements of **oldtype**

- Useful for sending entire matrix rows (C/C++) or columns (Fortran)

Vector Datatypes

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- Create a sequence of equally spaced blocks of elements

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

  - The new datatype represents a sequence of **count** blocks, each containing **blen** elements of the old datatype
  - Every two consecutive blocks are separated by **stride** elements each

- Useful for sending matrix columns (C/C++) or rows (Fortran)
  - **stride** = row (C/C++) | column (Fortran) length (in number of elements)
  - **blocklen** = 1 (or the number of consecutive rows/columns)
  - **count** = number of rows (C/C++) | columns (Fortran)

Vector Datatypes

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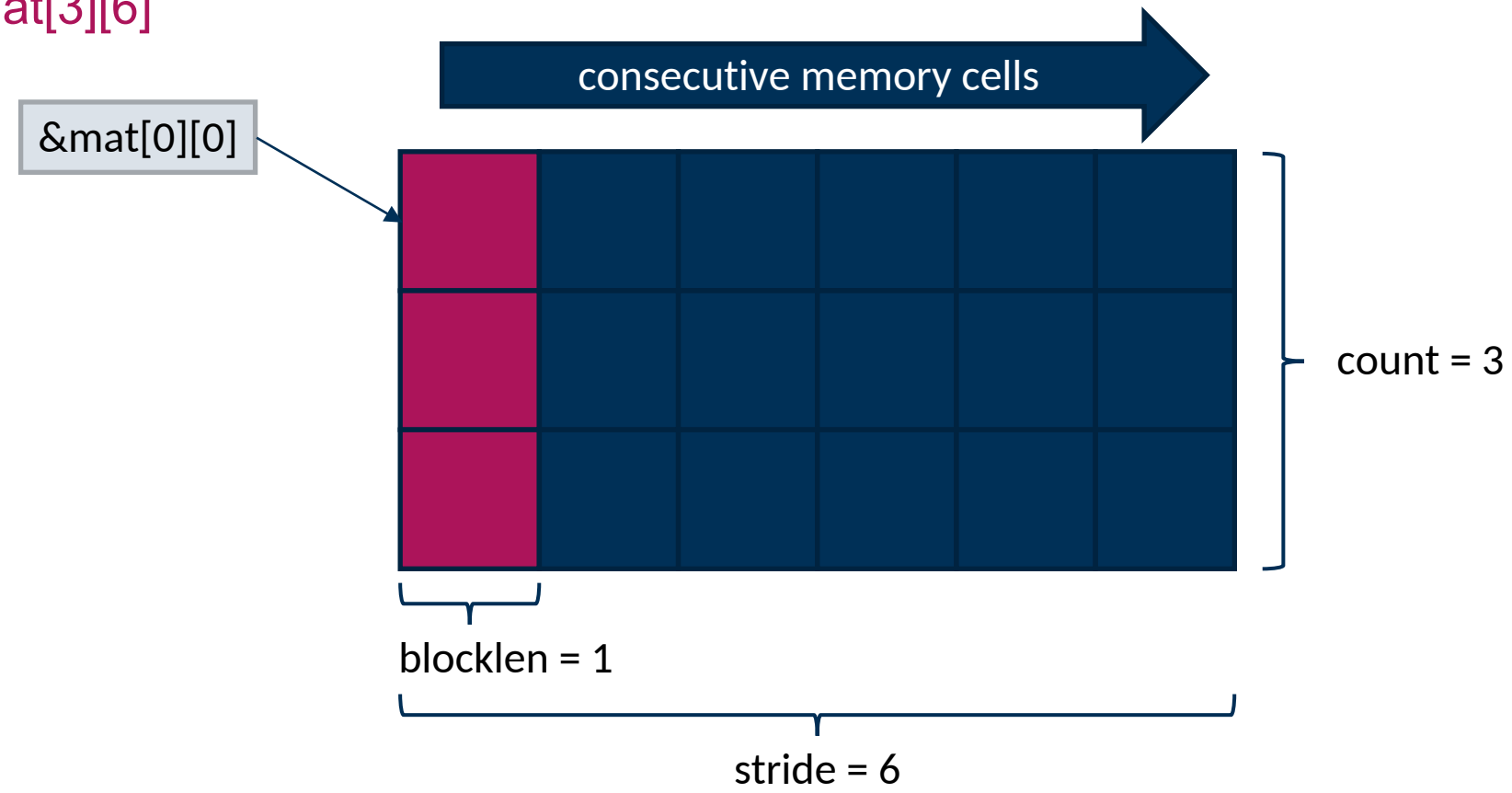
- Example: single column of a C/C++ matrix
  - mat[3][6]



Vector Datatypes

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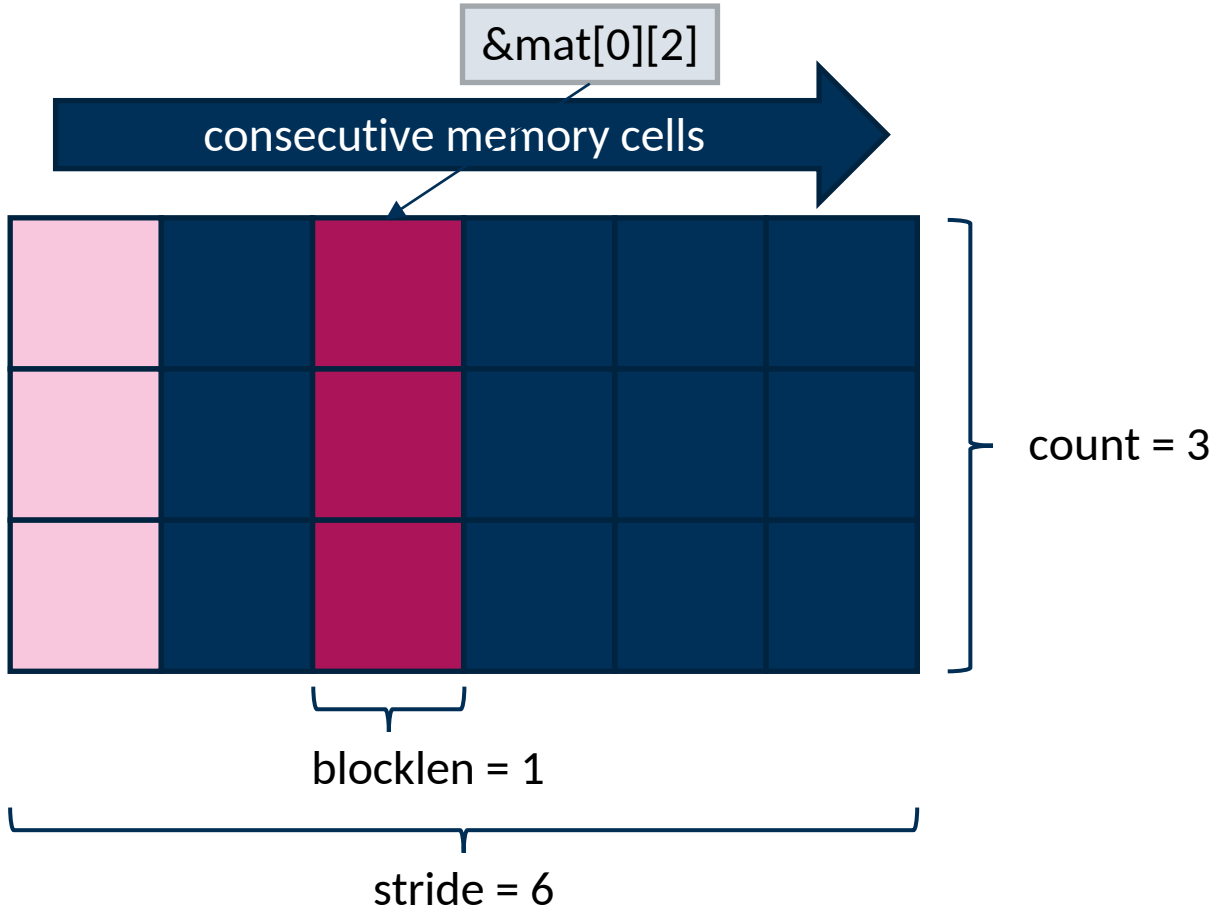
- Example: single column of a C/C++ matrix
  - mat[3][6]



Vector Datatypes

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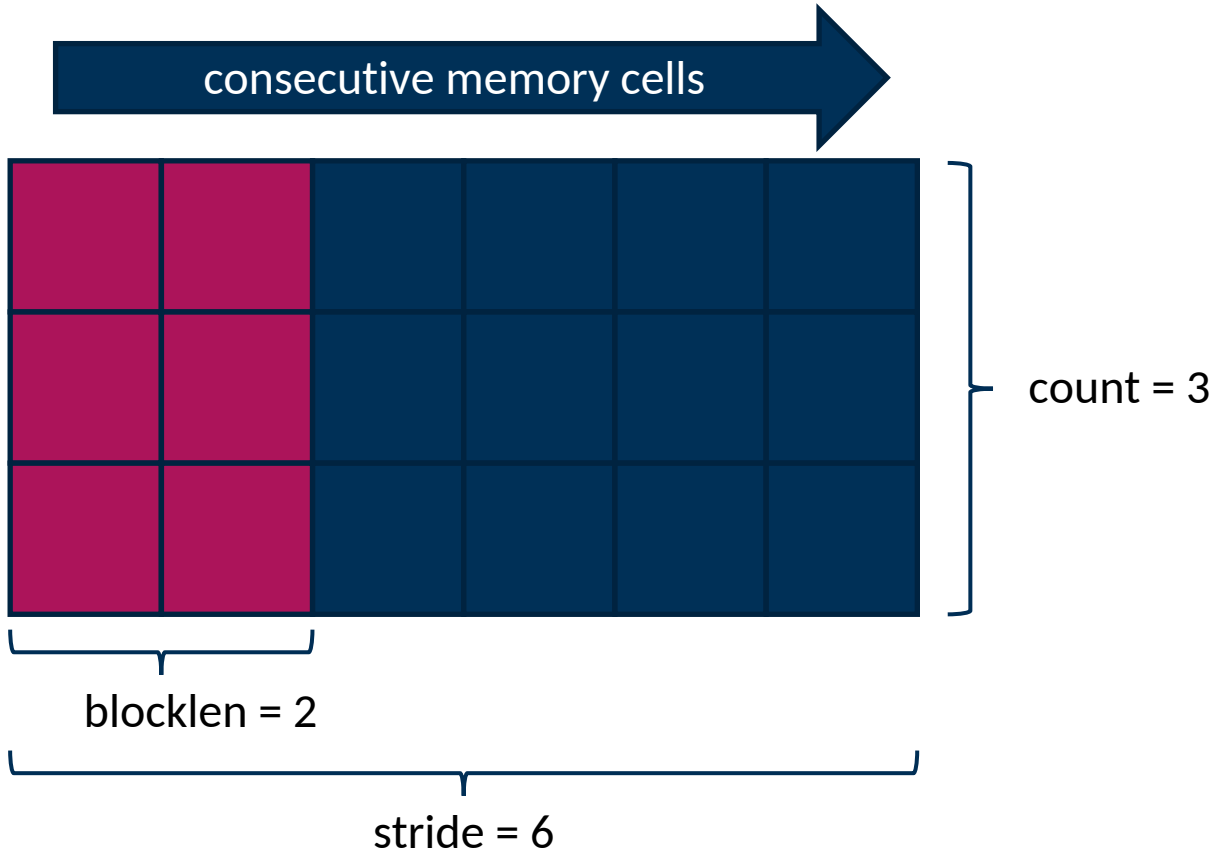
- Example: two consecutive columns of a C/C++ matrix
  - mat[3][6]



Indexed Datatypes

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- Indexed list of arbitrary-sized blocks within a matrix

```
MPI_Type_indexed (int count, const int array_of_blocklengths[],
                  const int array_of_displacements[], MPI_Datatype oldtype,
                  MPI_Datatype *newtype)
```

  - The new datatype represents a sequence of **count** blocks, where the *i*-th block
    - contains **array_of_blocklengths[i]** elements of the old datatype and
    - Every two consecutive blocks are separated by **stride** elements each

- Useful for custom shapes of data in fixed-sized matrices
  - Lower/upper triangle
    - Blocksizes increase with every block

Indexed Datatypes

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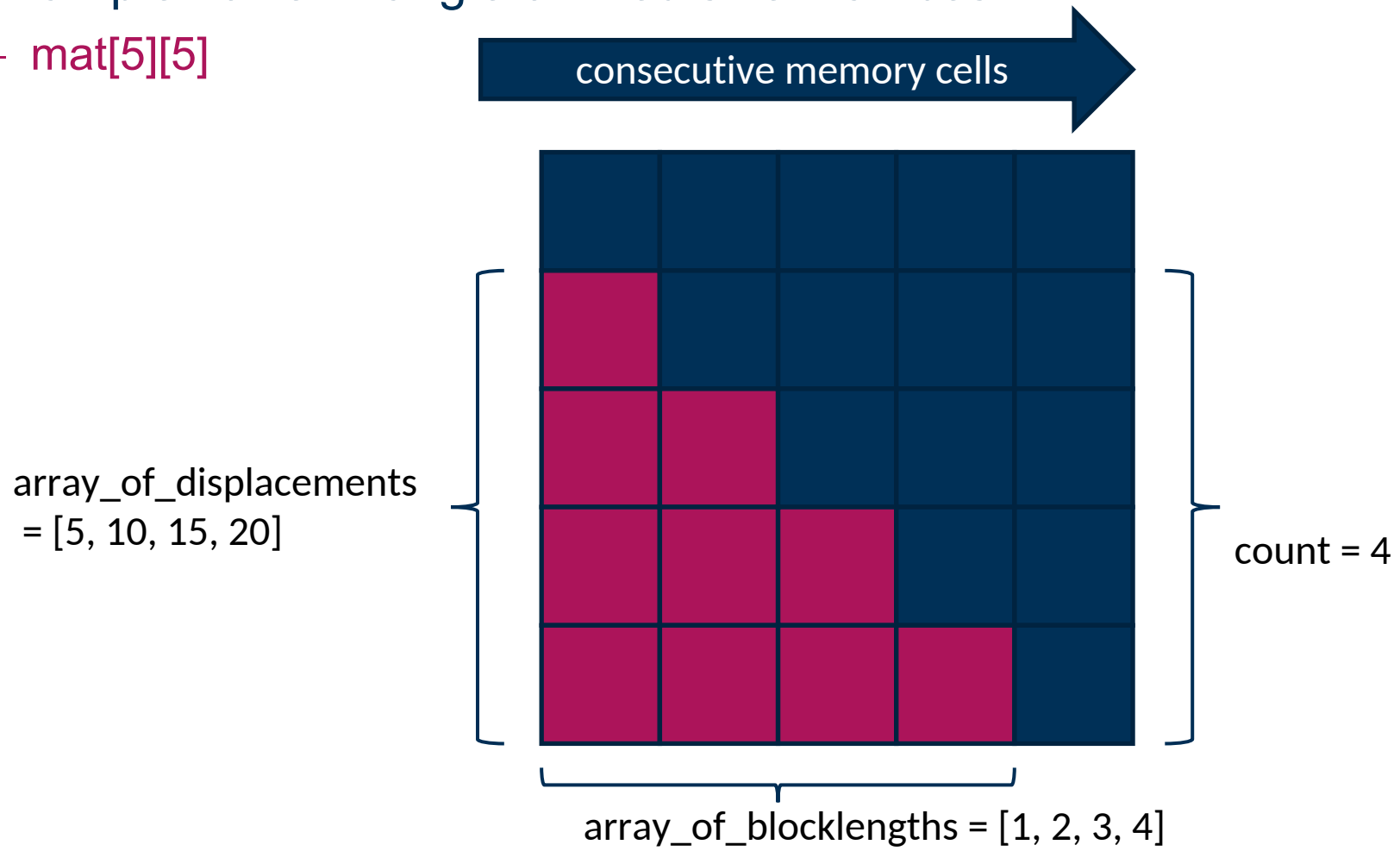
- Example: lower triangle of fixed size matrices
  - mat[5][5]



Structure Datatypes

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- The most generic datatype
  - Useful for C/C++ structures and Fortran derived data type / COMMON blocks

```
MPI_Type_create_struct (int count, const int array_of_blocklengths[],
                        MPI_Aint array_of_displacements[],
                        MPI_Datatype array_of_types[],
                        MPI_Datatype *datatype)
```

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

Structure Datatypes

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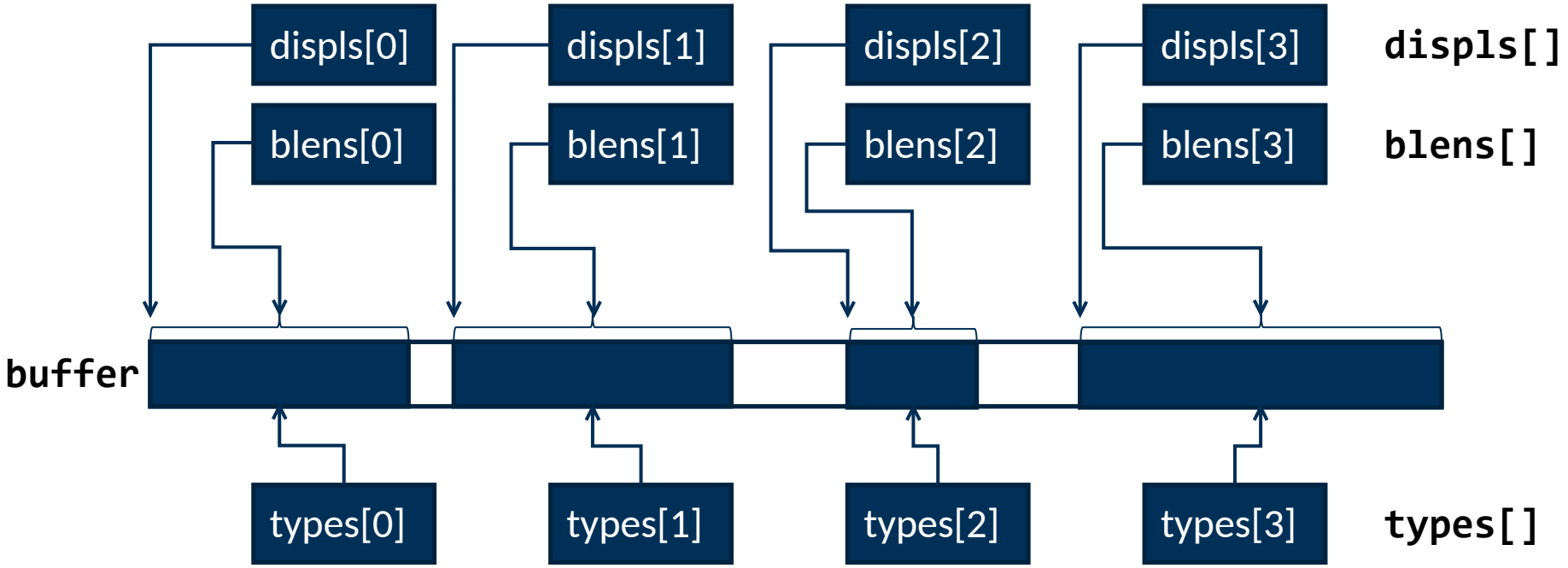
```
MPI_Type_create_struct (int count, int blens[], MPI_Aint displs[],
                        MPI_Datatype types[], MPI_Datatype *datatype)
```



Structure Datatypes

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- The most generic datatype
  - Corresponds to C/C++ struct

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

int blens[] = { 1, 3, 1 };
MPI_Aint displs[] = { offsetof(Particle, mass),
                      offsetof(Particle, pos),
                      offsetof(Particle, sym) };
MPI_Datatype types[] = { MPI_FLOAT, MPI_DOUBLE, MPI_CHAR };

MPI_Datatype particle_type;
MPI_Type_create_struct(3, blens, displs, types, &particle_type);
```

Using Derived Datatypes

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- Register a datatype for use with communication operations:

```
MPI_Type_commit (MPI_Datatype *datatype)
```

  - A datatype must be committed before it can be used in communications
  - All predefined datatypes are already committed
  - Intermediate datatypes, i.e. ones used for building more complex datatypes but not used in communication, can be left uncommitted

- Deregister and free a datatype:

```
MPI_Type_free (MPI_Datatype *datatype)
```

  - Derived datatypes, build from the freed datatype, are not affected
  - **datatype** set to **MPI_TYPE_NULL** upon successful return

Structure Datatypes – Example

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

int blens[] = { 1, 3, 1 };
MPI_Aint displs[] = { offsetof(Particle, mass),
                      offsetof(Particle, pos),
                      offsetof(Particle, sym) };
MPI_Datatype types[] = { MPI_FLOAT, MPI_DOUBLE, MPI_CHAR };

MPI_Datatype particle_struct;
MPI_Type_create_struct(3, blens, displs, types, &particle_struct);
MPI_Type_commit(&particle_struct);
```

– particle_struct can now be used to send a single Particle

Structure Datatypes

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– Resize to the true size of the structure

```
int blens[] = { 1, 3, 1 };
MPI_Aint displs[] = { offsetof(Particle, mass),
                      offsetof(Particle, pos),
                      offsetof(Particle, sym) };
MPI_Datatype types[] = { MPI_FLOAT, MPI_DOUBLE, MPI_CHAR };

MPI_Datatype particle_struct;
MPI_Type_create_struct(3, blens, displs, types, &particle_struct);
// No need to commit particle_struct - not used in communication

MPI_Aint true_extent = sizeof(Particle);
MPI_Type_create_resized(particle_struct, 0, true_extent, &particle_type);
MPI_Type_commit(&particle_type);
```

– MPI_Type_create_resized takes an existing datatype and creates a new one with modified lower bound and extent

Summary: Derived Datatypes

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- Local handles describing how to access memory
- Can be mixed and matched on both sides of a communication operation as long as their type signatures match
- Lower and upper bound can be manipulated to account for padding at beginning and end
- Need to be committed before use in communication or I/O
- Language-specific handles need to be used in mixed-language applications