703650 VO Parallel Systems WS2019/2020
MPI Derived Datatypes and Virtual Topologies

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Overview

- derived datatypes
  - allows to send user-specific datatypes
- virtual topologies
  - adds semantic position information to ranks
- tales from the proseminar
  - off-topic topics

Motivation

- we discussed using MPI for parallelization, but on a very basic level
  - we can only transfer contiguous ranges of arrays of the same element type
  - we need to manually compute rank numbers for talking to semantically significant and often-used ranks (e.g. left/right neighbor)

- what about
  - transferring (nested) structs/classes, arrays of tuples, columns of a 2 D matrix, etc.
  - ease of coding: “send temperature to my left neighbor” instead of “send `double` to `(myRank – 1 + numRanks) % numRanks`”

Derived Datatypes

Recap: MPI Datatypes

- several basic types predefined
  - `MPI_INT, MPI_FLOAT, MPI_DOUBLE, MPI_BYTE, …`
- what about something like on the right?
  - struct with 4 members
  - 3x 8 bytes + 4 bytes

```
struct Particle {
    double x;
    double y;
    double z;
    int species;
};
```

Issues With More Complex Data Structures

- MPI doesn't know how large a single element is
  - no predefined `MPI_(DATA_TYPE_THAT_DOESNT_EXIST_YET)`
  - what about nesting types? with differently-sized members?
  - sending individual elements blows up the code and causes performance overhead due to multiple messages

- issue of sending a single member of struct instances
  - bad solution: explicitly assemble send/receive buffers with single data type per message transfer
  - causes coding, memory footprint, and message overhead (at least one message per type)

Why not Just use MPI_BYTE/MPI_INT/MPI_... everywhere?

- adds strong typing to MPI library calls and allows automatic type handling
  - size of e.g. `int` is unknown (C standard only defines minimum requirements!)
  - `int` on machine A and `int` on machine B might have different size
  - machine A might be little-endian, machine B might be big-endian
  - saves a lot of explicit user-written `sizeof()` constructs
  - enables type-specific hardware optimizations for MPI

- using `MPI_BYTE/`... everywhere deprives you of all of the above

MPI Derived Datatypes

- composed of existing types
  - both basic and derived
- used to transfer high-level data structures
  - encodes more information in transfer, allows MPI to perform optimizations
  - more performance-efficient than individual transfer of data structure contents
  - less code, easier to read and maintain

MPI Derived Datatypes cont'd

- allow definition of new handles
  - e.g. MPI_FOOBAR

- require several steps
  - construction: declare and define new datatype
  - allocation / commit: needs to be done once by all ranks before using new datatype
  - usage (optional)
  - deallocation (optional): frees internal MPI storage, to be done once by all ranks

Selection of MPI Derived Datatype Facilities

- `MPI_Type_create_struct(…)`
  - specifies the data layout of user-defined structs (or classes)
- `MPI_Type_vector(…)`
  - specifies strided data, i.e. same-type data with missing elements
- `MPI_Type_create_subarray(…)`
  - specifies sub-ranges of multi-dimensional arrays
- `MPI_Type_contiguous(…)`
  - specifies a user-defined contiguous type comparable to C arrays

Structs

- `int MPI_Type_create_struct(int count, const int blocklengths[], const MPI_Aint displacements[], const MPI_Datatype types[], MPI_Datatype* newtype)`
  - `count`: number of blocks
  - `blocklengths`: number of elements per block (array)
  - `displacments`: starting address of first element of each block (array)
  - `types`: type of each block (array)
  - `newtype`: resulting derived datatype

- allows user-defined, aggregated types to be used in MPI communication directly

Structs: Block Lenghts, Displacements and Types

```
struct Particle {
    int posX;
    int posY;
    int posZ;
    double magneticForceX;
    double magneticForceY;
    double magneticForceZ;
};
```

block no 0, starts at byte 0,
12 bytes long, type is integer

block no 1, starts at byte 12,
24 bytes long, type is double

Careful with Displacements

- careful with manually specifying displacements
  - binary layout of your struct in memory is compiler-dependent!
  - e.g. struct members might be padded to multiples of 8 bytes
- use `offsetof()` instead!

```
MPI_Aint displacements[2] =
    { 0,
      12 };

// ===== vs =====

MPI_Aint displacements[2] =
    { offsetof(Foo, posX),
      offsetof(Foo, magneticForceX) };
```

Careful with Pointers

- don't transfer shallow copies of data
  - `double*  data` might be not available or at a different address on node B
- try to avoid
  - otherwise, make a deep copy and ensure proper pointers

```
struct Particle {
    int size;
    double* data;
};
```

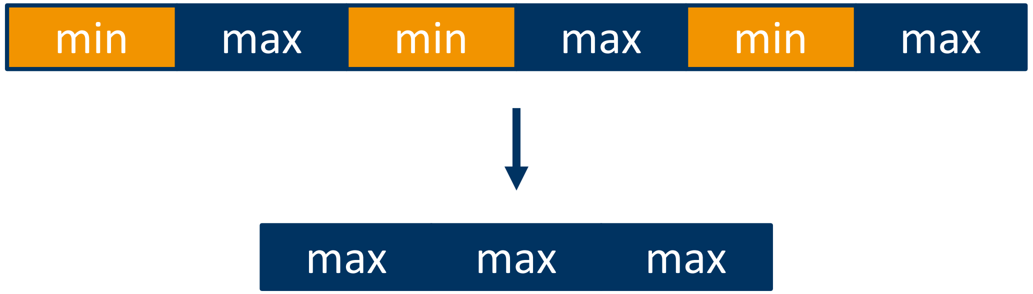
Struct Example

```c
typedef struct {
    int barInt;
    double barDoubleA;
    double barDoubleB;
} Foo;
MPI_Datatype myType;
int blocklengths[2] = { 1, 2 };
MPI_Aint displacements[2] =
    { offsetof(Foo, barInt),
      offsetof(Foo, barDoubleA) };
MPI_Datatype datatypes[2] =
    { MPI_INT, MPI_DOUBLE };
```

```c
MPI_Type_create_struct(2, blocklengths,
    displacements, datatypes, &myType);

if (myRank == 0) {
    Foo data[2] = ...
    MPI_Send(data, 2, myType, 1, 42,
        MPI_COMM_WORLD);
} else {
    Foo data[2] = ...
    MPI_Recv(data, 2, myType, 0, 42,
        MPI_COMM_WORLD,
        MPI_STATUS_IGNORE);
}
```

Non-Contiguous Data

- send all max values of an array of `(min, max)`-tuples to another rank

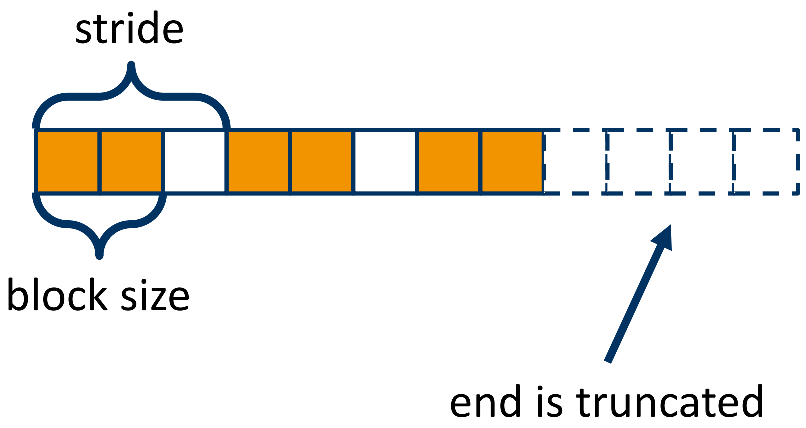


- send the column of a matrix

- do all of that without having to copy data to a contiguous buffer first!

Vectors

- Support strides (gaps in arrays)
  - e.g. take 2 elements, omit 1 element, repeat 3 times in total
  - useful for linear algebra



Vector Example

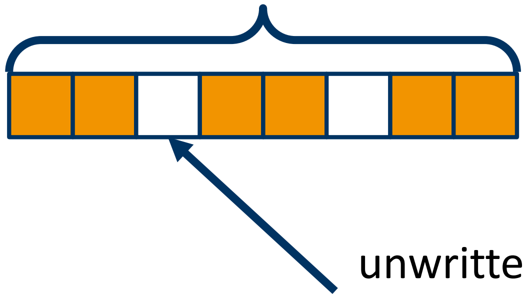
```
#define SIZE 20
#define STRIDE 3
#define COUNT 3
#define LENGTH 2

MPI_Datatype myType;
MPI_Type_vector(COUNT, LENGTH, STRIDE,
    MPI_CHAR, &myType);
MPI_Type_commit(&myType);
```

```
if (myRank == 0) {
    char data[SIZE] = ...;
    MPI_Send(data, 1, myType, 1, 42,
        MPI_COMM_WORLD);
} else {
    char data[SIZE];
    MPI_Recv(data, 1, myType, 0, 42,
        MPI_COMM_WORLD,
        MPI_STATUS_IGNORE);
}
```

Vector Variants

```c
char data[SIZE];
MPI_Recv(data, 1, myType,
    0, 42, MPI_COMM_WORLD,
    MPI_STATUS_IGNORE);
```

```c
char data[COUNT*LENGTH];
MPI_Recv(data, COUNT*LENGTH, MPI_CHAR,
    0, 42, MPI_COMM_WORLD,
    MPI_STATUS_IGNORE);
```



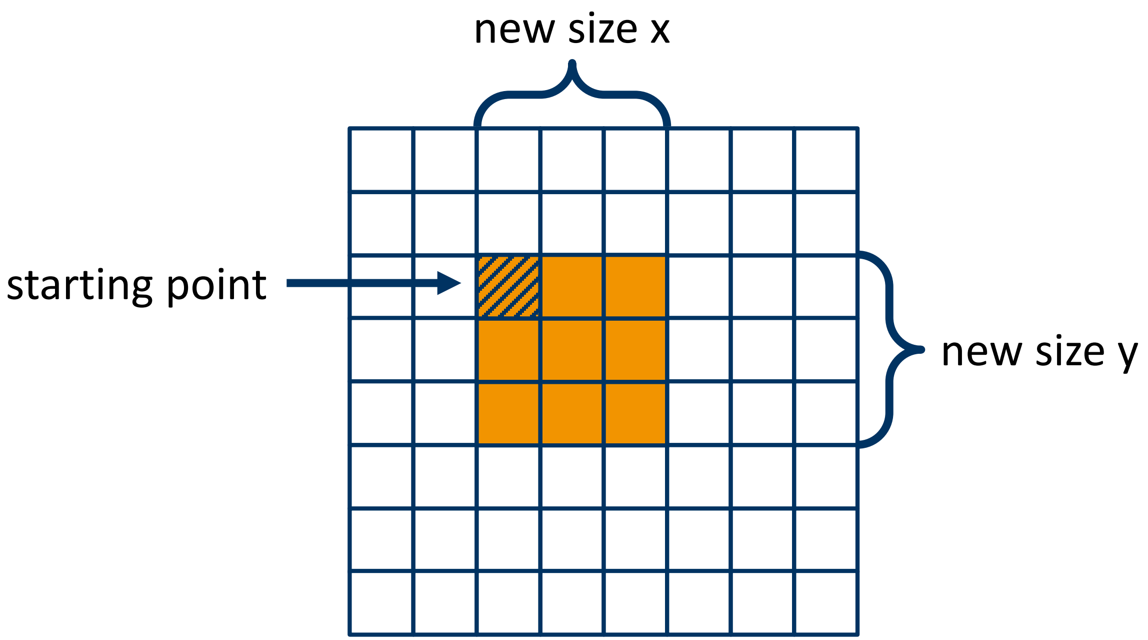
Use Case: Data Transposition

```
int data[SIZE][SIZE];
MPI_Type_vector(SIZE, 1, SIZE, MPI_INT,
    &myType);
MPI_Send(data, 1, myType,
    1, 42,
    MPI_COMM_WORLD);
```

```
int data[SIZE];
MPI_Recv(data, SIZE, MPI_INT,
    0, 42,
    MPI_COMM_WORLD, MPI_STATUS_IGNORE);
```

Subarrays

- Allows to address a multi-dimensional sub-range of array elements



Subarray Example in 2 D

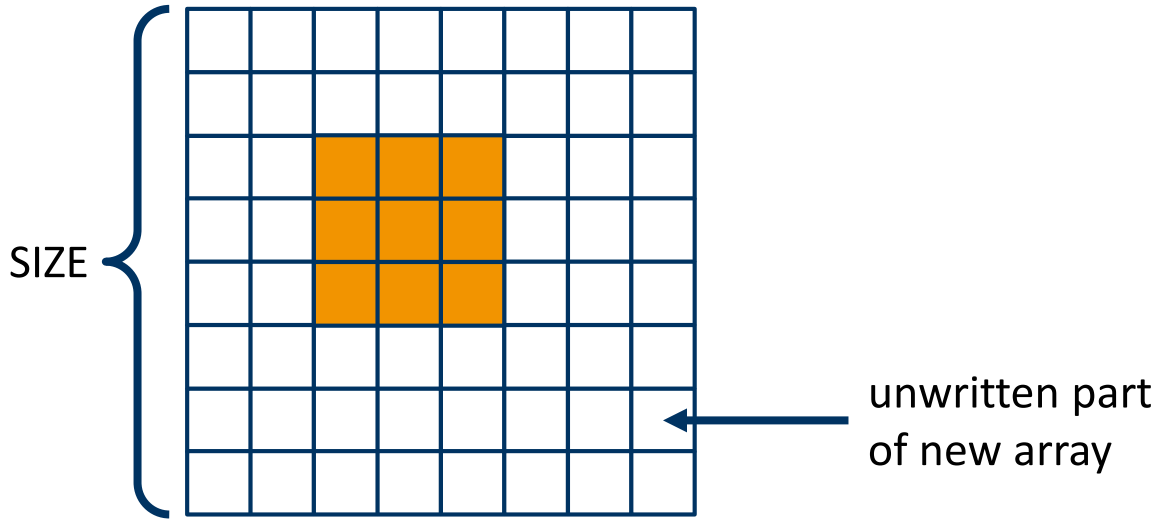
```c
#define SIZE 8
#define SUBSIZE 3

MPI_Datatype myType;
int size[2] = { SIZE, SIZE };
int subSize[2] = { SUBSIZE, SUBSIZE };
int start[2] = { 2, 2 };

MPI_Type_create_subarray(2, size,
    subSize, start, MPI_ORDER_C, MPI_INT,
    &myType);
MPI_Type_commit(&myType);
```

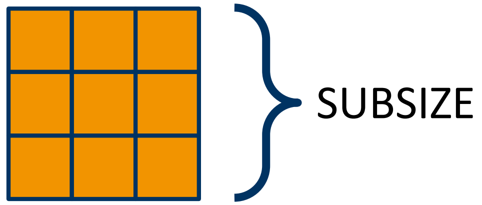
```c
if (myRank == 0) {
    int data[SIZE][SIZE] = ...;
    MPI_Send(data, 1, myType, 1, 42,
        MPI_COMM_WORLD);
} else {
    int subData[SUBSIZE][SUBSIZE];
    MPI_Recv(subData, SUBSIZE*SUBSIZE,
        MPI_INT, 0, 42, MPI_COMM_WORLD,
        MPI_STATUS_IGNORE);
}
```

Subarray Receive Variants

```c
int data[SIZE][SIZE];
MPI_Recv(data, 1,
    myType, 0, 42, MPI_COMM_WORLD,
    MPI_STATUS_IGNORE);
```

```c
int subData[SUBSIZE][SUBSIZE];
MPI_Recv(subData, SUBSIZE*SUBSIZE,
    MPI_INT, 0, 42, MPI_COMM_WORLD,
    MPI_STATUS_IGNORE);
```





Multiple Ways of Distributing Rows

- Allocate as a 1D array, use linearized indices
  - use 1D MPI vector with stride
  - (use nD MPI subarray with 1 dimension)
  - (use nD MPI darray with 1 dimension)

- Allocate as a nD array
  - use nested 1D MPI vectors
  - use nD MPI subarray
  - use nD MPI darray

- Same functional result for all of the above, but performance might differ
  - remember, MPI doesn't guarantee performance portability

Contiguous Derived Datatypes

- allows to aggregate same-type arrays into a single-count datatype

- has certain advantages
  - sending more than e.g. 2^{32}-1 elements (count parameter type in `MPI_Send/Recv/...` is only `int`!)
  - allows semantic grouping and naming of data

```
MPI_Datatype myType;
MPI_Type_contiguous(SIZE, MPI_CHAR, &myType);
MPI_Type_commit(&myType);

char data[SIZE] = { 0 };

if(myRank == 0) {
    MPI_Send(data, 1, myType, 1, 42,
        MPI_COMM_WORLD);
} else {
    MPI_Recv(data, 1, myType, 0, 42,
        MPI_COMM_WORLD, MPI_STATUS_IGNORE);
}

MPI_Type_free(&myType);
```

Packing/Unpacking

- MPI also offers `MPI_Pack(…)` and `MPI_Unpack(…)` functions
  - “Packs a datatype into contiguous memory” (MPICH documentation)
  - prefer this over derived datatypes? (hint: no)

- requires explicit copy of data from non-contiguous, user-defined form into a contiguous buffer to be sent with MPI
  - mostly superseded by MPI functions presented thus far, which directly access user-defined structures (no copy required)
  - pack/unpack still mostly offered for compatibility reasons, only very few edge cases

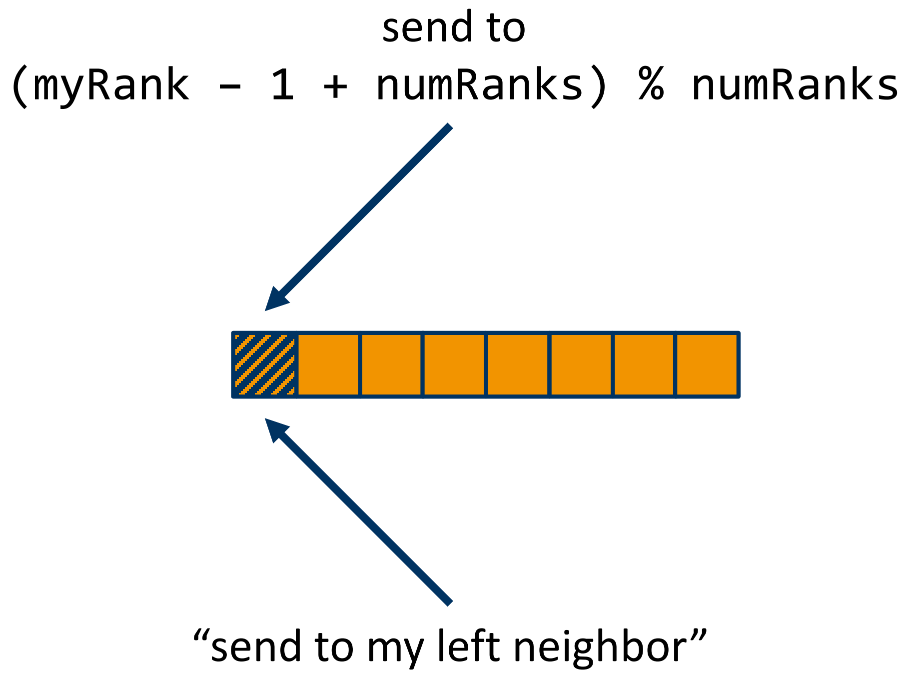
Free the Datatypes!

- call `MPI_Type_free(…)` once you no longer need the type
  - frees MPI-internal data storage for your custom type
  - reduces memory footprint for large numbers of datatypes
  - facilitates debugging
  - note: any pending communication using this type will continue and complete normally
  - omitted in most source code examples for obvious space reasons

Virtual Topologies

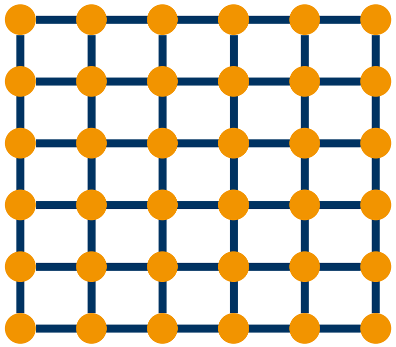
Virtual Topologies

- allows to “name” MPI ranks and provide addresses with semantics
  - high-level view of MPI ranks
  - simplifies implementation of complex algorithms
  - called “virtual” because it doesn’t necessarily match hardware topology
- naming scheme should fit communication pattern
  - and reflect the real-world topological relationship of parts of your problem
  - enables MPI to perform optimizations

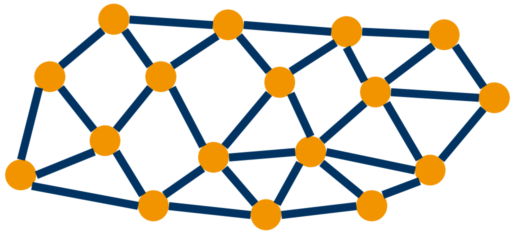


There are two Types of Topologies (According to MPI)

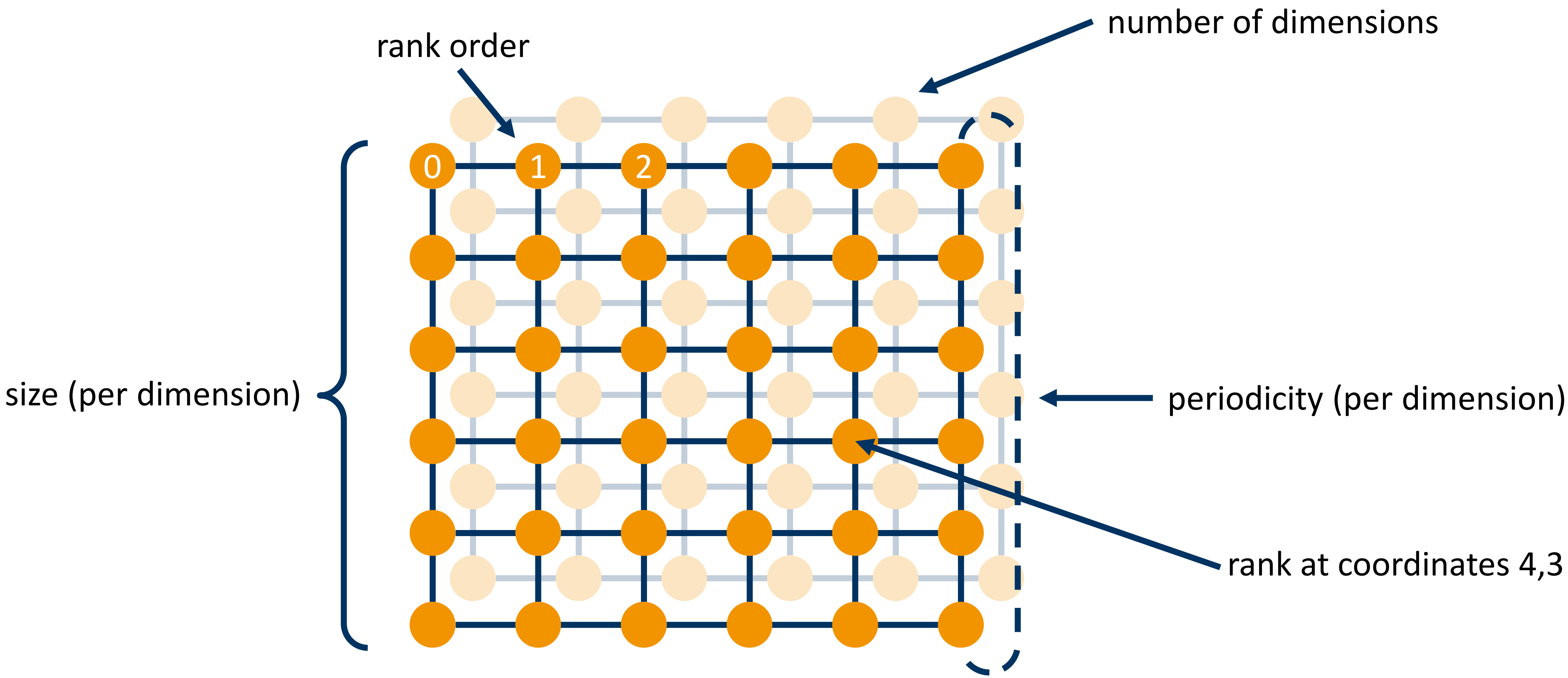
- Cartesian topologies
  - regular grids of squares/cubes/…
  - each rank is a node on the grid and connected to its neighbors
  - boundaries can be periodic
  - ranks can be identified via Cartesian coordinates instead of single index



- graph topologies
  - general graphs
  - each rank is a vertex in the graph
  - edges represent neighbor relationship
  - edge weights specify communication intensity (facilitates optimization)
  - not covered here



Properties of Cartesian Topologies



Working with Cartesian Topologies

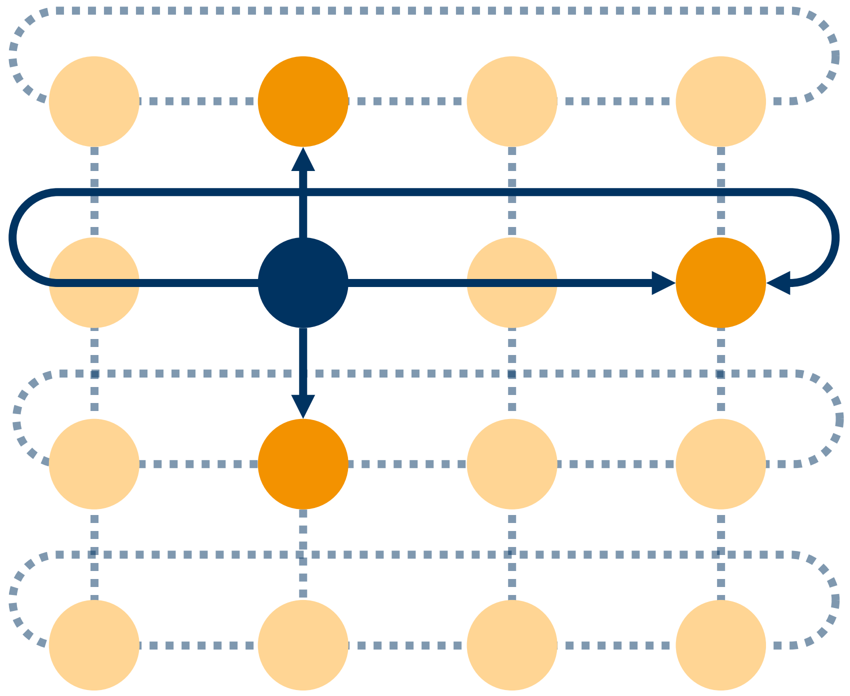
- create topology, resulting in new communicator
  - need to decide on dimensions, sizes, periodicity, etc…
  - per-dimension sizes can be computed using convenience function `MPI_Dims_create()`
  - new communicator implies ranks might have changed!
    - (remember MPI basics lecture: "[…] MPI semantics are relative to a *"communicator"* or *"group"*)
- compute rank numbers or coordinates as required
- communicate as you please
  - remember to specify correct communicator when using collective operations

Creating a Cartesian Topology

- ```
  int MPI_Cart_create(MPI_Comm comm_old, int ndims,
     const int dims[], const int periods[], int reorder,
     MPI_Comm* comm_cart)
  ```
  - `comm_old`: current communicator
  - `ndims`: number of dimensions
  - `dims`: size, per dimension
  - `periods`: periodicity (0 = open, 1 = periodic), per dimension
  - `reorder`: reorder rank numbers (0 = false, 1 = true)
  - `comm_cart`: new communicator with cartesian topology
  ```

Shifting

- computes rank numbers of neighbors
  - requires direction and displacement (=distance)
- example on the right
  - partially periodic 2D topology of 4x4
  - up/down shift with displacement 1
  - left/right shift with displacement 2

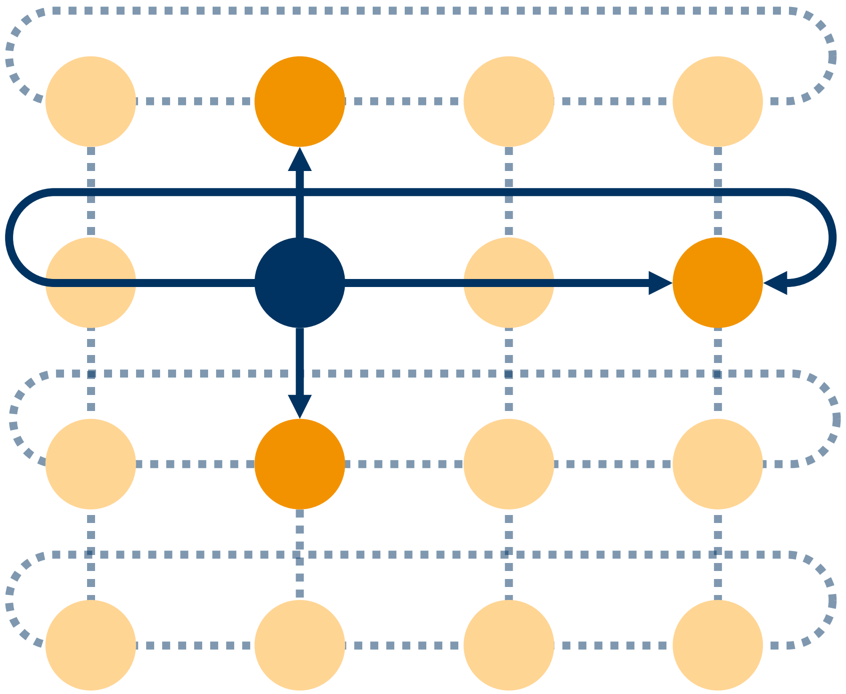


Shifting cont'd

- `int MPI_Cart_shift(MPI_Comm comm, int direction, int disp, int* rank_source, int* rank_dest)`
  - `comm`: communicator (must have cartesian topology!)
  - `direction`: dimension along which to select neighbors
  - `disp`: distance to neighbors
  - `rank_source`: neighbor for which the calling rank is the destination
  - `rank_dest`: requested neighbor for the calling rank

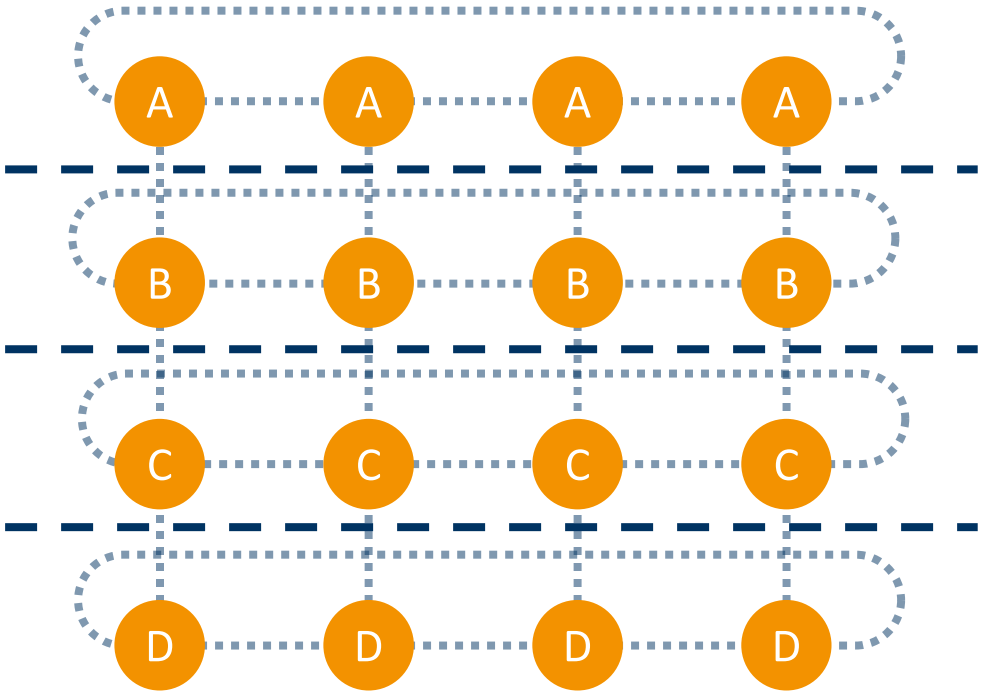
Shifting cont'd

```
MPI_Cart_shift(comm, 0, 1,
    &source, &dest);
// rank at 1,1:
// source is 1,0
// dest is 1,2
```



Slicing cont'd

- cuts a grid into slices
  - a new communicator is generated for each slice
  - enables slice-restricted collective communication
- example on the right
  - slicing a 2D topology horizontally
  - 4 new communicators A, B, C, and D with 4 ranks each
  - `MPI_Bcast(…,A)` only affects ranks of A



Slicing cont'd

- `int MPI_Cart_sub(MPI_Comm comm, const int remain_dims[], MPI_Comm* newcomm)`
  - `comm`: current communicator (must have cartesian topology!)
  - `remain_dims`: which dimensions to keep in sub-grid (0 = drop, 1 = include)
  - `newcomm`: new communicator holding only ranks of this slice

Additional Convenience Functions

- `MPI_Cart_coords(…)`
  - compute coordinates from a given rank (17 ➔ [4, 1])
- `MPI_Cart_rank(…)`
  - compute rank from given coordinates ([4,1] ➔ 17)
- `MPI_Cart_sub(…)`
  - partition grid into lower-dimension sub-grids (e.g. 2D square from 3D cube)
- `MPI_Cartdim_get(…)/MPI_Cart_get(…)`
  - get topology information for a given communicator

Tales from the Proseminar: Verification and Validation

- absolutely not the same thing, though often used synonymously

- verification means checking your implementation
  - ensure that implementation meets the specification
  - check that software output is correct

- validation means checking your specification
  - ensure that the specification meets requirements
  - check that software output serves the use case purpose

Summary

- derived data types can be very handy
  - no need to copy data to basic, contiguous buffers
  - allows to easily transpose data
  - arbitrary nesting possible
- virtual topologies add semantic position information to ranks
  - makes rank positions easily identifiable
  - allows direct neighbor communication
  - enables limited-scope collectives
- verification vs. validation