703308 VO High-Performance Computing
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 & semantics: “send temperature to my left neighbor” instead of “send `double` to `(myRank – 1 + numRanks) % numRanks`”

Derived Datatypes

Recap: MPI datatypes

- several predefined basic types
  - `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?

- derived datatypes add type information, allow 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
  - also does not carry any semantic information on the content

MPI derived datatypes

- composed of existing types
  - both basic and derived
  - can be nested
- 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: 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 lengths, 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 structs in memory is compiler-dependent (e.g. struct members might be padded to multiples of 8 bytes)
  - use `offsetof()` instead!
- also, do not confuse `MPI_Aint` (programming language data type) and `MPI_AINT` (MPI data type)
- additional option: use `MPI_BOTTOM` as the buffer argument, enables use of absolute addresses as displacements instead of offsets
  - rationale: MPI_Aint is a signed integer (overflow behavior is not defined), absolute addresses are unsigned (overflow is behavior is defined)

```
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 not be available or likely at a different memory address on node B

- try to avoid
  - otherwise, make a deep copy and adjust pointers at receiver side

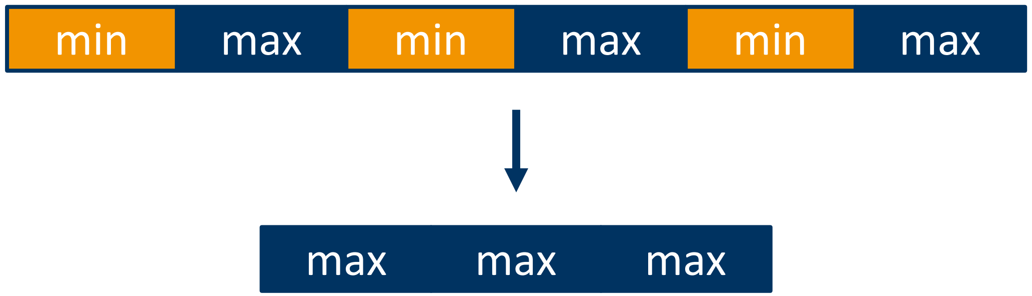
```
struct Particle {
    int size;
    double* data;
};
```

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);
MPI_Type_commit(&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



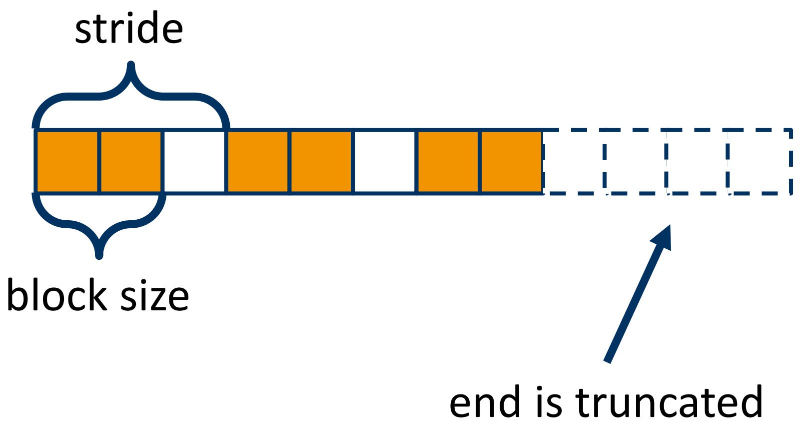
- send all max values of an array of `(min, max)`-tuples to another rank

- 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

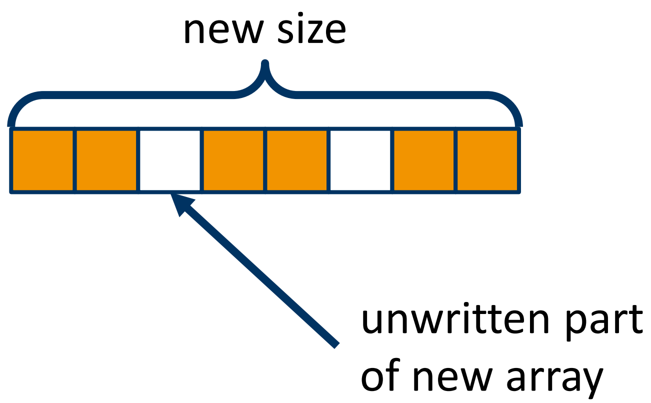
```c
#define SIZE 20
#define COUNT 3
#define LENGTH 2
#define STRIDE 3

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

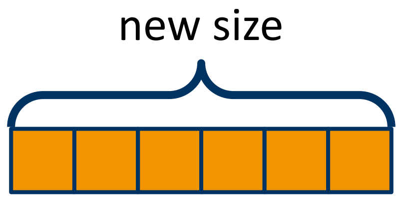
```c
if (myRank == 0) {
    char data[SIZE] = ...;
    MPI_Send(data, 1, myType, 1, 42,
        MPI_COMM_WORLD);
} else {
    char data[SIZE];
    MPI_Recv(data, 1, myType, 0, 42,
        MPI_COMM_WORLD,
        MPI_STATUS_IGNORE);
}
```

Vector variants: Use case compaction

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

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





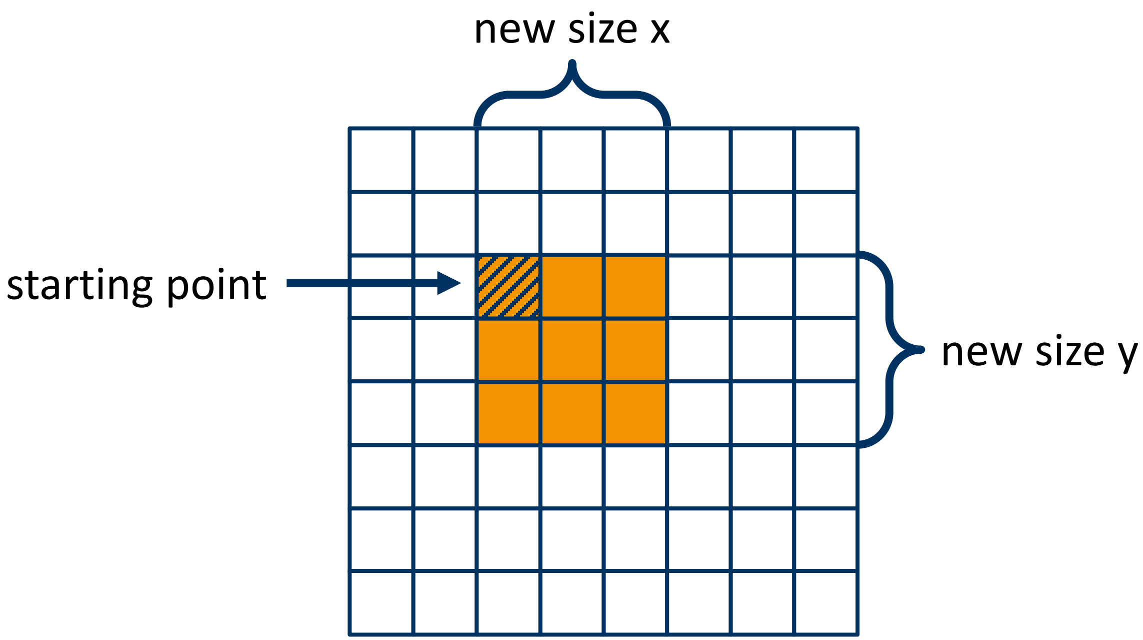
Vector variants: use case transposition

```
int data[SIZE][SIZE];
MPI_Type_vector(SIZE, 1, SIZE, MPI_INT,
    &myType);
MPI_Type_commit(&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 contiguous multi-dimensional sub-range of array elements



Subarray example in 2 D

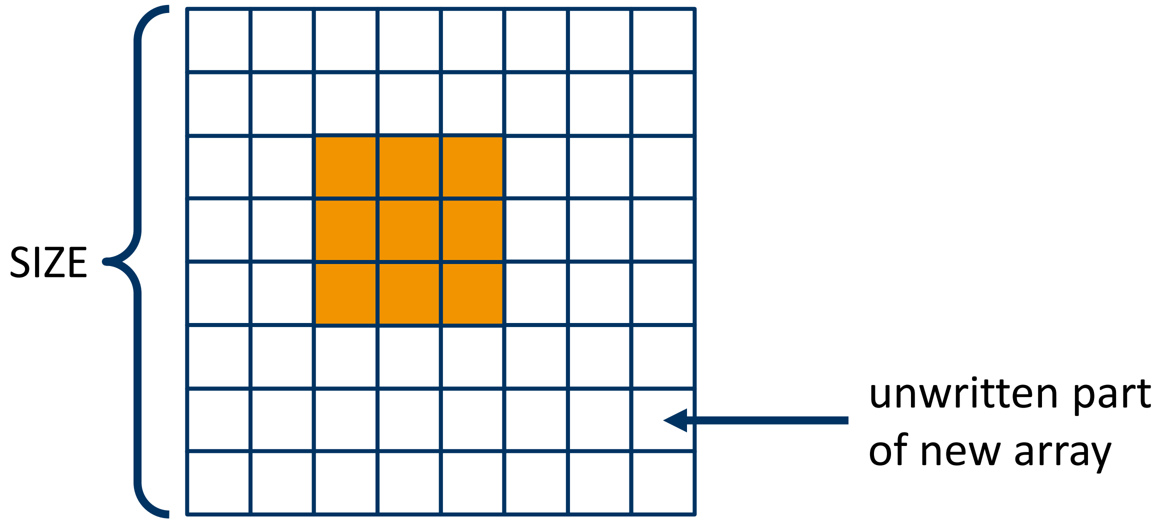
```c
#define SIZE 8
#define SUBSIZE 3

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);
```

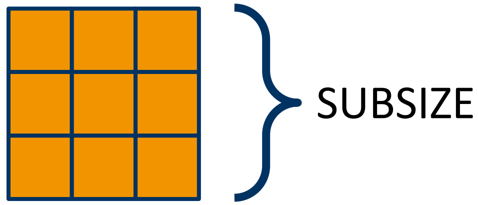
```c
if (myRank == 0) {
    int data[SIZE][SIZE] = ...;
    MPI_Send(data, 1, myType, 1, 42,
        MPI_COMM_WORLD);
} else {
    int subData[SUBSIZE][SUBSIZE];
    MPI_Recv(subData, SUBSIZE*SUBSIZE,
        MPI_INT, 0, 42, MPI_COMM_WORLD,
        MPI_STATUS_IGNORE);
}
```

Subarray receive variants

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

```
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 an 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 `INT_MAX` 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 user copy required)
  - pack/unpack still mostly offered for compatibility reasons, only very few edge cases

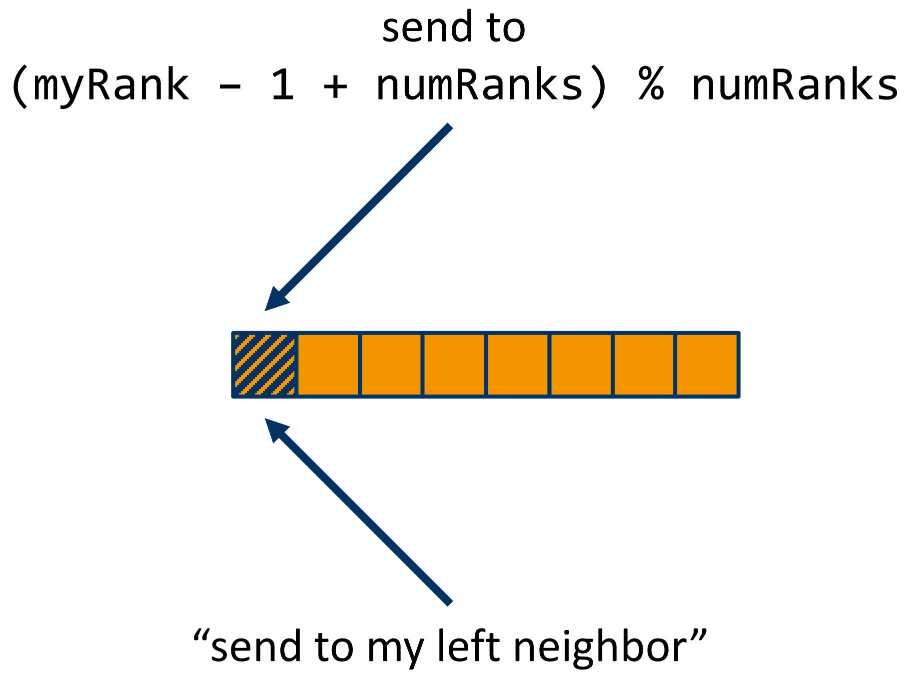
Free the datatypes!

- 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 many source code examples for obvious space reasons

Virtual Topologies

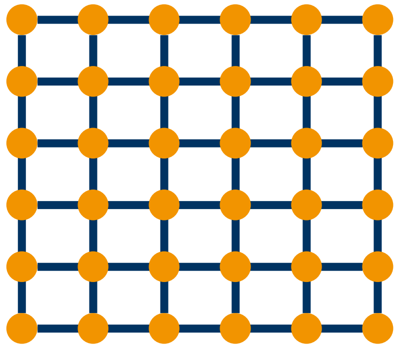
Virtual topologies

- 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's independent of the 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

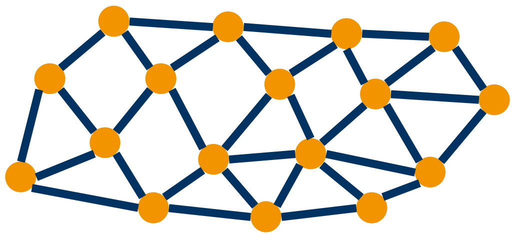


There are two types of topologies (according to MPI)

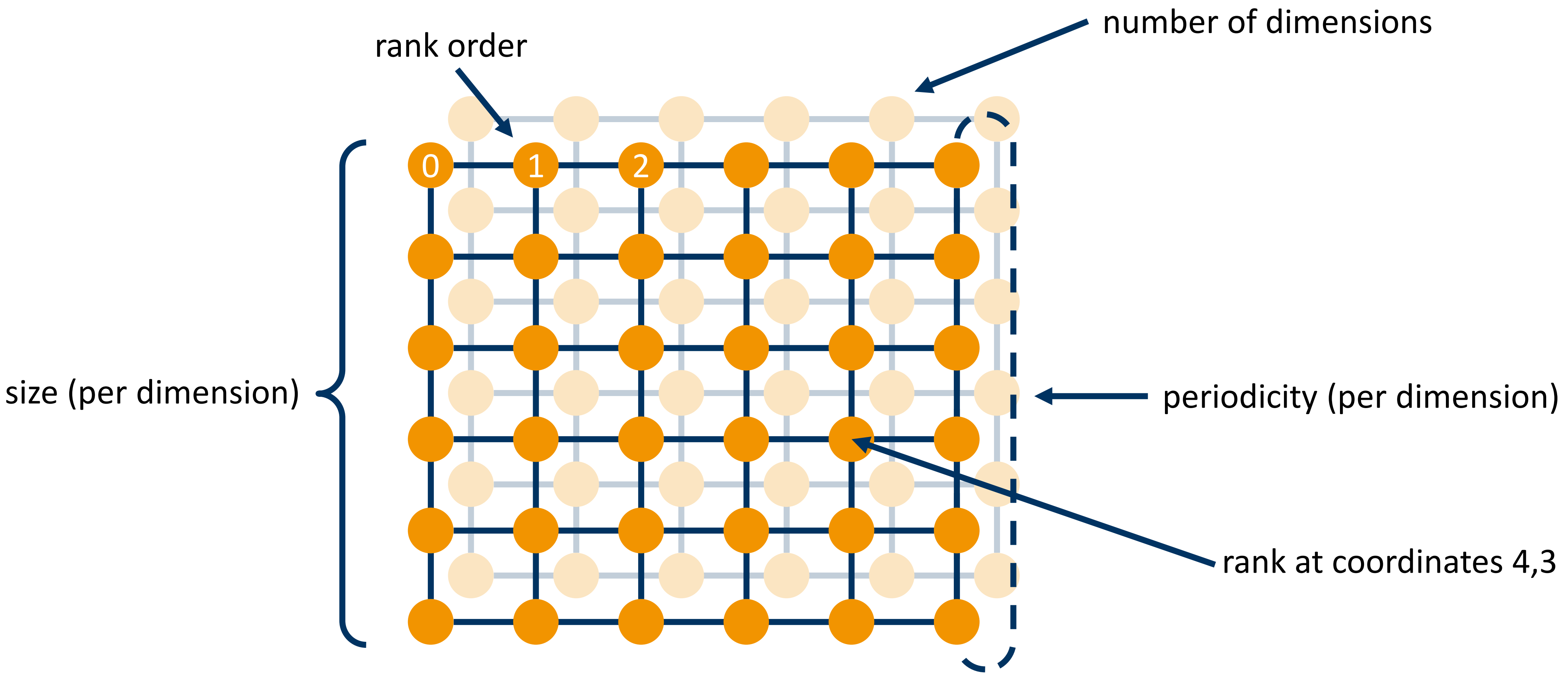
- Cartesian topologies
  - regular grids of squares/cubes/…
  - each rank is a node on the grid and connected to its neighbors
  - boundaries can be periodic
  - ranks can be identified via Cartesian coordinates instead of rank ID



- 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

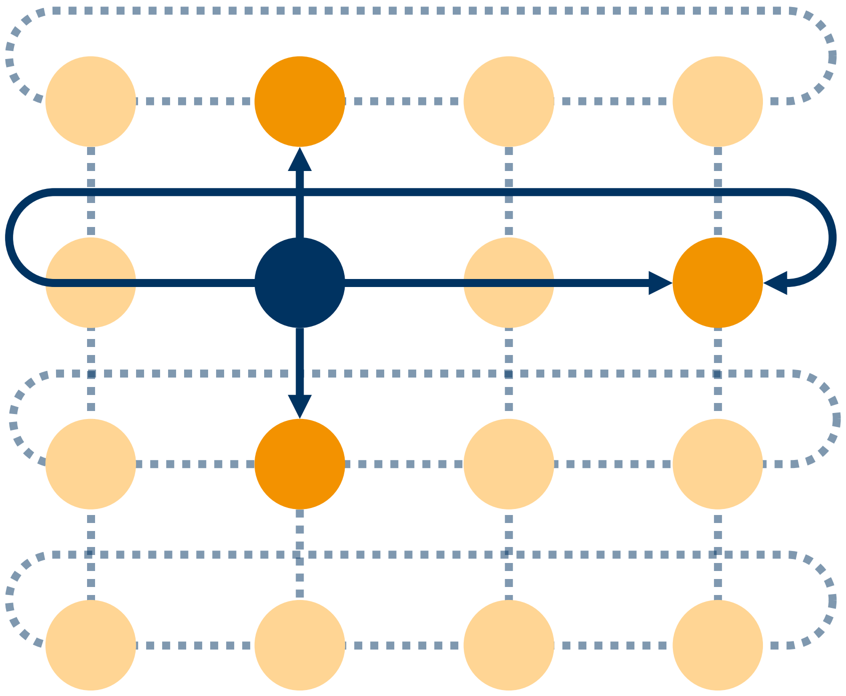
- create topology, resulting in new communicator
  - need to decide on dimensions, sizes, periodicity, etc…
  - per-dimension sizes can be computed using convenience function `MPI_Dims_create()`
  - new communicator implies rank IDs might have changed!
    - (remember MPI basics lecture: "[…] MPI semantics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

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 (`MPI_Cart_shift()`)

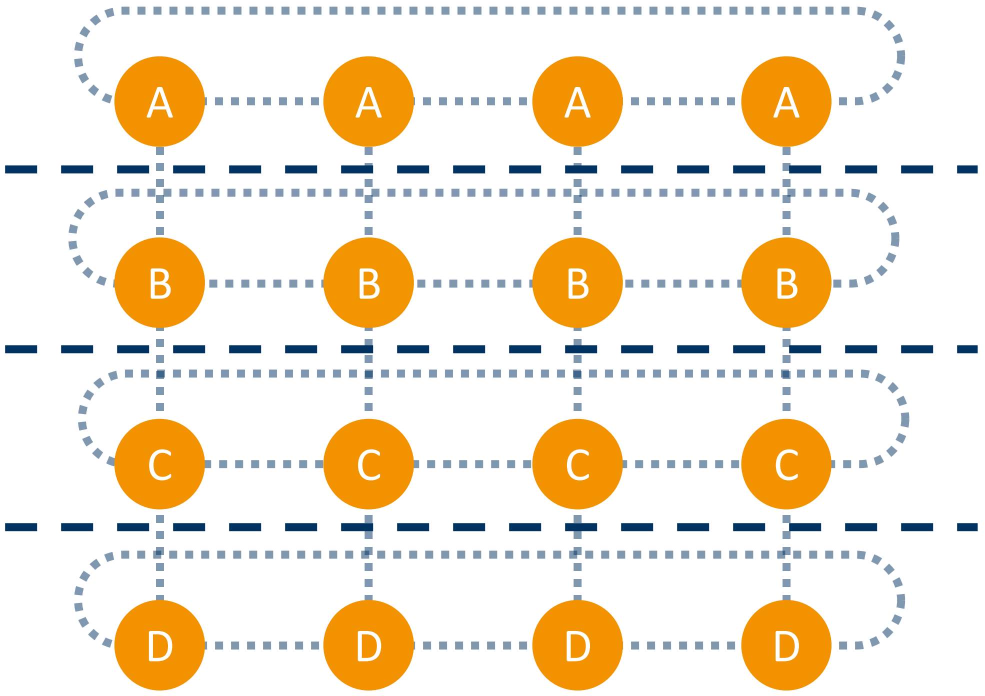
- computes rank numbers of neighbors
  - requires direction and displacement (=distance)
- example on the right
  - partially periodic 2D topology of 4x4
  - up/down shift with displacement 1
  - or left/right shift with displacement 2
- Can return `MPI_PROC_NULL` if neighbor does not exist
  - can be used in communication, will result in a no-op



Slicing (`MPI_Cart_sub()`)

- cuts a grid into slices
  - a new communicator is generated for each slice
  - enables slice-restricted collective communication

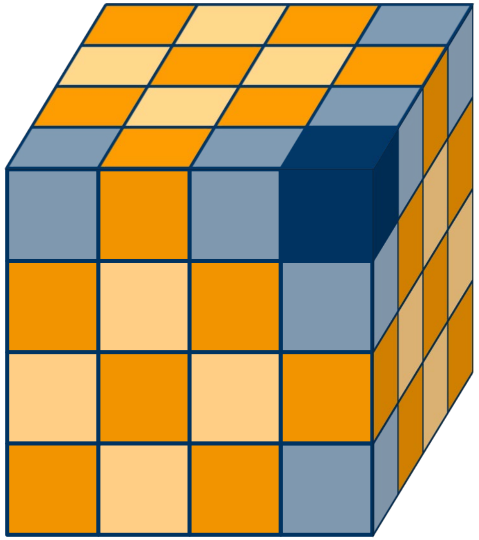
- example on the right
  - slicing a 2D topology horizontally
  - 4 new communicators A, B, C, and D with 4 ranks each
  - `MPI_Bcast(…,A)` only affects ranks of A



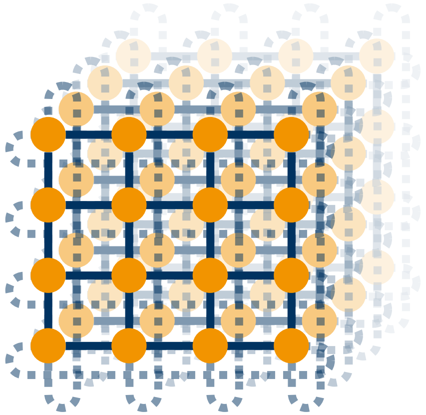
Convenience functions

- `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
- `MPI_Neighbor_allgather(…) / MPI_Neighbor_alltoall(…)`
  - sparse collective communication, exchanges data between neighbors if they are neighbors in the topology

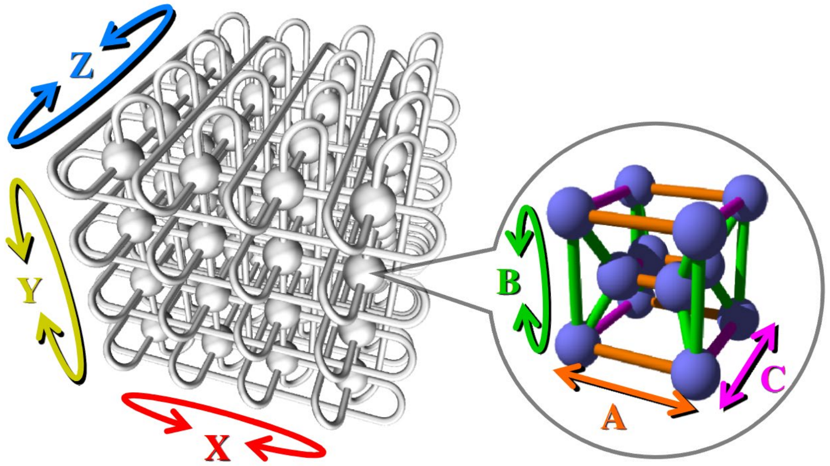
Usefulness of Cartesian topologies



Use case: 3D heat stencil with periodic boundary conditions



Implementation: 3D Cartesian topology with periodicity in all three dimensions



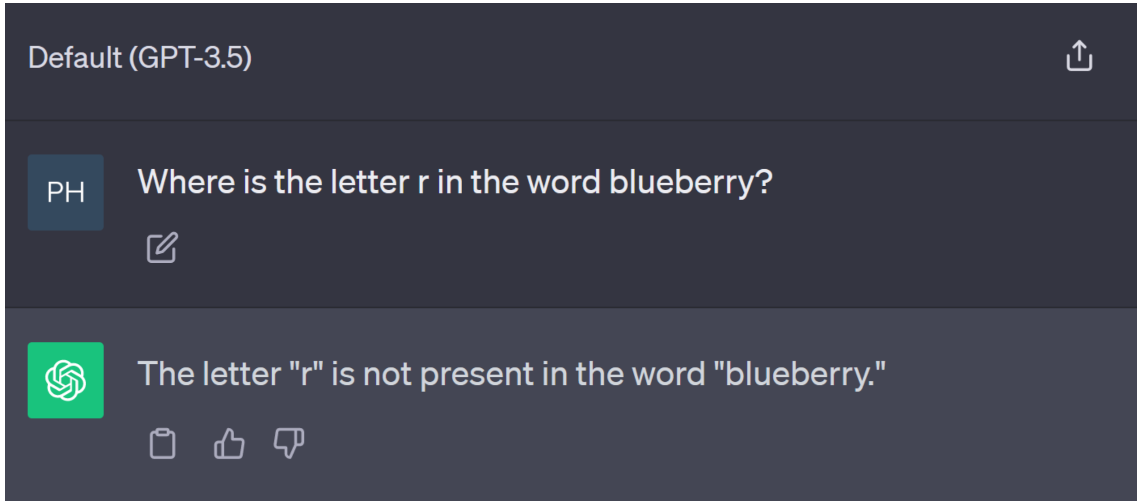
Mapped to hardware that uses (at least a 3D) torus interconnect (Image: Fugaku, Tofu D topology)

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 specification is correct

Tales from the proseminar: ChatGPT

- ChatGPT and other LLMs are absolutely useful
  - if you know their limitations
- Consider them an “unrealiable research assistant”
  - good for getting possibly new input/perspective/etc.
  - but always require their work to be checked



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 & ChatGPT

Image Sources

- Tofu D interconnect: https://link.springer.com/content/pdf/10.1007/978-3-319-07518-1_35.pdf