# An Introduction to Message Passing and Parallel Programming with MPI


Alireza Ghasemi and Georg Hager

Erlangen National High Performance Computing Center

Volker Weinberg

Leibniz Supercomputing Centre (LRZ)


**A collaborative course of NHR@FAU and LRZ Garching**

# Introduction to MPI: Agenda

- **Pint-to-point communication: Blocking**
- **Point-to-point communication: Nonblocking**
- **Helper functions**
- **Collectives**
- **Datatypes**

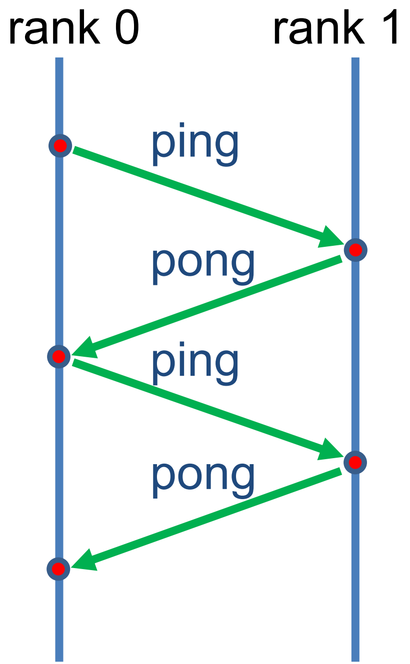
# Point-to-Point Communication
# Blocking

# Blocking communication

- Definition: a blocking communication does not return until the message data and envelope have been safely stored away so that the sender is free to modify the send buffer after return.
- The term blocking may be confusing. Indeed based on the definition above, one can infer:
  - The call to a send procedure does not obstruct the flow of the program at that line of the code up to the completion of the communication. Therefore, a blocking sender may return when the transmission of the message may be:
    - not yet started
    - ongoing
    - completed (less likely)

# Single-round ping-pong

```c
#include <mpi.h>
#include <stdio.h>
int main(int argc, char **argv) {
     int ierr, irank, nrank, COUNT=1000;
     MPI_Status status;
     double *d=malloc(COUNT * sizeof(double));
     ierr=MPI_Init(&argc,&argv);
     ierr=MPI_Comm_rank(MPI_COMM_WORLD,&irank);
     ierr=MPI_Comm_size(MPI_COMM_WORLD,&nrank);
     if(irank==0) for(int i=0;i<COUNT;i++) d[i]=100.0;
     if(irank==1) for(int i=0;i<COUNT;i++) d[i]=200.0;
     printf("BEFORE: nrank,irank,d = %5d%5d%8.1f\n",nrank,irank,d[0]);
     if(irank==0) {
         MPI_Send(d,COUNT,MPI_DOUBLE,1,0,MPI_COMM_WORLD);
         MPI_Recv(d,COUNT,MPI_DOUBLE,1,0,MPI_COMM_WORLD,&status);
     }
     else if(irank==1) {
         MPI_Recv(d,COUNT,MPI_DOUBLE,0,0,MPI_COMM_WORLD,&status);
         MPI_Send(d,COUNT,MPI_DOUBLE,0,0,MPI_COMM_WORLD);
     }
     printf("AFTER: nrank,irank,d = %5d%5d%8.1f\n",nrank,irank,d[0]);
     ierr=MPI_Finalize();
}
```




- First rank 0 sends and rank 1 receives, then the opposite:
  - Final value of d at rank 0?

# The message passing paradigm

Let’s consider changing the order of send and receive in rank 1, i.e. both ranks call first MPI_SEND and then MPI_RECV:

```
if(irank==0) {
    MPI_Send(d,COUNT,MPI_DOUBLE,1,0,MPI_COMM_WORLD);
    MPI_Recv(d,COUNT,MPI_DOUBLE,1,0,MPI_COMM_WORLD,&status);
}
else if(irank==1) {
    MPI_Send(d,COUNT,MPI_DOUBLE,0,0,MPI_COMM_WORLD);
    MPI_Recv(d,COUNT,MPI_DOUBLE,0,0,MPI_COMM_WORLD,&status);
}
```

- Is DEADLOCK expected?
  - Final value of d at rank 0?

Executing with different values of COUNT:

```
mpirun -n 2 ./a.out 10          # OK
mpirun -n 2 ./a.out 100         # OK
mpirun -n 2 ./a.out 1000        # OK
mpirun -n 2 ./a.out 10000       # OK
mpirun -n 2 ./a.out ????????    # at some array length DEADLOCK occurs
```

# Communication modes

- There are four send communication modes:

| Mode | Binding |
|---|---|
| Synchronous | MPI_Ssend |
| Buffered (asynchronous) | MPI_Bsend |
| Standard | MPI_Send |
| Ready | MPI_Rsend |

- There is only one receive communication mode:
  - Standard: MPI_Recv

# Synchronous send: MPI_Ssend

- It can be started whether or not a matching receive was posted
- It will complete successfully only if a matching receive is posted
  - Send buffer can be reused
  - Receiver has reached a certain point in its execution

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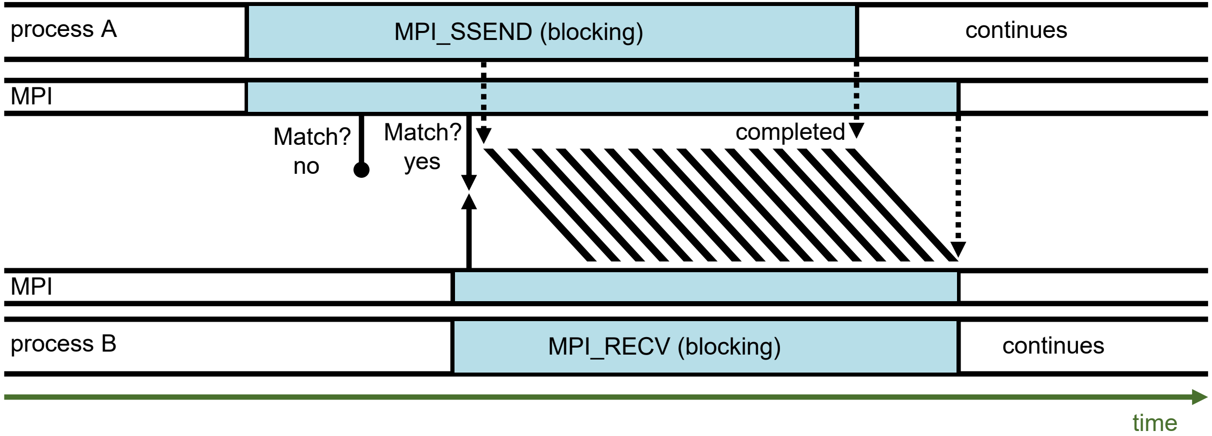
Tips

- Useful for debugging
- Serialization
- High latency
  (synchronization overhead)
- Best bandwidth



# Standard send: MPI_Send

- It can be started whether or not a matching receive was posted
- It may complete before a matching receive is posted
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  - The operation is local or nonlocal
  - It buffers or sends  synchronously: message size, MPI implementation, etc.

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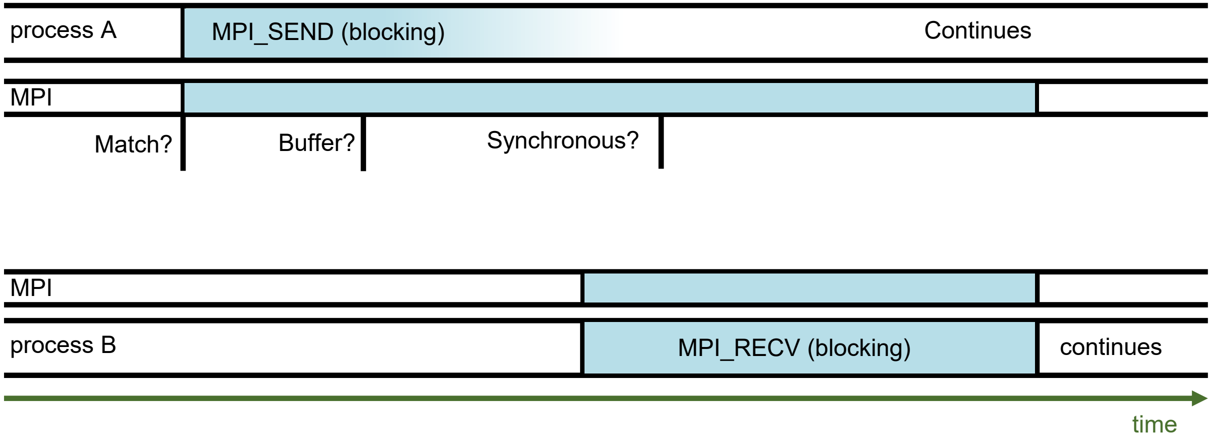
Tips

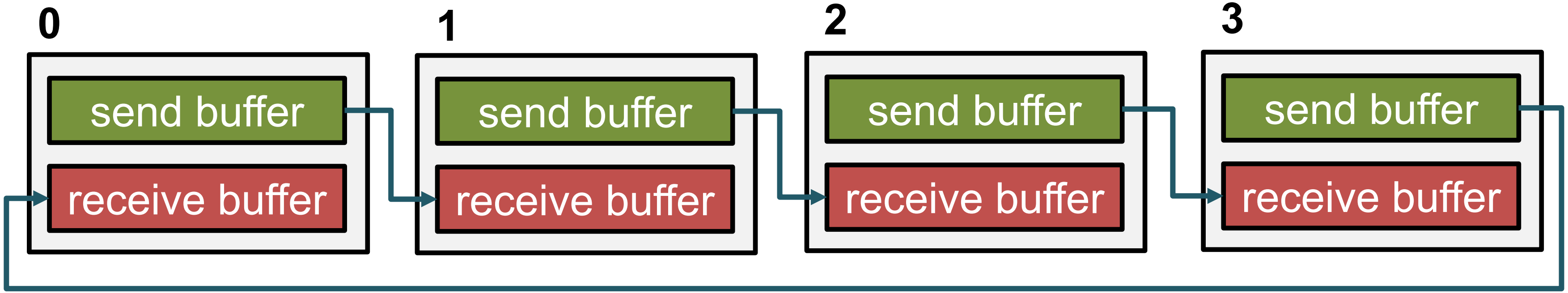
- Deadlock may occur
- Minimal transfer time

The standard send is the standard choice for you!



# Point-to-Point Communication MPI_SEND/MPI_RECV

- Sending/Receiving at the same time is a common use case
- e.g.: shift messages, ring topologies, ghost cell exchange




- MPI_Send/MPI_Recv: pairs are not reliable!

```
//my left neighbor
left=(rank-1)%size;
//my right neighbor
right=(rank+1)%size;
MPI_Send(sendbuf,n,type,right,tag,comm);
MPI_Recv(recvbuf,n,type,left,tag,comm,status);
```

- How to avoid potential deadlock?

# Point-to-Point Communication MPI_SENDRECV

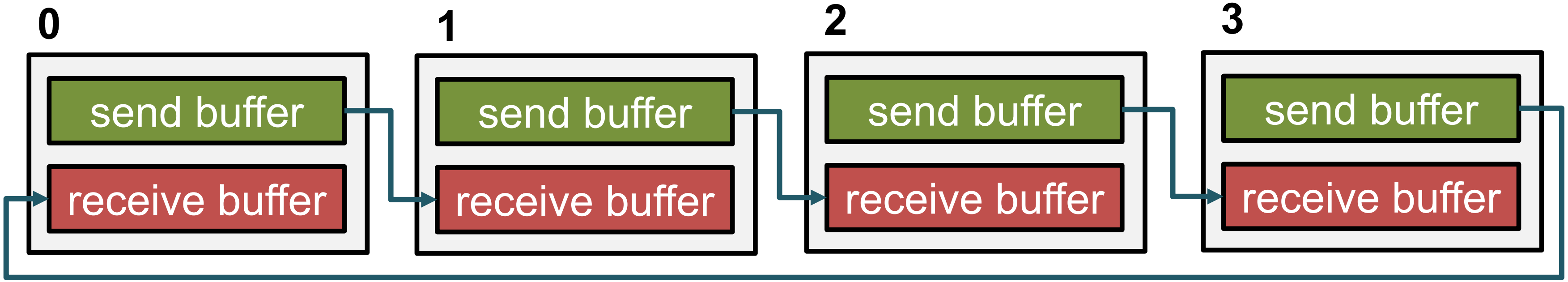
- Syntax: simple combination of send and receive arguments:

```
MPI_Sendrecv(buffer_send, sendcount, sendtype, dest,   sendtag,
             buffer_recv, recvcount, recvtype, source, recvtag,
             comm, MPI_Status * status)
```

- disjoint send/receive buffers
- can have different count & data type
- blocking call

- MPI takes care, thereby no deadlocks occur:

```
// Rank left from myself
left = (rank - 1 + size) % size;
// Rank right from myself
right = (rank + 1) % size;
MPI_Sendrecv(buffer_send, n, MPI_INT, right, 0,
             buffer_recv, n, MPI_INT, left,  0,
             MPI_COMM_WORLD, status);
```



# Point-to-Point Communication MPI_SENDRECV

- useful for open chains/non-circular shifts:

```
// Rank left from myself.
left = rank - 1; if (left < 0) { left = MPI_PROC_NULL; }
// Rank right from myself.
right = rank + 1; if (right >= size) {right = MPI_PROC_NULL; }
MPI_Sendrecv(buffer_send, n, MPI_INT, right, 0,
             buffer_recv, n, MPI_INT, left,  0, MPI_COMM_WORLD, &status);
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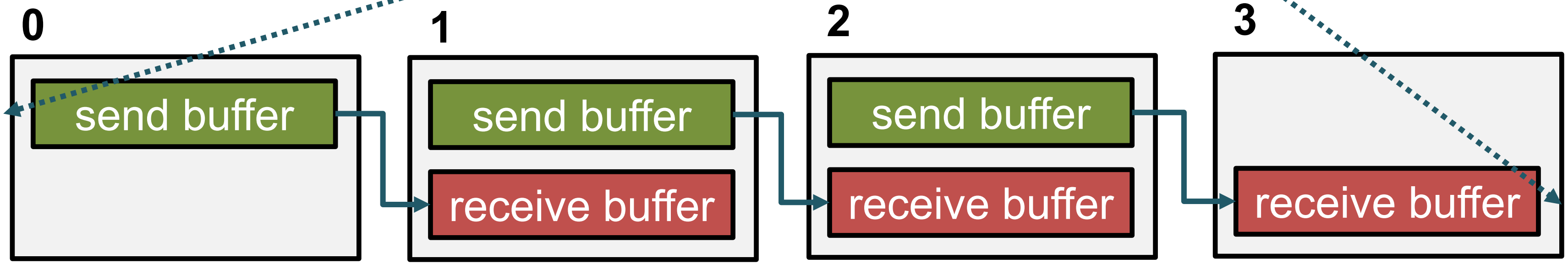
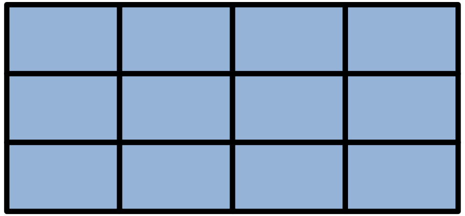



- MPI_PROC_NULL as source/destination acts as no-op
  - send/recv with MPI_PROC_NULL return immediately, buffers are not altered
- MPI_Sendrecv matches with simple *send/*recv point-to-point calls

# Ghost Cell Exchange with MPI_Sendrecv

Domain distributed to ranks here 4 x 3 ranks each rank gets one tile



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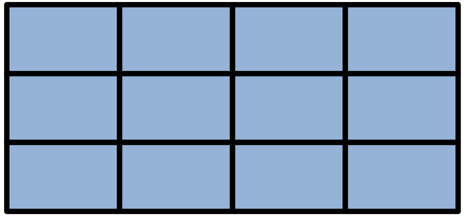
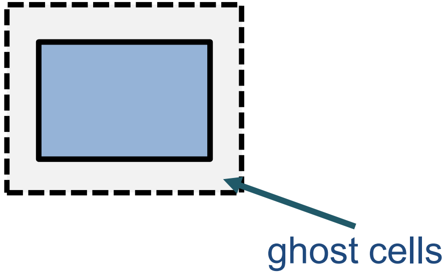


Each ranks tile is surrounded by ghost cells, representing the cells of the neighbors



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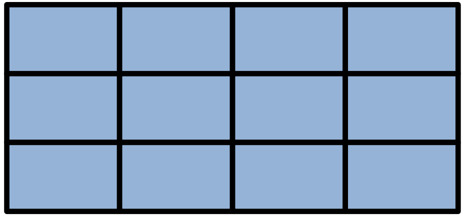

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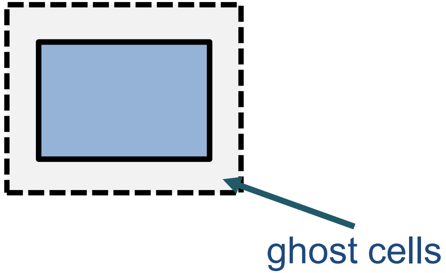
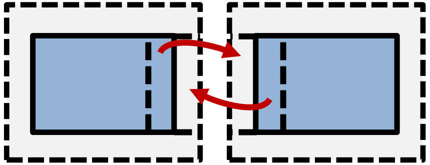



After each sweep over a tile perform ghost cell exchange, i.e. update ghost cells with new values of neighbor cells



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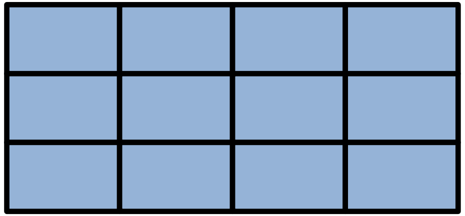

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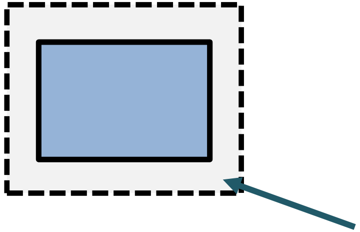

ghost cells

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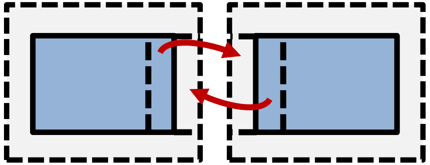
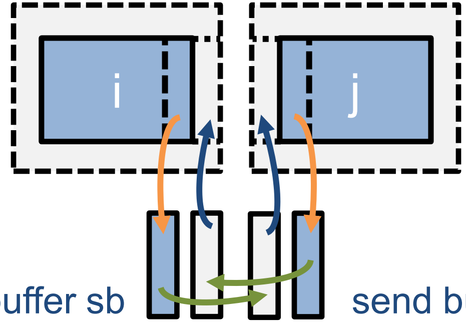


Possible implementation:

1. copy new data into contiguous send buffer
2. send/receive new data to/from the neighbor
3. copy new data into ghost cells

```
MPI_Sendrecv(
sb, …, j,
rb, …, j, …)
```

step 2




```
MPI_Sendrecv(
sb, …, i,
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step 2

# Blocking Point-to-Point Communication: Summary

- Blocking MPI communication calls:
  - send/receive buffer can safely be reused when a blocking call returns
  - Blocking send has 4 communication modes:
    1. Synchronous  2. Buffered  3. Standard  4. Ready
  - Blocking Receive has only one communication mode: MPI_Recv
  - Blocking calls can lead to deadlocks
- Shift operations: keep eye on deadlocks and serialization
- MPI_Sendrecv: combined send and receive
  - MPI ensures no deadlocks occur
  - MPI_Sendrecv_replace: useful when only one single buffer is required

# Point-to-Point Communication
# Nonblocking

# Nonblocking point-to-point communication

- Call to a nonblocking send/recv procedure returns straight away. It avoids synchronization so that the following opportunities can be exploited:
  - Avoiding certain deadlocks
  - Truly bidirectional commun.
  - Avoid idle time:
    - Overlapping communication and computation but not guaranteed by the standard

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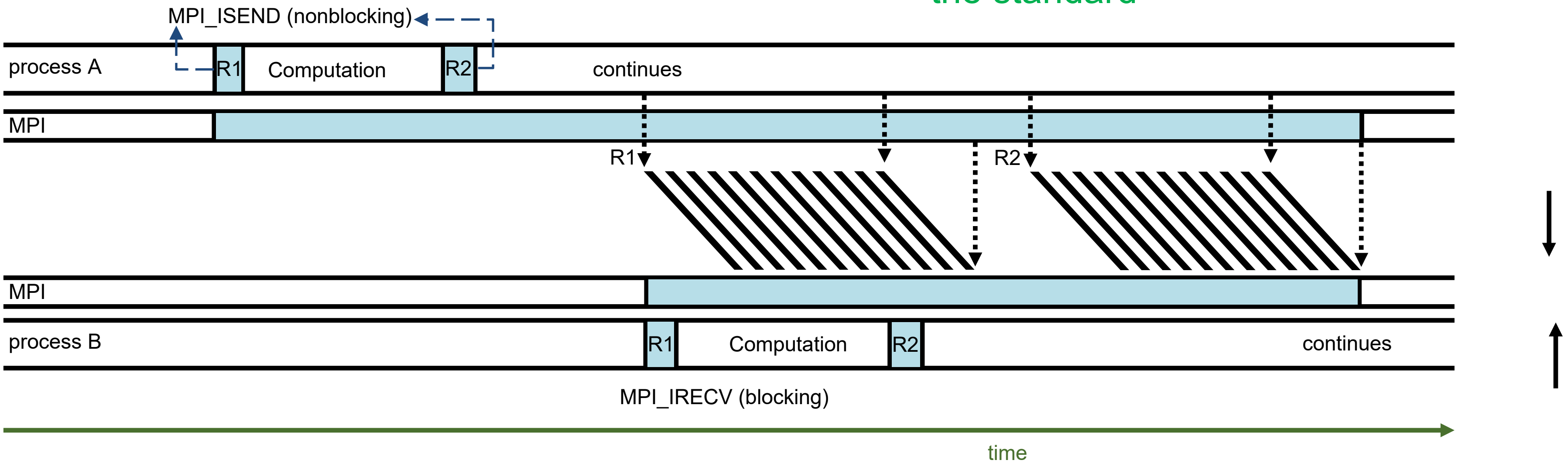


# Standard nonblocking send/receive

- ```
  MPI_Isend(sendbuf, count, datatype, dest,   tag,
                  comm, MPI_Request * request);

  MPI_Irecv(recvbuf, count, datatype, source, tag,
                  comm, MPI_Request * request);
  ```

  **request**: pointer to variable of type **MPI_Request**,
  will be associated with the corresponding operation
- **Do not reuse sendbuf/recvbuf before MPI_Isend/MPI_Irecv has been completed!**
  - Return of a nonblocking call does not imply completion ← Be careful!
- **MPI_Irecv** has no status argument
  - obtained later during completion via **MPI_Wait*/MPI_Test***
  ```

# Nonblocking send and receive variants

- Completion
  - Return of **`MPI_I*`** call does not imply completion
  - Check for completion via **`MPI_Wait* / MPI_Test*`**
  - Semantics identical to blocking call combined with a “wait”

| nonblocking MPI function | blocking MPI function | type | completes when |
|---|---|---|---|
| **`MPI_Isend`** | **`MPI_Send`** | synchronous or buffered | depends on type |
| **`MPI_Ibsend`** | **`MPI_Bsend`** | buffered | buffer has been copied |
| **`MPI_Issend`** | **`MPI_Ssend`** | synchronous | remote starts receive |
| **`MPI_Irecv`** | **`MPI_Recv`** | -- | message was received |

# Test for completion

Two test modes:

- Blocking
  - **`MPI_Wait*`**: Wait until the communication has been completed and buffer can safely be reused
- Nonblocking
  - **`MPI_Test*`**: Return true (false) if the communication has (not) completed

Despite the naming, the modes both pertain to nonblocking point-to-point communication!

# Test for completion – single request

- Test one communication handle for completion:

```
MPI_Wait(MPI_Request * request, MPI_Status * status);
MPI_Test(MPI_Request * request, int * flag,
         MPI_Status * status);
```

**request**: request handle of type **MPI_Request**

**status**: status object of type **MPI_Status** (cf. **MPI_Recv**)

**flag**: variable of type **int** to test for success

- MPI_Wait waits until the communication has been completed and buffer can safely be reused: Blocking
- MPI_Test returns TRUE (FALSE) if the communication has (not) completed: Nonblocking

# Use of wait/test

## MPI_Wait

```
MPI_Request request;
MPI_Status status;
MPI_Isend(send_buffer,count,MPI_CHAR,
    dst,0,MPI_COMM_WORLD,&request);

// do some work…
// do not use send_buffer
MPI_Wait(&request, &status);

// send_buffer can now be used safely
```

Nonblocking communication:

- Return from function != completion
- Each initiated operation must have a matching wait/test!

## MPI_Test

```
MPI_Request request;
MPI_Status status;
int flag;
MPI_Isend(send_buffer,count,MPI_CHAR,
    dst,0,MPI_COMM_WORLD,&request);

do {
    // do some work…
    // do not use send_buffer
    MPI_Test(&request, &flag, &status);
} while (!flag);

// send_buffer can now be used safely
```

loop

# Wait for completion – all requests in a list

- MPI can handle multiple communication requests
- Wait/Test for completion of multiple requests:

```
MPI_Waitall(int count, MPI_Request requests[],
                       MPI_Status statuses[]);

MPI_Testall(int count, MPI_Request requests[],
            int *flag, MPI_Status statuses[]);
```

- Waits for/Tests if all provided requests have been completed

# Use of MPI_Waitall

```
MPI_Request requests[2];
MPI_Status  statuses[2];

MPI_Isend(send_buffer, …, &(requests[0]));
MPI_Irecv(recv_buffer, …, &(requests[1]));

// do some work…

MPI_Waitall(2, requests, statuses)
// Isend & Irecv have been completed
```

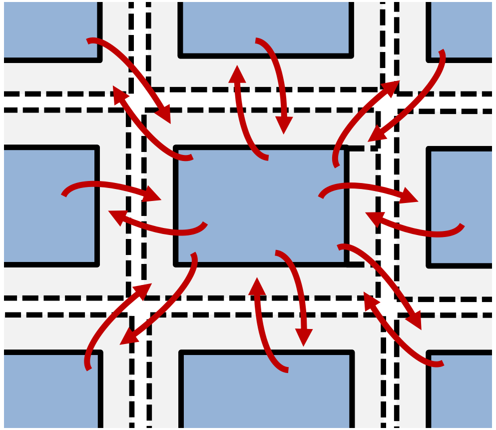
Arrays of requests and statuses

number of elements in the arrays

Requests can be from one or multiple send/receive operations or combination of them!

# Ghost Cell Exchange: nonblocking PtP Communication

- Ghost cell exchange: communication using nonblocking send/recv can be initiated with all neighbors at once.



**Possible implementation:**

1. Copy new data into contiguous send buffers
2. Start nonblocking receives/sends from/to corresponding neighbors
3. Wait with MPI_Waitall for all obtained requests to complete
4. Copy new data into ghost cells

# Other Ways of Testing for Completion

- Examine the completion of multiple requests:
  - MPI_Waitall
  - MPI_Testall
  - MPI_Waitany
  - MPI_Testany
  - MPI_Waitsome
  - MPI_Testsome

- Completed requests are automatically set to MPI_REQUEST_NULL

# Helper functions and Semantics

# Semantics

- Message order preservation (guaranteed inside a communicator)

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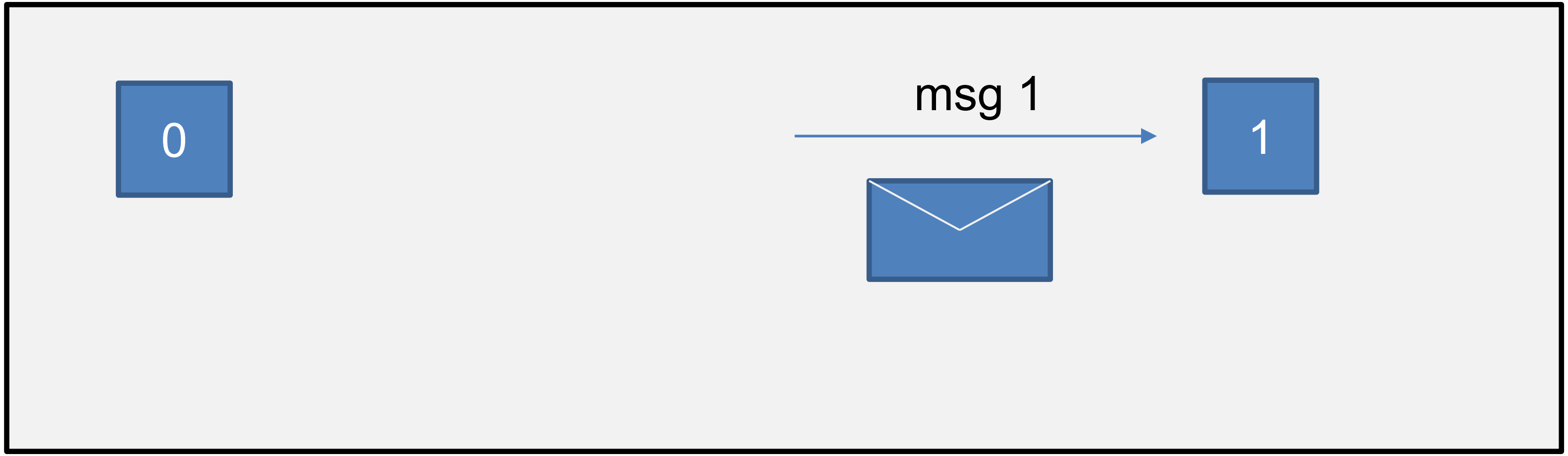

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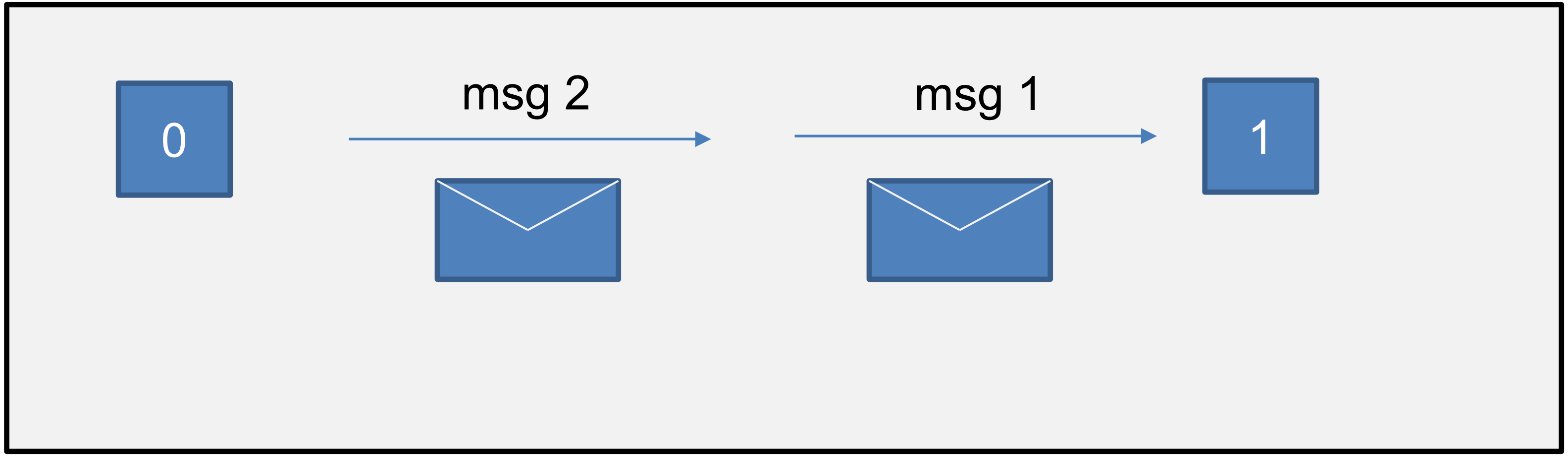

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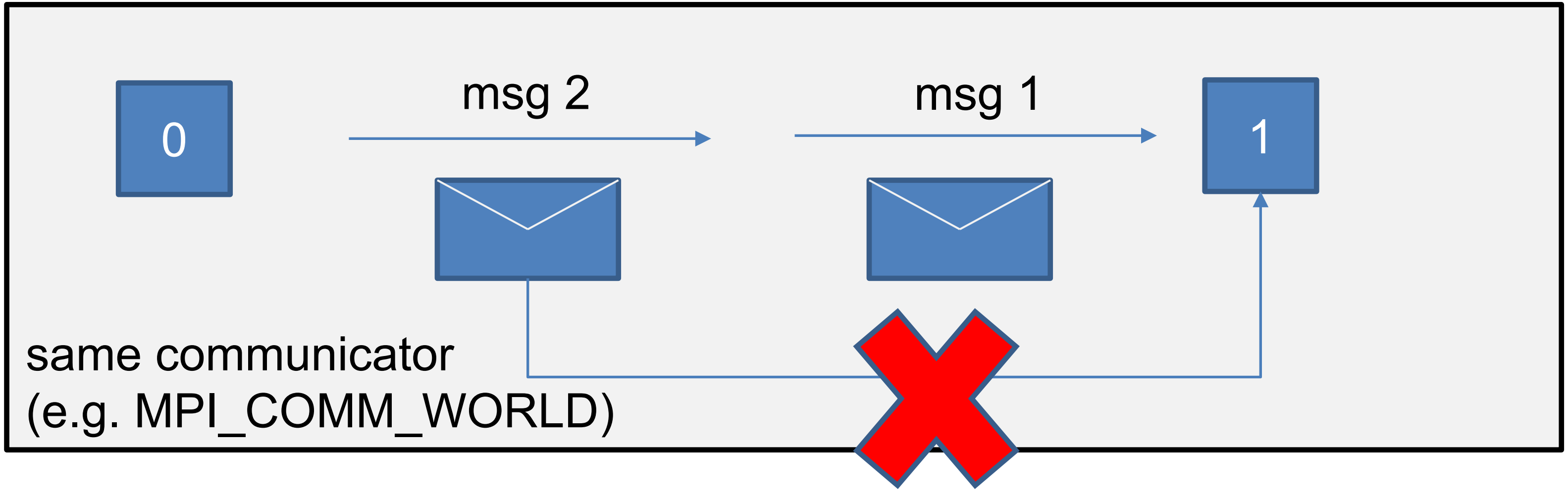


# Useful MPI Calls: MPI_WTIME

- Returns seconds since one point in past time

```
double MPI_Wtime()
```

- Use only for computation of time differences

```
time_start = MPI_Wtime()
// … working …
duration = MPI_Wtime() - time_start
```

- Returns time resolution in seconds,

```
double MPI_Wtick()
```

  - e.g. if resolution is 1ms `MPI_Wtick()` returns `1e-3`
- No `ierror` argument in Fortran: both modules mpi and mpi _f08
- Typically clocks from different ranks are not synchronized

# Useful MPI Calls: MPI_ABORT

- MPI_Abort forces an MPI program to terminate:

```
int MPI_Abort(MPI_Comm comm, int errorcode)
```

- Aborts all processes in communicator
- `errorcode` will be handed as exit value to calling environment
- Safe and well-defined way of terminating an MPI program (if implemented correctly)
- In general, if something unexpected happens, try to shut down your MPI program the standard way (MPI_Finalize())

# Questions?

# Collective Communication in MPI

# Collective Communication Introduction

- Operations including all ranks of a communicator
  - All ranks must call the function!
- Blocking calls: buffer can be reused after return
- Nonblocking calls with MPI-3.0
- Cannot interfere with point-to-point communication
  - Completely separate modes of operation!
- Data type matching
- No tags
- Sent message must fill receive buffer (count is exact)
- Typically MPI libraries provide optimized implementations for operations
  - Do not write your own collectives using PtP calls!

# Collective Communication Introduction

- May or may not synchronize the processes
- Types of collective calls:
  - Synchronization (barrier)
  - Data movement (broadcast, scatter, gather, all to all)
  - Collective computation/operations (reduction)
- MPI_*v bindings: allow for unequal data size across ranks

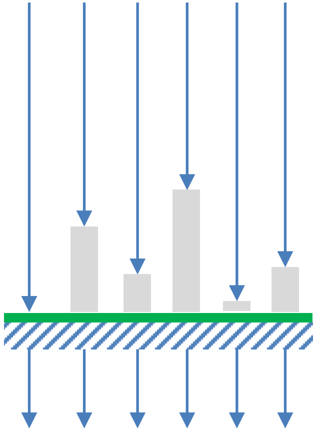
# Collective Communication Synchronization

- Explicit synchronization of all ranks from specified communicator

  ```
  MPI_Barrier(comm);
  ```

- Ranks only return from call after every rank has called the function

- `MPI_Barrier:` rarely needed
  - Debugging



# Collective Communication Broadcast

- Send buffer contents from one rank ("`root`") to all ranks

```
MPI_Bcast(buf, count, datatype, int root, comm);
```

- No restrictions on which rank is root – often rank 0

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| | rank | 0 | 1 (root) | 2 | 3 |
|---|---|---|---|---|---|
| Before -> | buffer | [ ][ ][ ] | [1][2][3] | [ ][ ][ ] | [ ][ ][ ] (int) |
| | | count = 3 | | | |
| After -> | buffer | [1][2][3] | [1][2][3] | [1][2][3] | [1][2][3] |

```
MPI_Bcast(buffer, 3, MPI_INT, 1, MPI_COMM_WORLD)
```

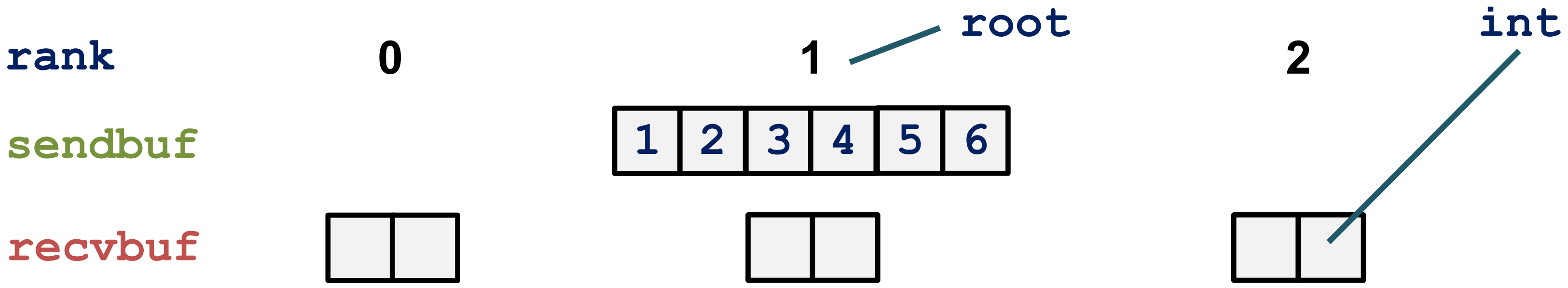
# Collective Communication Scatter

- Send every i-th chunk of an array to the i-th rank

```
MPI_Scatter(sendbuf, sendcount, sendtype,
            recvbuf, recvcount, recvtype,
            root, comm);
```

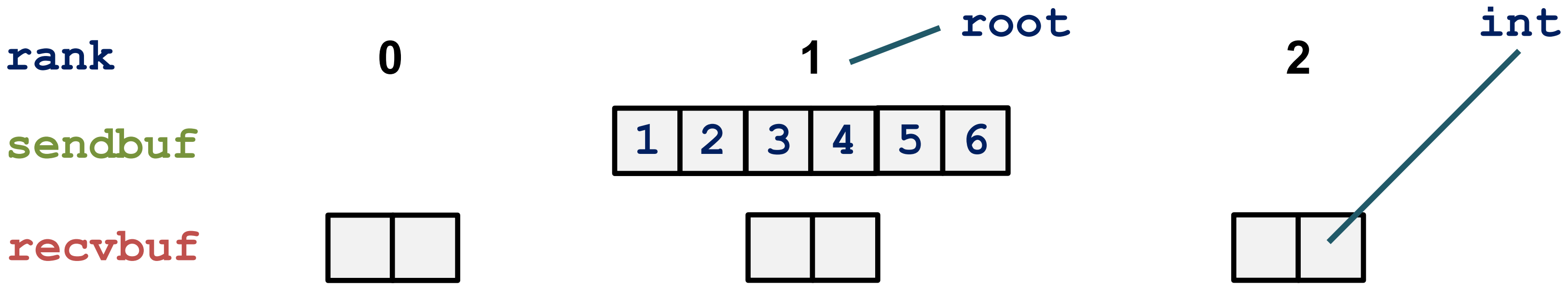
- Root and comm must be the same on all processes
- Type signature of send and receive variables must match
- Usually, **`sendcount`** = **`recvcount`** because **`sendtype = recvtype`**
  - This is the length of the chunk
- **`sendbuf`** is ignored on non-root ranks because there is nothing to send

# MPI_Scatter




```
MPI_Scatter(sendbuf, 2, MPI_INT, recvbuf, 2, MPI_INT,
            root, MPI_COMM_WORLD)
```

# MPI_Scatter




```
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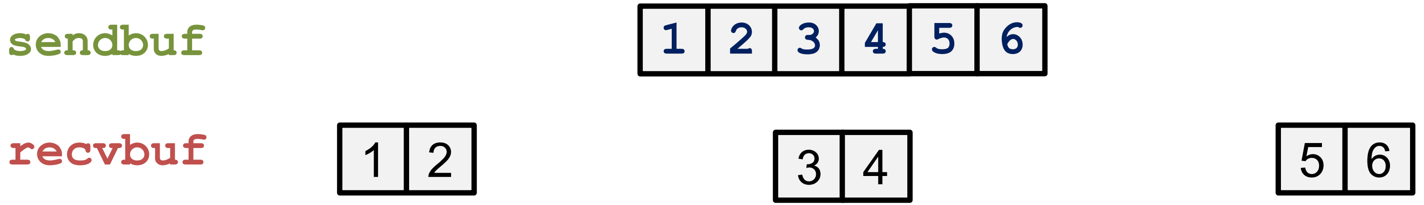
```



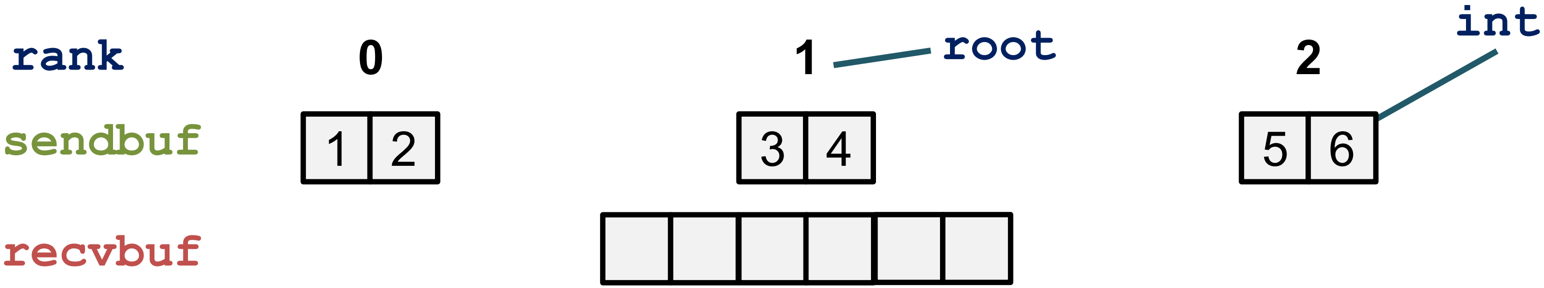
# Collective Communication Gather

- Receive a message from each rank and place i-th rank's message at i-th position in receive buffer

```
MPI_Gather(sendbuf, sendcount, sendtype,
           recvbuf, recvcount, recvtype,
           root, comm)
```

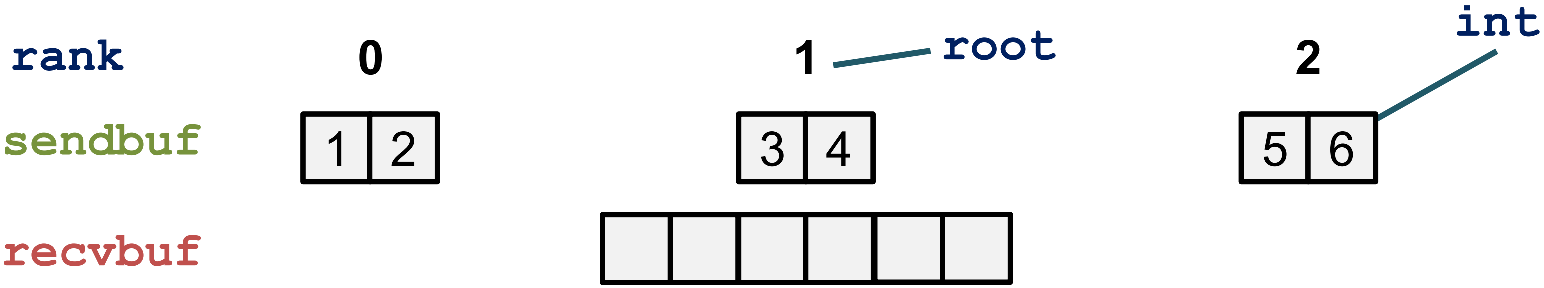
- Root and comm must be the same on all processes
- Type signature of send and receive variables must match
- Usually, `sendcount` = `recvcount` because `sendtype = recvtype`
- `recvbuf` is ignored on non-root ranks because there is nothing to receive

# MPI_Gather

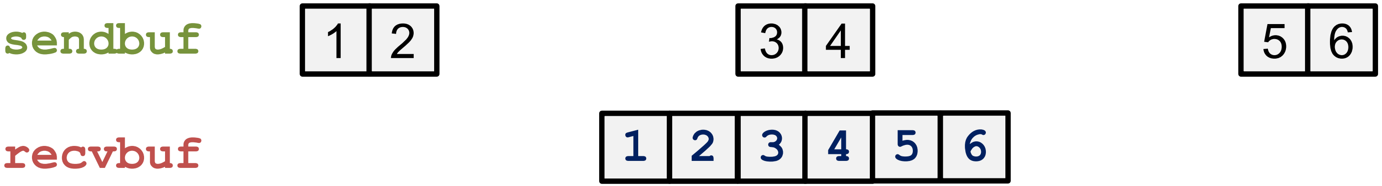



```
MPI_Gather(sendbuf, 2, MPI_INT, recvbuf, 2, MPI_INT,
           root, MPI_COMM_WORLD)
```

# MPI_Gather




```
MPI_Gather(sendbuf, 2, MPI_INT, recvbuf, 2, MPI_INT,
                root, MPI_COMM_WORLD)
```



# Collective Communication MPI_ALLGATHER

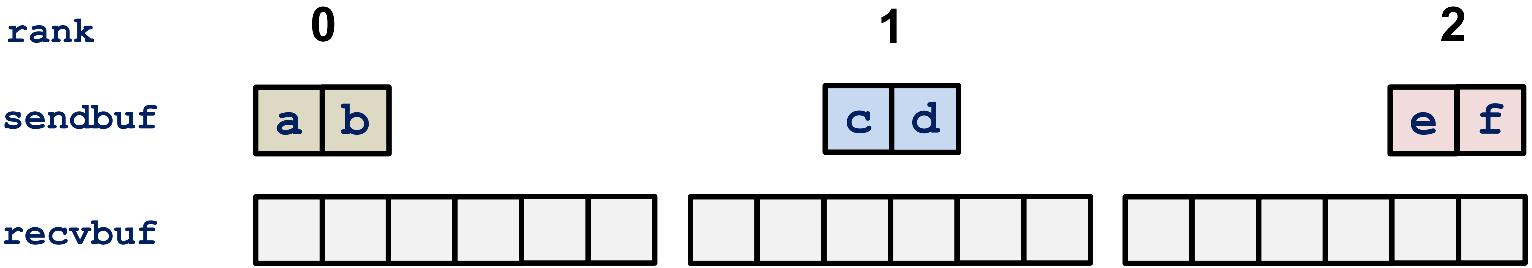
- Combination of gather and broadcast

```
MPI_Allgather(sendbuf, sendcount, sendtype,
              recvbuf, recvcount, recvtype,
              comm);
```

- Why not just use gather followed by a broadcast instead?
  - `MPI_Gather(…,root=i,…)` then `MPI_Bcast(…,root=i,…)`
  - MPI library has more options for optimization
  - General assumption: `MPI_Allgather` is faster than using separate `MPI_Gather` followed by `MPI_Bcast`

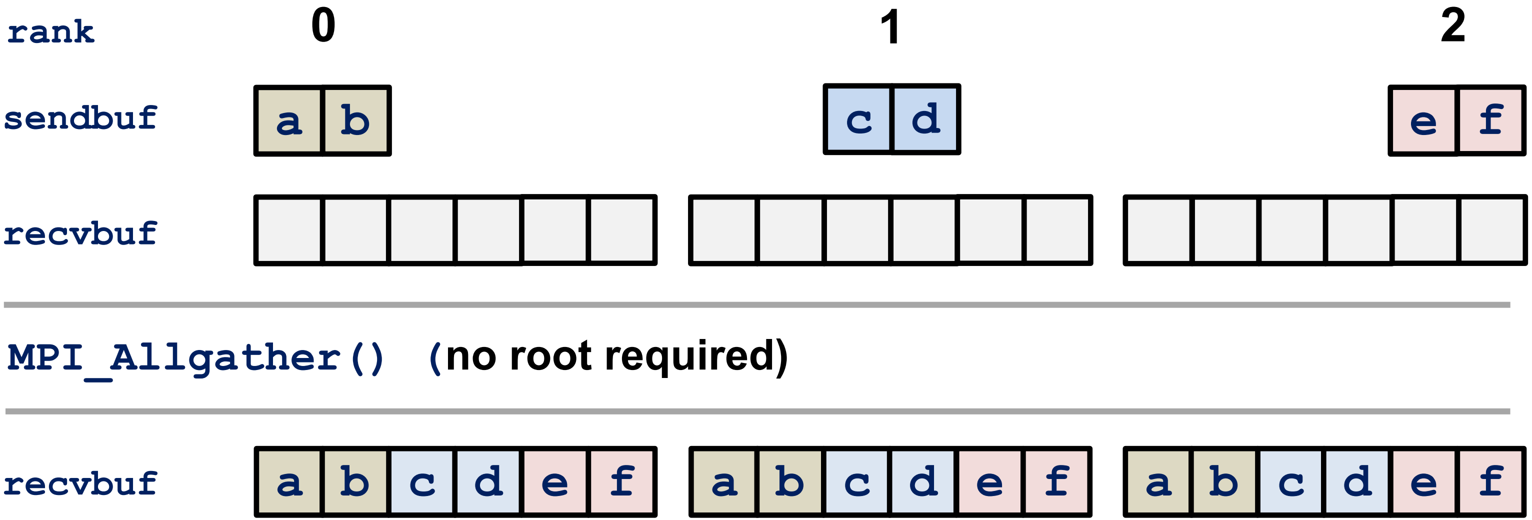
There is no MPI_Allscatter!!!

# MPI_Allgather




**`MPI_Allgather()` (no root required)**

# MPI_Allgather



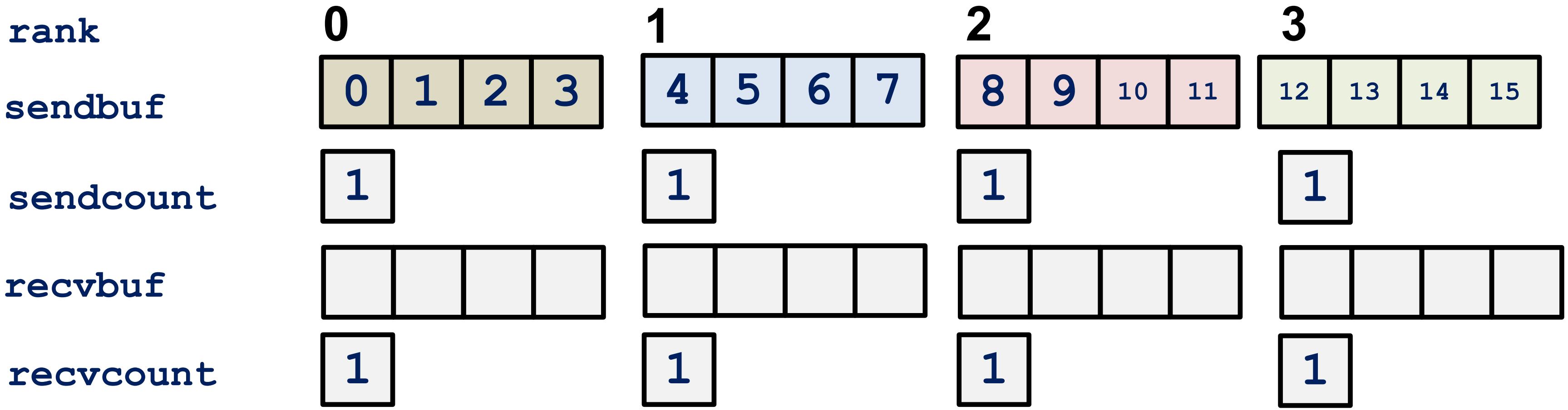

In this example: `sendcount=recvcount=2`

# Collective Communication MPI_ALLTOALL

- **MPI_Alltoall**: For all ranks, send i-th chunk to i-th rank

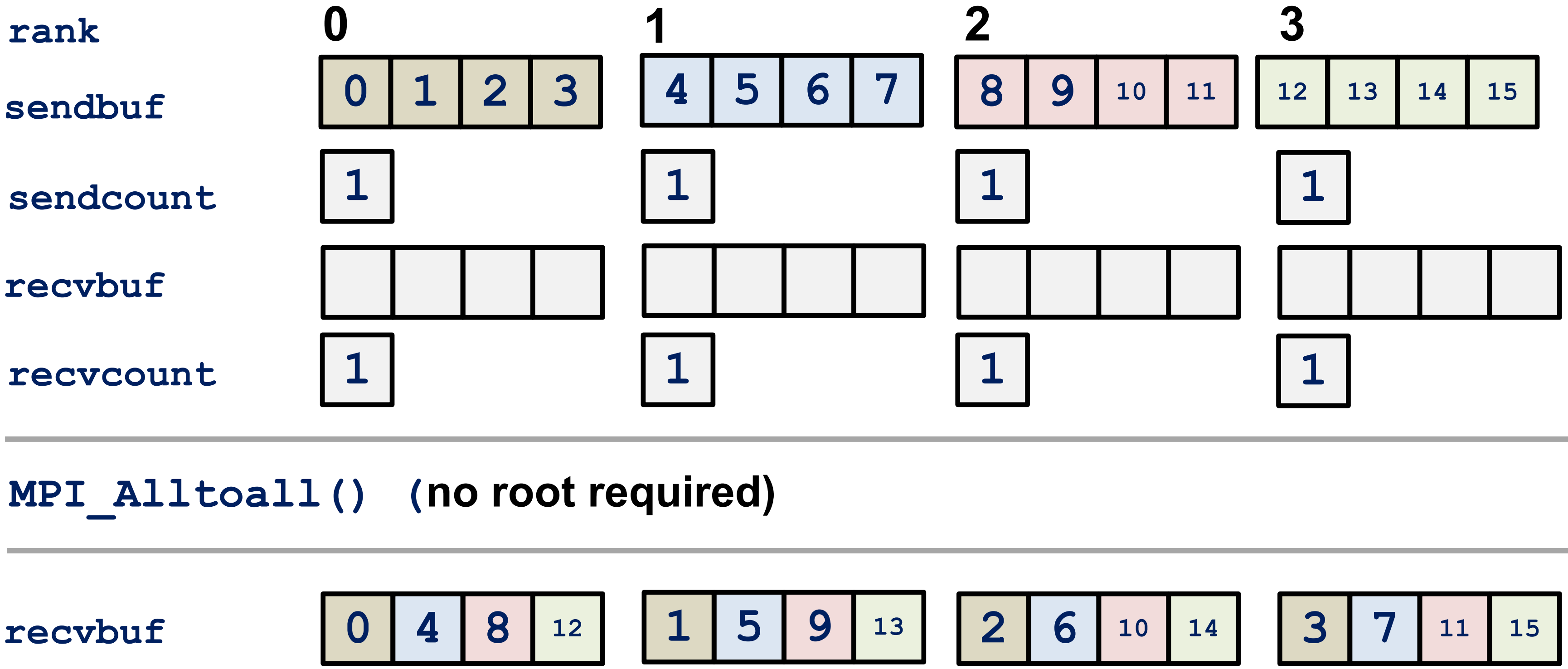
```
MPI_Alltoall(sendbuf, sendcount, sendtype,
             recvbuf, recvcount, recvtype,
             comm);
```

# MPI_Alltoall




`MPI_Alltoall()` (no root required)

# MPI_Alltoall



# Summary of MPI Collective Communications

- MPI (blocking) collectives
  - All ranks in communicator must call the function
- Communication and synchronization
  - Barrier, broadcast, scatter, gather, and combinations thereof
- In-place buffer specification **`MPI_IN_PLACE`**
  - Save some space if need be

# Global Operations Syntax

- Compute results over distributed data

```
MPI_Reduce(sendbuf, recvbuf, count,
           datatype, MPI_Op op,
           root, comm);
```

- Result in `recvbuf` only available on root process
- Perform operation on all `count` elements of an array
- If all ranks need the result, then use `MPI_Allreduce()`
- There are 12 predefined operations
- If the predefined operations are not enough, then use `MPI_Op_create`/`MPI_Op_free` to create own ops

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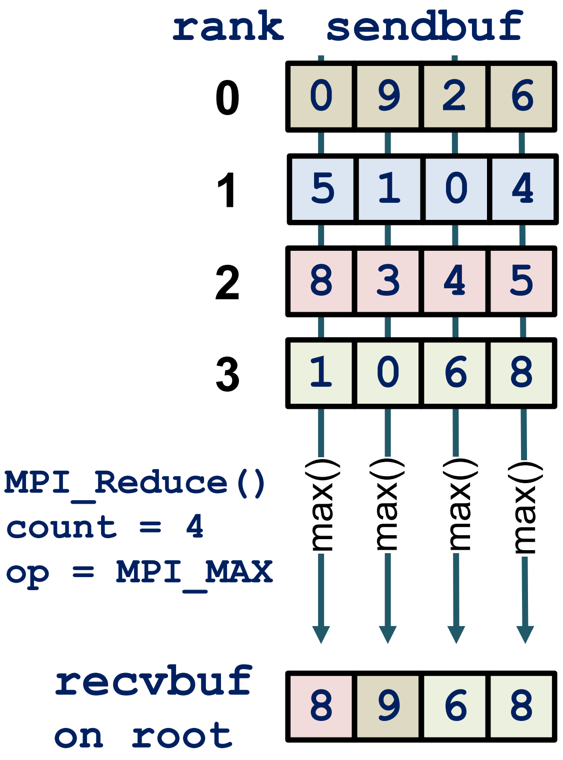


# Global operations – predefined operators

| Name | Operation | Name | Operation |
|---|---|---|---|
| `MPI_SUM` | Sum | `MPI_PROD` | Product |
| `MPI_MAX` | Maximum | `MPI_MIN` | Minimum |
| `MPI_LAND` | Logical AND | `MPI_BAND` | Bit-AND |
| `MPI_LOR` | Logical OR | `MPI_BOR` | Bit-OR |
| `MPI_LXOR` | Logical XOR | `MPI_BXOR` | Bit-XOR |
| `MPI_MAXLOC` | Maximum+Position | `MPI_MINLOC` | Minimum+Position |

- Define own operations with `MPI_Op_create`/`MPI_Op_free`
- MPI assumes that the operations are associative
  → be careful with floating-point operations, as floating-point arithmetic is not associative due to rounding

# "In-place" buffer specification

- Override local input buffer with a result

**MPI_Reduce**

```
// out-of-place
int partial_sum, total_sum;
MPI_Reduce(&partial_sum, &total_sum,
           1, MPI_INT, MPI_SUM, root, comm);

// in-place
int partial_sum, total_sum;
if (rank == root) {
  total_sum = partial_sum;
  MPI_Reduce(MPI_IN_PLACE, &total_sum,
             1, MPI_INT, MPI_SUM,
             root, comm);
}
else {
  MPI_Reduce(&partial_sum, &total_sum,
             1, MPI_INT, MPI_SUM,
             root, comm);
}
```

**MPI_Allreduce**

```
// out-of-place
int partial_sum, total_sum;
MPI_AllReduce(&partial_sum, &total_sum,
              1, MPI_INT, MPI_SUM, comm);


// in-place
int partial_sum, total_sum;

total_sum = partial_sum;
MPI_AllReduce(MPI_IN_PLACE, &total_sum,
              1, MPI_INT, MPI_SUM, comm);
```

# MPI_IN_PLACE Cheat Sheet

| Function | MPI_IN_PLACE argument | At which rank(s) | Comment [MPI 3.0] |
|---|---|---|---|
| MPI_GATHER | send buffer | root | Recv value at root already in the correct place in receive buffer. |
| MPI_GATHERV | send buffer | root | Recv value at root already in the correct place in receive buffer. |
| MPI_SCATTER | receive buffer | root | Root-th segment of send buffer is not moved. |
| MPI_SCATTERV | receive buffer | root | Root-th segment of send buffer is not moved. |
| MPI_ALLGATHER | send buffer | all | Input data at the correct place were process would receive its own contribution. |
| MPI_ALLGATHERV | send buffer | all | Input data at the correct place were process would receive its own contribution. |
| MPI_ALLTOALL | send buffer | all | Data to be send is taken from receive buffer and replaced by received data, data send/received must be of the same type map specified in receive count/receive type. |
| MPI_ALLTOALLV | send buffer | all | Data to be send is taken from receive buffer and replaced by received data. Data send/received must be of the same type map specified in receive count/receive type. The same amount of data and data type is exchanged between two processes. |
| MPI_REDUCE | send buffer | root | Data taken from receive buffer, replaced with output data. |
| MPI_ALLREDUCE | send buffer | all | Data taken from receive buffer, replaced with output data. |

# Derived Data Types in MPI

# Why do we need data types in MPI?

- Example: Root reads configuration and broadcasts it to all others

```
// root: read configuration from
// file into struct config
MPI_Bcast(&cfg.nx, 1, MPI_INT, …);
MPI_Bcast(&cfg.ny, 1, MPI_INT, …);
MPI_Bcast(&cfg.du, 1, MPI_DOUBLE,…);
MPI_Bcast(&cfg.it, 1, MPI_INT, …);
```

Want to do something like:

```
MPI_Bcast(
   &cfg, 1, <type cfg>,…);
```

```
MPI_Bcast(&cfg, sizeof(cfg),
MPI_BYTE, ..)
```

is **not** a solution. Its not portable as no data conversion can take place

MPI is supposed to support parallel computations across heterogeneous environments and communication in such environments may require data conversions.

# Why do we need data types in MPI?

- Example: Send column of matrix (noncontiguous in C):
  - Send each element alone?
  - Manually copy elements out into a contiguous buffer and send it?

| | | | | |
|---|---|---|---|---|
| 0 | 1 | 2 | 3 | 4 |
| 5 | 6 | 7 | 8 | 9 |
| 10 | 11 | 12 | 13 | 14 |
| 15 | 16 | 17 | 18 | 19 |
| 20 | 21 | 22 | 23 | 24 |
| 25 | 26 | 27 | 28 | 29 |

# Creating an MPI data type

Three steps:

1. Construct with

   ```
   MPI_Type_*(...);
   ```

2. Commit new data type with

   ```
   MPI_Type_commit(MPI_Datatype * nt);
   ```

3. After use, deallocate the data type with

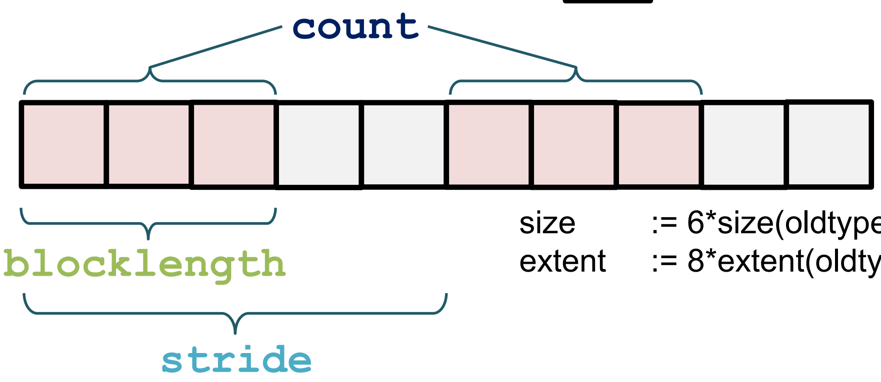
   ```
   MPI_Type_free(MPI_Datatype * nt);
   ```

All local, non-collective calls

# A flexible, vector-like type: MPI_Type_vector

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

| | |
|---|---|
| `count` | `2 (no. of blocks)` |
| `blocklength` | `3 (no. of elements in each block)` |
| `stride` | `5 (no. of elements b/w start of each block)` |
| `oldtype` | `MPI_INT` |




size := 6*size(oldtype)
extent := 8*extent(oldtype)

# A flexible, vector-like type: MPI_Type_vector

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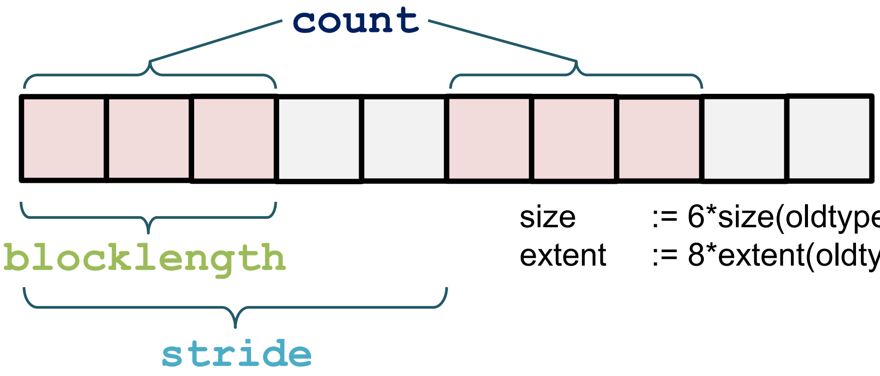

| | |
|---|---|
| `count` | `2 (no. of blocks)` |
| `blocklength` | `3 (no. of elements in each block)` |
| `stride` | `5 (no. of elements b/w start of each block)` |
| `oldtype` | `MPI_INT` |



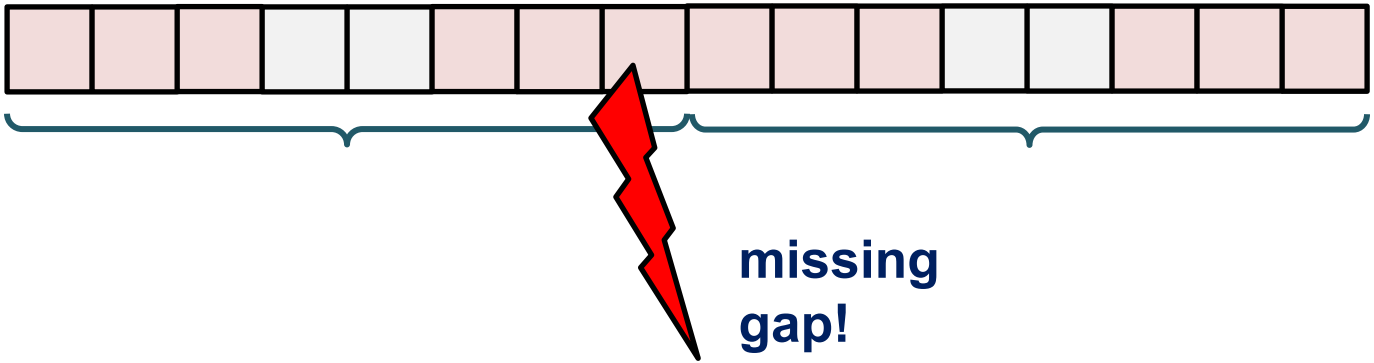

size := 6*size(oldtype)
extent := 8*extent(oldtype)

```
MPI_Datatype nt;
MPI_Type_vector(
2, 3, 5, MPI_INT, &nt);

MPI_Type_commit(&nt);
// use nt…
MPI_Type_free(&nt);
```

# Caveat when using a type

- Caution: Concatenating such types in a send operation can lead to unexpected results!
- `count` argument to `send` and others must be handled with care:

`MPI_Send(buf, 2, nt,...)` with `nt` (newtype from prev. slide)



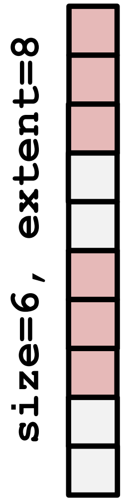
# Data type size and extent

- Get the total **size** (in bytes) of datatype in a message

```
int MPI_type_size(MPI_Datatype newtype, int *size);
```

- Get the lower bound and the **extent** (span from the first byte to the last byte) of datatype

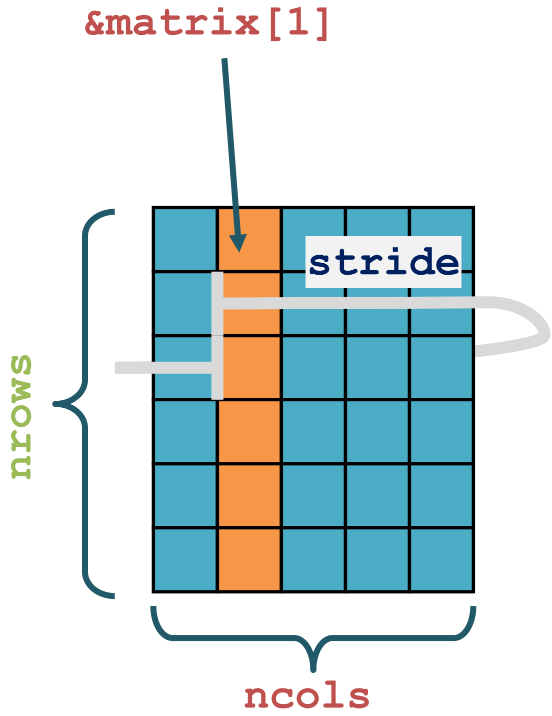
```
int MPI_type_get_extent(MPI_Datatype newtype,
                        MPI_Aint *lb,
                        MPI_Aint *extent);
```




- MPI allows to change the extent of a datatype using
  - **MPI_Type_create_resized**
    - **Sizeof**
    - **MPI_Get_address/MPI_Aint_diff**

# Sending a column of a matrix in C

## Row-major data layout in C → cannot use plain array




```c
double matrix[30];
MPI_Datatype nt;

// count = nrows, blocklength = 1,
// stride = ncols
MPI_Type_vector(nrows, 1, ncols,
                MPI_DOUBLE, &nt);
MPI_Type_commit(&nt);

// send column
MPI_Send(&matrix[1], 1, nt, …);

MPI_Type_free(&nt);
```

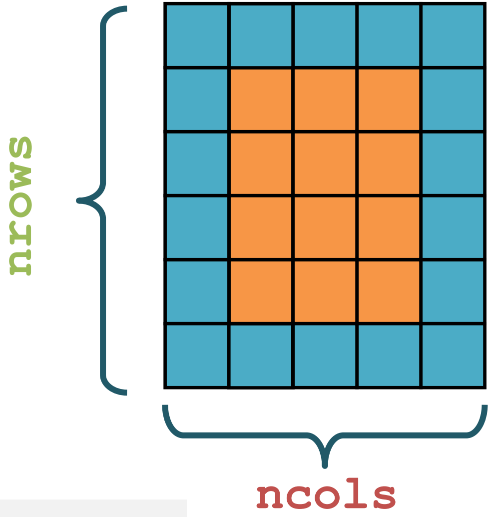
# Sub-array Data Type

```
MPI_Type_create_subarray(int dims,
   int ar_sizes[], int ar_subsizes[], int ar_starts[],
   int order, MPI_Datatype oldtype, MPI_Datatype * newtype);
```

- `dims`: dimension of the array
- `ar_sizes`: array with sizes of array (dims entries)
- `ar_subsizes`: array with sizes of subarray (dims entries)
- `ar_starts`: start indices of the subarray inside array (dims entries), start at 0 (also in Fortran)
- `order`
  - row-major: **`MPI_ORDER_C`**
  - column-major: **`MPI_ORDER_FORTRAN`**

# Example for a sub-array type: “bulk” of a matrix

| | |
|---|---|
| `dims` | `2` |
| `ar_sizes` | `{ncols, nrows}` |
| `ar_subsizes` | `{ncols-2, nrows-2}` |
| `ar_starts` | `{1, 1}` |
| `order` | `MPI_ORDER_C` |
| `oldtype` | `MPI_INT` |




```
MPI_Type_create_subarray(dims, ar_sizes, ar_subsizes,
                 ar_starts, order, oldtype, &nt);
MPI_Type_commit(&nt);
// use nt...
MPI_Send(&buf[0], 1, nt, …); // etc.
MPI_Type_free(&nt);
```

# A Short List of MPI Bindings to Create Data Type

| Function | Description |
|---|---|
| MPI_Type_contiguous | Creates a new data type that is a concatenation of a number of elements of an existing data type. |
| MPI_Type_vector | Creates a vector consisting of a number of elements of the same datatype repeated with a certain stride. |
| MPI_Type_indexed | Creates a new data type that consists of a specified number of blocks of arbitrary size. |
| MPI_Type_create_subarray | Creates a new data type that consists of an n-dimensional subarray of an n-dimensional array. |
| MPI_Type_create_darray | Creates a data type corresponding to a distributed, multidimensional array. It supports block, cyclic and no distribution for each dimension. |
| MPI_Type_create_struct | Creates an MPI datatype from a general set of datatypes, displacements, and block sizes. |

There exist more bindings, not all listed here!

- Remarks to Fortran programmers:
  - Arrays in Fortran are stored in column-major order
  - It requires special care for derived datatypes (**`MPI_Type_create_struct`**) because of some sort of optimizations such as reordering elements of a derived datatype

# Questions?