New Features in MPI 4.0

Rolf Rabenseifner, Tobias Haas
rabenseifner@hlrs.de **tobias.has@hlrs.de**

University of Stuttgart
High-Performance Computing-Center Stuttgart (HLRS)
www.hlrs.de

MPI Forum

- **MPI-1 Forum**
  - MPI-1.0 — May 1994
  - MPI-1.1 — June 1995
- **MPI-2 Forum**
  - MPI-1.2 — July 18, 1997: mainly clarifications.
  - MPI-2.0 — July 19, 1997: extensions to MPI-1.2.
- **MPI-3 Forum → MPI-4 Forum**
  - Started Jan. 14-16, 2008 (1st meeting in Chicago)
  - MPI-2.1 — June 23, 2008
    — mainly combining MPI-1 and MPI-2 books to one book
  - MPI-2.2 — September 4, 2009: Clarifications and a few new functions
  - MPI-3.0 — September 21, 2012: Important new functionality
  - MPI-3.1 — June 4, 2015: Errata & new: Nonblocking I/O, MPI_AINT_DIFF / _ADD
  - MPI-4.0 — June 9, 2021: Several new functionalities
    (not printed)
  - MPI-4.1 — scheduled for end 2023

Topics 1-19

Topics 20-24

**Only a short overview:
1-2 Minutes/topic
+
many background slides**

Acknowledgments for the HLRS MPI course

This talk is based on our HLRS MPI-3.1/4.0 five-day course

→ All course slides + exercises: https://www.hlrs.de/training/self-study-materials/mpi-course-material

→ Used in many training courses: https://www.hlrs.de/training/ & https://vsc.ac.at/training

→ Course acknowledgments also apply:

- The MPI-1.1 part of this course is partially based on the MPI course developed by the EPCC Training and Education Centre, Edinburgh Parallel Computing Centre, University of Edinburgh.
- Thanks to the EPCC, especially to Neil MacDonald, Elspeth Minty, Tim Harding, and Simon Brown.
- Course Notes and exercises of the EPCC course can be used together with these slides.
- The MPI-2.0 part is partially based on the MPI-2 tutorial at the MPIDC 2000 by Anthony Skjellum, Purushotham Bangalore, Shane Hebert (High Performance Computing Lab, Mississippi State University, and Rolf Rabenseifner (HLRS)
- Some MPI-3.0 detailed slides are provided by the MPI-3.0 ticket authors, chapter authors, or chapter working groups, Richard Graham (chair of MPI-3.0), and Torsten Hoefler (additional example about new one-sided interfaces)
- Thanks to Claudia Blaas-Schenner from TU Wien (Vienna) and many other trainers and participants for all their helpful hints for optimizing this course over so many years.
- **Thanks to Tobias Haas from HLRS for his Python binding of the exercises.** Thanks to Claudia Blaas-Schenner and David Fischak from TU Wien (Vienna) for their additional hints on the Python bindings. Additional background was a first draft from the HiDALGO project at HLRS.

Large counts

Large Counts with MPI_Count, …

New in MPI-3.0

- MPI uses different integer types
  - int and INTEGER
  - MPI_Aint = INTEGER(KIND=MPI_ADDRESS_KIND)
  - MPI_Offset = INTEGER(KIND=MPI_OFFSET_KIND)
  - MPI_Count = INTEGER(KIND=MPI_COUNT_KIND) — New in MPI-3.0
- sizeof(int) ≤ sizeof(MPI_Aint) / sizeof(MPI_Offset) ≤ sizeof(MPI_Count)
- All count arguments are int or INTEGER.
- Real message sizes may be larger due to datatype size.
- MPI_Type_get_extent, MPI_Type_get_true_extent,
  MPI_Type_size, MPI_Type_get_elements
  return **MPI_UNDEFINED** if value is too large — New in MPI-3.0
- New in MPI-3.0: MPI_Type_get_extent_**x**, MPI_Type_get_true_extent_**x**,
  MPI_Type_size_**x**, MPI_Type_get_elements_**x**
  return values as **MPI_Count**
- **New in MPI-4.0:** **MPI_Xxxx_c(…)** in C: additional interfaces with large counts
  MPI_Xxxx(…) !(_c) in Fortran: overloaded interfaces with large counts

Two exceptions with explicit _c in Fortran:
MPI_Op_create_c & MPI_Register_datarep_c

MPI 3.1 page 28
MPI 4.0 page 37

- **Language independent definition**

3.2.4 Blocking Receive

The syntax of the blocking receive operation is given below.

MPI_RECV (buf, count, datatype, source, tag, comm, status)

OUT	buf	initial address of receive buffer (choice)
IN	count	number of elements in receive buffer (non-negative integer)
IN	datatype	datatype of each receive buffer element (handle)
IN	source	rank of source or MPI_ANY_SOURCE (integer)
IN	tag	message tag or MPI_ANY_TAG (integer)
IN	comm	communicator (handle)
OUT	status	status object (Status)

- **C interface**

New in MPI-4.0

```
int MPI_Recv(void* buf, int count, MPI_Datatype datatype, int source,
             int tag, MPI_Comm comm, MPI_Status *status)
```

- **Fortran 2008** interface through **mpi_f08** module

```
MPI_Recv(buf, count, datatype, source, tag, comm, status, ierror)
    TYPE(*), DIMENSION(..) :: buf
    INTEGER, INTENT(IN) :: count, source, tag
    TYPE(MPI_Datatype), INTENT(IN) :: datatype
    TYPE(MPI_Comm), INTENT(IN) :: comm
    TYPE(MPI_Status) :: status
    INTEGER, OPTIONAL, INTENT(OUT) :: ierror
```

Large count version in **MPI-4.0**
MPI_Recv_c(…) in C
with MPI_Count count
MPI_Recv(…) !(_c) in Fortran
with INTEGER(KIND=MPI_COUNT_KIND) :: count

- Old **Fortran** interface through **mpi** module and **mpif.h**

```
MPI_RECV(BUF, COUNT, DATATYPE, SOURCE, TAG, COMM, STATUS, IERROR)
    <type> BUF(*)
    INTEGER COUNT, DATATYPE, SOURCE, TAG, COMM, STATUS(MPI_STATUS_SIZE),
    IERROR
```

No large count in mpi / mpif.h

https://www.mpi-forum.org/docs/mpi-3.1/mpi31-report.pdf#page=60
https://www.mpi-forum.org/docs/mpi-4.0/mpi40-report.pdf#page=77

background

The Fortran support methods

In MPI-4.0, new large count interfaces only in mpi_f08 !

Fortran

Fortran support method	MPI-1.1	MPI-2	MPI-3	MPI-4.0	MPI-next	MPI-…	far future
USE mpi_f08	x	x	5	5	5	5	5
USE mpi	x	3	4	4 / 2b	2b	1	0
INCLUDE ´mpif.h´	3	3	2a	2a/b	1	0	0

Past (MPI-1.1 – MPI-3) — Today (MPI-4.0) — Maybe in the future (MPI-next – far future)

<u>Level of Quality:</u>

- 5 – valid and consistent with the Fortran standard (Fortran 2008 + TS 29113) [1)]
- 4 – valid and only partially consistent
- 3 – valid and small consistency (e.g., without argument checking)
- 2 – use is strongly (a) discouraged or (b) partially frozen (i.e., not with all new functions)
- 1 – deprecated
- 0 – removed
- x – not yet existing

1) For full consistency, Fortran 200**<u>3</u>** + TS29113 is enough.
Fortran 2018 and later versions include TS 29113.
Without TS29113, same partial consistency as with the mpi module.

background

MPI_Put

C

- C/C++: int MPI_Put(const void *origin_addr, int origin_count,
  MPI_Datatype origin_datatype, int target_rank, MPI_Aint target_disp,
  int target_count, MPI_Datatype target_datatype, MPI_Win win)

  int MPI_Put_c(const void *origin_addr, MPI_Count origin_count,
  MPI_Datatype origin_datatype, int target_rank, MPI_Aint target_disp,
  MPI_Count target_count, MPI_Datatype target_datatype, MPI_Win win)

  Large count version, new in MPI-4.0

Fortran

- Fortran: MPI_Put(origin_addr, origin_count, origin_datatype, target_rank,
  target_disp, target_count, target_datatype, win, ierror)

```
mpi_f08:       TYPE(*), DIMENSION(..), INTENT(IN), ASYNCHRONOUS :: origin_addr
               INTEGER, INTENT(IN)                          :: origin_count, target_count
          or   INTEGER(KIND=MPI_COUNT_KIND), INTENT(IN)     :: origin_count, target_count
               INTEGER, INTENT(IN)                          :: target_rank
               TYPE(MPI_Datatype), INTENT(IN)               :: origin_datatype, target_datatype
               INTEGER(KIND=MPI_ADDRESS_KIND), INTENT(IN)   :: target_disp
               TYPE(MPI_Win), INTENT(IN)                    :: win
               INTEGER, OPTIONAL, INTENT(OUT)               :: ierror
mpi & mpif.h:  <type> ORIGIN_ADDR(*)
               INTEGER ORIGIN_COUNT, ORIGIN_DATATYPE, TARGET_RANK,
               INTEGER TARGET_COUNT, TARGET_DATATYPE, WIN, IERROR
               INTEGER(KIND=MPI_ADDRESS_KIND) TARGET_DISP
```

Overloaded large count version since MPI-4.0

Python

- Python: win.Put((origin_buf, origin_count, origin_datatype), target_rank,
  (target_disp, target_count, target_datatype))

The course-slides include also the mpi4py binding, which are not part of the MPI standard

background

Window Creation with MPI_Win_create

C

- C/C++:
```
int MPI_Win_create(void *base, MPI_Aint size,
                   int disp_unit, MPI_Info info,
                   MPI_Comm comm, MPI_Win *win)

int MPI_Win_create_c(void *base, MPI_Aint size,
                   MPI_Aint disp_unit, MPI_Info info,
                   MPI_Comm comm, MPI_Win *win)
```
Large count version, new in MPI-4.0

Fortran

- Fortran: MPI_Win_create(base, size, disp_unit, info, comm, *win*, ierror)

mpi_f08:
```
      TYPE(*), DIMENSION(..), ASYNCHRONOUS          :: base
      INTEGER(KIND=MPI_ADDRESS_KIND), INTENT(IN)    :: size
      INTEGER, INTENT(IN)                           :: disp_unit
   or INTEGER(KIND=MPI_ADDRESS_KIND), INTENT(IN)    :: disp_unit
      TYPE(MPI_Info), INTENT(IN)                    :: info
      TYPE(MPI_Comm), INTENT(IN)                    :: comm
      TYPE(MPI_Win), INTENT(OUT)                    :: win
      INTEGER, OPTIONAL, INTENT(OUT)                :: ierror
```
Overloaded large count version since MPI-4.0

mpi & mpif.h:
```
      <type> base(*)
      INTEGER(KIND=MPI_ADDRESS_KIND) size
      INTEGER  disp_unit, info, comm, win, ierror
```

Python

- Python: *win* = MPI.Win.Create(memory, disp_unit, info, comm)

e.g., a numpy array

New persistent collectives
→ new terms „*nonblocking & co*“

Non-Blocking Communications

Separate communication into **three phases**:

- Initiate nonblocking communication
  - returns immediately
  - routine name starting with MPI_**I**…

  → it is local,
  i.e., it returns independently of any other process' activity
- Do some work (perhaps involving other communications?)
- Wait for nonblocking communication to **complete**, i.e.,
  - the send buffer is read out, or
  - the receive buffer is filled in

"I" stands for
- Immediate (=local)
- and Incomplete

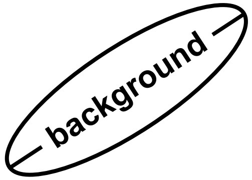
} = nonblocking[1)]

1) The definition of nonblocking is clarified

Complete rewording of MPI-4.0
Section 2.4 Semantic Terms
2.4.1 MPI Operations
2.4.2 MPI Procedures

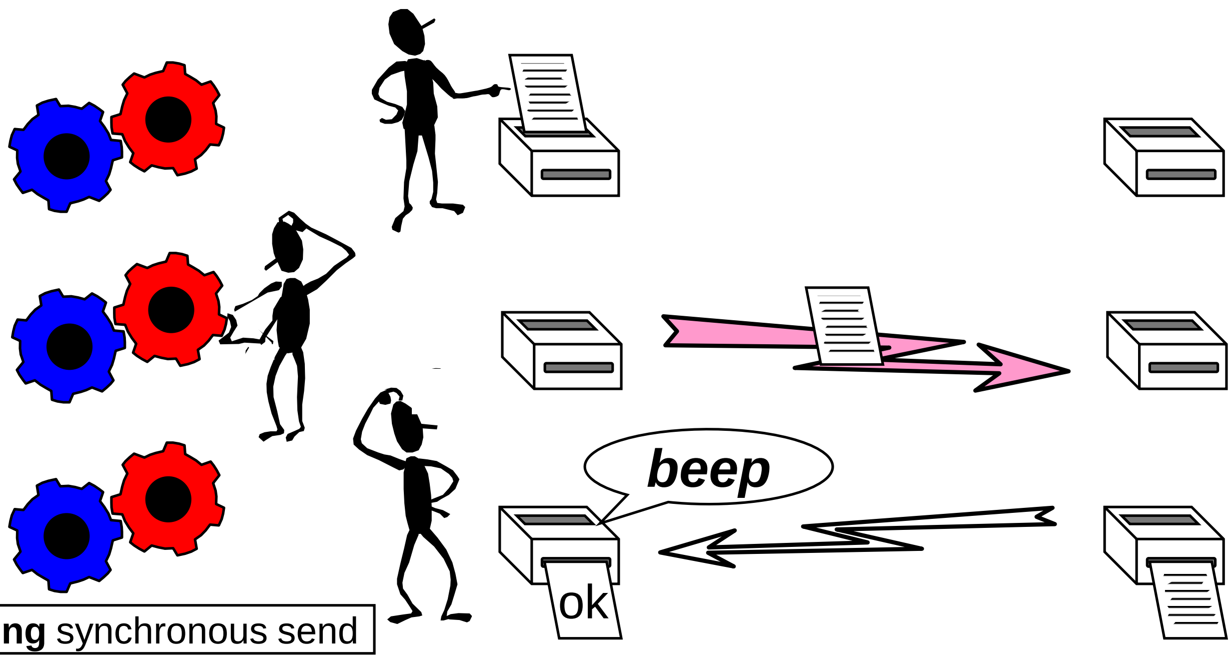
MPI-1.1 – MPI-3.1:
→ nonblocking = incomplete
MPI-4.0:
→ nonblocking = incomplete AND local

Nonblocking Operations



Nonblocking operations consist of:

- A nonblocking procedure call: it returns immediately and allows the sub-program to perform other work
- At some later time the sub-program must ***test*** or ***wait*** for the completion of the nonblocking operation



The basis of MPI

Visiting MPI Chapter 2 Terms and Conventions

Clarified in MPI-4.0

Operations and Procedures, (non)blocking / (non-)local

- **MPI operations** consist of four stages:
  - Initialization, starting, completion, freeing
- **MPI operations** can be
  - **Blocking**: all four stages are combined in a single complete/blocking procedure. → which returns when operation has completed.
  - **Nonblocking**: → next slide
  - **Persistent**: → 2nd next slide
- **MPI procedures** can be
  - **Non-local:** returning may require, during its execution, some specific semantically-related MPI procedure to be called on another MPI process.
  - **Local:** is not non-local. (See also discussion of *"weak local"*)
- **MPI procedures** (if they implement an operation or parts of it) can be
  - **Completing:** on return, all resources (e.g., buffers or array arg.s) can be reused.
  - **Incomplete:** return before resources can be reused.
  - **Nonblocking:** incomplete AND local / **Blocking:** Completing OR non-local.

Orthogonal concept, although in most cases:
- Incomplete/nonblocking communication proc. → local
- Complete/blocking communication proc. → non-local

(with some exceptions)

- **Examples**:
  - Nonblocking: • Incomplete & local: MPI_Isend, MPI_Irecv, MPI_Ibcast, MPI_Send_init
  - Blocking: • Completing & non-local: MPI_Send, MPI_Recv, MPI_Bcast
    - • Incomplete & non-local: MPI_Mprobe, MPI_Bcast_init (**New in MPI-4.0**)
    - • Completing & local: MPI_Bsend, MPI_Rsend, MPI_Mrecv

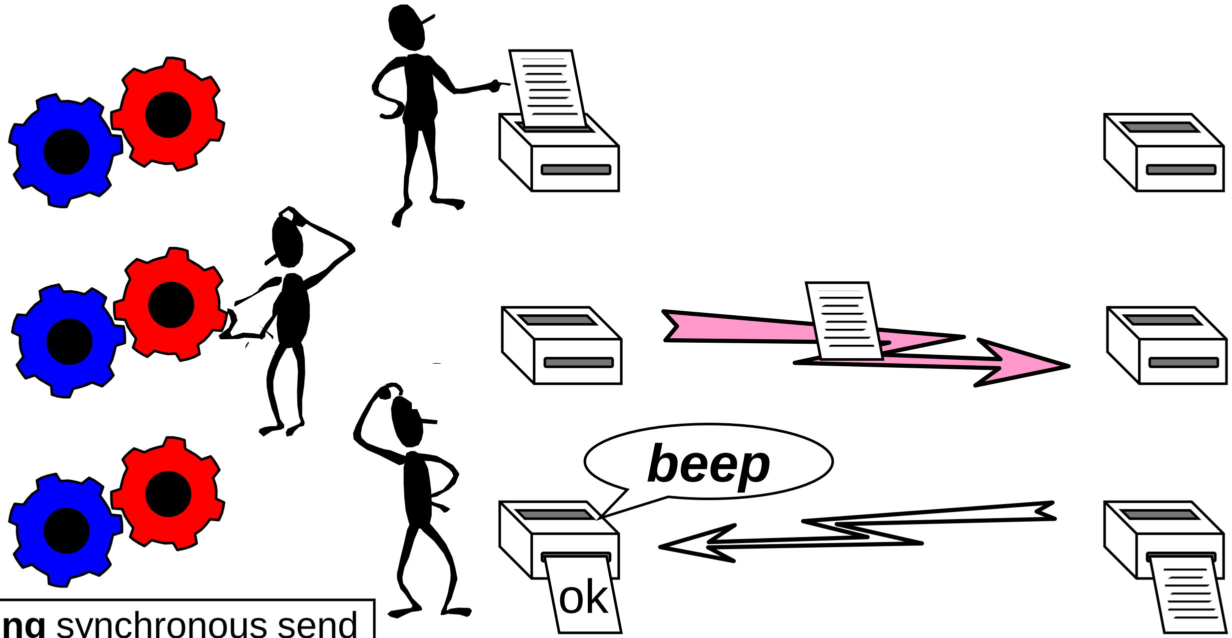
The semantics of all operation-related MPI procedures is listed in **Annex A.2** (since MPI-4.0)

Nonblocking Operations

Nonblocking operations consist of:

New in MPI-4.0

- A nonblocking procedure call: it is **incomplete** & returns **immediately** and allows the sub-program to perform other work → stages **initialization** + **starting** = initiation
- At some later time the sub-program must ***test*** or ***wait*** for the completion of the nonblocking operation → stages **completion** + **freeing**



nonblocking synchronous send

Goal:
Enables **additional optimizations** within the MPI library

Persistent Requests

For communication calls with identical argument lists in each loop iteration (only buffer content changes):

New in MPI-4.0 — Stage

- **MPI_(,B,S,R)Send_init** and **MPI_Recv_init** — ***initialization***
  - Creates a persistent MPI_Request handle
  - Status of the handle is initiated as *inactive*
  - Local calls (does not communicate)
  - It only setups the argument list
- **MPI_Bcast_init** …, also for collective operations
  - Blocking & collective calls (may communicate)
- **MPI_Start**(request [,ierror]) / **MPI_Startall**(cnt, requests [,ierror]) — ***starting***
  - Starts the communication call(s) as nonblocking call(s), i.e., handle gets *active*
- To be completed with regular MPI_Wait… / MPI_Test… calls → *inactive* — ***completion***
- MPI_Request_free to finally free such a handle — ***freeing***
- Usage sequence: init Loop(Start Wait/Test) Request_free

New in MPI-4.0

Caused all these new definitions of the terms

Recommendation:
Never free an **active** request handle.
Active request handles should be completed with WAIT or TEST

Persistent inactive request → **active**

Completes an active request handle → **in**active

Free the **in**active persistent request handle

Partitioned Point-to-Point Communication

New in MPI-4.0

Partitioned Point-to-Point Communication

- MPI-4.0:
  Partitioned communication is “partitioned“ because it allows for multiple contributions of data to be made, potentially, from multiple actors (e.g., threads or tasks) in an MPI process to a single communication operation.
- A point-to-point operation (i.e., send or receive)
  - can be split into partitions,
  - and each partition is filled and then “send” with MPI_Pready by a thread;
  - And same for receiving.
- Technically provided as a new form of persistent communication.

background

Partitioned Communication Example

```
#define PARTITIONS 8
#define COUNT 6
double message[PARTITIONS*COUNT];
MPI_Count count_send = COUNT, count_recv=COUNT/2;
int source = 0, dest = 1, tag = 1, flag = 0, rank, thread_provided;
MPI_Request request;

MPI_Init_thread(NULL,NULL,MPI_THREAD_MULTIPLE, &thread_provided);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);

/* Sender part (rank 0) */
if (rank == 0){
        MPI_Psend_init(message, PARTITIONS, count_send, MPI_DOUBLE, dest, tag,
                MPI_COMM_WORLD, MPI_INFO_NULL, &request);
        MPI_Start(&request);
#pragma omp parallel for shared(request) num_threads(8)
        for(int i = 0; i < PARTITIONS; ++i){ /* 1 partition per thread */
            /* compute and fill partition message[COUNT*i…COUNT*(i+1)-1], then mark ready: */
            MPI_Pready(i, request);
        }
        while(!flag){
            /* Do useful work */
            MPI_Test(&request, &flag, MPI_STATUS_IGNORE);
            /* Do useful work */
        }
        MPI_Request_free(&request);
}
```

background

Partitioned Communication Example

```
/* Receiver part (rank 1) */
else if (rank == 1){
        /* We split every partition by half, i.e. count per partition divided by two, number or partitions increased by 2 */
                MPI_Precv_init(message, PARTITIONS*2, count_recv, MPI_DOUBLE, source, tag,
                                MPI_COMM_WORLD, MPI_INFO_NULL, &request);
                MPI_Start(&request);
 #pragma omp parallel for shared(request) num_threads(NUM_THREADS)
        for (int j=0; j< PARTITIONS*2; j+=2){
                int part1_complete = 0, part2_complete = 0;
                int work1_complete = 0, work2_complete = 0;
                while(work1_complete == 0 || work2_complete == 0){
                  /* test partition #j and #j+1 */
                       if(!part1_complete){ MPI_Parrived(request, j, &part1_complete);}
                       if(part1_complete && !work1_complete){
                               /* Do work using partition j data */
                               work1_complete = 1;
                        }
                       if(!part2_complete){ MPI_Parrived(request, j+1, &part2_complete);}
                       if(part2_complete && !work2_complete){
                               /* Do work using partition j+1 data */
                               work2_complete = 1;
                        }
                }
        }
        /* Need to complete request since MPI_PARRIVED doesn‘t. */
        MPI_Wait(&request, MPI_STATUS_IGNORE); /* Alternative: MPI_Test in loop and do useful work, see previous slide*/
        MPI_Request_free(&request);
}
```

background

Comments on Partitioned Communication

- Sequence is

  Init (Start Pready/Rarrived Wait/Test)∗ Free

  e.g.

  MPI_Psend[recv]_init (MPI_Pstart MPI_Pready MPI_Wait)* MPI_Request_free

- MPI_PSEND_INIT must be combined with MPI_PRECV_INIT.
- Matching rules are the same as for normal pt-to-pt communication.
  In doubt, order of initialization is used to break ties.
- Buffers must have **same** size for send and receive.
- Partitioning on sender/receiver may differ (as in the example).
- PREADY **must** be used to mark partition to be sent.
- MPI_PARRIVED(request,partition,flag) **may** be used to check
  - if partition is complete,
  - but does not complete the request (must be done with MPI_TEST/MPI_WAIT).

The new sessions model

Since MPI-1

New in MPI-4.0

World Model and *Sessions Model*

Since MPI-2.0: duplicates **with** associated key values, topology and **info hints**. **Since MPI-4.0:** Now **without info hints**

- ***The World Model***
  - MPI_COMM_WORLD can be used between MPI_Init and MPI_Finalize
  - Exactly one call to MPI_Init and MPI_Finalize
  - Problem, if several independent software layers want to use MPI:
    - **Each layer can duplicate MPI_COMM_WORLD using MPI_COMM_DUP()**
    - **But there is no rule on which layer calls MPI_Init and which one MPI_Finalize**
- ***The Sessions Model***
  - Each independent software layer **xxx** can initialize and finalize MPI, e.g., as follows:
    - **As part of layer_xxx_init**
      - **MPI_Session_init**(MPI_INFO_NULL, MPI_ERRORS_ARE_FATAL, &session);
      - **MPI_Group_from_session_pset**(session, "mpi://WORLD", &xxx_world_group);
      - **MPI_Comm_create_from_group**(xxx_world_group, "stringtag_xxx", MPI_INFO_NULL, MPI_ERRORS_ARE_FATAL, &xxx_world_comm);
      - **MPI_Group_free**(&xxx_world_group);
    - **As part of layer_xxx_finalize**
      - **MPI_Comm_free**(&xxx_world_comm);
      - **MPI_Session_finalize**(&session);
  - **Caution:** MPI objects derived from different MPI Session handles shall **not** be intermixed with each other in a single MPI procedure call.
- An MPI application may use the World Model (not more than once) together with the Sessions Model (with several overlapping or non-overlapping sessions)

e.g., each independent software layer initiates its own session and communicator

Environment inquiry – implementation information (1)

New in MPI-3.0

<u>Inquire start environment</u>

- Predefined info object **MPI_INFO_ENV** (in the World Model)
  or info handle created with **MPI_Info_create_env** (in the Sessions Model)
  holds arguments from
  - mpiexec, or
  - MPI_COMM_SPAWN

New in MPI-4.0

see a few slides later

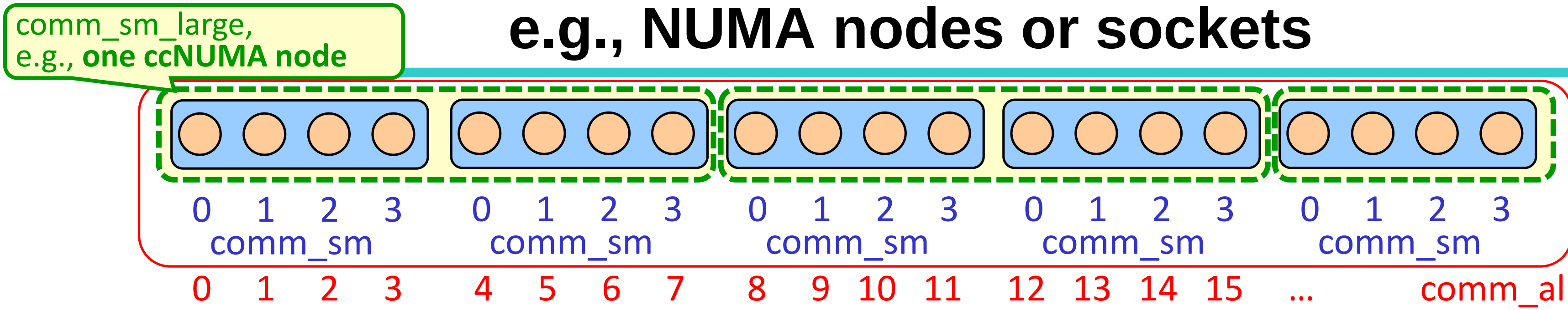
Sessions Model – Summary

New in MPI-4.0

- The Sessions Model → a method to init/finalize MPI within independent application components / software layers

New ways for hardware-based split of communicators

Splitting into smaller shared memory islands, e.g., NUMA nodes or sockets



- Subsets of shared memory nodes, e.g., one comm_sm on each socket with size_sm cores **(requires also sequential ranks in comm_all for each socket!)**

```
MPI_Comm_split_type (comm_all, MPI_COMM_TYPE_SHARED, 0, MPI_INFO_NULL, &comm_sm_large);
MPI_Comm_rank (comm_sm_large, &my_rank_sm_large); MPI_Comm_size (comm_sm_large, &size_sm_large);
MPI_Comm_split (comm_sm_large, /*color*/ my_rank_sm_large / size_sm, 0, &comm_sm);
MPI_Win_allocate_shared (..., comm_sm, ...);
```

or (size_sm_large /number_of_sockets) — here 2

- Most MPI libraries have an non-standardized method to split a communicator into NUMA nodes (e.g., sockets): (see also Current support for split types in MPI implementations or MPI based libraries)
  - **OpenMPI:** choose split_type as OMPI_COMM_TYPE_NUMA
  - **HPE:** MPI_Info_create (&info); MPI_Info_set(info, "shmem_topo", "numa"); // or "socket"
    MPI_Comm_split_type(comm_all, MPI_COMM_TYPE_SHARED, 0, info, &comm_sm);
  - **mpich:** split_type=MPIX_COMM_TYPE_NEIGHBORHOOD, info_key= "SHMEM_INFO_KEY“ and value= "machine", "socket", "package", **"numa"**, "core", "hwthread", "pu", "l1cache", …, or "l5cache"

May not work with Intel-MPI

New in MPI-4.0

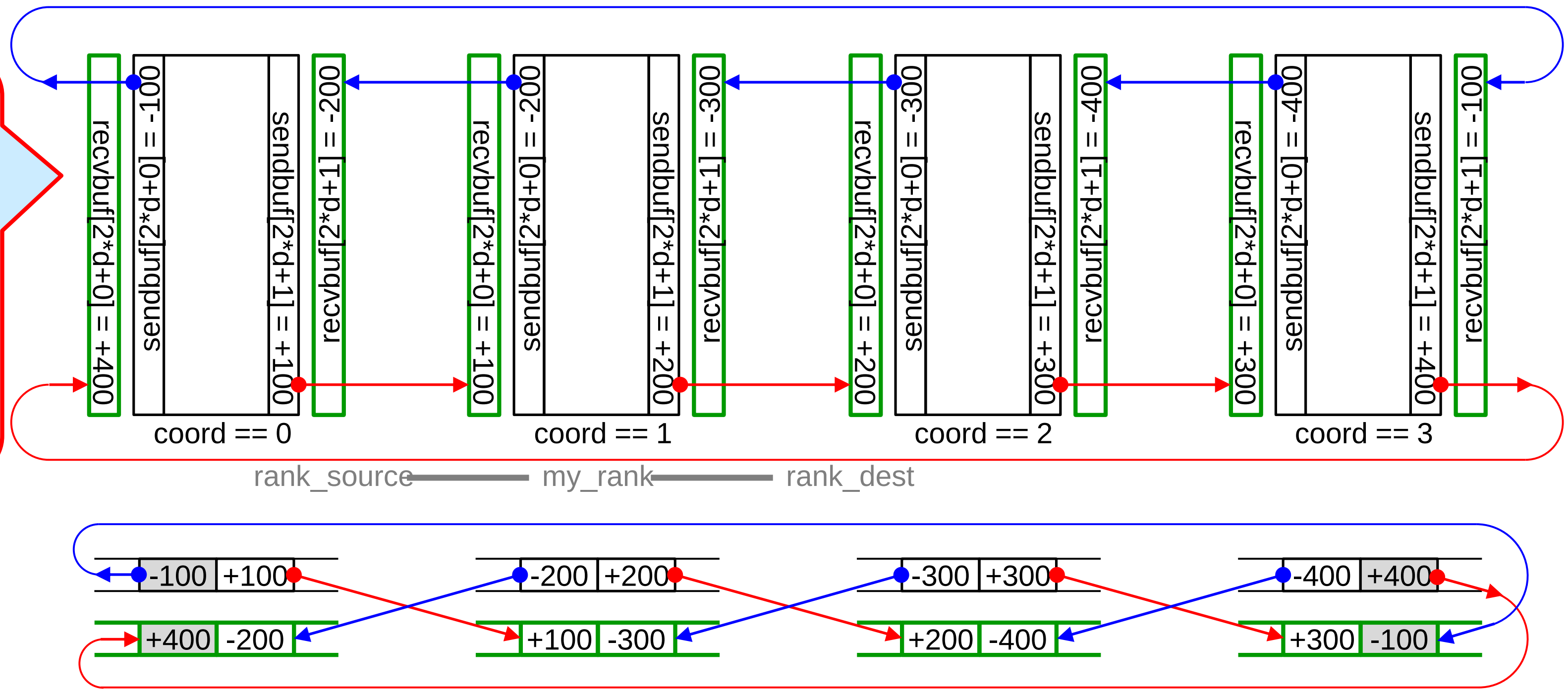
- **Two additional standardized split types:**
  - **MPI_COMM_TYPE_HW_GUIDED and**
  - **MPI_COMM_TYPE_HW_UNGUIDED**
- See also Exercise 3.

MPI_Neighbor communication: Examples / bug-fixes

Clarified in MPI-4.0

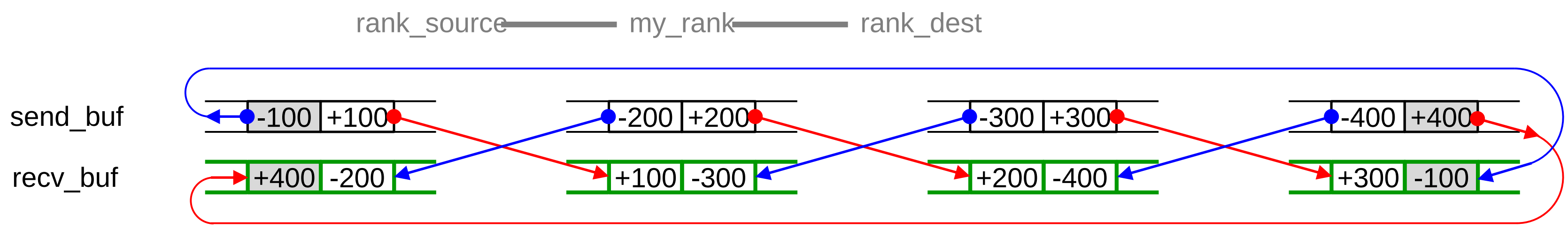
Periodic MPI_NEIGHBOR_ALLTOALL in direction *d* with 4 processes

This figure represents one direction *d*. Of course, it is valid for any direction



… grey array entries are used only if periods[d] == non-zero in C or .TRUE. in Fortran

As if …

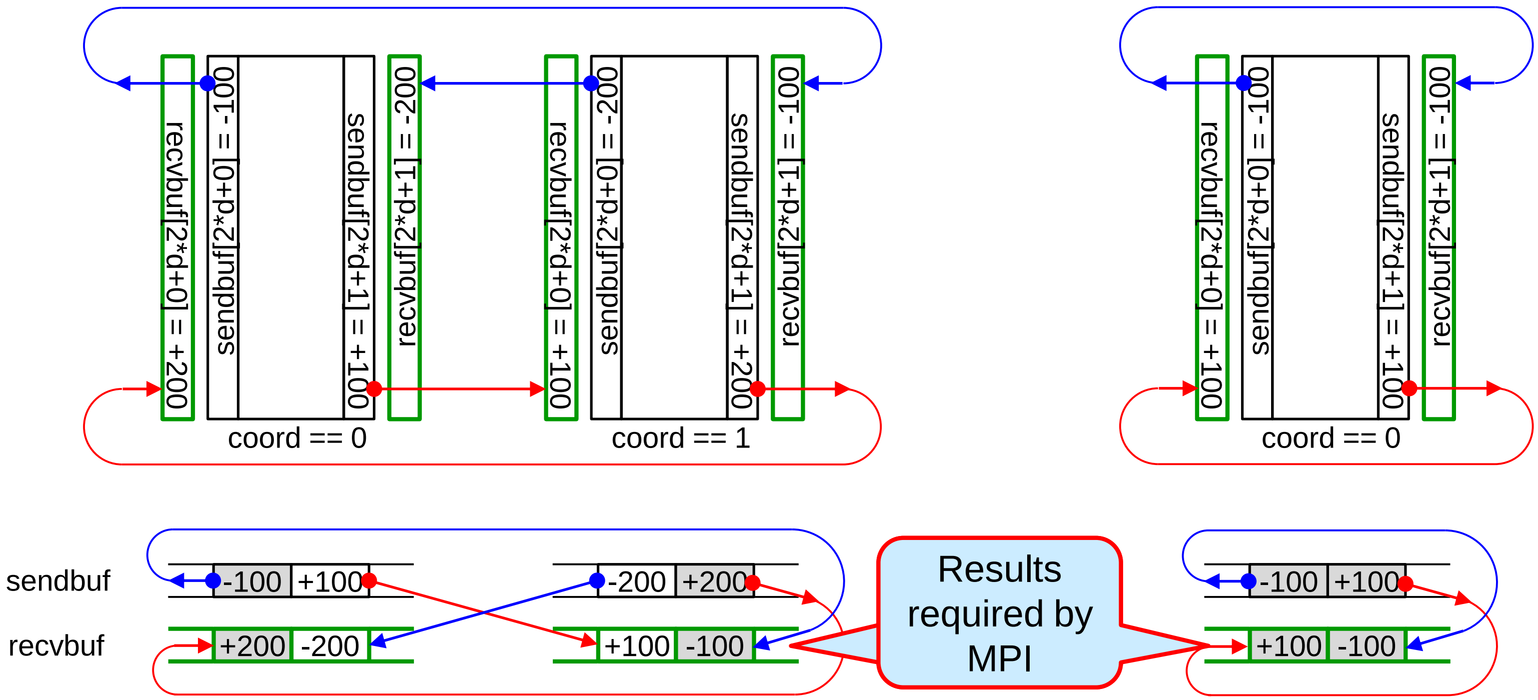


After MPI_NEIGHBOR_ALLTOALL on a Cartesian communicator returned, the content of the `recvbuf` is **as if** the following code is executed:

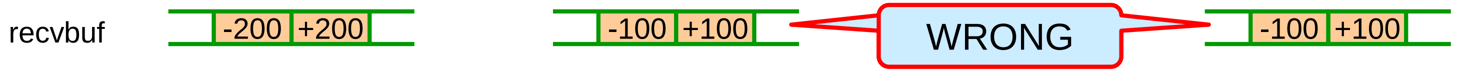
```
MPI_Cartdim_get(comm, &ndims);
for( /*direction*/ d = 0; d < ndims; d++) {
   MPI_Cart_shift(comm, /*direction*/ d, /*disp*/ 1, &rank_source, &rank_dest);
   MPI_Sendrecv(sendbuf[d*2+0], sendcount, sendtype, rank_source, /*sendtag*/ d*2,
                recvbuf[d*2+1], recvcount, recvtype, rank_dest,   /*recvtag*/ d*2,
                comm, &status); /* 1st communication in direction of displacment -1 */
   MPI_Sendrecv(sendbuf[d*2+1], sendcount, sendtype, rank_dest,   /*sendtag*/ d*2+1,
                recvbuf[d*2+0], recvcount, recvtype, rank_source, /*recvtag*/ d*2+1,
                comm, &status); /* 2nd communication in direction of displacment +1 */
}
```

The tags are chosen to guarantee that both communications (i.e., in negative and positive direction) cannot be mixed up, even if the MPI_SENDRECV is substituted by nonblocking communication and the MPI_ISEND and MPI_IRECV calls are started in any sequence.

Wrong implementations of periodic MPI_NEIGHBOR_ALLTOALL with only 2 and 1 processes



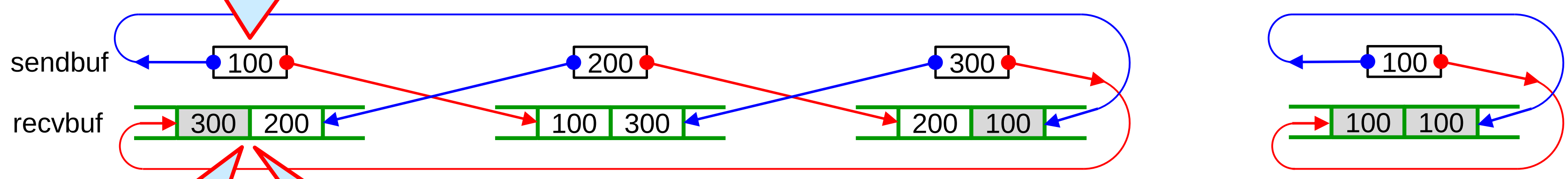
Wrong results with **openmpi/4.0.1-gnu-8.3.0** and **cray-mpich/7.7.6** with 2 and 1 processes:



Clarified in MPI-4.0

Communication pattern of MPI_NEIGHBOR_ALLGATHER

The send_buf is only one element, which is sent to the neighbor processes in all directions



… grey array entries are used only if periods[d] == non-zero in C or .TRUE. In Fortran

The recv_buf represents one direction *d*. Of course, this figure is valid for any direction

The green recv_buf elements are recvbuf[2**d*+0] and recvbuf[2**d*+1]

Other small new MPI-4 features

Info handles revisited

- New nonblocking MPI_Comm_**i**dup_with_info (New in MPI-4.0) complementing blocking MPI_Comm_dup_with_info (Was new in MPI-3.0)

- Use MPI_Info_get_string (New in MPI-4.0) instead of deprecated MPI_Info_get_valuelen and MPI_Info_get

- MPI_Comm|File|Win_**set**_info + MPI_Comm|File|Win_**get**_info were clarified:
  - The MPI library may or may not set or recognize some (system specific) hints (Additional text in MPI-4.0)

skipped

MPI_Info Object

A general service for many MPI procedures

- An **`MPI_Info`** is an opaque object that consists of a set of (key,value) pairs
  - Both key and value are **strings**
  - A **key** should have a **unique** name within one info handle
  - Several keys are reserved by standard / implementation
  - Portable programs may use **`MPI_INFO_NULL`** as the info argument
  - Vendor keys are also portable, may be ignored by other libraries
  - Several sets of vendor-specific keys may be used

Info handle →

key1	value1
key2	value2
…	…

Internally stored in the MPI library

- Allows applications to **pass environment-specific information**
- Allow applications to **provide assertions** regarding their usage of MPI objects and operations → to improve performance or resource utilization

New in MPI-4.0

- Several functions provided to manipulate the info objects
- Used in:
  - *Process Creation*,
  - *Window Creation*,
  - *MPI-I/O*,
  - *MPI_Comm_(i)dup_with_info*, **New in MPI-4.0**
  - *MPI_INFO_ENV*

Example:

```
MPI_Info  info_noncontig;
MPI_Info_create (&info_noncontig);
MPI_Info_set (info_noncontig,
                  "alloc_shared_noncontig", "true");
MPI_Win_allocate_shared (…,  info_noncontig, …);
```

Creates the list with 0 entries (MPI_Info_create)

Adds 1 new entry, or modifies the value if key already exists (MPI_Info_set)

- The key/value list returned by MPI_**Comm|File|Win_get**_info in the handle may differ from a those set by the application during Comm|File|Win creation or stored with MPI_Comm|File|Win_**set**_info: The MPI library may or may not set or recognize some (system specific) hints.

New in MPI-4.0: Use MPI_Info_get_string instead of deprecated MPI_Info_get_valuelen and MPI_Info_get.

 Slide ~230 in the HLRS MPI course

Wildcarding

- Receiver can wildcard.
- To receive from any source — source = MPI_ANY_SOURCE
- To receive from any tag — tag = MPI_ANY_TAG
- Actual source and tag are returned in the receiver's *status* parameter.

- With info assertions **New in MPI-4.0**
  - "mpi_assert_no_any_source" = "true" and/or
  - "mpi_assert_no_any_tag" = "true"

  stored on the communicator using MPI_Comm_set_info(),
  - an MPI application can tell the MPI library that it will never use MPI_ANY_SOURCE and/or MPI_ANY_TAG **on this communicator**

  → may enable lower latencies.
- Other assertions:
  - "mpi_assert_exact_length" = "true" → receive buffer must have exact length
  - "mpi_assert_allow_overtaking" = "true" → message order need not to be preserved

Error handler revisited

New in MPI-4.0

- "*MPI calls that are not related to any MPI objects are considered to be attached to the communicator **MPI_COMM_SELF** when using the World Model*"
  - If you want to change the initial error handler
    - MPI_ERRORS_ARE_FATAL is the default
    - **May be changed when calling mpirun / mpiexec** (New in MPI-4.0)

  then you must change it for both,
  MPI_COMM_WORLD and MPI_COMM_SELF

New in MPI-4.0

- New error handler MPI_ERRORS_ABORT
  - aborts only all processes of the related communicator

New in MPI-4.0

- Many other small additions / clarifications / …, see
  - MPI-4.0 Appendix B.1.2 *Changes in MPI-4.0*, items 4, 19-21, 26-27

skipped

Error Handling → "assembler for parallel computing"

2-level-concept with **error codes** and **error classes**, see MPI-3.1/MPI-4.0 Sect. 8.3-5/9.3-5

Most important aspects:

- The communication should be reliable (same rule as for processor and memory)
- If the MPI program is erroneous → no warranties:
  - by default: abort, if error detected by MPI library
    otherwise, unpredictable behavior

    i.e., error handler MPI_ERRORS_ARE_FATAL is the default
  - C/C++: MPI_Comm_set_errhandler (comm, MPI_ERRORS_RETURN);
    Fortran: call MPI_Comm_set_errhandler(comm, MPI_ERRORS_RETURN, ierr)

    Newly added in MPI-4.0

    directly after MPI_INIT with both comm = MPI_COMM_WORLD and MPI_COMM_SELF, then
    - **ierror returned by each MPI routine (except MPI window and MPI file routines)**
    - **undefined state after an erroneous MPI call has occurred**
      (only MPI_Abort(…) should be still callable)
  - Exception: MPI-I/O has default MPI_ERRORS_RETURN
    - Default can be changed through MPI_FILE_NULL:
    - MPI_File_set_errhandler (MPI_FILE_NULL, MPI_ERRORS_ARE_FATAL)
    - See MPI-3.1 Sect. 13.7, page 555 / MPI-4.0 Sect. 14.7, page 719, and course Chapter 7
  - MPI_ERRORS_ARE_FATAL aborts the process and all connected processes
  - MPI_ERRORS_ABORT aborts only all processes of the related communicator

    New in MPI-4.0

Send-Receive in one routine

- MPI_Sendrecv & MPI_Sendrecv_replace
  - Combines the triple "MPI_Irecv + Send + Wait" into one routine

New in MPI-4.0

- Nonblocking MPI_**I**sendrecv & MPI_**I**sendrecv_replace
  - Whereas blocking MPI_Sendrecv was used to prevent
    - **serializations and**
    - **deadlocks,**
  - the nonblocking MPI_Isendrecv can be used, e.g.,
    to parallelize the existing communication calls in multiple directions
    → e.g., to minimize idle times if only some neighbors are delayed

Use cases for nonblocking operations

- To prevent **serializations** and **deadlocks**
  (as if overlapping of communication with other communication)
  - Now also described in the intro of MPI-4.0 Section 3.7 Nonblocking Communication

New in MPI-4.0

> 3.7 Nonblocking Communication
>
> Nonblocking communication is important both for reasons of correctness and performance. For complex communication patterns, the use of only blocking communication (without buffering) is difficult because the programmer must ensure that each send is matched with a receive in an order that avoids ***deadlock***. For communication patterns that are determined only at run time, this is even more difficult. Nonblocking communication can be used to avoid this problem, allowing programmers to express complex and possibly dynamic communication patterns without needing to ensure that all sends and receives are issued in an order that prevents deadlock (see Section 3.5 and the discussion of "safe" programs). Nonblocking communication also allows for the ***overlap*** of communication with different communication operations, e.g., to prevent the ***serialization*** of such operations, and for the ***overlap*** of communication with computation. Whether an implementation is able to accomplish an effective (from a performance standpoint) overlap of operations depends on the implementation itself and the system on which the implementation is running.
> Using nonblocking operations ***permits*** an implementation to overlap communication with computation, but does not require it to do so.

Window creation or allocation

Four different methods

- Using existing memory as windows
  - **MPI_Alloc_mem, MPI_Win_create, MPI_Win_free, MPI_Free_mem**
- Allocating new memory as windows
  - **MPI_Win_allocate**
- Allocating shared memory windows – usable only within a shared memory node
  - **MPI_Win_allocate_shared, MPI_Win_shared_query**
- Using existing memory dynamically
  - **MPI_Win_create_dynamic, MPI_Win_attach, MPI_Win_detach**

New in MPI-3.0

MPI_Alloc_mem, MPI_Win_allocate, and MPI_Win_allocate_shared:

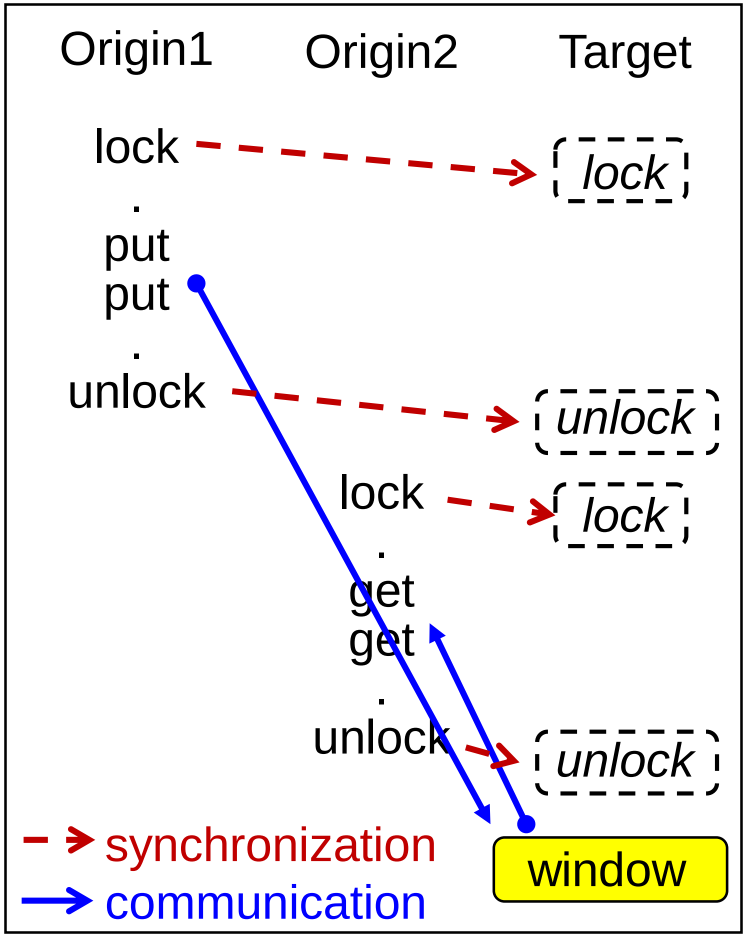
New in MPI-4.0

- Memory alignment must fit to all predefined MPI datatypes
  - alternative minimum alignment through info key "mpi_minimum_memory_alignment"

Lock/Unlock

- Does not guarantee a sequence
- agent may be necessary on systems without (virtual) shared memory
- Portable programs can use lock calls to windows in memory allocated **only** by **`MPI_Alloc_mem`**, **`MPI_Win_allocate`**, or **`MPI_Win_attach`** or **`MPI_Win_allocate_shared`**

  New in MPI-4.0
- RMA completed after **`MPI_Unlock`** at both origin and target
- No concept of an exposure epoch
  - → *like window is permanently exposed*
  - → local load/stores must be enclosed in a local lock/unlock epoch



Clarified in MPI-4.0

MPI_Request_free

- MPI_Request_free for *active* communication request:
  - Marks a request handle for deallocation
  - Deallocation will be done after *active* communication completion
  - May be used only for *active* send-request to substitute MPI_Wait, but *strongly discouraged* and dangerous when there is no other 100% guarantee that the send-buffer can be reused.
    - **Active send handle is produced with MPI_I(,s,b,r)send or MPI_(,S,B,R)send_init + MPI_Start**

New in MPI-4.0

  - *Should never be used* for *active* receive requests.

- Conclusion:
  MPI_Request_free really useful only for *inactive* persistent requests
  i.e., after such Loop(Start Wait/Test),
  i.e., not after Start

MPI_Cancel

- Marks a active nonblocking communication handle for cancellation.
- MPI_Cancel is a local call, i.e., returns immediately.
- **Subsequent call to MPI_Wait must return irrespective of the activities of other processes.**
- **Either** the **cancellation** or the **communication** succeeds, but not both.
- MPI_Test_cancelled(wait_status, flag [,ierror])
  - flag = true → cancellation succeeded, communication failed
  - flag = false → cancellation failed, communication succeeded

- **Comment: Do not use it – may be reason for worse performance**

New in MPI-4.0

- **MPI_Cancel of send requests is deprecated**

MPI_SIZEOF(…) – Fortran only API

- MPI_SIZEOF(…) was introduced in MPI-2.0
  - in combination with MPI_Type_match_size
  - as alternative to (recommended)
    - **MPI_TYPE_CREATE_F90_INTEGER**
    - **MPI_TYPE_CREATE_F90_REAL**
    - **MPI_TYPE_CREATE_F90_COMPLEX**

    to generate basic datatype handles
    for KIND-parameterized Fortran types

New in MPI-4.0

- **MPI_SIZEOF is deprecated**

Other changes …

- Tools chapter

New in MPI-4.0

  - MPI-4.0 Appendix B.1.2 *Changes in MPI-4.0*, items 30-32

Semantic changes & warnings

Removed / Semantic changes & warnings / Errata

Chapter 16+17 – Deprecated + Removed Interfaces

…

Nothing new in MPI-4.0

New in MPI-4.0

Chapter 18 – Semantic Changes and Warnings

18.1 Semantic Changes

This section describes semantics that have changed in a way that would potentially cause an **MPI program to behave differently when using this version of the MPI Standard** without changing the program's code.

18.1.1 Semantic Changes Starting in MPI-4.0

MPI_COMM_DUP and MPI_COMM_IDUP no longer propagate info hints from the input communicator to the output communicator. This behavior can be achieved using MPI_COMM_DUP_WITH_INFO and MPI_COMM_IDUP_WITH_INFO.

The default communicator where errors are raised when not involving a communicator, window, or file was changed from MPI_COMM_WORLD to MPI_COMM_SELF.

18.2 Additional Warnings

This section describes additional changes that could potentially cause a program that relies on the semantics described in a previous version of the MPI Standard to behave differently than with this version of MPI. The changes in this section are limited in scope and **unlikely to impact most programs**.

18.2.1 Warnings Starting in MPI-4.0

Impact only for tool-providers: most be prepared for longer names in MPI

The limit for length of MPI identifiers was removed. Prior to MPI-4.0, MPI identifiers were limited to 30 characters (31 with the profiling interface). This limitation was initially introduced to avoid exceeding the limit on some compilation systems.

Annex B – Change-Log

New subsection in each MPI version

18.x.1 Fixes to Errata in Previous Versions of MPI

Some future MPI-4.1 / 5.0 plans

Active Working Groups → Important efforts

- Collective, Communicators, Context, Persistent, Partitioned, Groups, Topologies
  → e.g. partitioned collectives, partitioned arrival / any / some
- Fault Tolerance
  → new chapter on User Level Failure Mitigation / Fault Tolerance (ULFM/FT)
- Hardware-Topologies
  → standardized levels for MPI_COMM_TYPE_HW_GUIDED
- Hybrid & Accelerator **See next slide**
- Languages → side documents (other timeline), e.g., for other bindings (e.g. C++, Python)
- Remote Memory Access → bug fixes **See next slides**
  → completely new API allowing, e.g., offloading to the network interface controller (NIC)
  → simplifying existing interface
  → MPI_WIN_SHARED_QUERY also for the shared memory-part of regular windows
- Semantic Terms
  → apply them to RMA; differentiation between a procedure and a specific call to it
  → Progress **See next slides**
- Sessions
  → Adding functionality for features currently supporting only for the World Model
  → e.g. dynamic resources, buffered send, …
- Tools → QMPI + handling introspection and debugging interface

See https://www.mpi-forum.org/mpi-41/

Hybrid & Accelerator

https://github.com/mpiwg-hybrid/hybrid-issues/wiki

- **Active Topics**
- Continuations proposal #6
- Clarification of thread ordering rules #117
- Integration with accelerator programming models:
  - Accelerator info keys #3
  - Stream/Graph Based MPI Operations #5
  - Accelerator bindings for partitioned communication #4
  - Partitioned communication buffer preparation (shared with Persistence WG) #264
- Asynchronous operations #585

Errata to MPI shared memory

Errata to MPI shared memory

- Problem with MPI-3.0 to MPI-4.0:
  The role of assertions in RMA synchronization used for direct shared memory accesses (i.e., without RMA calls) is not clearly defined!
  - Detected & communicated about March 01, 2015
  - Implications for **all RMA function on a shared memory window**:
    - **Users: Always use assert=0**
    - **Implementors: Always ignore the assert values**
    - **MPI Forum: Specify valid assertions for shared memory windows**

- MPI_Win_sync + any other process-to-process synchronization
  - Rules are unclear
  - AtoUsers in MPI-3.1/MPI-4.0, page 456 lines 22-29/ page 613 line 46 – 614 line 5
  - And through Example MPI-3.1/MPI-4.0, pages 468f/626f, Exa. 11.21/12.21

  → See next slides (skip them)

background

General MPI shared memory synchronization rules

(based on MPI-3.1/MPI-4.0, MPI_Win_allocate_shared, page 408/560, lines 43-47/22-26: ***“A consistent view …”***)

Defining	Proc 0	Proc 1			Proc 0		Proc 1
	Sync-from →	Sync-to		**being**	MPI_Win_post[1]	→	MPI_Win_start[1]
				or	MPI_Win_complete[1]	→	MPI_Win_wait[1]
				or	MPI_Win_fence[1]	↔	MPI_Win_fence[1]
				or	MPI_Win_sync Any-process-sync[2]	→	Any-process-sync[2] MPI_Win_sync
				or[3]	MPI_Win_unlock[1]	→	MPI_Win_lock[1]

and the lock on process 0 is granted first

and A, B, C are shared variables

and having …		**then it is guaranteed that …**
A=val_1 Sync-from → Sync-to load(A)	⇒	**… the load(A) in P1 loads val_1** (this is the write-read-rule)
load(B) Sync-from → Sync-to B=val_2	⇒	**… the load(B) in P0 is not affected by the store of val_2 in P1** (read-write-rule)
C=val_3 Sync-from → Sync-to C=val_4 load(C)	⇒	**… that the load(C) in P1 loads val_4** (write-write-rule)

See next slide

[1] Must be paired according to the general one-sided synchronization rules.
[2] "Any-process-sync" may be done with methods from MPI (e.g. with send→recv as in MPI-3.1/MPI-4.0 Example 11/12.21, but also with some synchronization through MPI shared memory loads and stores, e.g. with C++11 atomic loads and stores).
[3] No rule for MPI_Win_flush (according current forum discussion)

background

"Any-process-sync" & MPI_Win_sync on shared memory

- If the shared memory data transfer is done without RMA operation, then the synchronization can be done by other methods.
- This example demonstrates the rules for the unified memory model if the **data transfer** is implemented **only with load and store** (instead of MPI_Get or MPI_Put)
- and the **synchronization** between the processes is done **with MPI communication** (instead of RMA synchronization routines).

→ See Exercise 3

```
Process A                         Process B
MPI_WIN_LOCK_ALL(                 MPI_WIN_LOCK_ALL(
MPI_MODE_NOCHECK,win)             MPI_MODE_NOCHECK,win)
DO ...                            DO ...
 X=...
 MPI_F_SYNC_REG(X) 1)
 MPI_Win_sync(win)
 MPI_Send
                                   MPI_Recv
                                   MPI_Win_sync(win)
                                   MPI_F_SYNC_REG(X) 1)
                                   local_tmp = X
                                   MPI_F_SYNC_REG(X) 1)
                                   MPI_Win_sync(win)
                                   MPI_Send
                                   print local_tmp
 MPI_Recv
 MPI_Win_sync(win)
 MPI_F_SYNC_REG(X) 1)
                                           1) Fortran only.
END DO                            END DO
MPI_WIN_UNLOCK_ALL(win)           MPI_WIN_UNLOCK_ALL(win)
```

X is part of a shared memory window and should be **the same** memory location **in both processes**.

A new value is **written** in X

For MPI_WIN_SYNC, a passive target epoch is established with **MPI_WIN_LOCK_ALL**.

Data exchange in this direction, therefore **MPI_Win_sync** is needed in both processes: **Write-read-rule**

Message telling that X is filled

MPI_WIN_SYNC acts only locally as a processor-memory-fence.

X is **read** out

Message telling that X is read out and can be refilled

2nd pair of MPI_Win_sync is needed to guarantee the **read-write-rule**

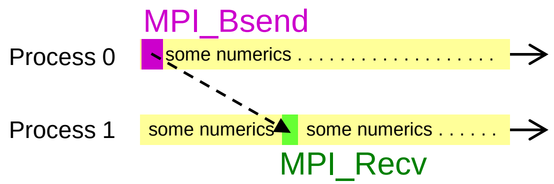
At begin of next iteration: Next **write** of X

Is missing in MPI-3.1/MPI-4.0, pages 468f/626f, Exa. 11/12.21 (i,.e., page 469/627, line 31/14)

Progress text / functionality update → delayed until MPI-5

What is progress

- To internally finish a started operation
  - the process that started the operation, and/or other related processes may need to make **progress** from the viewpoint of the underlying MPI system.
  - Example:
    - **Process 1:** Operation MPI receive, e.g., started with MPI_Recv or MPI_Irecv
    - **Process 0:** Is other related process
      - Called MPI_Bsend, already returned,
      - but data still buffered (from the viewpoint of the underlying MPI system)
    - **That process 1 can internally finish the receive operation, process 0 needs to make progress, i.e., to really send the buffered data**



- Which rules apply that process 0 provides progress? See next slide

Use cases for nonblocking operations

- Real overlapping of
  - several communications
  - communication and computation

General progress rule of MPI

- MPI is mainly defined in a way that **progress** on communication (and …) is **required only during MPI procedure calls.**
- But then, progress is required
  - for **all** outstanding (incomplete/nonblocking) communications
  - together with operation of the current communication (…) procedure call.
- See, e.g., in MPI-4.0
  - Sect. 3.5, page 54, and 3.7.4, page 75; Paragraphs "Progress", esp. progress of repeated MPI_Test, p.$75_{38\text{-}40}$
  - Sect. 3.8.1 and 3.8.2 about MPI_(I)(M)PROBE
  - Sect. 3.8.4 Cancel, esp. page 94 lines 8-16 & MPI_Finalize Example 11.6, page $496_{26\text{-}48}$ & MPI_Session_finalize, esp. page $502_{30\text{-}47}$ and Example 11.8 on page 503
  - Sect. 4.2.2 MPI_Parrived: Same progress rule as for repeated MPI_Test, see page $111_{31\text{-}34}$
  - Sect. 5.12: Nonblocking collectives: Same rules as for nonblocking pt-to-pt
  - Sect. 12.7.3: Progress with one-sided communication, especially the **rationale at the end**
  - Sect. 11.6: MPI and Threads
  - Sect. 14.6.3: Progress with MPI-I/O
- Non of these rules require progress outside of called MPI routines,
  - But MPI_Test and each MPI routine that blocks must do progress on any ongoing (i.e. nonblocking) communication
- Additional progress
  - By several calls to MPI_Test(), which enables progress
  - Use non-standard extensions to switch on asynchronous progress
    - E.g., with MPICH: export MPICH_ASYNC_PROGRESS=1

Implies a helper thread and MPI_THREAD_MULTIPLE (?)

Progress / weak local

An MPI procedure is **non-local** if returning may require, during its execution, some *specific* semantically-related MPI procedure to be called on another MPI process.

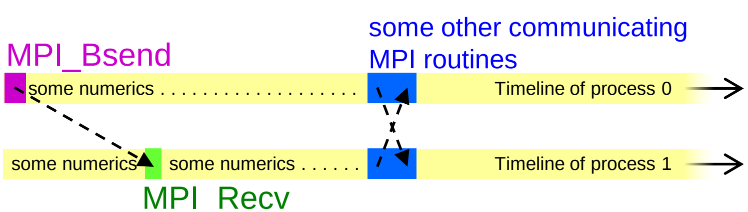
An MPI procedure is **local** if it is not *non-local*.

- Local MPI procedures may be implemented as *"weak local"*:
  - To complete its work locally, it may require an *unspecific* MPI call on another process

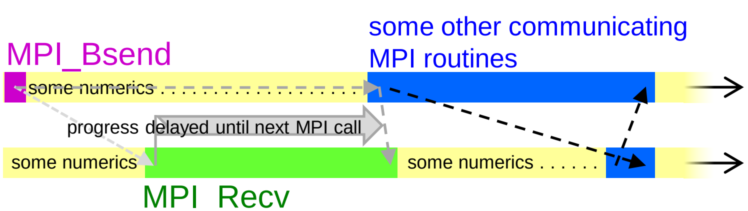
Normally perfect ☺
Always correct ☺
But may also lead to negative surprises ☹

- Examples (always tested with **large** messages):
  - Bsend is local.
    - **Corresponding MPI_Recv may require progress in the sending process ➔ may be blocked until the sending process calls another unspecific MPI procedure**

Progress happens **independent from** / …

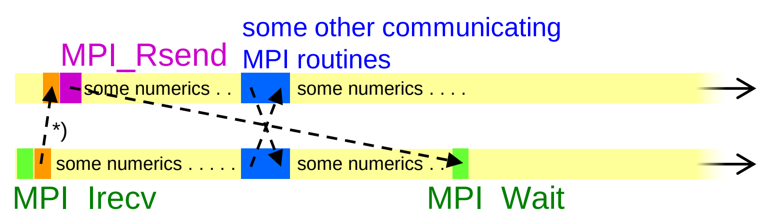


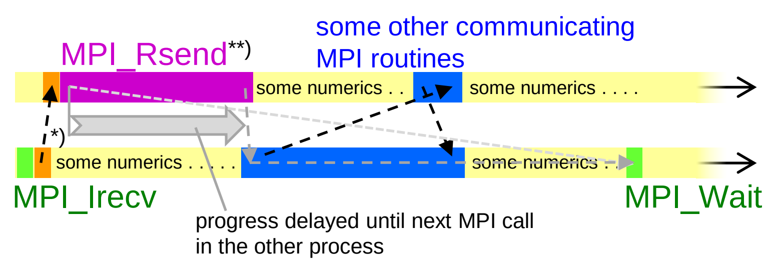
… / **only within MPI calls**



Experiments, see
MPI/tasks/**C/Ch18**/progress-test-**b**send.c + progress-test-**b**send-output.txt
progress-test-**r**send.c + progress-test-**r**send-output.txt

- Rsend is local, since the corresponding MPI_(I)Recv must already be called.
  - **But the MPI_Rsend may require progress in the receiving process ➔ may be blocked until the receiving process calls another unspecific MPI routine**





*) Additional communication that guarantees that MPI_Rsend is called after the corresponding MPI_Irecv is already started.
**) Same for MPI_Ssend and MPI_Send.

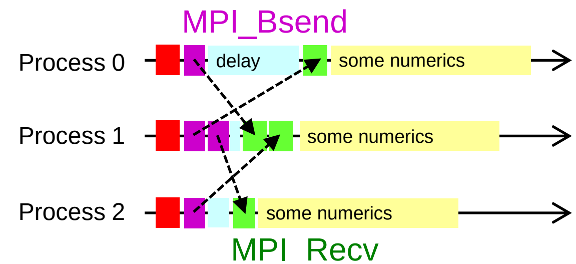
Possible consequences with MPI_Bsend

MPI/tasks/C/Ch18/progress-test-bsend-3-processes.c

```
MPI_Buffer_attach(…)
MPI_Barrier(…);           ← Only for starting the experiment together
for (iter=1; iter <=3; iter++ ){
  if(my_rank>0)              MPI_Bsend(…, my_rank-1, …);
  if(my_rank<numprocs-1) MPI_Bsend(…, my_rank+1, …);
  sleep(…);  // some small delay
  if(my_rank>0)              MPI_Recv (…, my_rank-1, …);
  if(my_rank<numprocs-1) MPI_Recv (…, my_rank+1, …);
  sleep(20); // simulating 20 sec of numerical work
}
MPI_Barrier(…);
MPI_Buffer_detach(…)
```

Not needed because the blocking non-collective buffer detach would cause the same result

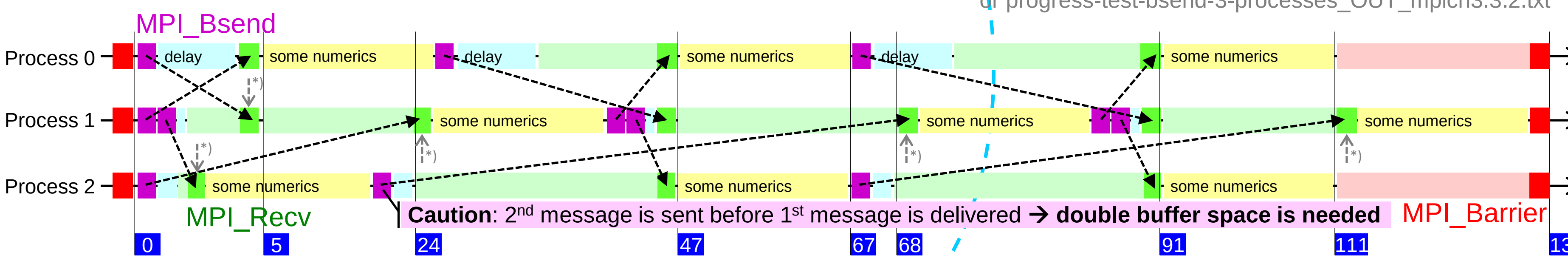
Expected behavior with independent progress



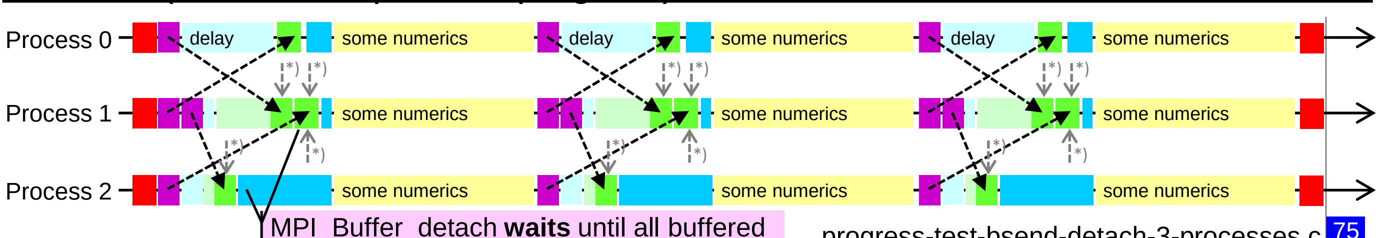
Newer versions, e.g. OpenMPI **3**.1.6, have partially fixed the reported problem, but portable applications should still be aware of it. See progress-test-bsend-3-processes_OUT_openmpi3.1.6_COMMENTED.txt

Real behavior without independent progress

(timing of 1st experiment, see progress-test-bsend-3-processes_OUT_openmpi2.1.6.txt or progress-test-bsend-3-processes_OUT_mpich3.3.2.txt)



Solution (without independent progress): add buffer detach/attach before numerics



The programs and protocols contain also a 2nd experiment:

It is without the "*small delays*" and reports 120 sec vs. 60 sec, i.e., **two times slower** without detaching + re-attaching the buffer after each comm. step

*) The receive of the buffered message is delayed until another unspecific MPI call in the sending process can implement the data transfer: MPI_Recv or MPI_Buffer_detach (2nd example).

MPI Progress Rule

Of course,
more progress is always allowed!
E.g., through a progress thread ☺

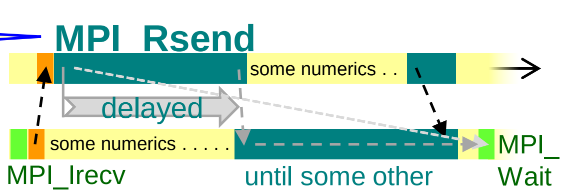
- MPI library must provide the following **minimal** progress:
  1. ***Blocked MPI procedure calls*** must provide progress on **all** enabled MPI operations.
  2. Test procedures will eventually return flag=true once the matching operation has been started:
     - **MPI_Test, MPI_Iprobe, MPI_Improbe,**
     - **MPI_Request_get_status, MPI_Win_test (specification is missing in MPI-3.1/MPI-4.0, may be clarified in MPI-4.1)**
     - **MPI_Parrived (new procedure in MPI-4.0)**
  3. MPI finalization must guarantee that all required progress will be provided before the process exits.
  4. Further rules, e.g., on collectives, I/O, …

References in MPI-4.0:

1. Sect. 3.5, page 54, and 3.7.4, page 75. Paragraphs "Progress".
   Sect. 11.6: MPI and Threads.
   Sect. 12.7.3: Progress with one-sided communication, especially the rationale at the end.
2. Sect. 3.7.4 on MPI_Test, esp. p.75 $_{38\text{-}40}$
   Sect. 3.8.1 & 3.8.2: MPI_(I)(M)PROBE,
   Sect. 4.2.2 MPI_Parrived p. 111 $_{31\text{-}34}$
3. Sect. 3.8.4 Cancel, p. 94 lines 8-16.
   MPI_Finalize Example 11.6, p. 496 $_{26\text{-}48}$,
   MPI_Session_finalize, esp. p. 502 $_{30\text{-}47}$
   and Example 11.8 , p. 804
4. Sect. 5.12: Nonblocking Collectives.
   Sect. 14.6.3: MPI-I/O

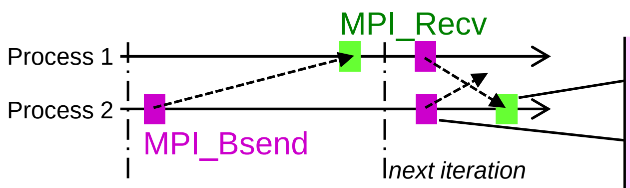
- ***A blocked MPI procedure call*** *can be:*
  - **Non-local MPI procedure**
    (e.g., MPI_Send, MPI_Recv, MPI_Wait for a receive/send request handle)
    waits for a specific semantically-related MPI call on another MPI process
    (e.g., MPI_(I)Recv, MPI_(I)Send, MPI_(I)Send / MPI_(I)Recv)
  - **Local MPI procedure** (see also references 3.)
    (e.g., MPI_Rsend)
    waits for some unspecific MPI call on another MPI process
    (e.g., any other MPI call that must do progress → see above 1. or 2. or 3
    but it may be also a related routine, e.g., the MPI_Wait in the example).

Blocked call



Progress / weak local – summary

- → In principle, program as if your MPI library provides independent progress
- → But weak progress can lead to very unexpected performance behavior
- → Hopefully fixed in many MPI libraries
- → MPI_THREAD_MULTIPLE instead of …_SINGLE usually makes no difference
  - – Test with progress-test-bsend_init.c & progress-test-bsend_init-thread-multiple.c
- → Nevertheless, make sure that your programs are correct & portable, e.g.:



Back to our ***loop(bsend left+right; recv left+right)*** example:
Only by receiving this (*response)* message, process 2 logically knows now (and not earlier) that its 1st message is received.
Therefore here (still without this knowledge), process 2 must have attached enough buffer space for both the 1st and 2nd message together.
This logical consideration is independent of weak or strong progress.

Weighted Cartesian Toplogies

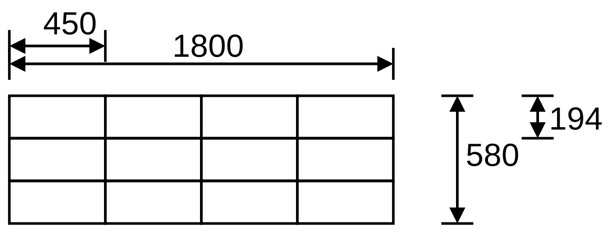
The problems

1. All MPI libraries provide the necessary interfaces ☺ ☺ ☺,
   but **without** re-numbering in nearly all MPI-libraries ☹ ☹ ☹
   - **You may substitute MPI_Cart_create() by Bill Gropp’s solution**
     William D. Gropp, Using Node [and Socket] Information to Implement MPI Cartesian Topologies, Parallel Computing, 2019, and in: Proceedings of the 25th European MPI User' Group Meeting, EuroMPI'18, ACM, New York, NY, USA, 2018, pp. 18:1-18:9. doi:10.1145/3236367.3236377. Slides: http://wgropp.cs.illinois.edu/bib/talks/tdata/2018/nodecart-final.pdf.
2. The existing MPI-3.1 and MPI-4.0 interfaces are not optimal
   – for cluster of ccNUMA node hardware,
     - We substitute MPI_Dims_create() + MPI_Cart_create()
       by MPIX_Cart_weighted_create(… MPIX_WEIGHTS_EQUAL …)

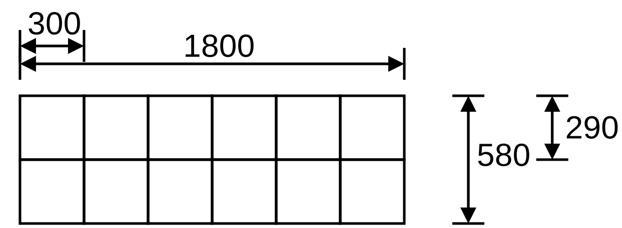
   – nor for application specific data mesh sizes
     or direction-dependent bandwidth
     - by MPIX_Cart_weighted_create(… weights ….)
3. Caution: The application must be prepared for rank re-numbering
   - All communication through the newly created
     Cartesian communicator with re-numbered ranks!
   - One must not load data based on MPI_COMM_WORLD ranks!

Examples

- Application topology awareness
  - 2-D example with 12 MPI processes and data mesh size 1800x580
    - **MPI_Dims_create → 4x3**
    - **data mesh aware → 6x2 processes**

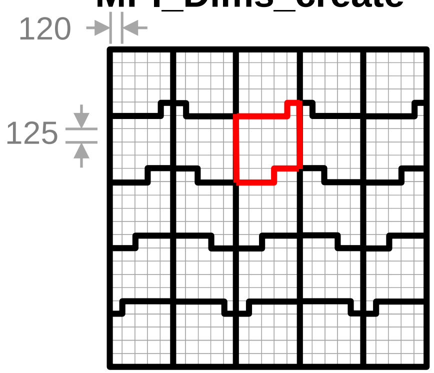


Boundary of a subdomain = 2(450+194) = **1288** ☹



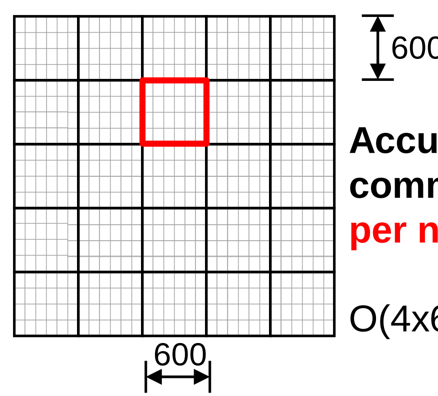
Boundary of a subdomain = 2(300+290) = **1180** ☺

- Hardware topology awareness
  - 2-D example with 25 nodes x 24 cores and data mesh size 3000x3000
    - **MPI_Dims_create → 25 x 24**
    - **Hardware aware → 30 x 20**
      = (5 nodes x 6 cores) X (5 nodes x 4 cores)



Accumulated communication per node

O(10x120+12x125)
= O(**2700**) ☹



Accumulated communication per node

O(4x600) = O(**2400**) ☺

Other small functionality / changes

Environment inquiry – implementation information (2)

Environmental inquiries

C

Fortran

Python

- C: MPI_Comm_get_attr(MPI_COMM_WORLD, keyval, *&p*, *&flag*)
  - Will return in *p* a pointer to an int containing the *attribute_val*
- Fortran: MPI_Comm_get_attr(MPI_COMM_WORLD, keyval, *attribute_val*, *flag*, *ierror*)
- Python: *attribute_val* = MPI.COMM_WORLD.Get_attr(keyval)

C: **pointer** based attributes
Fortran: **integer(kind=MPI_ADDRESS_KIND)** based attributes

- with keyval =
  - **MPI_TAG_UB**

    Python: MPI.TAG_UB

    → returns upper bound for tag values in *attribute_val*

    → must be at least 32767
  - **MPI_HOST**

    May be deprecates in MPI-4.1

    → returns host-rank (if exists) or MPI_PROC_NULL (if there is no host)
  - **MPI_IO**

    → returns MPI_ANY_SOURCE in *attribute_val* (if every process can provide I/O)
  - **MPI_WTIME_IS_GLOBAL**

    → returns 1 in *attribute_val* (if clocks are synchronized), otherwise, 0

Examples: see MPI-3.1, Sect. 17.2.7, page 664, line 43 – page 665, line 13 or
MPI-4.0, Sect. 19.3.7, page 852, line 29-47

Summary

MPI-4.0 has a lot **for better service / better performance**

- Large counts
- Sessions Model
- Better error handling
- More consistent standard:
  - Revisited terms & semantics
  - New introduction for nonblocking operations
  - Removed / Semantic changes & warnings / Errata

- Persistent collectives
- **Partitioned Point-to-Point Communication**
  → MPI + OpenMP
- New ways for hardware-based split of communicators
  → shared memory on ccNUMA domains instead of whole ccNUMA node
- Neighbor communication now usable
- Pt-to-pt assertion info for wildcards, message order not preserving, and using exact receive buffer count
- Nonblocking MPI_**I**sendrecv

Outlook on MPI-4.1 / 5.0