



# 703650 VO Parallel Systems WS2020/2021

## MPI Groups, Communicators and One-Sided Communication

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# Overview

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- ▶ communicators and groups
- ▶ one-sided communication
- ▶ error handling

# Motivation

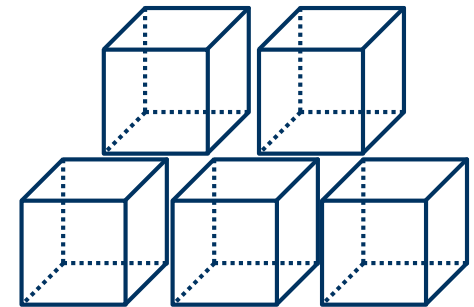
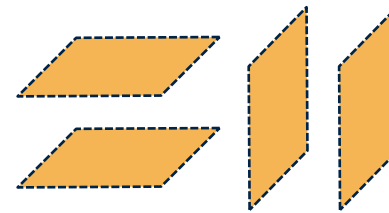
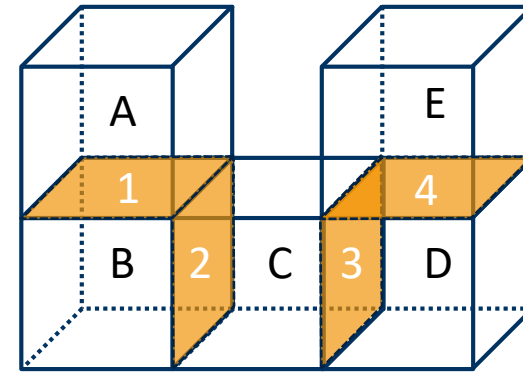
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- ▶ Real-world applications are rarely a single component
  - ▶ often MPMD
  - ▶ usually combination of libraries (e.g. molecular mechanics and linear algebra)
- ▶ Adds several new complexities compared to single-component software
  - ▶ collective communication via `MPI_COMM_WORLD`?
  - ▶ how to identify sub-programs?
  - ▶ how to specifically communicate between and within programs?
- ▶ And what about NUMA?
  - ▶ virtual topologies do not reflect e.g. shared memory address spaces

## Motivation cont'd

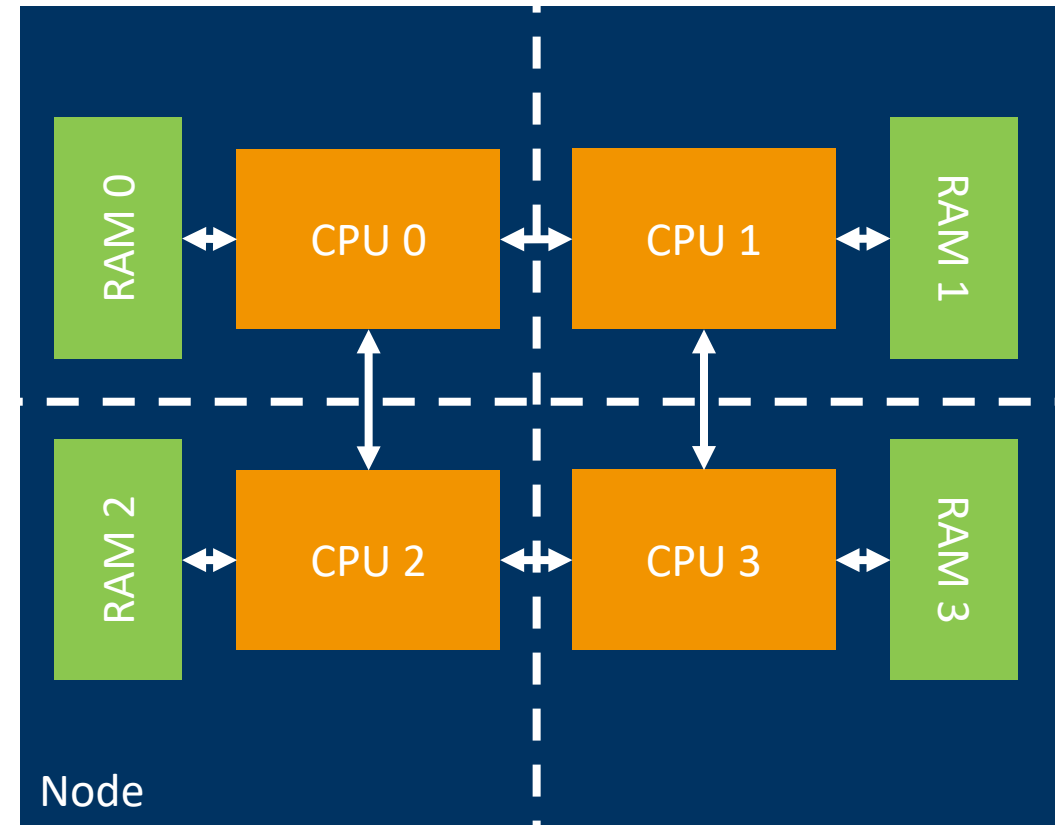
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- ▶ unstructured grid with cell and face element types
  - ▶ assume both require global communication among their types
- ▶ a communicator per element type would be useful
  - ▶ but how?



## Motivation cont'd

- ▶ consider shared memory node with 4 CPUs and many cores per CPU
- ▶ local collective communication among cores of a CPU is cheap
  - ▶ how to limit?
  - ▶ construct a communicator per CPU?
  - ▶ do this in hardware-independent way?



# Communicators and Groups

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- ▶ Communicators and groups hold sets of ranks
  - ▶ directly used for e.g. collective communication
  - ▶ also required for identifying single ranks
  - ▶ remember MPI basics lecture: everything in MPI is relative to a communicator or group
- ▶ Why not stick to `MPI_COMM_WORLD`?
  - ▶ isolate application sub-programs
    - ▶ individual processing steps (MPMD)
    - ▶ domain decomposition (SPMD, c.f. slicing Cartesian topologies)
    - ▶ libraries (portability)
  - ▶ usability
    - ▶ add user-defined attributes such as topologies
  - ▶ performance
    - ▶ re-numbering of ranks (virtual topology vs. hardware topology)

# Communicators and Groups cont'd

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## ▶ MPI\_Group

- ▶ holds ordered set of ranks
- ▶ ordering is given by mapping process identifier (e.g. PID) on rank number
- ▶ construction of and operations on groups are always **local** operations

## ▶ MPI\_Comm

- ▶ holds an MPI\_Group
  - ▶ transitively holds ordered set of ranks
- ▶ can hold attributes (e.g. topology)
- ▶ constructed from groups
- ▶ construction of communicators are **global** operations

# Operations on MPI\_Group

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## ► Constructors

- MPI\_Comm\_group(...)
- MPI\_Group\_union(...)
- MPI\_Group\_intersection(...)
- MPI\_Group\_difference(...)
- MPI\_Group\_incl(...)
- MPI\_Group\_excl(...)
- MPI\_Group\_range\_incl(...)
- MPI\_Group\_range\_excl(...)

## ► Accessors

- MPI\_Group\_size(...)
- MPI\_Group\_rank(...)
- MPI\_Group\_compare(...)
  - result is MPI\_IDENT, MPI\_SIMILAR or MPI\_UNEQUAL

## ► Destructors

- MPI\_Group\_free(...)



# Operations on MPI\_Comm

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## ► Constructors

- MPI\_Comm\_dup(...)
- MPI\_Comm\_create(...)
- MPI\_Comm\_split(...)
- Convenience constructors such as MPI\_Cart\_sub(...)

## ► Accessors

- MPI\_Comm\_size(...)
- MPI\_Comm\_rank(...)
- MPI\_Comm\_compare(...)
  - result is MPI\_IDENT, MPI\_SIMILAR, MPI\_CONGRUENT or MPI\_UNEQUAL

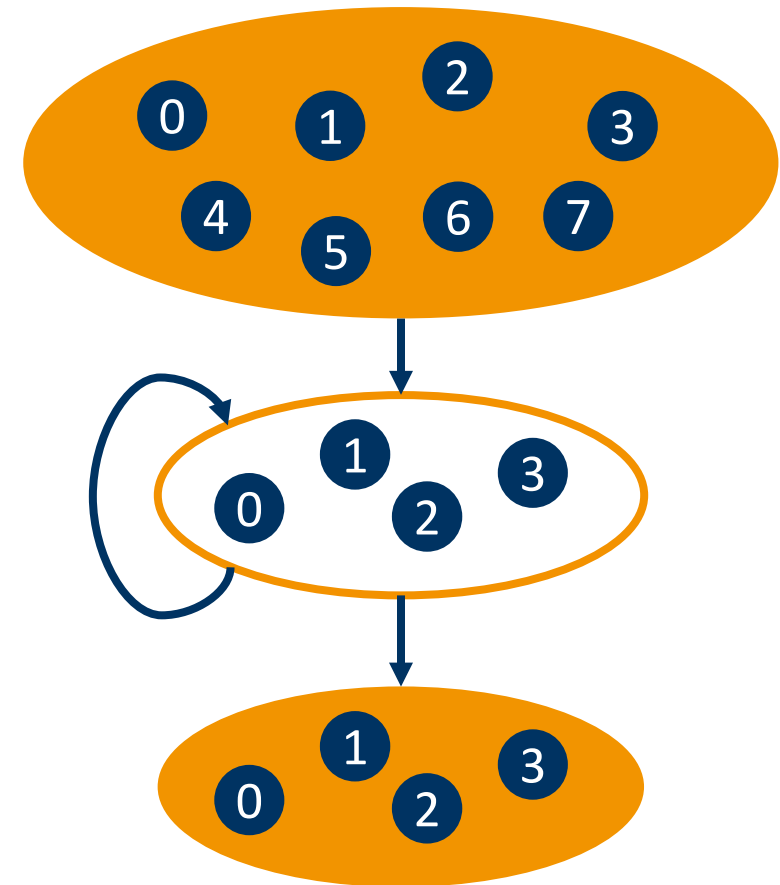
## ► Destructors

- MPI\_Comm\_free(...)

# Group and Communicator Workflow

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- ▶ start with `MPI_COMM_WORLD`
- ▶ construct group(s) of rank subsets and modify as required
  - ▶ `MPI_Group_union()`,  
`MPI_Group_range_incl()`, ...
- ▶ create new communicator from group and use for communication



# Splitting Communicators

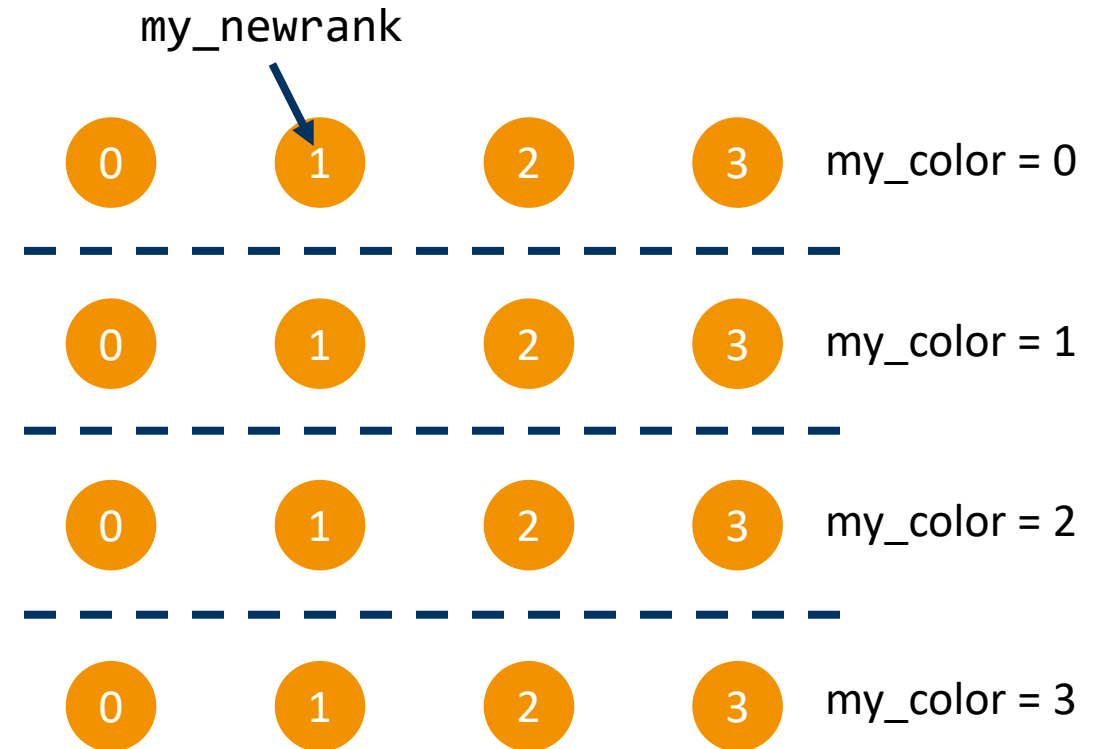
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- ▶ `int MPI_Comm_split(MPI_Comm comm, int color, int key, MPI_Comm* newcomm)`
  - ▶ `comm`: current communicator
  - ▶ `color`: control of subset assignment (same color: same new communicator)
  - ▶ `key`: control of rank assignment (0: sorted as in `comm`; otherwise according to ascending key values)
  - ▶ `newcomm`: new communicator
- ▶ `MPI_Comm_split_type(...)`
  - ▶ allows to split dependent on hardware properties

# MPI\_Comm\_split Example

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```
MPI_Comm newComm;  
MPI_Comm_rank(MPI_COMM_WORLD, &myRank);  
int myColor = myRank / 4;  
MPI_Comm_split(MPI_COMM_WORLD, myColor,  
               myRank, &newComm);  
MPI_Comm_rank(newComm, &newRank);
```



## Solutions to Motivation Examples

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```
MPI_Comm newComm;  
MPI_Comm_rank(MPI_COMM_WORLD, &rank);  
int color =  
    (elementType == TYPE_FACES);  
MPI_Comm_split( MPI_COMM_WORLD,  
    color, rank, &newComm);
```

```
MPI_Comm newComm;  
MPI_Comm_rank(MPI_COMM_WORLD, &rank);  
MPI_Comm_split_type( MPI_COMM_WORLD,  
    MPI_COMM_TYPE_SHARED, rank,  
    MPI_INFO_NULL, &newComm);  
// also: OMPI_COMM_TYPE_CORE,  
// OMPI_COMM_TYPE_L1CACHE,  
// OMPI_COMM_TYPE_L2CACHE,  
// OMPI_COMM_TYPE_L3CACHE, ...
```

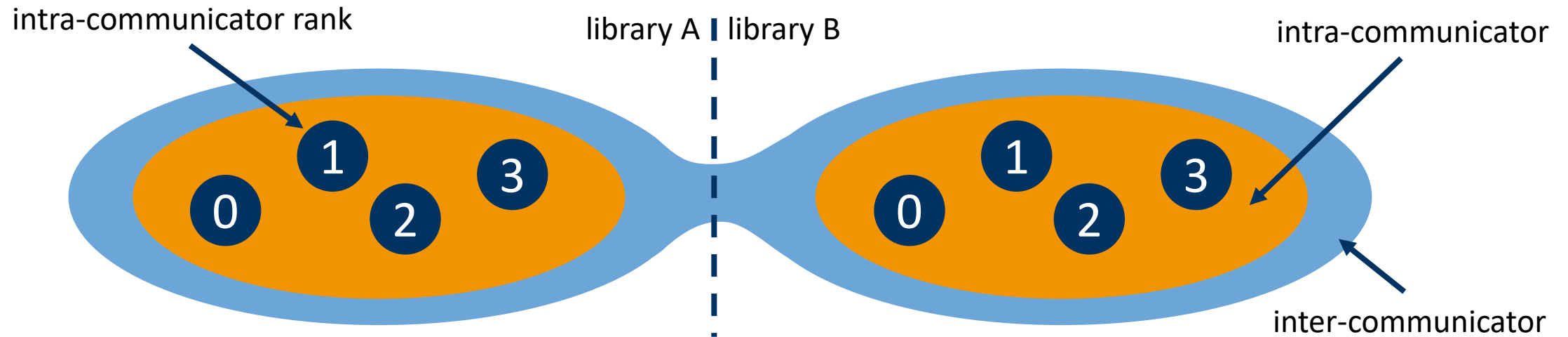
# Intra- and Inter-Communicators

## ▶ intra-communicator

- ▶ collection of ranks that can send messages to each other via point-to-point and collectives
- ▶ e.g. `MPI_COMM_WORLD`

## ▶ inter-communicator

- ▶ collection of ranks from disjoint intra-communicators
- ▶ allows sending messages between communicators





## One-sided Communication



# Motivation

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- ▶ message-passing paradigm
  - ▶ fits distributed memory systems well
  - ▶ data transfers among distinct address spaces require network communication
  - ▶ requires explicit communication
  - ▶ little control over message aggregation
- ▶ shared memory paradigm
  - ▶ no message passing required
  - ▶ data transfer aggregation possible – write multiple bytes, elements, ... in one go
  - ▶ much more convenient from a user and performance perspective
    - ▶ does not necessarily require receiving side to participate
  - ▶ also, messages are needless overhead on shared-memory systems
    - ▶ sending/receiving messages just for writing to a different memory address in the same address space?



# MPI's Solution: One-sided Communication

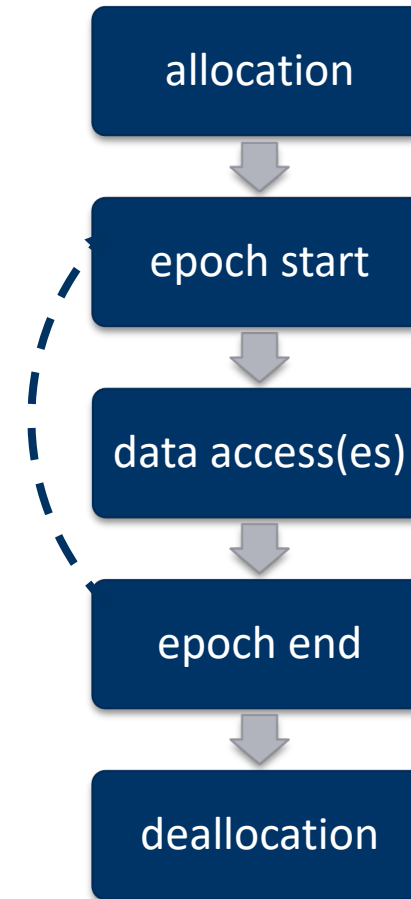
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- ▶ classic point-to-point (*“two-side”*) communication implies synchronization
  - ▶ at every data transfer action
  - ▶ incurs a lot of overhead in the presence of many messages
- ▶ one-sided communication decouples data movement and synchronization
  - ▶ ranks expose a *“window”* of rank-local memory
  - ▶ can be accessed by other ranks using remote memory access (RMA)
  - ▶ data accesses do not necessarily require action on the rank exposing memory
  - ▶ both read and write are possible
    - ▶ ranks no longer identify as *“sender”* and *“receiver”* but as *“origin”* and *“target”* instead

# One-sided Communication Workflow

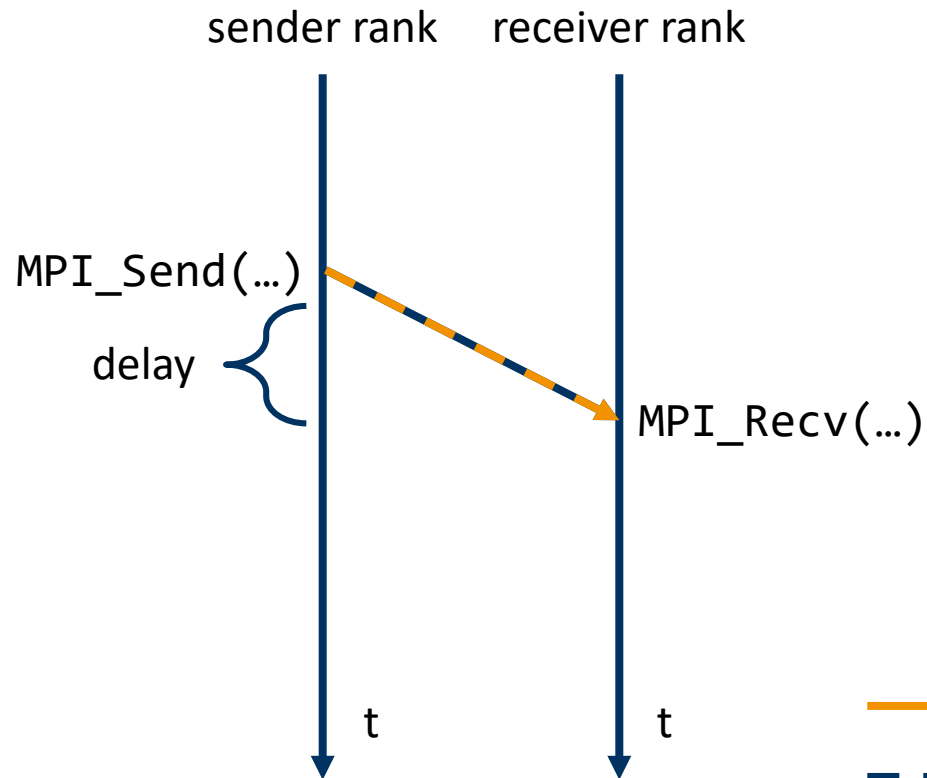
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- ▶ allocate buffer and window
  - ▶ can ask MPI to allocate fast memory
- ▶ open window (*“start epoch”*)
  - ▶ synchronization point
  - ▶ allows data access by remote ranks
- ▶ close window (*“end epoch”*)
  - ▶ synchronization point
  - ▶ commits data accesses
- ▶ deallocate window and buffer

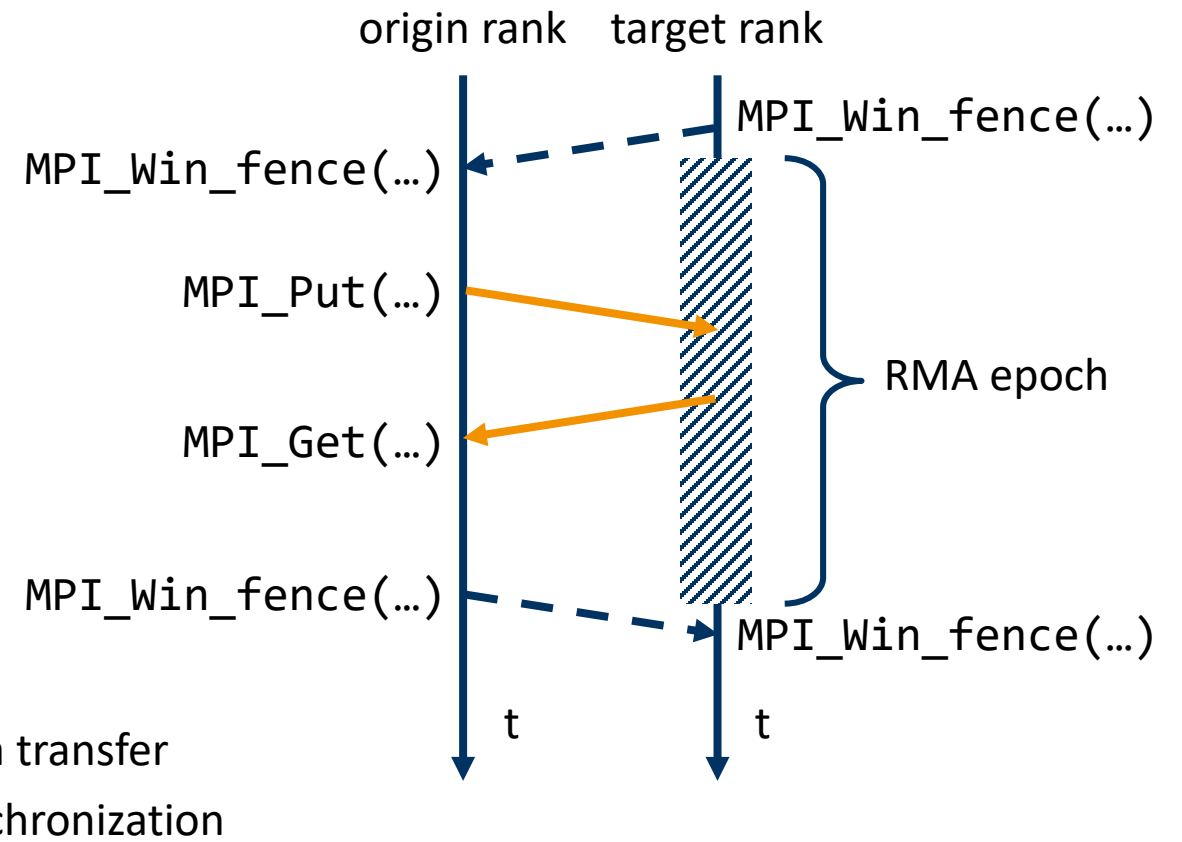


# MPI One-sided Communication cont'd

## ► two-sided



## ► one-sided



# Means of Synchronization

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## ▶ active target synchronization

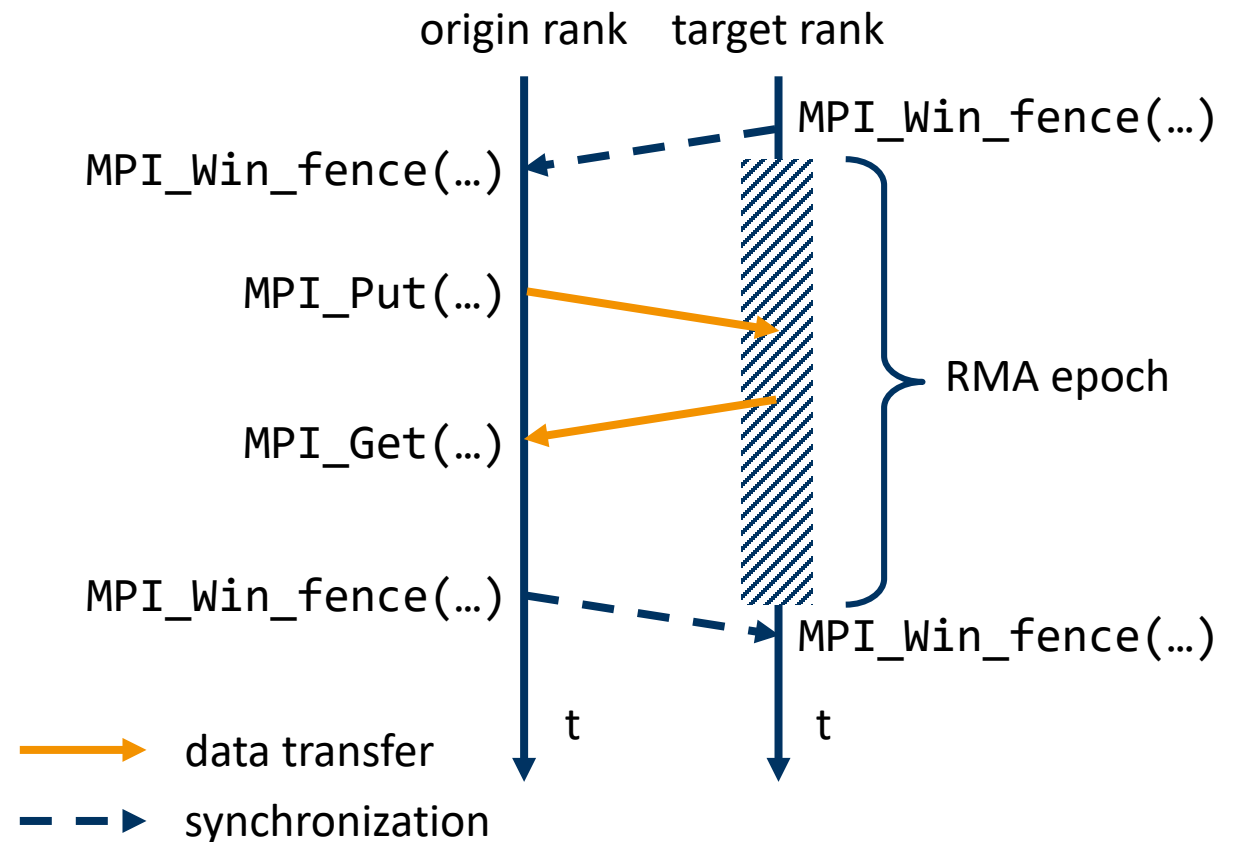
- ▶ target participates in synchronization
- ▶ similar to message-passing paradigm
- ▶ uses `MPI_Win_fence()` or `post-start-complete-wait`
- ▶ works well for bulk-synchronous parallel programs
  - ▶ e.g. structured grid with ghost cell exchange

## ▶ passive target synchronization

- ▶ target does not synchronize
- ▶ similar to shared memory paradigm
- ▶ uses `MPI_Win_lock()` and `MPI_Win_unlock()`
- ▶ works well for dynamic, independent access patterns

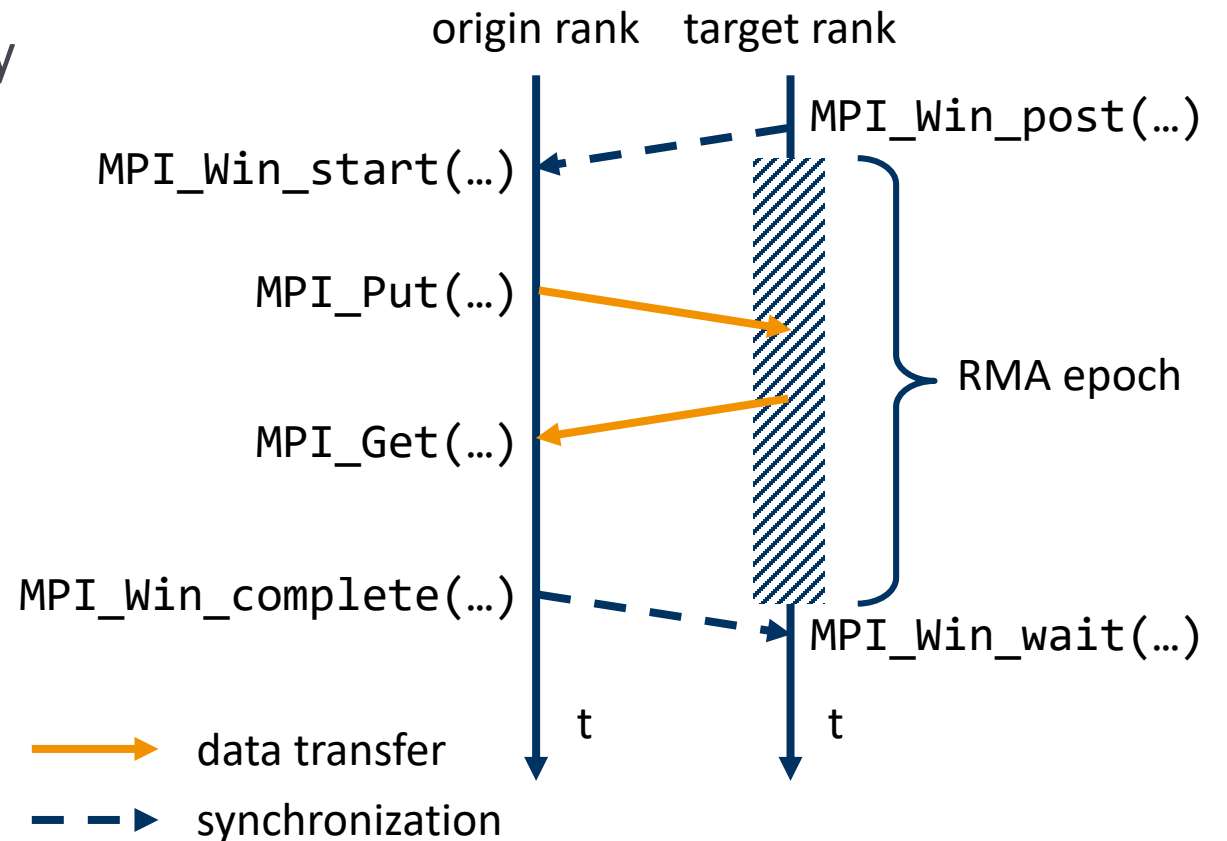
# Active Target Synchronization: Fence

- ▶ collective synchronization
  - ▶ origin/target not specified
- ▶ all control the epoch
  - ▶ starts/ends all epochs on all participating ranks
- ▶ fence enforces synchronization



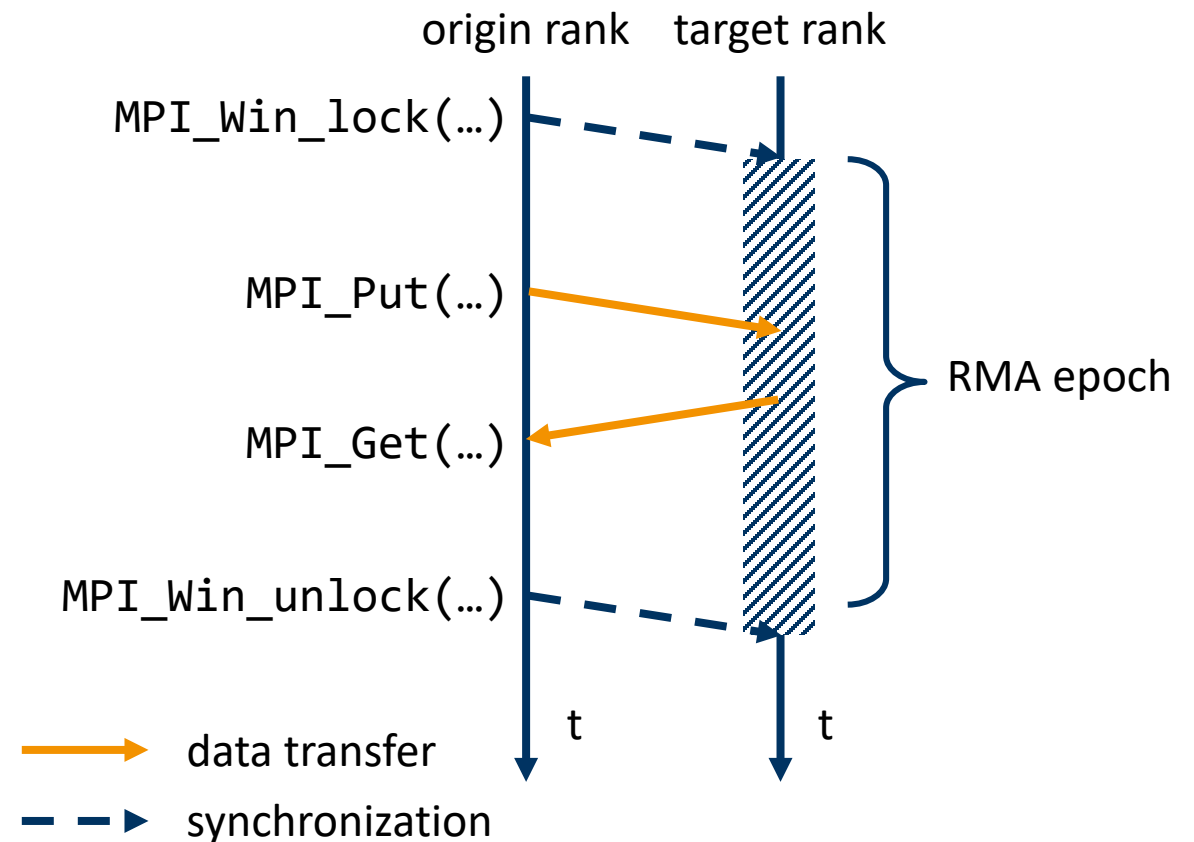
# Active Target Synchronization: Post/Start/Complete/Wait

- ▶ selective synchronization
  - ▶ origin and target specify a group they communicate with
- ▶ both control their epochs
  - ▶ origin: start/complete
  - ▶ target: post/wait
- ▶ synchronization calls may block to enforce ordering



## Passive Target Synchronization: Lock/Unlock

- ▶ target neither involved in data transfer, nor in synchronization
- ▶ origin has full control over epoch
- ▶ resembles shared memory programming models (e.g. Pthreads, std::mutex, ...)
  - ▶ but not the same
  - ▶ no critical section!



# Implications of One-sided Communication

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## ▶ several benefits

- ▶ allows dynamic access patterns (e.g. when target rank does not know number and ranks of origins)
- ▶ reduce synchronization overhead for multiple data transfers
- ▶ reduce management overhead on receiver side (e.g. tag matching)
- ▶ performance gain
- ▶ reduce coding effort on receiver side

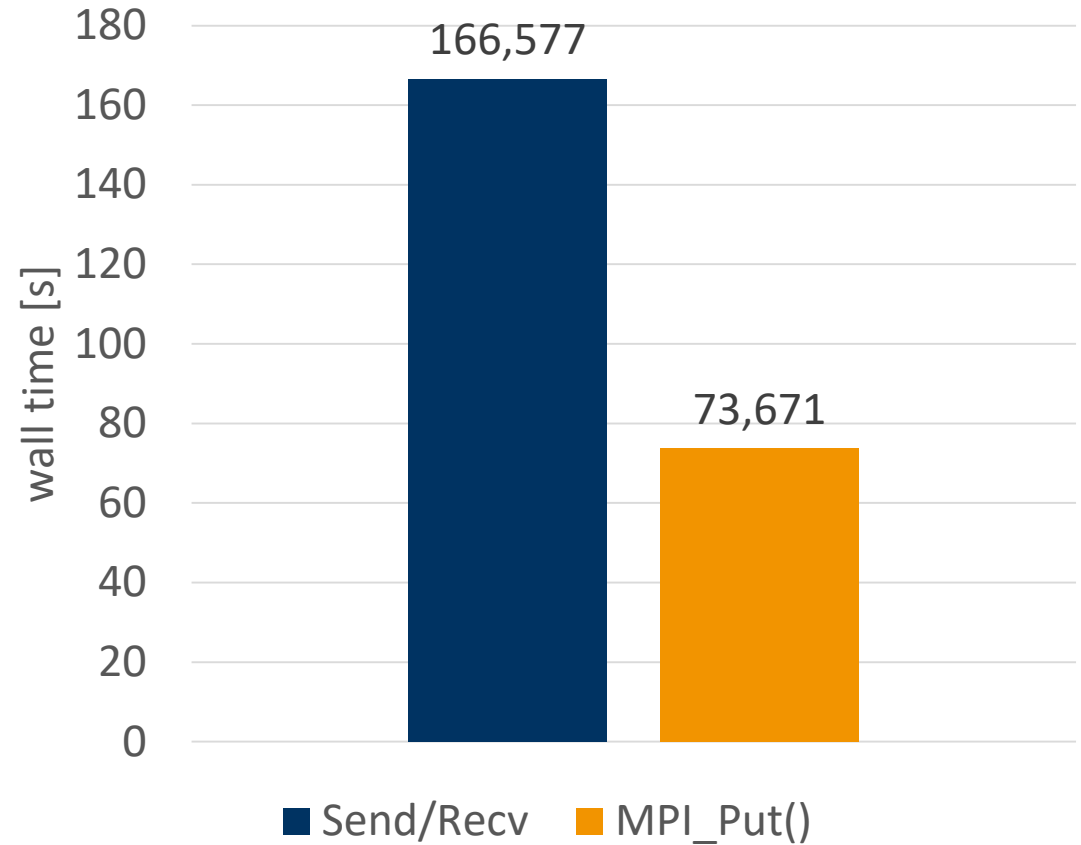
## ▶ drawbacks

- ▶ no send/receive matching
- ▶ operations are not explicitly visible on the receiver side
- ▶ user often responsible for correct order of reads/writes (race conditions)
- ▶ only non-blocking communication



# Performance Comparison

- ▶ LCC2, openmpi/3.1.1  
openmpi-1perhost 2
- ▶ rank 0 sends  $10^8$  int to rank 1
  - ▶ once using plain  $10^8$  send/recv calls
  - ▶ once using  $10^8$  MPI\_Put() calls with MPI\_Fence() synchronization
- ▶ execution time reduced by 2.26x
  - ▶ only between two ranks
  - ▶ but an edge case stress test



## Optional Window Fence Assertions

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- ▶ **MPI\_MODE\_NOSTORE**
  - ▶ local window was not updated by local store, local get or receive calls since last fence
- ▶ **MPI\_MODE\_NOPUT**
  - ▶ local window will not be updated by put or accumulate until next fence
- ▶ **MPI\_MODE\_NOPRECEDE**
  - ▶ fence does not complete any sequence of locally issued RMA calls
- ▶ **MPI\_MODE\_NOSUCCEED**
  - ▶ fence does not start any sequence of locally issued RMA calls
- ▶ none of these are required, but they can improve performance

# Four Window Models

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- ▶ `MPI_Win_create(...)`
  - ▶ private memory buffer already allocated, use as window
- ▶ `MPI_Win_allocate(...)`
  - ▶ allocate buffer and use as window
- ▶ `MPI_Win_create_dynamic(...)`
  - ▶ expose a buffer which is not available yet
  - ▶ use later with `MPI_Win_attach()/MPI_win_detach()`
- ▶ `MPI_Win_allocate_shared(...)`
  - ▶ allocate and use buffer in shared memory segment of the OS
  - ▶ only works for `MPI_COMM_TYPE_SHARED`

# Transferring Data: Put & Get

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- ▶ `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)`
  - ▶ `origin_addr`: local address of data to put
  - ▶ `origin_count`: number of elements on origin side
  - ▶ `origin_datatype`: type of elements on origin side
  - ▶ `target_rank`: rank of target process
  - ▶ `target_disp`: offset of target address to base address of target window
  - ▶ `target_count`: number of elements on target side
  - ▶ `target_datatype`: type of elements on target side
  - ▶ `win`: window handle
  
- ▶ `MPI_Get(...)`
  - ▶ transfer data from target to origin

## Transferring Data: Accumulate

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### ▶ `MPI_Accumulate(...)`

- ▶ transfer data from origin and accumulate atomically at target
- ▶ can only use predefined operations of `MPI_Reduce(...)` (e.g. `MPI_SUM`)
- ▶ use `MPI_REPLACE` to get atomic put

### ▶ `MPI_Get_accumulate(...)`

- ▶ same as `MPI_Accumulate(...)` but store target buffer data in result buffer before accumulating
- ▶ use with `MPI_NO_OP` to get atomic get or `MPI_REPLACE` to get atomic swap

# Transferring Data: Single-element Atomics

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- ▶ `MPI_Compare_and_swap(...)`
  - ▶ atomic swap if data at target buffer matches comparison value
  - ▶ must be single element
  - ▶ must be predefined integer, logical or byte type
- ▶ `MPI_Fetch_and_op(...)`
  - ▶ variant of `MPI_Get_accumulate(...)`, available for hardware optimization
  - ▶ must be single-element
  - ▶ must be predefined data type

# MPI One-sided Communication Example

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```
// rank 0
MPI_Win window;
int buffer[SIZE] = ... ;
MPI_Win_create(&buffer, sizeof(int)*SIZE,
    sizeof(int), MPI_INFO_NULL,
    MPI_COMM_WORLD, &window);
MPI_Win_fence(MPI_MODE_NOSTORE |
    MPI_MODE_NOPUT | MPI_MODE_NOPRECEDE,
    window);
MPI_Put(&buffer, SIZE, MPI_INT, 1, 0,
    SIZE, MPI_INT, window);
MPI_Win_fence(MPI_MODE_NOSTORE |
    MPI_MODE_NOPUT | MPI_MODE_NOSUCCEED,
    window);
MPI_Win_free(&window);
```

```
// rank 1
MPI_Win window;
int buffer[SIZE] = { 0 };
MPI_Win_create(&buffer, sizeof(int)*SIZE,
    sizeof(int), MPI_INFO_NULL,
    MPI_COMM_WORLD, &window);
MPI_Win_fence(MPI_MODE_NOSTORE |
    MPI_MODE_NOPRECEDE |
    MPI_MODE_NOSUCCEED, window);
// window open, buffer is being written to
MPI_Win_fence(MPI_MODE_NOPUT |
    MPI_MODE_NOPRECEDE |
    MPI_MODE_NOSUCCEED, window);
// use buffer here
MPI_Win_free(&window);
```

# RMA Semantics

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- ▶ order of Get and Put/Accumulate is not guaranteed
  - ▶ race condition
  - ▶ same for multiple Put operations (use Accumulate instead)
- ▶ no local access to window during access epoch
  - ▶ use an RMA operation if absolutely required
- ▶ local vs. remote completion of operation
  - ▶ no send buffer re-use after Put until end of access epoch
- ▶ no concurrent passive synchronization epochs to same target
  - ▶ only relevant in multi-threading context
- ▶ lot's of MPI fence optimizations
  - ▶ where to place, which assertions to use

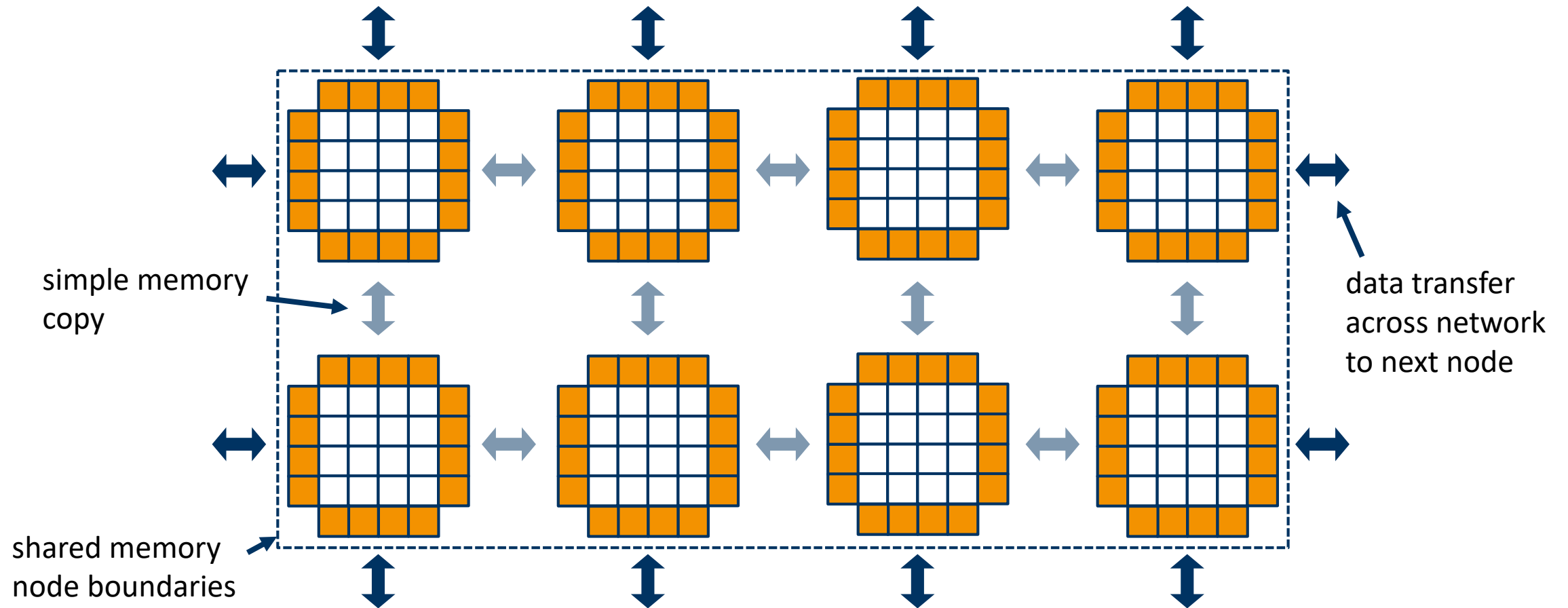


# Shared-memory One-sided Communication

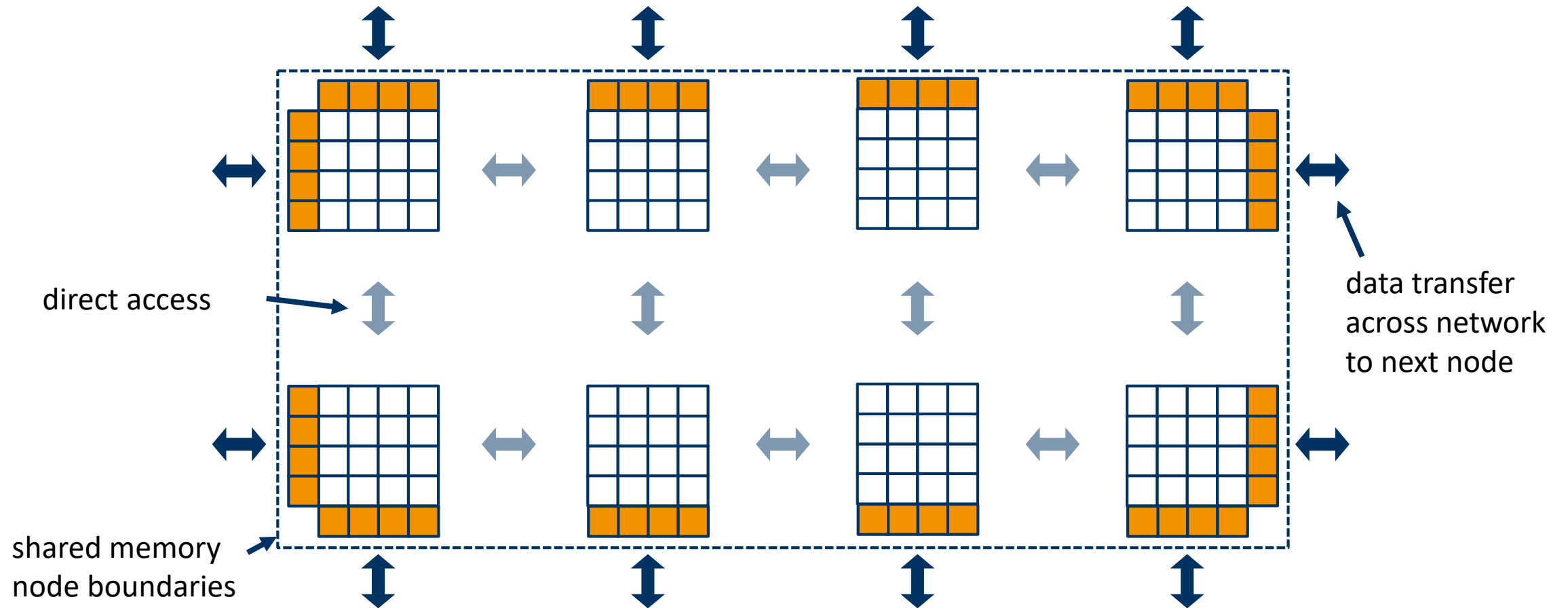
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- ▶ one-sided communication also available in a truly shared memory fashion
  - ▶ origin of data transfer will get a pointer to access target memory
  - ▶ naturally only works for ranks in the same physical address space
  - ▶ c.f. POSIX shared memory segments
- ▶ allows to share memory between ranks
  - ▶ reduces memory footprint (e.g. no extra buffer for ghost cell exchange of a stencil)
  - ▶ even more efficient for intra-node communication than one-sided communication

# Ghost Cell Exchange (Message Passing in Shared Memory)



# Ghost Cell Exchange (MPI Shared Memory Access)



## Example for Shared Memory One-Sided Communication

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```
MPI_Comm_split_type(MPI_COMM_WORLD, MPI_COMM_TYPE_SHARED,  
    0, MPI_INFO_NULL, &comm_sm);  
MPI_Win_allocate_shared((MPI_Aint)(sizeof(int)),  
    sizeof(int), MPI_INFO_NULL, comm_sm, &rcv_buf_ptr,  
    &win);  
MPI_Win_fence(0, win);  
*rcv_buf_ptr = ...; // replaces the MPI_Put() call!  
MPI_Win_fence(0, win);  
MPI_Win_free(&win);
```

# MPI and Multithreading

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- ▶ one-sided shared memory communication can become quite complex
  - ▶ there are alternatives: MPI + OpenMP or `std::thread` or Pthreads or TBB or ...
  - ▶ these are known as *hybrid programming models*
  - ▶ both paradigms have their ups and downs (number of programming models, compiler support, ...)
- ▶ MPI+threads needs to be supported by MPI, indicated by one of four safety levels
  - ▶ `MPI_THREAD_SINGLE`: only a single thread per rank
  - ▶ `MPI_THREAD_FUNNELED`: multithreaded ranks, but only the main thread calls MPI
  - ▶ `MPI_THREAD_SERIALIZED`: multithreaded, but only one per time calls MPI
  - ▶ `MPI_THREAD_MULTIPLE`: multithreaded, any thread can call MPI any time (with restrictions)
  - ▶ MPI implementations are not required to support more than `MPI_THREAD_SINGLE`
    - ▶ always check beforehand and call `MPI_Init_thread()` instead of `MPI_Init()`



# Error Handling



# Error Handling

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- ▶ MPI introduces additional hassle
  - ▶ imagine everything that can go wrong with a sequential process
  - ▶ add the fact that multiple processes are interacting, across the network
- ▶ default behavior: communication errors cause abort of MPI operation
  - ▶ causes respective process to exit
  - ▶ causes all other MPI processes of the same application to exit
- ▶ this only relates to halting crashes
  - ▶ also consider deadlocks or hangs

## Error Handling cont'd

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- ▶ all MPI routines return error codes
  - ▶ `MPI_SUCCESS` if everything went well
- ▶ should always check and act accordingly
  - ▶ consider action to take when MPI calls fail
  - ▶ compare to a failing malloc in sequential program
  - ▶ make sure to free allocated resources (e.g. file handles)



## Error Handling cont'd

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- ▶ error behavior can be altered with `MPI_Comm_set_errhandler(...)`
  - ▶ `MPI_ERRORS_FATAL`: abort if error detected (default)
  - ▶ `MPI_ERRORS_RETURN`: return error code to user program
- ▶ user-defined error handlers can be installed
  - ▶ `MPI_Comm_create_errhandler(...)`
  - ▶ `MPI_Comm_set_errhandler(...)`
  - ▶ `MPI_Comm_get_errhandler(...)`

# Additional Topics

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- ▶ File I/O
  - ▶ data file partitioning among processes, strided file access (derived data types!)
  - ▶ asynchronous data transfers
- ▶ process management
  - ▶ process spawning
  - ▶ socket-style communication
- ▶ Fortran-specific issues
  - ▶ slight differences in MPI function signatures
- ▶ profiling support
  - ▶ MPI\_... vs. PMPI\_...

# Summary

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- ▶ communicators and groups
  - ▶ offers high-level control over sets of ranks
- ▶ one-sided communication
  - ▶ can improve performance, but can be tricky to use
- ▶ error handling
  - ▶ graceful exits