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MPI Tutorial – Part 2

Design of Parallel and High-Performance Computing – Recitation Session

Slides credits: Pavan Balaji, Torsten Hoefler
https://htor.inf.ethz.ch/teaching/mpi_tutorials/isc16/hoefler-balaji-isc16-advanced-mpi.pdf

MPI – Q&A

What if a processes receives a message before posting a matching receive?

What if this message is very big?

How does all of this work in non-blocking collectives?

MPI Datatypes

MPI Datatypes – Basic Types

- **Basic Types: MPI_INT, MPI_CHAR, MPI_FLOAT, MPI_DOUBLE …**
- **Use them (and the count argument) to send the corresponding types in C.**

- **Now assume we have a 2D matrix of N*N doubles in C**
- **C does not have multi-dimensional arrays built in**
- **Can emulate it using 1D array.**
- **mat[i,j] = m[i*N+j] (row major layout) or mat[i, j] = m[j*N+i] (column major layout)**

```
double* m = malloc(N*N*sizeof(double));

// fill with random data
for (int i=0; i<N; i++)
   for (int j=0; i<N; i++)
     m[i*N+j] = rand();
```

MPI Datatypes – Small messages

Now we want to send a column of our matrix stored in row-major layout to another process

```
for (int row=0; i<N; i++)
  MPI_Send(&m[row*N+col], 1, MPI_DOUBLE, peer, tag, comm);
```

This will send N separate small messages

Each message has to be matched by the receiver, and usually there is some overhead when sending small messages (i.e., minimum packet size on the network)

So this will give bad performance! Do NOT do this!

MPI Datatypes – Manual Packing

So how about packing the column data into a send buffer?

```
double* buf = malloc(N*sizeof(double));
for (int row=0; i<N; i++) {
    sendbuf[row] = m[row*N+col];
}
MPI_Send(buf, 1, MPI_DOUBLE, peer, tag, comm);
```

Works better in many cases

Sadly, many people do this in real applications

We added an extra copy of our data! Copying is not free! But what if your network is very good with small messages?

Maybe a hybrid approach would be best, i.e., send in chunks of 100 doubles? Or 500?

Idea: Let MPI decide how to handle this!

MPI Datatypes – Type creation

We need to tell MPI how the data is laid out

MPI_Type_vector(count, blocklen, stride, basetype, newtype) will create a new datatype, which consists of count instances of blocklen times basetype, with a space of stride in between.

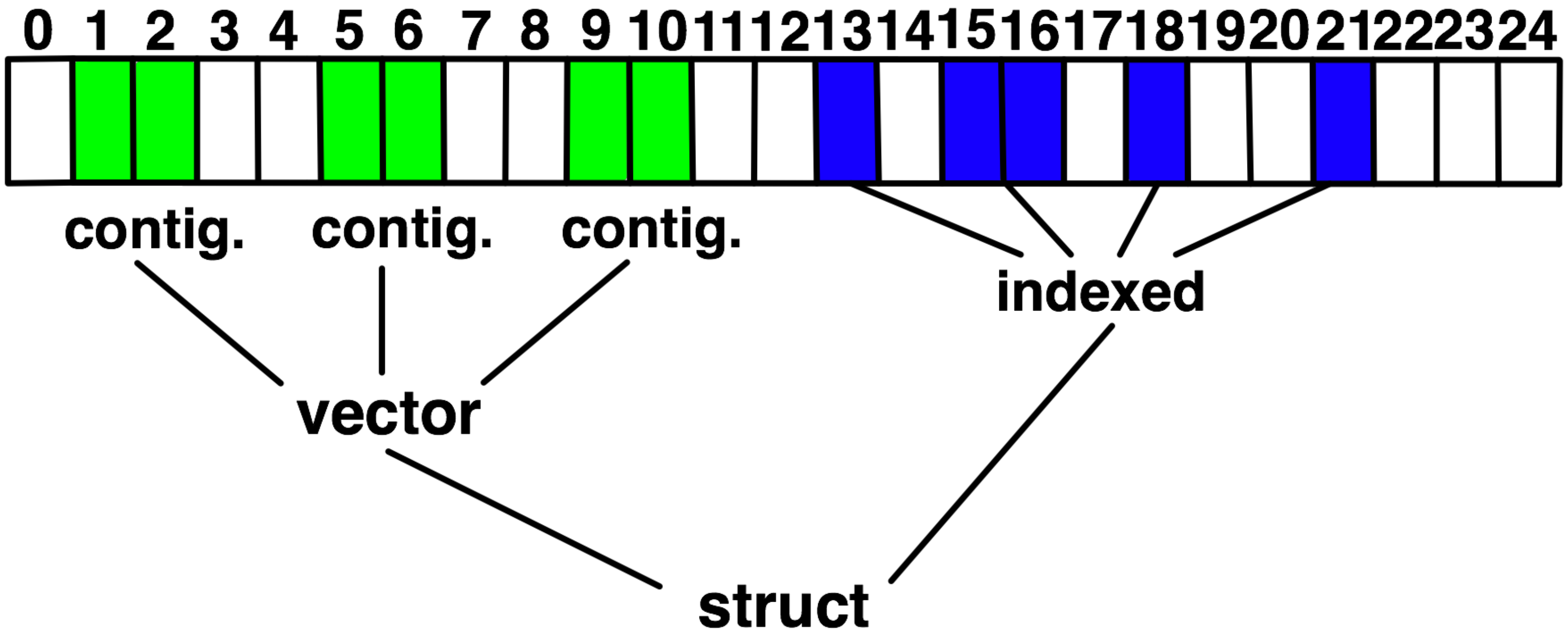
stride = 4
count = 5
blocklen = 1

Before a new type can be used it has to be committed with MPI_Type_commit(MPI_Datatype* newtype)

```
MPI_Datatype newtype;
MPI_Type_vector(N, blocklen, N, MPI_DOUBLE, &newtype);
MPI_Type_commit(&newtype);
MPI_Send(m, 1, newtype, peer, tag, comm);
```

MPI Datatypes – Composable

- **MPI Datatypes can are composable! - So you can create a vector of a vector datatype! (Useful for 3D matrices!)**
- **The MPI_Type_vector() is not the only type creation function**
  - MPI_Type_indexed() allows non-uniform strides
  - MPI_Type_struct() allows to combine different datatypes into one "object" See
  - Check the MPI standard for complete list/definition if you need them!



Type map vs. Type signature

- Type signature is the sequence of basic datatypes used in a derived datatype, e.g.

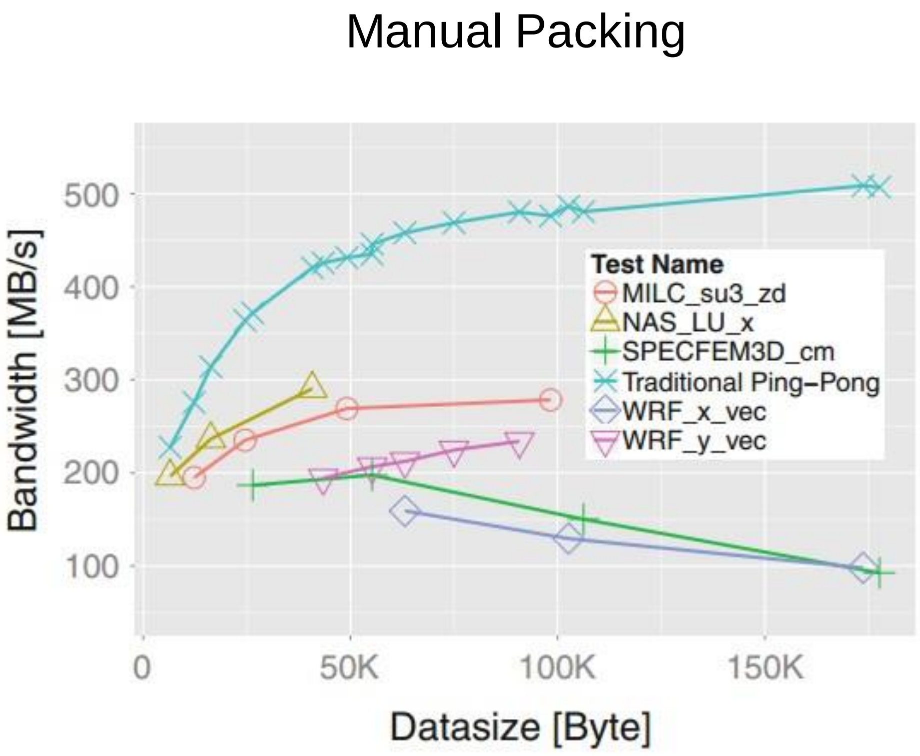
```
typesig(mystruct) = {char, int, double}
```

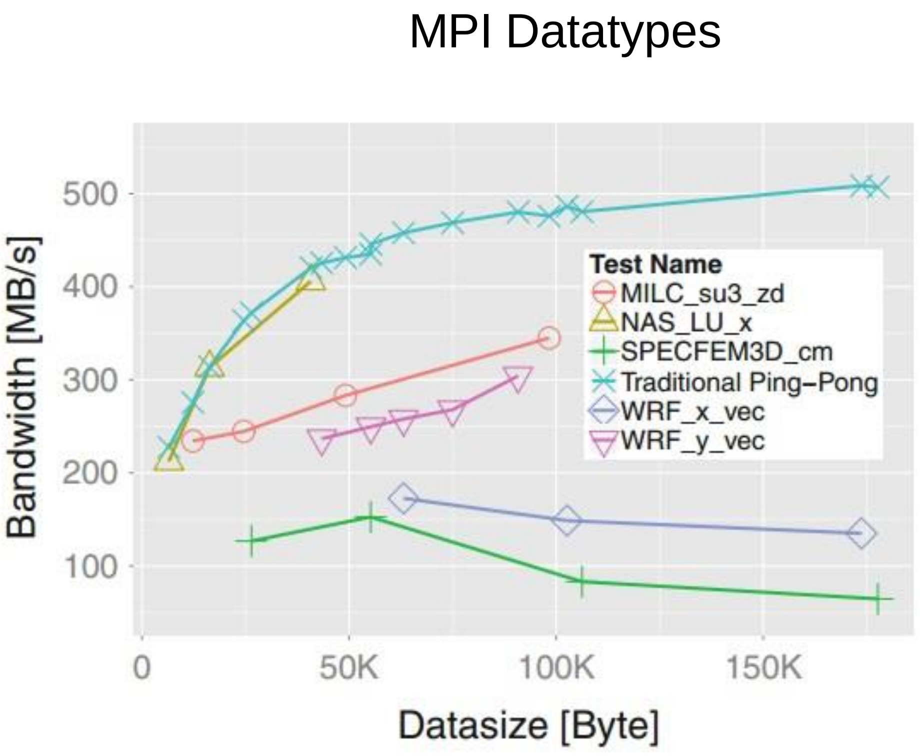
- Type map is sequence of basic datatypes + sequence of displacements

```
typemap(mystruct) = {(char,0),(int,8),(double,16)}
```

- Type matching rule of MPI: type signature of sender and receiver has to match
  - Including the count argument in Send and Recv operation (e.g. unroll the description)
  - Receiver must not define overlapping datatypes
  - The message does not need to fill the whole receive buffer

Datatypes - Performance





Schneider/Gerstenberger: Application-oriented ping-pong benchmarking: how to assess the real communication overheads

Non-blocking Collectives

Nonblocking Collective Communication

- **Nonblocking (send/recv) communication**
  - Deadlock avoidance
  - Overlapping communication/computation
- **Collective communication**
  - Collection of pre-defined optimized routines
- **→ Nonblocking collective communication**
  - Combines both techniques (more than the sum of the parts ☺)
  - System noise/imbalance resiliency
  - Semantic advantages

Nonblocking Collective Communication

- **Nonblocking variants of all collectives**
  - MPI_Ibcast(<bcast args>, MPI_Request *req);
- **Semantics**
  - Function returns no matter what
  - No guaranteed progress (quality of implementation)
  - Usual completion calls (wait, test) + mixing
  - Out-of order completion
- **Restrictions**
  - No tags, in-order matching
  - Send and vector buffers may not be touched during operation
  - MPI_Cancel not supported
  - No matching with blocking collectives

Hoefler et al.: Implementation and Performance Analysis of Non-Blocking Collective Operations for MPI

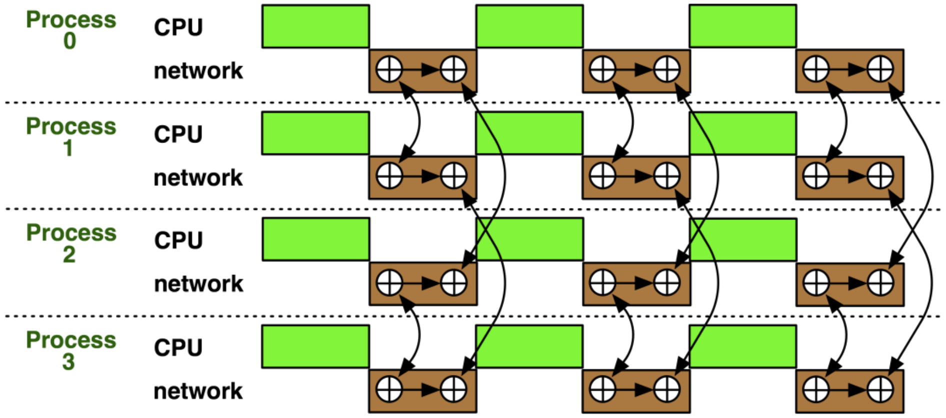
Nonblocking Collective Communication

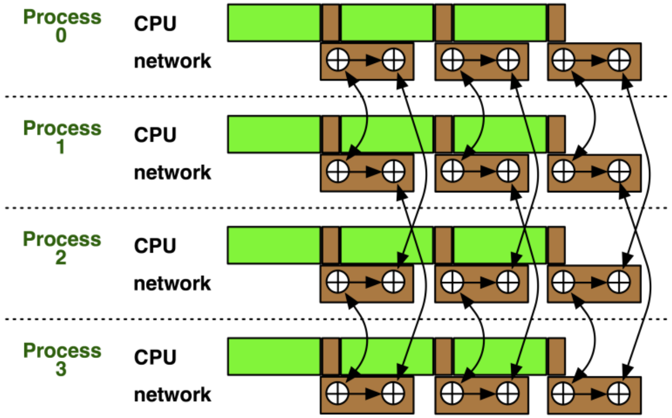
- **Semantic advantages**
  - Enable asynchronous progression (and manual)
    Software pipelining
  - Decouple data transfer and synchronization
    Noise resiliency!
  - Allow overlapping communicators
    See also neighborhood collectives
  - Multiple outstanding operations at any time
    Enables pipelining window

Hoefler et al.: Implementation and Performance Analysis of Non-Blocking Collective Operations for MPI

Nonblocking Collectives Overlap

- **Software pipelining**
  - More complex parameters
  - Progression issues
  - Not scale-invariant



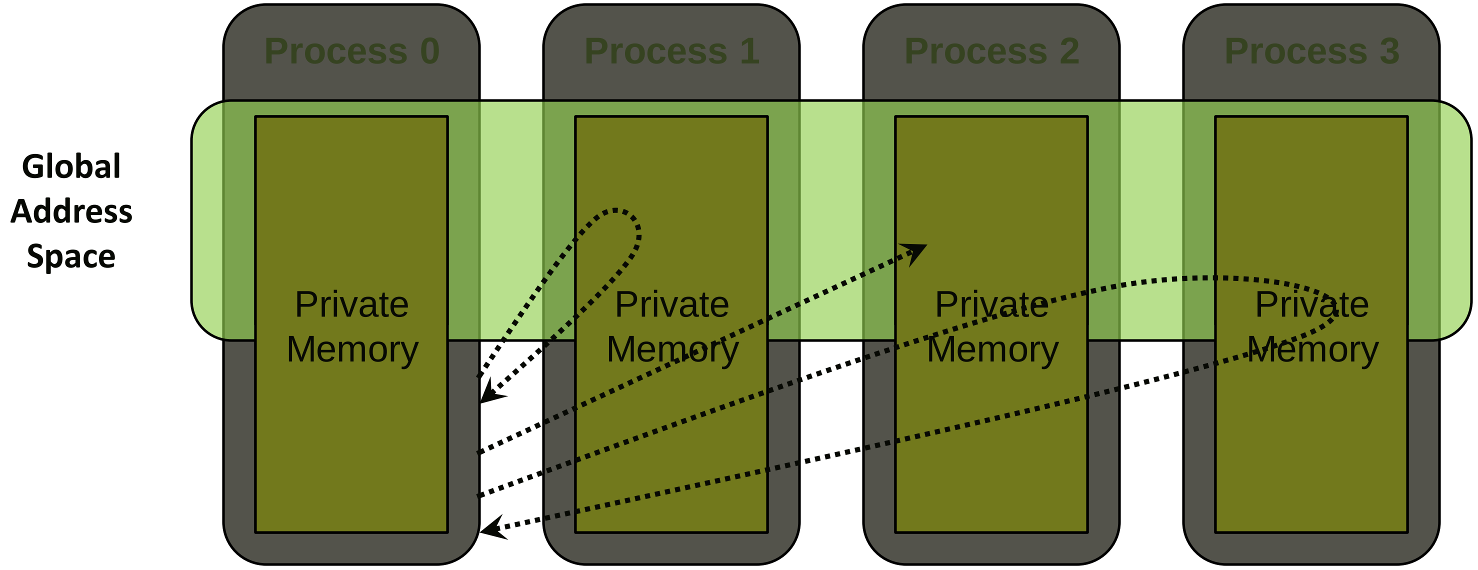


Hoefler: Leveraging Non-blocking Collective Communication in High-performance Applications

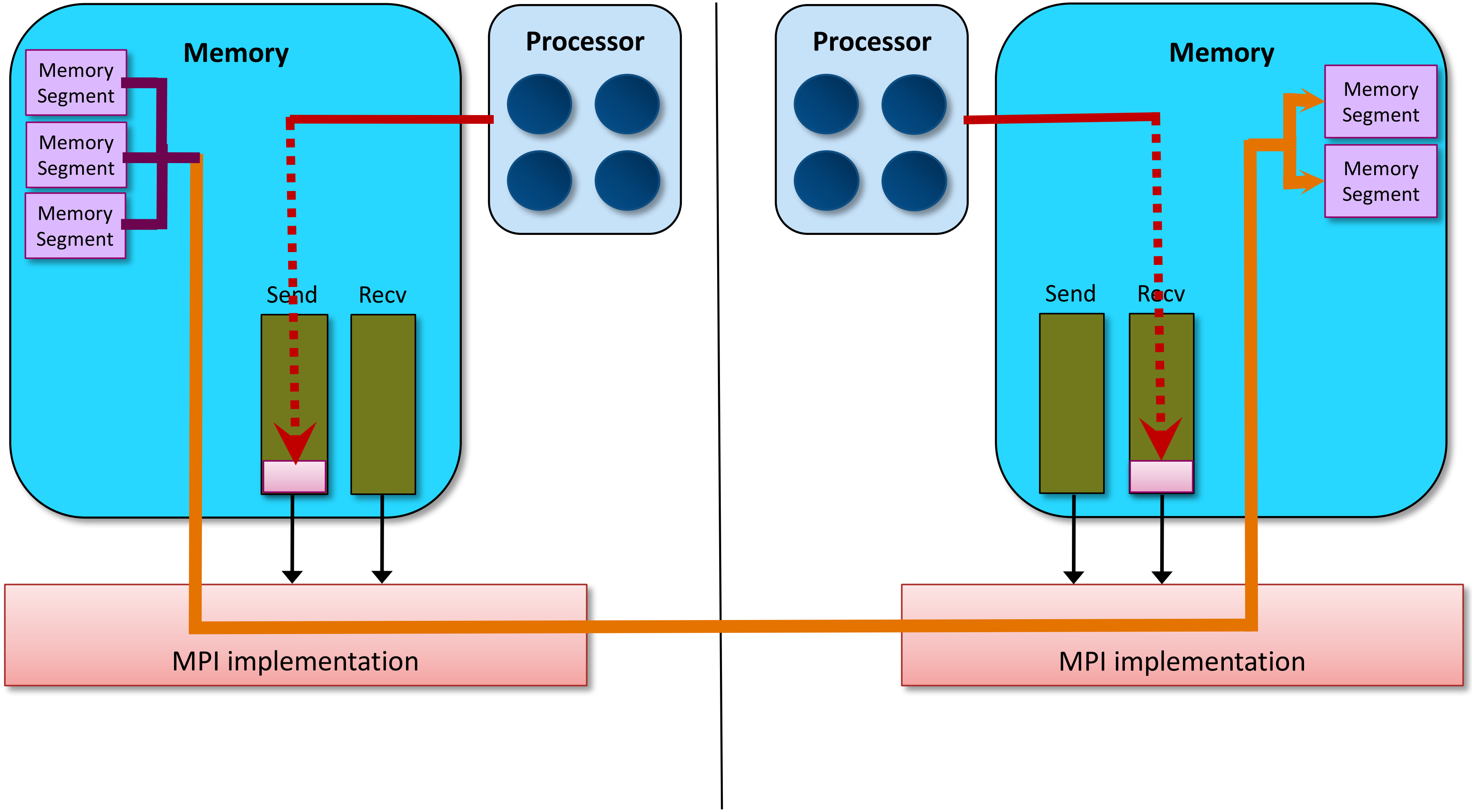
MPI One-sided

One-sided Communication

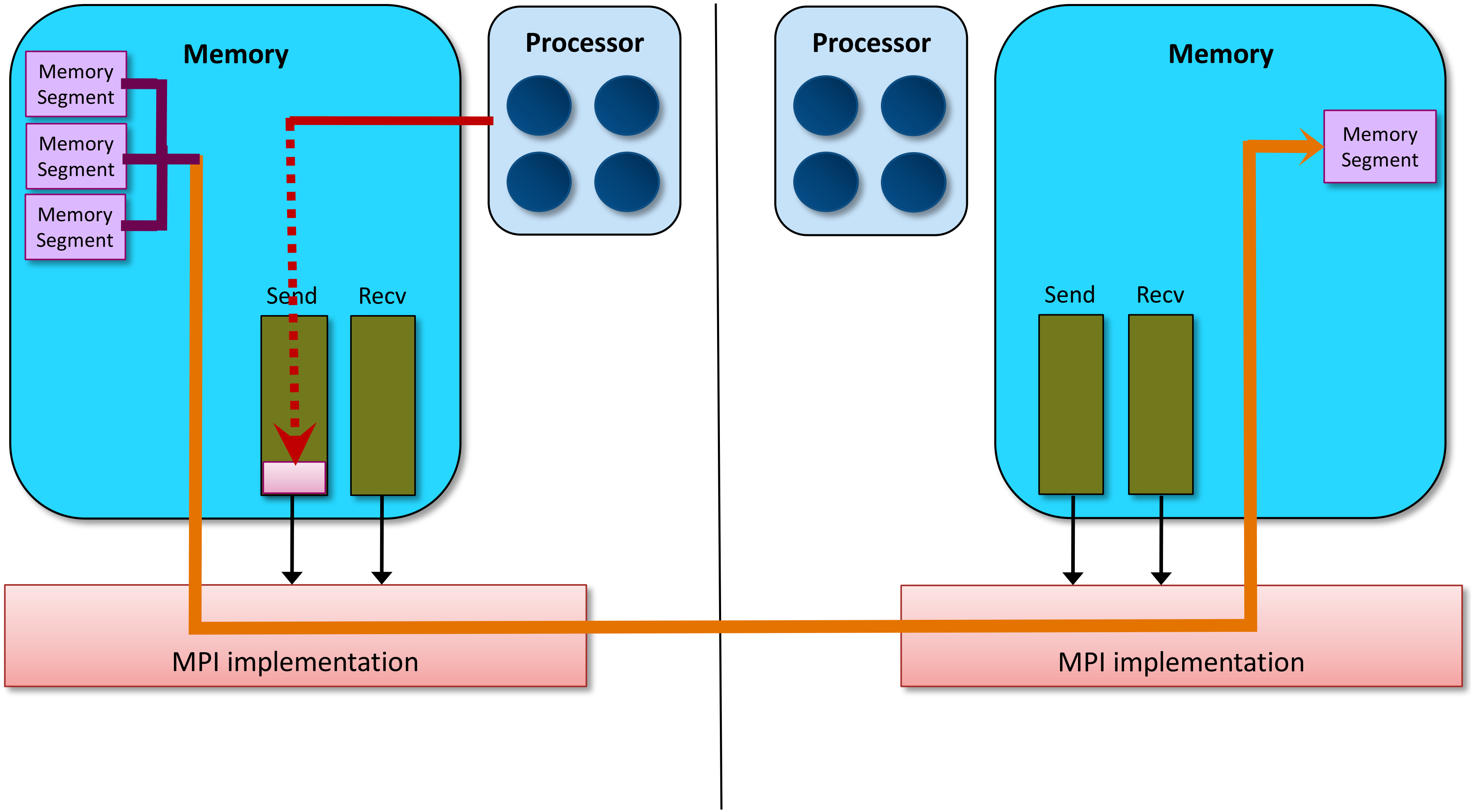
- **The basic idea of one-sided communication models is to decouple data movement with process synchronization**
  - Should be able move data without requiring that the remote process synchronize
  - Each process exposes a part of its memory to other processes
  - Other processes can directly read from or write to this memory



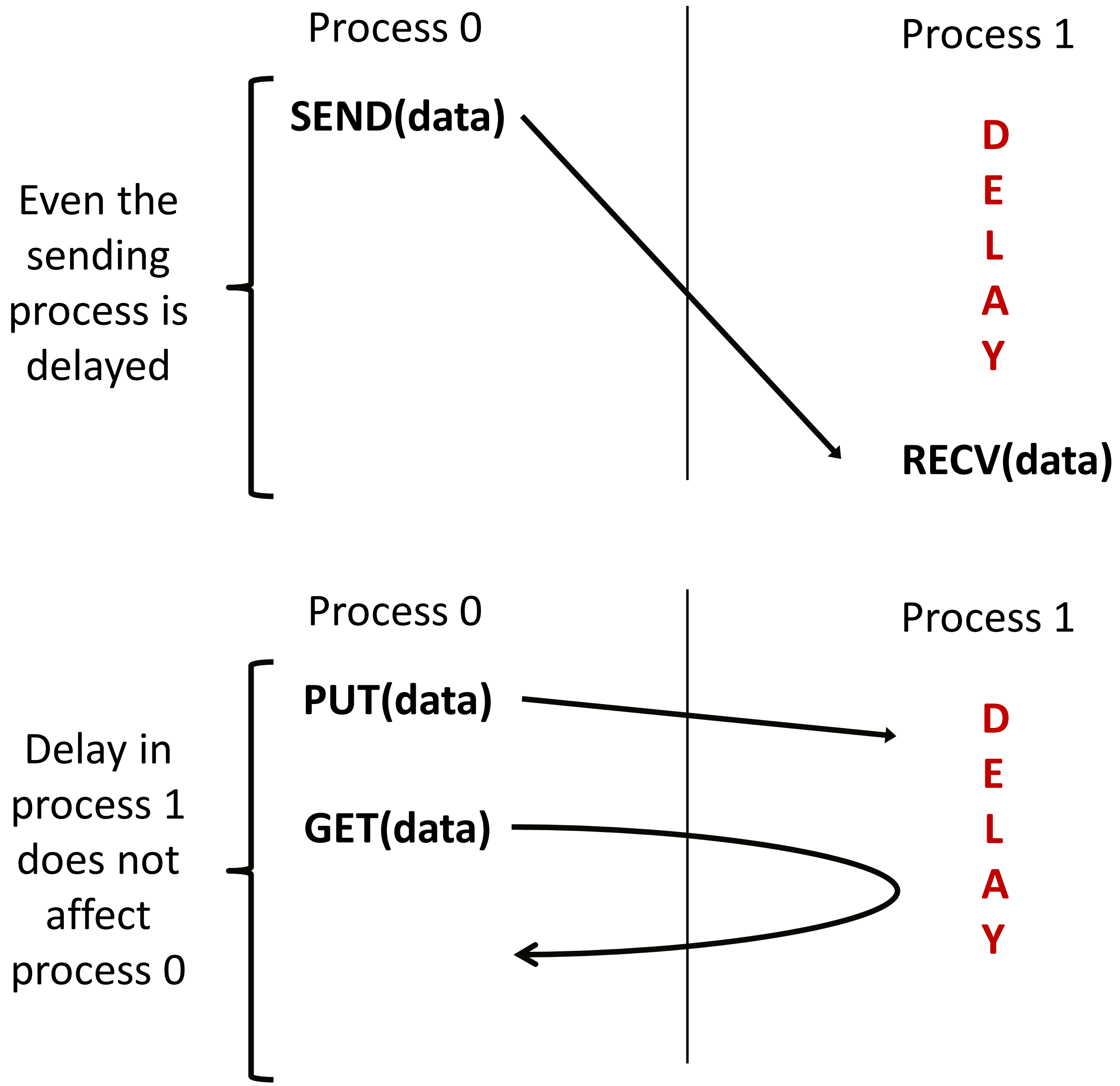
Two-sided Communication Example



One-sided Communication Example



Comparing One-sided and Two-sided Programming

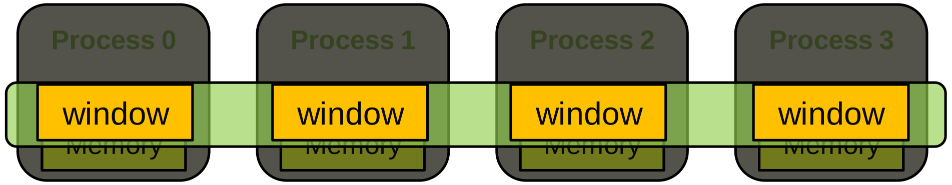


What we need to know in MPI RMA

- How to create remote accessible memory?
- Reading, Writing and Updating remote memory
- Data Synchronization
- Memory Model

Creating remotely accessible memory

- **Any memory used by a process is, by default, only locally accessible**
  - X = malloc(100);



- **Once the memory is allocated, the user has to make an explicit MPI call to declare a memory region as remotely accessible**
  - MPI terminology for remotely accessible memory is a "**window**"
  - A group of processes collectively create a "window"
- **Once a memory region is declared as remotely accessible, all processes in the window can read/write data to this memory without explicitly synchronizing with the target process**

Window creation models

- **Four models exist**
  - MPI_WIN_CREATE

    You already have an allocated buffer that you would like to make remotely accessible
  - MPI_WIN_ALLOCATE

    You want to create a buffer and directly make it remotely accessible
  - MPI_WIN_CREATE_DYNAMIC

    You don’t have a buffer yet, but will have one in the future

    You may want to dynamically add/remove buffers to/from the window
  - MPI_WIN_ALLOCATE_SHARED

    You want multiple processes on the same node share a buffer

MPI_WIN_CREATE

```
MPI_Win_create(void *base, MPI_Aint size,
               int disp_unit, MPI_Info info,
               MPI_Comm comm, MPI_Win *win)
```

- **Expose a region of memory in an RMA window**
  - Only data exposed in a window can be accessed with RMA ops.
- **Arguments:**
  - base - pointer to local data to expose
  - size - size of local data in bytes (nonnegative integer)
  - disp_unit - local unit size for displacements, in bytes (positive integer)
  - info - info argument (handle)
  - comm - communicator (handle)
  - win - window (handle)

Example with MPI_WIN_CREATE

```
int main(int argc, char ** argv)
{
    int *a;    MPI_Win win;

    MPI_Init(&argc, &argv);

    /* create private memory */
    MPI_Alloc_mem(1000*sizeof(int), MPI_INFO_NULL, &a);
    /* use private memory like you normally would */
    a[0] = 1;  a[1] = 2;

    /* collectively declare memory as remotely accessible */
    MPI_Win_create(a, 1000*sizeof(int), sizeof(int),
                         MPI_INFO_NULL, MPI_COMM_WORLD, &win);

    /* Array ‘a’ is now accessibly by all processes in
     * MPI_COMM_WORLD */

    MPI_Win_free(&win);
    MPI_Free_mem(a);
    MPI_Finalize(); return 0;
}
```

MPI_WIN_ALLOCATE

```
MPI_Win_allocate(MPI_Aint size, int disp_unit,
                 MPI_Info info, MPI_Comm comm,
                 void *baseptr, MPI_Win *win)
```

- **Create a remotely accessible memory region in an RMA window**
  - Only data exposed in a window can be accessed with RMA ops.
- **Arguments:**
  - size - size of local data in bytes (nonnegative integer)
  - disp_unit - local unit size for displacements, in bytes (positive integer)
  - info - info argument (handle)
  - comm - communicator (handle)
  - baseptr - pointer to exposed local data
  - win - window (handle)

Example with MPI_WIN_ALLOCATE

```
int main(int argc, char ** argv)
{
    int *a;    MPI_Win win;

    MPI_Init(&argc, &argv);

    /* collectively create remote accessible memory in a window */
    MPI_Win_allocate(1000*sizeof(int), sizeof(int), MPI_INFO_NULL,
                     MPI_COMM_WORLD, &a, &win);

    /* Array ‘a’ is now accessible from all processes in
     * MPI_COMM_WORLD */

    MPI_Win_free(&win); // will also free the buffer memory

    MPI_Finalize(); return 0;
}
```

MPI_WIN_CREATE_DYNAMIC

```
MPI_Win_create_dynamic(MPI_Info info, MPI_Comm comm,
                       MPI_Win *win)
```

- **Create an RMA window, to which data can later be attached**
  - Only data exposed in a window can be accessed with RMA ops
- **Initially "empty"**
  - Application can dynamically attach/detach memory to this window by calling MPI_Win_attach/detach
  - Application can access data on this window only after a memory region has been attached
- **Window origin is MPI_BOTTOM**
  - Displacements are segment addresses relative to MPI_BOTTOM
  - Must tell others the displacement after calling attach

Example with MPI_WIN_CREATE_DYNAMIC

```
int main(int argc, char ** argv)
{
    int *a;    MPI_Win win;

    MPI_Init(&argc, &argv);
    MPI_Win_create_dynamic(MPI_INFO_NULL, MPI_COMM_WORLD, &win);

    /* create private memory */
    a = (int *) malloc(1000 * sizeof(int));
    /* use private memory like you normally would */
    a[0] = 1;  a[1] = 2;

    /* locally declare memory as remotely accessible */
    MPI_Win_attach(win, a, 1000*sizeof(int));

    /* Array ‘a’ is now accessible from all processes */

    /* undeclare remotely accessible memory */
    MPI_Win_detach(win, a);  free(a);
    MPI_Win_free(&win);

    MPI_Finalize(); return 0;
}
```

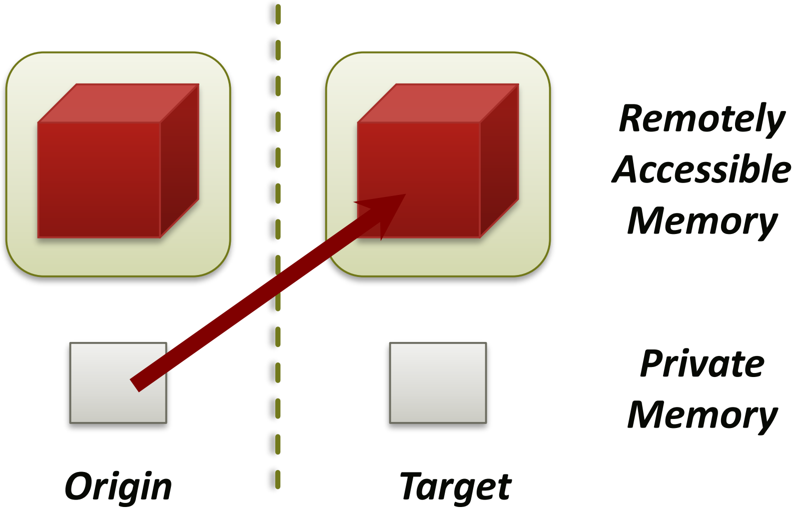
Data movement

- **MPI provides ability to read, write and atomically modify data in remotely accessible memory regions**
  - MPI_PUT
  - MPI_GET
  - MPI_ACCUMULATE (atomic)
  - MPI_GET_ACCUMULATE (atomic)
  - MPI_COMPARE_AND_SWAP (atomic)
  - MPI_FETCH_AND_OP (atomic)

Data movement: *Put*

```
MPI_Put(void *origin_addr, int origin_count,
        MPI_Datatype origin_dtype, int target_rank,
        MPI_Aint target_disp, int target_count,
        MPI_Datatype target_dtype, MPI_Win win)
```

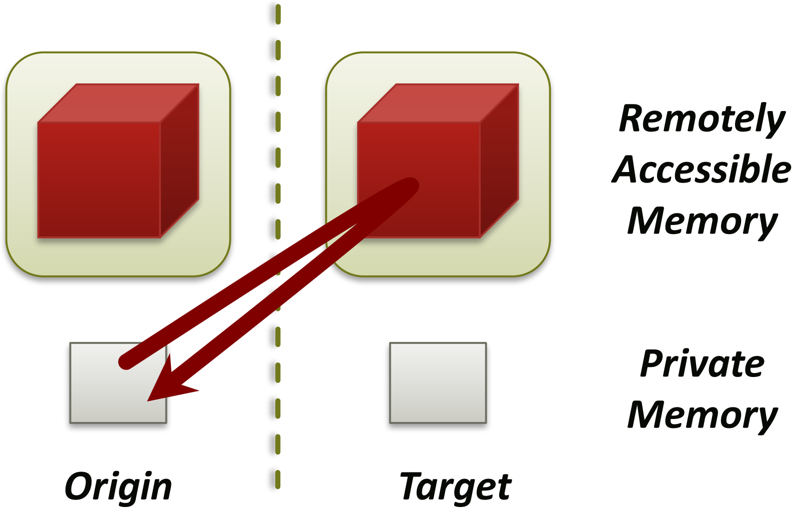
- Move data from origin, to target
- Separate data description triples for origin and target



Data movement: *Get*

```
MPI_Get(void *origin_addr, int origin_count,
        MPI_Datatype origin_dtype, int target_rank,
        MPI_Aint target_disp, int target_count,
        MPI_Datatype target_dtype, MPI_Win win)
```

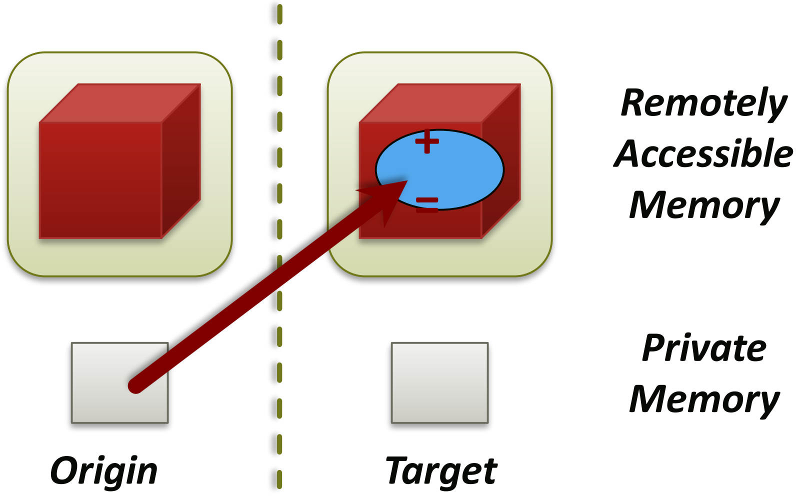
- Move data to origin, from target
- Separate data description triples for origin and target



Atomic Data Aggregation: *Accumulate*

```
MPI_Accumulate(void *origin_addr, int origin_count,
        MPI_Datatype origin_dtype, int target_rank,
        MPI_Aint target_disp, int target_count,
        MPI_Datatype target_dtype, MPI_Op op, MPI_Win win)
```

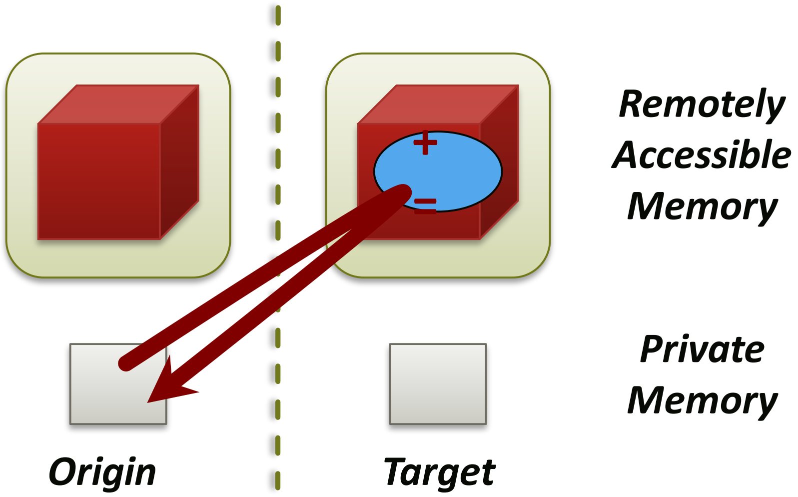
- **Atomic update operation, similar to a put**
  - Reduces origin and target data into target buffer using op argument as combiner
  - Op = MPI_SUM, MPI_PROD, MPI_OR, MPI_REPLACE, …
  - Predefined ops only, no user-defined operations
- **Different data layouts between target/origin OK**
  - Basic type elements must match
- **Op = MPI_REPLACE**
  - Implements *f(a,b)=b*
  - Atomic PUT



Atomic Data Aggregation: *Get Accumulate*

```
MPI_Get_accumulate(void *origin_addr, int origin_count,
        MPI_Datatype origin_dtype, void *result_addr,
        int result_count, MPI_Datatype result_dtype,
        int target_rank, MPI_Aint target_disp,
        int target_count, MPI_Datatype target_dype,
        MPI_Op op, MPI_Win win)
```

- **Atomic read-modify-write**
  - Op = MPI_SUM, MPI_PROD, MPI_OR, MPI_REPLACE, MPI_NO_OP, …
  - Predefined ops only
- **Result stored in target buffer**
- **Original data stored at result_add**
- **Different data layouts between target/origin OK**
  - Basic type elements must match
- **Atomic get with MPI_NO_OP**
- **Atomic swap with MPI_REPLACE**



Atomic Data Aggregation: *CAS and FOP*

```
MPI_Fetch_and_op(void *origin_addr, void *result_addr,
       MPI_Datatype dtype, int target_rank,
       MPI_Aint target_disp, MPI_Op op, MPI_Win win)
```

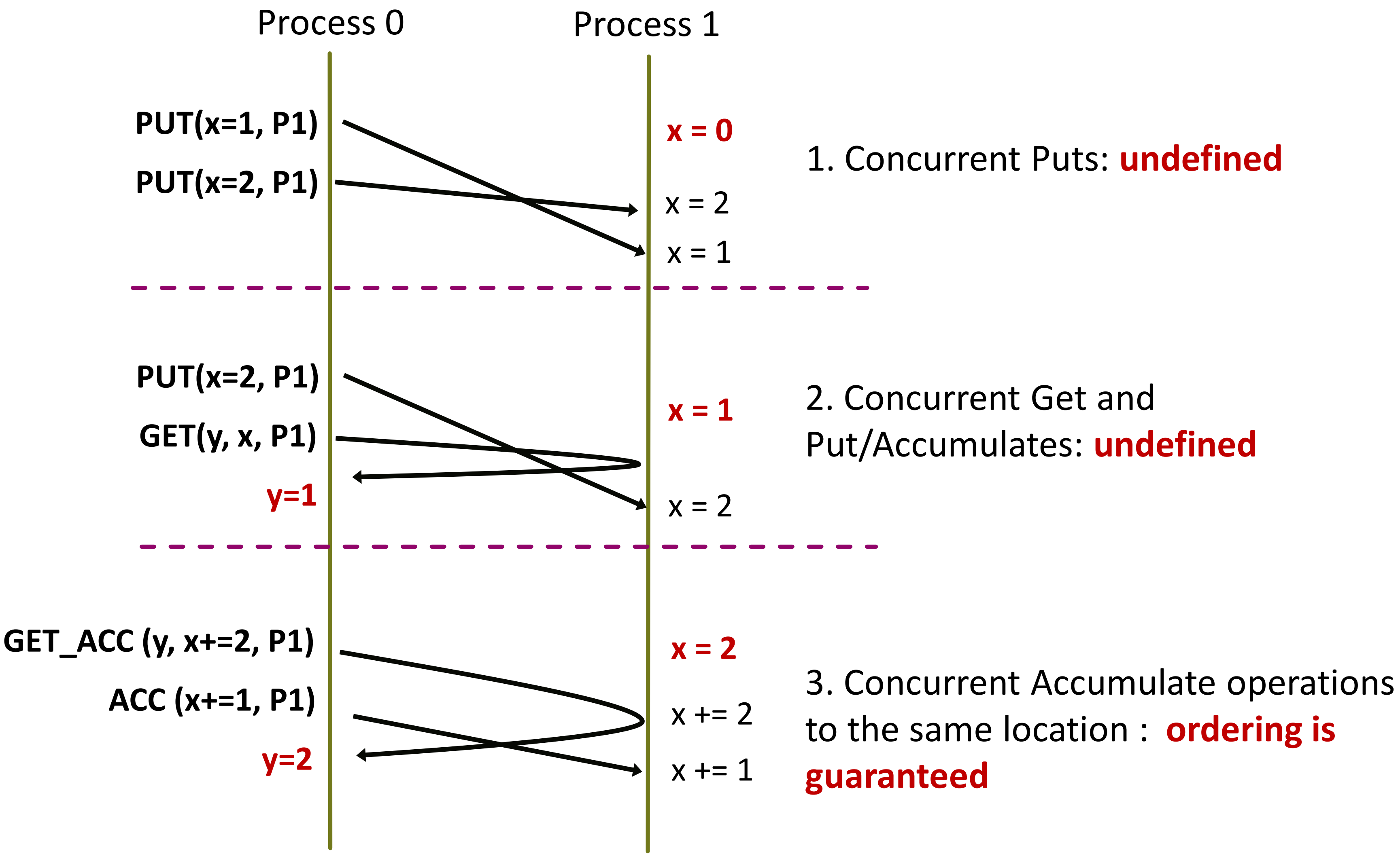
```
MPI_Compare_and_swap(void *origin_addr, void *compare_addr,
       void *result_addr, MPI_Datatype dtype, int target_rank,
       MPI_Aint target_disp, MPI_Win win)
```

- **FOP: Simpler version of MPI_Get_accumulate**
  - All buffers share a single predefined datatype
  - No count argument (it’s always 1)
  - Simpler interface allows hardware optimization
- **CAS: Atomic swap if target value is equal to compare value**

Ordering of Operations in MPI RMA

- **No guaranteed ordering for Put/Get operations**
- **Result of concurrent Puts to the same location undefined**
- **Result of Get concurrent Put/Accumulate undefined**
  - Can be garbage in both cases
- **Result of concurrent accumulate operations to the same location are defined according to the order in which the occurred**
  - Atomic put: Accumulate with op = MPI_REPLACE
  - Atomic get: Get_accumulate with op = MPI_NO_OP
- **Accumulate operations from a given process are ordered by default**
  - User can tell the MPI implementation that (s)he does not require ordering as optimization hint
  - You can ask for only the needed orderings: RAW (read-after-write), WAR, RAR, or WAW

Examples with operation ordering



RMA Synchronization Models

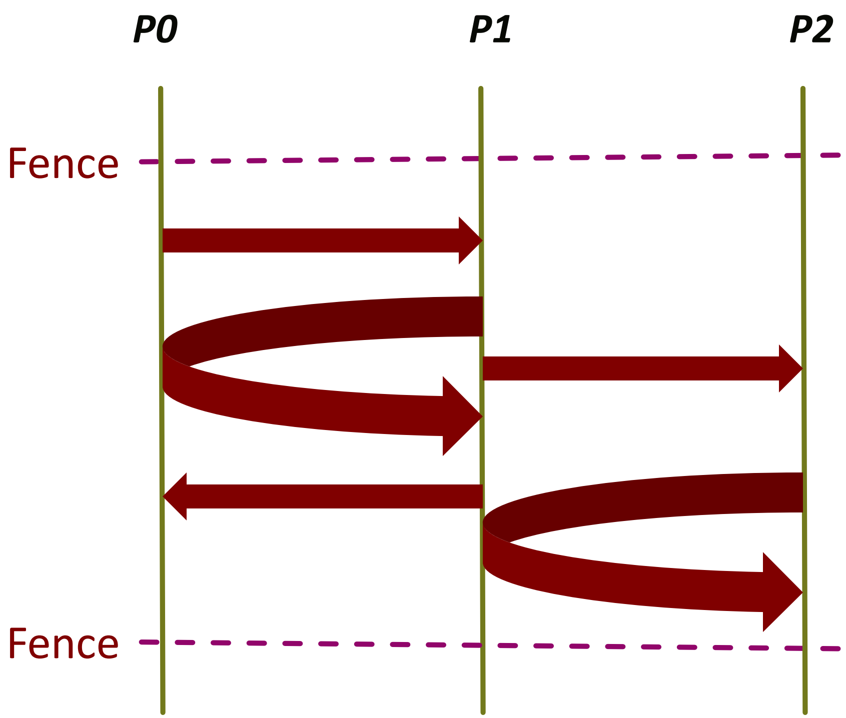
- **RMA data access model**
  - When is a process allowed to read/write remotely accessible memory?
  - When is data written by process X is available for process Y to read?
  - RMA synchronization models define these semantics
- **Three synchronization models provided by MPI:**
  - Fence (active target)
  - Post-start-complete-wait (generalized active target)
  - Lock/Unlock (passive target)
- **Data accesses occur within "epochs"**
  - *Access epochs*: contain a set of operations issued by an origin process
  - *Exposure epochs*: enable remote processes to update a target's window
  - Epochs define ordering and completion semantics
  - Synchronization models provide mechanisms for establishing epochs

    E.g., starting, ending, and synchronizing epochs

Fence: Active Target Synchronization

```
MPI_Win_fence(int assert, MPI_Win win)
```

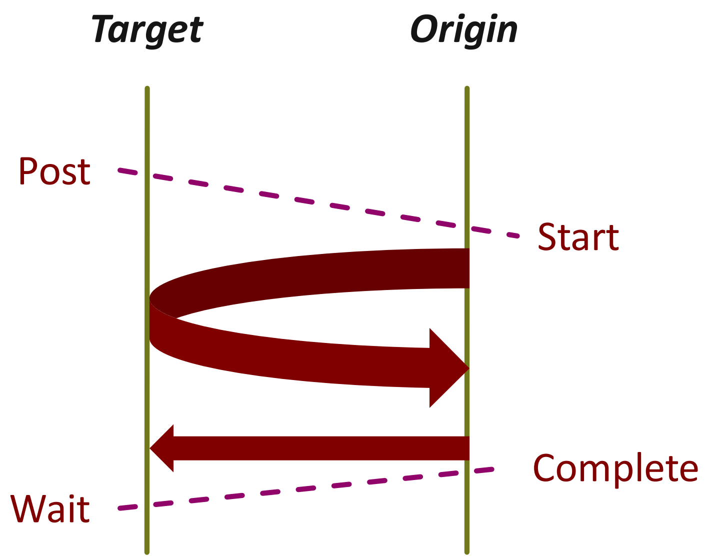
- Collective synchronization model
- Starts *and* ends access and exposure epochs on all processes in the window
- All processes in group of “win” do an MPI_WIN_FENCE to open an epoch
- Everyone can issue PUT/GET operations to read/write data
- Everyone does an MPI_WIN_FENCE to close the epoch
- All operations complete at the second fence synchronization



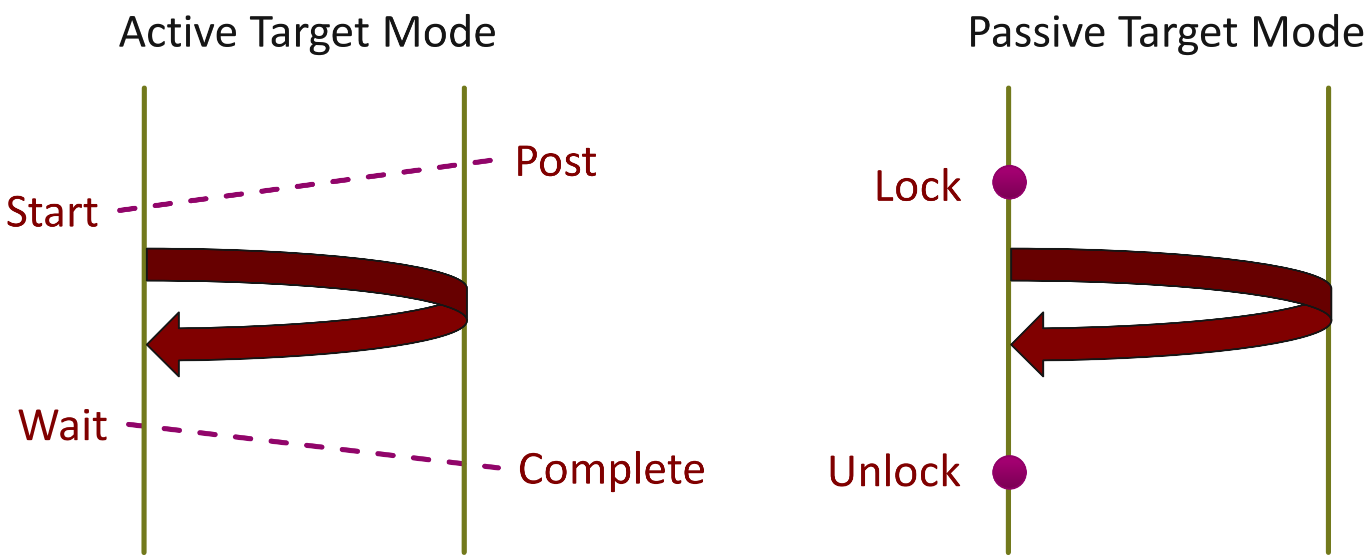
PSCW: Generalized Active Target Synchronization

```
MPI_Win_post/start(MPI_Group grp, int assert, MPI_Win win)
MPI_Win_complete/wait(MPI_Win win)
```

- **Like FENCE, but origin and target specify who they communicate with**
- **Target: Exposure epoch**
  - Opened with MPI_Win_post
  - Closed by MPI_Win_wait
- **Origin: Access epoch**
  - Opened by MPI_Win_start
  - Closed by MPI_Win_complete
- **All synchronization operations may block, to enforce P-S/C-W ordering**
  - Processes can be both origins and targets



Lock/Unlock: Passive Target Synchronization



- **Passive mode: One-sided, *asynchronous* communication**
  - Target does **not** participate in communication operation
- **Shared memory-like model**

Passive Target Synchronization

```
MPI_Win_lock(int locktype, int rank, int assert, MPI_Win win)
```

```
MPI_Win_unlock(int rank, MPI_Win win)
```

```
MPI_Win_flush/flush_local(int rank, MPI_Win win)
```

- **Lock/Unlock: Begin/end passive mode epoch**
  - Target process does not make a corresponding MPI call
  - Can initiate multiple passive target epochs to different processes
  - Concurrent epochs to same process not allowed (affects threads)
- **Lock type**
  - SHARED: Other processes using shared can access concurrently
  - EXCLUSIVE: No other processes can access concurrently
- **Flush: Remotely complete RMA operations to the target process**
  - After completion, data can be read by target process or a different process
- **Flush_local: Locally complete RMA operations to the target process**

Advanced Passive Target Synchronization

```
MPI_Win_lock_all(int assert, MPI_Win win)
```

```
MPI_Win_unlock_all(MPI_Win win)
```

```
MPI_Win_flush_all/flush_local_all(MPI_Win win)
```

- **Lock_all: Shared lock, passive target epoch to all other processes**
  - Expected usage is long-lived: lock_all, put/get, flush, …, unlock_all
- **Flush_all – remotely complete RMA operations to all processes**
- **Flush_local_all – locally complete RMA operations to all processes**

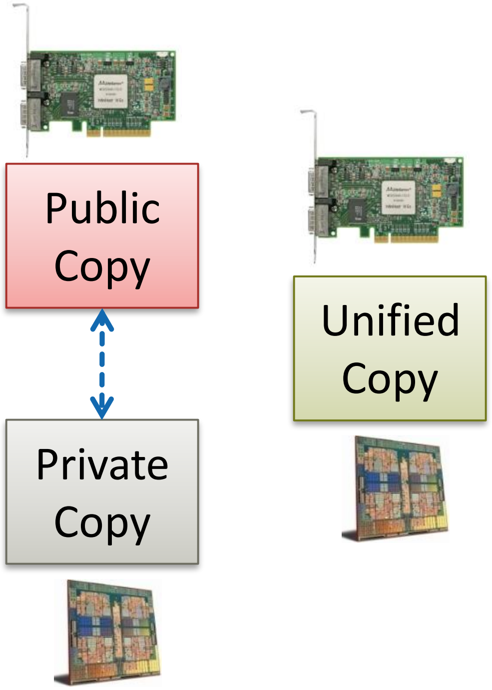
Which synchronization mode should I use, when?

- **RMA communication has low overheads versus send/recv**
  - Two-sided: Matching, queuing, buffering, unexpected receives, etc…
  - One-sided: No matching, no buffering, always ready to receive
  - Utilize RDMA provided by high-speed interconnects (e.g. InfiniBand)
- **Active mode: bulk synchronization**
  - E.g. ghost cell exchange
- **Passive mode: asynchronous data movement**
  - Useful when dataset is large, requiring memory of multiple nodes
  - Also, when data access and synchronization pattern is dynamic
  - Common use case: distributed, shared arrays
- **Passive target locking mode**
  - Lock/unlock – Useful when exclusive epochs are needed
  - Lock_all/unlock_all – Useful when only shared epochs are needed

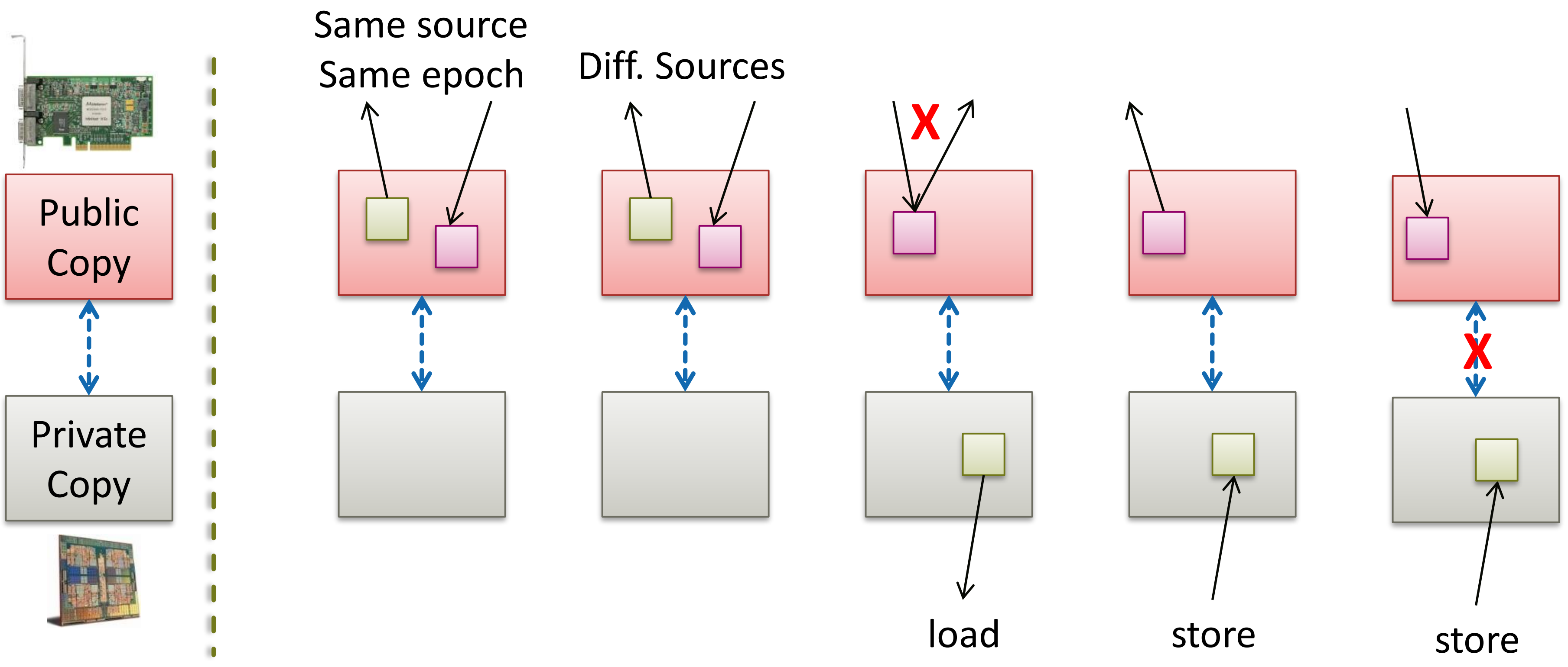
MPI RMA Memory Model

- **MPI-3 provides two memory models: separate and unified**
- **MPI-2: Separate Model**
  - Logical public and private copies
  - MPI provides software coherence between window copies
  - Extremely portable, to systems that don't provide hardware coherence
- **MPI-3: New Unified Model**
  - Single copy of the window
  - System must provide coherence
  - Superset of separate semantics

    E.g. allows concurrent local/remote access
  - Provides access to full performance potential of hardware

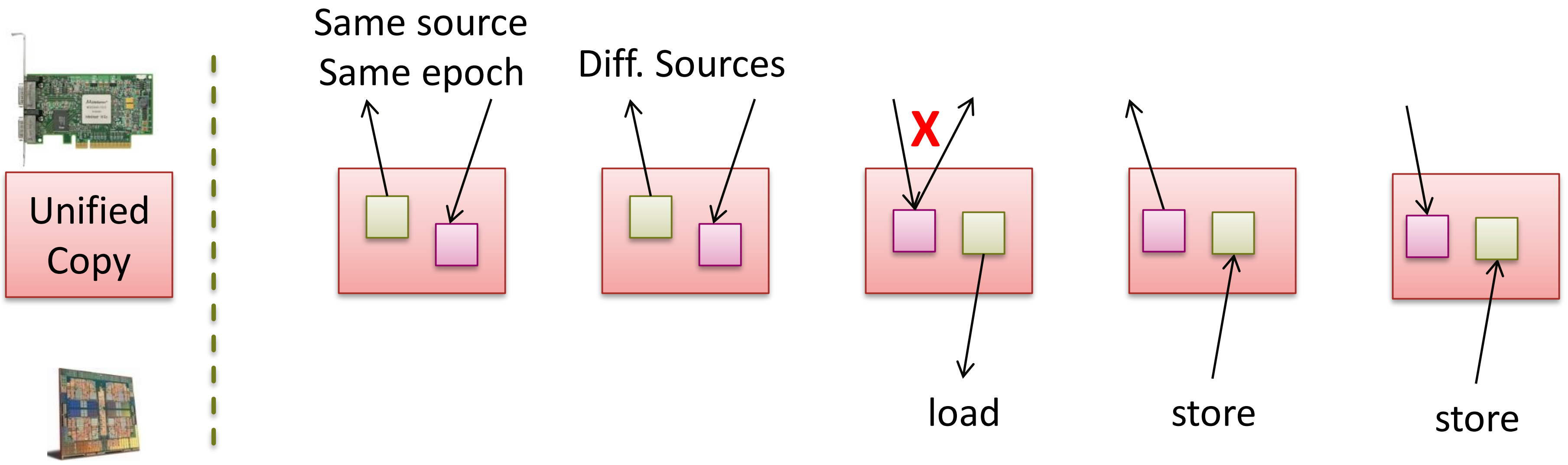


MPI RMA Memory Model (separate windows)



- **Very portable, compatible with non-coherent memory systems**
- **Limits concurrent accesses to enable software coherence**

MPI RMA Memory Model (unified windows)



- **Allows concurrent local/remote accesses**
- **Concurrent, conflicting operations are allowed (not invalid)**
  - Outcome is not defined by MPI (defined by the hardware)
- **Can enable better performance by reducing synchronization**