Advanced MPI

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Nonblocking and collective communications

- Nonblocking communication
  - Prevent deadlocks related to message ordering
  - Overlapping communication/computation
    - If communication progress is provided by the implementation/hardware

- Collective communication
  - Collection of pre-defined routines for generalist communication patterns
    - Optimized by the implementations

- Nonblocking collective communication
  - Combines both advantages
  - System noise/imbalance resiliency
  - Semantic advantages
Nonblocking communications

• Semantics are simple:
  • Function returns immediately
  • No requirement for progress (more complicated than point-to-point communications)

• E.g.: MPI_Isend(..., MPI_Request *req);

• Nonblocking tests:
  • Test, Testany, Testall, Testsome

• Blocking wait:
  • Wait, Waitany, Waitall, Waitsome

• Blocking vs. nonblocking communication
  • Mostly equivalent, nonblocking has constant request management overhead
  • Nonblocking may have other non-trivial overheads
Nonblocking communications

• An important technical detail
  • Eager vs. Rendezvous
    small eager rest of data

• Most/All MPIs switch protocols
  • Small messages are copied to internal remote buffers
    • And then copied to user buffer
    • Frees sender immediately (cf. bsend)
    • Usually below MTU
    • Large messages divided in multiple pieces
    • wait until receiver is ready yo prevent temporary memory allocations on the receiver due to unexpected communication
    • Blocks sender until receiver arrived

• Hint: in many cases you can tune these limits (for your environment) and your application
  • Not only for performance reasons but also to minimize the memory used by the MPI library (for internal storage)
Software Pipelining - Motivation

```c
if( 0 == rank ) {
    for( int i = 0; i < MANY; i++ ) {
        buf[i] = compute(buf, size, i);
    }
    MPI_Send(buf, size, MPI_DOUBLE, 1, 42, comm);
} else {
    MPI_Recv(buf, size, MPI_DOUBLE, 0, 42, comm, &status);
    compute(buf, size);
}
```

![Diagram showing CPU and network activities over time](diagram.png)
Software Pipelining - Implementation

MPI_Request req = MPI_REQUEST_NULL;
if( 0 == rank ) {
    for( int b = 0; b < (size / BSIZE); b++ ) {
        MPI_wait( req, &status); /* complete previous step */
        for( int i = b * BSIZE; i < ((b+1) * BSIZE); i++ )
            buf[i] = compute(buf, size, i);
        MPI_Isend(&buf[b * BSIZE], BSIZE, MPI_DOUBLE, 1, 42, comm, &req);
    }
} else {
    for( int b = 0; b < (size / BSIZE); b++ ) {
        MPI_Recv(&buf[b*BSIZE], BSIZE, MPI_DOUBLE, 0, 42, comm, &status);
        compute(&buf[b*BSIZE], BSIZE);
    }
}

What if the computation is more expensive than the communication?
Software Pipelining - Implementation

```c
MPI_Request req = MPI_REQUEST_NULL;
if( 0 == rank ) {
    for( int b = 0; b < (size / BSIZE); b++ ) {
        MPI_wait( req, &status); /* complete previous step */
        for( int i = b * BSIZE; i < ((b+1) * BSIZE); i++ )
            buf[i] = compute(buf, size, i);
        MPI_Isend(&buf[b * BSIZE], BSIZE, MPI_DOUBLE, 1, 42, comm, &req);
    }
} else {
    for( int b = 0; b < (size / BSIZE); b++ ) {
        MPI_Recv(&buf[b*BSIZE], BSIZE, MPI_DOUBLE, 0, 42, comm, &status);
        compute(&buf[b*BSIZE], BSIZE);
    }
}
```

Computation more expensive than the communication.
MPI_Request req[2] = {MPI_REQUEST_NULL};
if( 0 == rank ) {
    /* keep the same send code */
} else {
    idx = 0;
    MPI_Irecv(&buf[0*BSIZE], BSIZE, MPI_DOUBLE, 0, 42, comm, &req[idx]);
    for( int b = 0; b < (size / BSIZE); b++ ) {
        MPI_Wait(&req[idx], &status);
        if( (b+1)*BSIZE < size ) {
            idx = (idx + 1) % 2;
            MPI_Irecv(&buf[(b+1)*BSIZE], BSIZE, ..., comm, &req[idx]);
        }
        compute(&buf[b*BSIZE], BSIZE);
    }
}
Computation more expensive than the communication.
Software pipelining - modelization

- No pipeline
  \[ T = T_{\text{comp}}(s) + T_{\text{comm}}(s) + T_{\text{startc}}(s) + T'_{\text{comp}}(s) \]

- Pipeline
  \[ T = T_{\text{comp}}(bs) + T_{\text{comm}}(bs) + T_{\text{startc}}(bs) + \text{nblocks} \times \max(T_{\text{comp}}(bs), T_{\text{comm}}(bs), T_{\text{startc}}(bs), T'_{\text{comp}}(bs)) \]
Communicators - Collectives

- Simple classification by operation class

- **One-To-All** (simplex mode)
  - One process contributes to the result. All processes receive the result.
    - MPI_Bcast
    - MPI_Scatter, MPI_Scatterv

- **All-To-One** (simplex mode)
  - All processes contribute to the result. One process receives the result.
    - MPI_Gather, MPI_Gatherv
    - MPI_Reduce

- **All-To-All** (duplex mode)
  - All processes contribute to the result. All processes receive the result.
    - MPI_Allgather, MPI_Allgatherv
    - MPI_Alltoall, MPI_Alltoallv
    - MPI_Allreduce, MPI_Reduce_scatter

- **Other**
  - Collective operations that do not fit into one of the above categories.
    - MPI_Scan
    - MPI_Barrier

- **Common semantics:**
  - Blocking semantics (return when complete)
  - Therefore no tags (communicators can serve as such)
  - Not necessarily synchronizing (only barrier and all*)
Collective Communications

- Most algorithms are $\log(P)$
- They classify in 3 major communication patterns
  - Scatter, Gather, Reduce
  - Barrier, AllReduce, Allgather, Alltoall
  - Scan, Exscan
Nonblocking collectives

• Nonblocking variants of all collectives
  • MPI_Ibcast(&amp;#123; , 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
Nonblocking collectives

- 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

- Complex progression
  - MPI’s global progress rule!
  - Higher CPU overhead (offloading?)
  - Differences in asymptotic behavior
    - Collective time often
    - Computation
    - Performance modeling (more complicated than for blocking)
    - One term often dominates and complicates overlap
- Rank reordering (transform the original, resource manager provided allocation) and map the processes on it based on the communication pattern

Courtesy to Torsten Hoefler
MPI topologies support

- **MPI-1**: Basic support Convenience functions
  - Create and query a graph
  - Useful especially for Cartesian topologies
  - Query neighbors in n-dimensional space
  - Non-scalable: the graph knowledge must be global as each rank must specify the full graph

- **MPI-2.2**: Scalable Graph topology
  - Distributed Graph: each rank specifies its neighbors or arbitrary subset of the graph

- **MPI-3.0**: Neighborhood collectives
  - Adding communication functions defined on graph topologies (neighborhood of distance one)
Cartesian topology creation

- Specify ndims-dimensional topology
  - Optionally periodic in each dimension (Torus)

- Some processes may return MPI_COMM_NULL
  - Product sum of dims must be $\leq P$

- Reorder argument allows for topology mapping
  - Each calling process may have a new rank in the created communicator
  - Application must adapt to rank changing between the old and the new communicator, i.e. data must be manually remapped

- MPI provides support for creating the dimensions array ("square" topologies via MPI_Dims_create)
  - Non-zero entries on the dims array will not be changed

```c
MPI_Cart_create(MPI_Comm old_comm, int ndims, const int*dims, const int*periods,
                int reorder, MPI_Comm *comm)
MPI_Dims_create(int nnodes, int ndims, int *dims)
```
Graph Creation

• nnodes is the total number of nodes in the graph
• index[i] stores the total number of neighbors for the first i nodes (sum)
  • Acts as offset into edges array
• edges stores the edge list for all processes
  • Edge list for process j starts at index[j] in edges
  • Process j has index[j+1]-index[j] edges

• Each process must know the entire topology

```c
MPI_Graph_create(MPI_Comm comm_old, int nnodes,
                 const int *index, const int *edges, int reorder,
                 MPI_Comm *comm_graph)
```
Distributed graph creation

- Scalable, allows distributed graph specification
  - Each node specifies either the local neighbors or any edge in the graph (knowledge is now globally distributed)

- Specify edge weights
  - Optimization opportunity for reordering despite the fact that the meaning is undefined
  - Each edge must be specified twice, once as out-edge (at the source) and once as in-edge (at the dest)

- Info arguments
  - Communicate assertions of semantics to the MPI library
  - E.g., semantics of edge weights
Distributed graph creation

MPI_Dist_graph_create_adjacent(MPI_Comm old_comm
    int indegree, const int sources[], const int sourceweights[],
    int outdegree, const int destinations[], const int destweights[],
    MPI_Info info, int reorder, MPI_Comm *comm_dist_graph)

- n – number of source nodes
- sources – n source nodes
- degrees – number of edges for each source
- destinations, weights – dest. processor specification
- info, reorder – as usual
- MPI_Dist_graph_create requires global communications to redistribute the information (as each process will eventually need to know it’s neighbors)

MPI_Dist_graph_create(MPI_Comm comm_old, int n,
    const int sources[], const int degrees[], const int destinations[],
    const int weights[], MPI_Info info, int reorder,
    MPI_Comm*comm_dist_graph)
Example: distributed graph creation

- MPI_Dist_graph_create_adjacent
- MPI_Dist_graph_create

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- The order is not important, but it must reflect on how the topology will be used
- Define the buffers order in the neighborhood collectives
- MPI_Dist_graph_create can be any permutation of the same edges representation
Distributed Graph query functions

- Query information (the number of neighbors and the neighbors) about the calling process
  - MPI_Dist_graph_neighbors_count return counts for the indegree, outdegree and weight.

\[
\begin{align*}
\text{MPI}_\text{Dist}\_\text{graph}\_\text{neighbors}\_\text{count} & (\text{MPI}_\text{Comm}\ \text{comm}, \\
& \text{int } \*\text{indegree} , \text{int } \*\text{outdegree} , \text{int } \*\text{weighted} ) \\
\text{MPI}_\text{Dist}\_\text{graph}\_\text{neighbors} & (\text{MPI}_\text{Comm}\ \text{comm}, \\
& \text{int } \text{maxindegree} , \text{int } \text{sources}[], \text{int } \text{sourceweights}[], \\
& \text{int } \text{maxoutdegree} , \text{int } \text{destinations}[], \text{int } \text{destweights}[] )
\end{align*}
\]

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Neighborhood Collectives

• Collective communications over topologies
  • They are still collective (all processes in the communicator must do the call, including processes without neighbors)
  • Buffers are accessed in the neighbors sequence
    • Order is determined by order of neighbors as returned by the corresponding query functions ([dist_]graph_neighbors).
    • Defined by order of dimensions, first negative, then positive
    • Cartesians 2*ndims sources and destinations
    • Distributed graphs are directed and may have different numbers of send/recv neighbors
    • Processes at borders (MPI_PROC_NULL) leave holes in buffers (will not be updated or communicated)!
  • Every process is root in its own neighborhood (!)
MPI_Neighbor_allgather

• Each process send the same message to all neighbors (the sendbuf)
• Each process receives indegree messages, one from each neighbors in their corresponding order from the query functions
• Similar to MPI_gather where each process is the root on the neighborhood

```c
MPI_Neighbor_allgather(
    const void* sendbuf, int sendcount, MPI_Datatype sendtype,
    void* recvbuf, int recvcount, MPI_Datatype recvtype,
    MPI_Comm comm)
```
MPI_Neighbor_allgather(
    const void* sendbuf, int sendcount, MPI_Datatype sendtype,
    void* recvbuf, int recvcount, MPI_Datatype recvtype,
    MPI_Comm comm)

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Nonblocking versions

• Full support for all nonblocking neighborhood collectives
  • Same collective invocation requirement
  • Matching will be done in order of the collective post for each collective
    • As each communicator can only have a single topology

• Think about the Jacobi where the communications are done with neighbor collectives
One-sided communications

• In MPI we are talking about epoch: a window of memory updates
  • Somewhat similar to memory transactions
  • Everything in an epoch is visible at once on the remote peers
  • Allow to decouple data transfers and synchronizations

• Terms:
  • Origin process: Process with the source buffer, initiates the operation
  • Target process: Process with the destination buffer, does not explicitly call communication functions
  • Epoch: Virtual time where operations are in flight. Data is consistent after new epoch is started.
    • Access epoch: rank acts as origin for RMA calls
    • Exposure epoch: rank acts as target for RMA calls
  • Ordering: only for accumulate operations: order of messages between two processes (default: in order, can be relaxed)
  • Assert: assertions about how the one sided functions are used, “fast” optimization hints, cf. Info objects (slower)
Overview

• Window creation
  • Static
    • Expose allocated memory: MPI_Win_create
    • Allocate and expose memory: MPI_Win_allocate
  • Dynamic
    • MPI_Win_create_dynamic

• Communications
  • Data movements: Put, Rput, Get, Rget
  • Accumulate (acc, racc, get_acc, rget_acc)
  • Atomic operations (fetch&op, compare and swap)

• Synchronizations
  • Active: Collective (fence); Group
  • Passive: P2P (lock/unlock); One epoch (lock _all)
Memory Exposure

- Collective calls (attached to a communicator)

- Info
  - no_locks – user asserts to not lock win
  - accumulate_ordering – comma-separated rar, war, raw, waw
  - accumulate_ops – same_op or same_op_no_op (default) – assert used ops for related accumulates
  - same_size – if true, user asserts that size is identical on all calling processes (only for MPI_Win_allocate)

- MPI_Win_allocate is preferred, as the implementation is allowed to prepare the memory (pinning and co.)

- MPI_Win_free will free the memory allocated by the MPI library (special care for MPI_Win_allocate)

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

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

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

MPI_Win_attach(MPI_Win win, void *base, MPI_Aint size)

MPI_Win_detach(MPI_Win win, const void *base)

MPI_Win_free(MPI_Win *win)
```
One Sided communications
• Put and Get have symmetric behaviors
• Nonblocking, they will complete at the end of the epoch
• Conflicting accesses (for more than one byte) are allowed, but their outcome is undefined
• The request-based version can be waited using any MPI completion mechanism (MPI_Test* or MPI_Wait*)
• Similarly to MPI_Ssend completion of the request only has a local meaning
  • GET: the data is stored in the local buffer
  • PUT: The local buffer can be safely reused (no remote completion)

```c
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)
MPI_Rput(..., MPI_Request *request)
```
One Sided Accumulate

- Atomic update of remote memory based on a combination of the existing data and local data
  - Except if OP is MPI_REPLACE (when it is equivalent to MPI_Put)
  - Non overlapping entries at the target (because memory consistency and ordering accesses)
- MPI_Get_accumulate similar behavior to fetch_and_* operations
  - Accumulate origin into target, returns content before accumulate in result
  - The accumulate operation is atomic
- Order between operations can be relaxed with info (accumulate_ordering = raw, waw, rar, war) during window creation

```c
MPI_Accumulate(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_Op op, MPI_Win win)

MPI_Get_accumulate(const void *origin_addr, int origin_count, MPI_Datatype origin_datatype,
                    void *result_addr, int result_count, MPI_Datatype result_datatype,
                    int target_rank, MPI_Aint target_disp, int target_count, MPI_Datatype target_datatype,
                    MPI_Op op, MPI_Win win)
```
One Sided Atomic Operations

• Similar to the atomic operations on the processor

• Fetch_and_op common use case for single element
  • Supposed to be a faster version of the MPI_Get_accumulate because of the restriction on the datatype and count

• Compare and swap
  • Compares compare buffer with target and replaces value at target with origin if compare and target are identical. Original target value is returned in result.

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

MPI_Compare_and_swap(const void *origin_addr, const void *compare_addr, void *result_addr, MPI_Datatype datatype, int target_rank, MPI_Aint target Disp, MPI_Win win)
```
One Sided Synchronizations

- **Active / Passive**
  
  ```c
  MPI_Win_fence(int assert, MPI_Win win)
  ```

- **Collective Synchronization:** all operations started before will complete by the time we return
  - Ends the exposure epoch for the entire window
  - Optimization possible via the MPI_MODE_NOPRECEDE assert (no local or remote operations with target the local processor exists)

  ```c
  MPI_Win_post(MPI_Group group, int assert, MPI_Win win)
  MPI_Win_start(MPI_Group group, int assert, MPI_Win win)
  MPI_Win_complete(MPI_Win win)
  MPI_Win_wait(MPI_Win win)
  ```

- **Specification of access/exposure epochs separately:**
  - Post: start exposure epoch to group, nonblocking
  - Start: start access epoch to group, may wait for post
  - Complete: finish prev. access epoch, origin completion only (not target)
  - Wait: will wait for complete, completes at (active) target

- **As asynchronous as possible**
One Sided Synchronizations

- Initiates RMA access epoch to rank
  - No concept of exposure epoch
- Unlock closes access epoch
  - Operations have completed at origin and target
- Type:
  - Exclusive: no other process may hold lock to rank
  - More like a real lock, e.g., for local accesses
  - Shared: other processes may also hold lock

```
MPI_Win_lock(int lock_type, int rank, int assert, MPI_Win win)
MPI_Win_unlock(int rank, MPI_Win win)

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

- Starts a shared access epoch from origin to all ranks!
  - Not collective!
- Does not really lock anything
  - Opens a different mode of use
More advanced MPI and mixed programming topics
Extracting messages from MPI

- MPI_Recv delivers each message from a peer in the order in which these messages were send
  - No coordination between peers is possible

- Take a scenario where we have a ring of processors with \((P-1)\) participants, and a lone process that centralize messages from all peers.
- Each processor (except 0) waits for a message from its predecessor in the ring before sending a message to the coordinator.
- In which order the messages are received at the coordinator?
- How we can implement this if each ring participant send a message of a different length?
- What if we assume a large number of processes?

- Missing functionality: the capability to peek (but not alter) into the network to extract what message will be the next to be locally received
  - Functionality that behaves as MPI_Recv but without altering the matching queue
MPI Probe

- MPI_ANY_SOURCE and MPI_ANY_TAG can be used as markers for unnamed receives
- The usual usage scenario is probe, memory allocation and then receive
  - How can we use this functionality in a thread safe application when all threads work on the same communicator?
  - Assume 2 threads (X,Y) doing the probe (P), alloc (A) and receive (R) operation each one on its own context
    - $X_P \rightarrow X_A \rightarrow X_R \rightarrow Y_P \rightarrow Y_A \rightarrow Y_R$
    - What happens if the order of the operations is $X_P \rightarrow X_A \rightarrow Y_P \rightarrow Y_A \rightarrow Y_R \rightarrow X_R$
- The access to the matching queue need to be protected for concurrent accesses
Message Probe

- Functionality that extracts the message from the matching queue but without receiving it
  - Supported by functionality to extract the content of the message into a user provided buffer
  - Any partial ordering between our threads X and Y is now correct:
    \[ X_{P'} \rightarrow X_A \rightarrow Y_{P'} \rightarrow Y_A \rightarrow Y_{R'} \rightarrow X_{R'} \]

```c
int MPI_Mprobe(int source, int tag, MPI_Comm comm, MPI_Status *status);
int MPI_Improbe(int source, int tag, MPI_Comm comm, int *flag, MPI_Message *message,
                 MPI_Status *status);
int MPI_Mrecv(void *buf, int count, MPI_Datatype type, MPI_Message *message,
              MPI_Status *status);
int MPI_Imrecv(void *buf, int count, MPI_Datatype type, MPI_Request *request);
```
Collective Communication with threads

• What is happening if multiple threads issue in the same communicator in same time
  • Multiple blocking collectives?
  • Multiple non-blocking collective with the same datatype and count?
  • Multiple non-blocking collective with the different datatype and count?
Shared Memory

• Potential for memory reduction as initialization data can be shared between processes
  • Avoid recomputing the same initial state by multiple applications (on the same node)
  • POSIX provides shared memory regions but (1) not all Oses have support for them and (2) it does not integrate with MPI functionality

• Need functionality to split a communicator in disjoint groups with shared capabilities
  • Similar to MPI_Comm_split with architecture aware color (key will then be the rank in the original communicator)
  • Single info key standardized: MPI_COMM_TYPE_SHARED
  • Some MPI implementations provide support for different granularities of sharing (Open MPI)

```c
int MPI_Comm_split_type(MPI_Comm comm, int split_type, int key, MPI_Info info, MPI_Comm *newcomm);
```
Shared Memory Window

- Allocates shared memory regions in win
  - Collective call resulting in a fully capable RMA window
  - Constraint: all processes in the communicator must be capable of physically sharing memory (usually same node)
  - The call returns a pointer to the local part
  - The info key define how the global shared memory region is defined:
    - Contiguous: process i memory starts right after the end of process i-1
    - Non contiguous (key alloc_shared_noncontig): allow the MPI to provide NUMA-aware optimizations.
  - One way to create the communicator needed is to use MPI_Comm_split_type

```c
int MPI_Win_allocate_shared (MPI_Aint size, int disp_unit, MPI_Info info, MPI_Comm comm,
                           void *baseptr, MPI_Win *win);
```
Shared Memory Window

- In non-contiguous cases, we need to extract the remote address in order to complete RMA operations.
  - As the memory region might be mapped at different addresses in different processes, each process's local address has no meaning.
  - Unlike in Open SHMEM, where the RMA operations are applied on symmetric memory (!).
  - Only works for windows of type MPI_WIN_FLAVOR_SHARED (aka. created via MPI_Win_allocate_shared).

```c
int MPI_Win_shared_query (MPI_Win win, int rank, MPI_Aint *size, int *disp_unit, void *baseptr);
```
RMA and pt2pt puzzle?

• Assuming a correctly initialized window what is the outcome of the following code?

```c
for(i = 0; i < len; a[i] = (double)(10*me+i), i++);
if (me == 0) {
    MPI_Win_lock(MPI_LOCK_EXCLUSIVE, 1, 0, win);
    MPI_Send(NULL, 0, MPI_BYTE, 2, 1001, MPI_COMM_WORLD);
    MPI_Get(a,len,MPI_DOUBLE,1,0,len,MPI_DOUBLE,win);
    MPI_Win_unlock(1, win);
    for(i = 0; i < len; i++) printf("a[%d] = %d\n", a[i]);
} else if (me == 2) { /* this should block till 0 releases the lock. */
    MPI_Recv(NULL, 0, MPI_BYTE, 0, 1001, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
    MPI_Win_lock(MPI_LOCK_EXCLUSIVE, 1, 0, win);
    MPI_Put(a,len,MPI_DOUBLE,1,0,len,MPI_DOUBLE,win);
    MPI_Win_unlock(1, win);
}
```