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-topoint 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

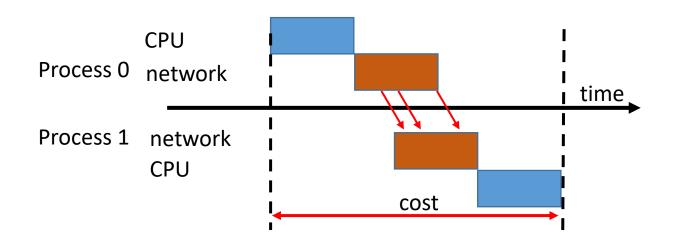
- An important technical detail
 - Eager vs. Rendezvous

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

```
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);
}</pre>
```



Software Pipelining - Implementation

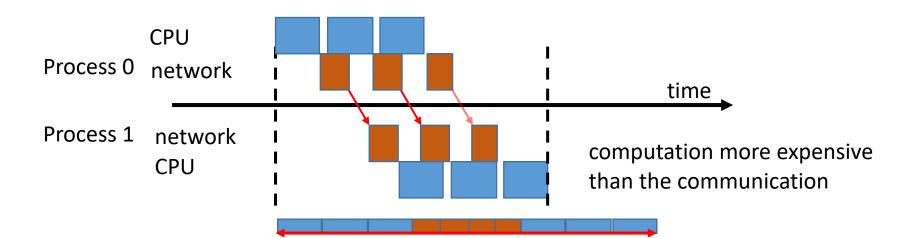
```
MPI Request reg = MPI REQUEST NULL;
    if( 0 == rank ) {
      for( int b = 0; b < (size / BSIZE); b++) {
         MPI_wait( req, &status); /* complete previous step */
         for(int i = b * BSIZE; i < ((b+1) * BSIZE); i++)
           buf[i] = compute(buf, size, i);
         MPI_Isend(&buf[b * 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);
          CPU
Process 0
          network
                                                               time
Process 1
           network
                                                        What if the computation is more
           CPU
                                                        expensive than the
                                                        communication?
                                original cost
```

Software Pipelining - Implementation

```
MPI Request reg = 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);
          CPU
Process 0
          network
                                                               time
Process 1
           network
                                                       computation more expensive
           CPU
                                                       than the communication
```

Software Pipelining - Implementation

```
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);
    }
}</pre>
```



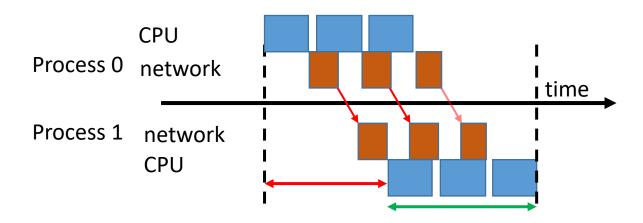
Software pipelining - modelization

No pipeline

•
$$T = T_{comp}(s) + T_{comm}(s) + T_{startc}(s) + T'_{comp}(s)$$

Pipeline

•
$$T = T_{comp}(bs) + T_{comm}(bs) + T_{startc}(bs) + nblocks * max(T_{comp}(bs), T_{comm}(bs), T_{startc}(bs), T'_{comp}(bs))$$



Communicators - Collectives

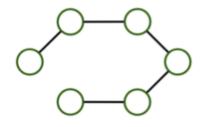
- Simple classification by operation class
- One-To-All (simplex mode)
 - One process contributes to the result. All processes receive the result.
 - MPI Bcast
 - MPI_Scatter, MPI_Scatterv
- All-To-One (simplex mode)
 - All processes contribute to the result. One process receives the result.
 - MPI_Gather, 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_lbcast(, 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

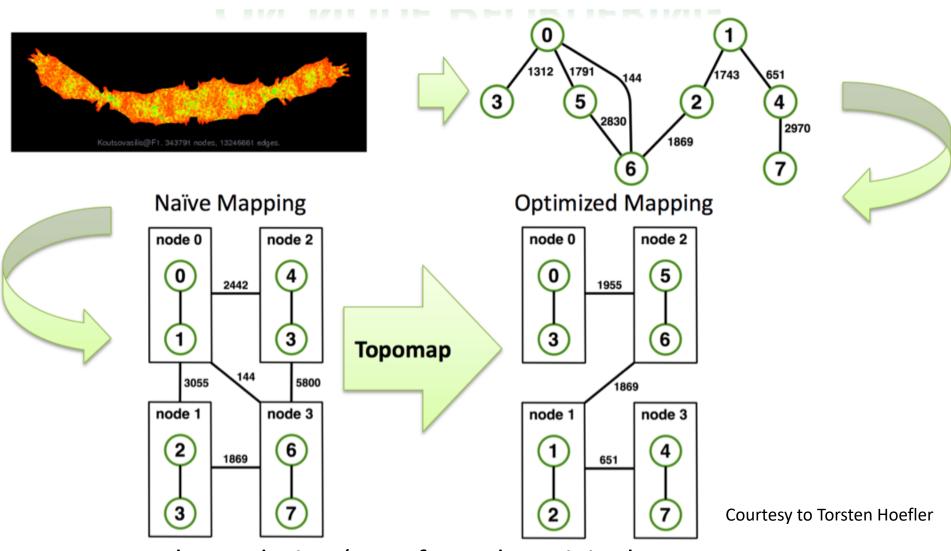
• Restrictions:

- 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 pipelinling
 - 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

Topologies and Neighborhood



 Rank reordering (transform the original, resource manager provided allocation) and map the processes on it based on the communication pattern

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 <= 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

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
 - Not scalable

```
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 nodes 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

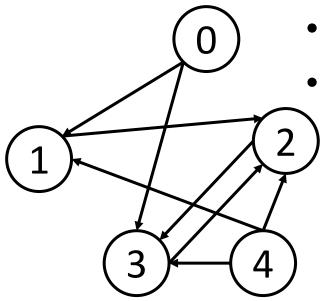
Distributed graph creation

```
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



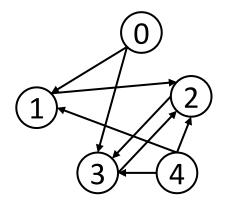
- MPI_Dist_graph_create_adjacent
- MPI_Dist_graph_create

	P0	P1	P2	Р3	P4
indegree	{0}	{2}	{3}	{3}	{0}
sources	{}	{0, 4}	{1, 3, 4}	{0, 2, 4}	{}
outdegree	{2}	{1}	{1}	{1}	{3}
destinations	{1, 3}	{2}	{3}	{2}	{1, 2, 3}

- 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.



	P0	P1	P2	Р3	P4
indegree	{O }	{ <mark>2</mark> }	{3 }	{3 }	{ <mark>0</mark> }
sources	{}	{0, 4}	{1, 3, 4}	{0, 2, 4}	{}
outdegree	{ <mark>2</mark> }	{ 1 }	{ <mark>1</mark> }	{ <mark>1</mark> }	{3 }
destinations	{1, 3}	{2}	{3}	{2}	{1, 2, 3}

MPI_Dist_graph_neighbors_count

MPI_Dist_graph_neighbors

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 (!)

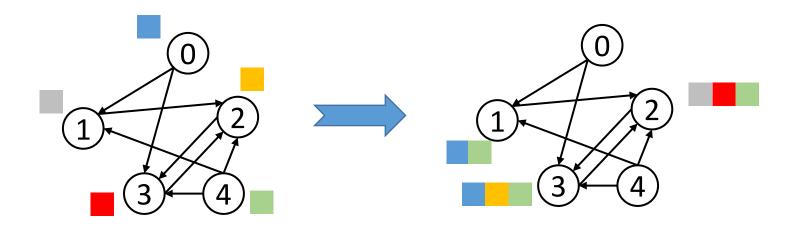
MPI_Neighbor_allgather

- 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
 - Despite the fact that name starts with all

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

MPI_Neighbor_allgather

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



	Р0	P1	P2	Р3	P4
indegree	{0}	{2}	{3}	{3}	{0}
sources	{}	{0, 4}	{1, 3, 4}	{0, 2, 4}	{}
outdegree	{2}	{1}	{1}	{1}	{3}
destinations	{1, 3}	{2}	{3}	{2}	{1, 2, 3}

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)

```
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_Send 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)

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

```
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.

```
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

```
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)

```
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

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

- 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

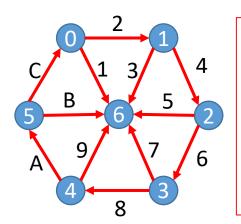
```
MPI_Win_lock_all(int assert, MPI_Win win)
MPI Win unlock_all(MPI_Win win)
```

- 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

```
int MPI_Probe(int source, int tag, MPI_Comm comm, MPI_Status *status);
int MPI_Iprobe(int source, int tag, MPI_Comm comm, int *flag, MPI_Status *status);
Int MPI_Get_count( MPI_Status* status, MPI_Datatype datatype, int* count);
MPI_Status a structure containing the fields MPI_SOURCE, MPI_TAG and MPI_ERROR
```

- 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
 - $X_P \longrightarrow X_A \longrightarrow X_R \longrightarrow Y_P \longrightarrow Y_A \longrightarrow Y_R$
 - What happens if the order of the operations is $X_P \longrightarrow X_A \longrightarrow Y_P \longrightarrow Y_A \longrightarrow Y_R \longrightarrow X_R$
- 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: $X_{P'} \longrightarrow X_A \longrightarrow Y_{P'} \longrightarrow Y_A \longrightarrow Y_{R'} \longrightarrow X_{R'}$

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)

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

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 local address has no meaning
 - Unlike in Open SHMEM where the RMA operations applied on symmetric memory (!)
 - Only works for windows of type MPI_WIN_FLAVOR_SHARED (aka. created via MPI_Win_allocate_shared)

RMA and pt2pt puzzle?

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

```
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);
```