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

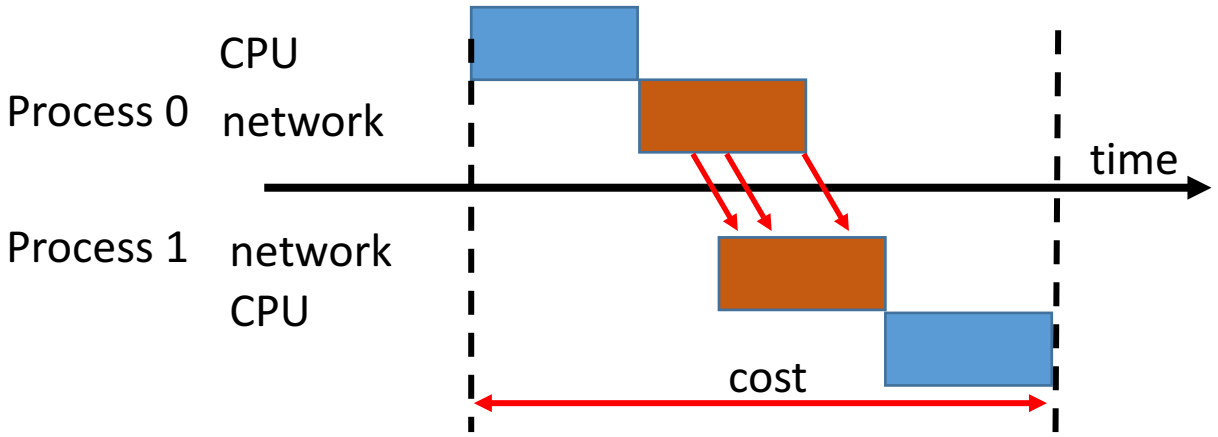
Nonblocking communications

- An important technical detail
  - Eager vs. Rendezvous

- 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)

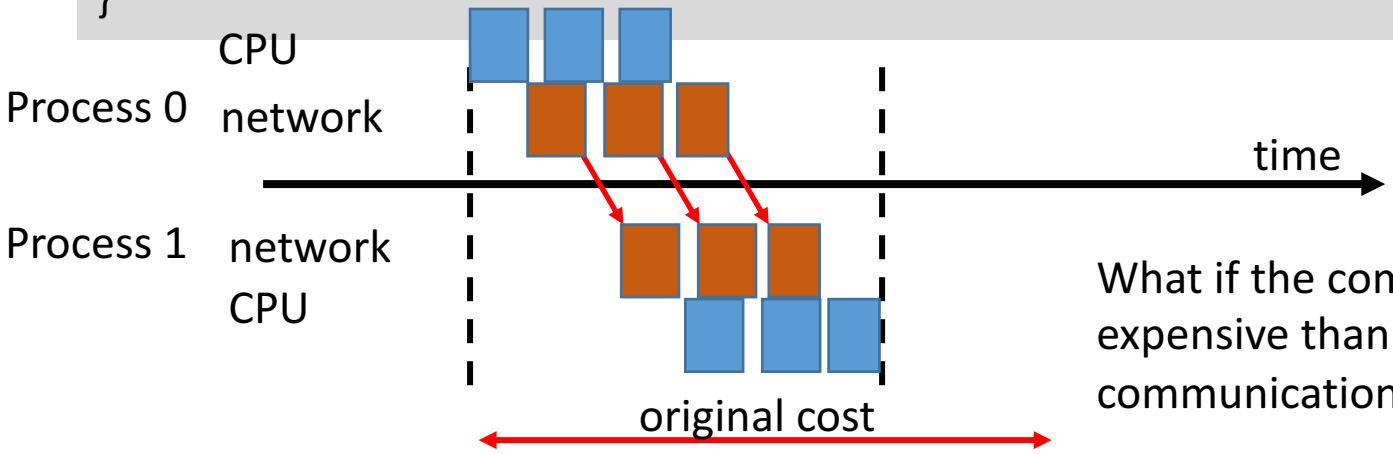
Software Pipelining - Motivation

```
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);
}
```



Software Pipelining - Implementation

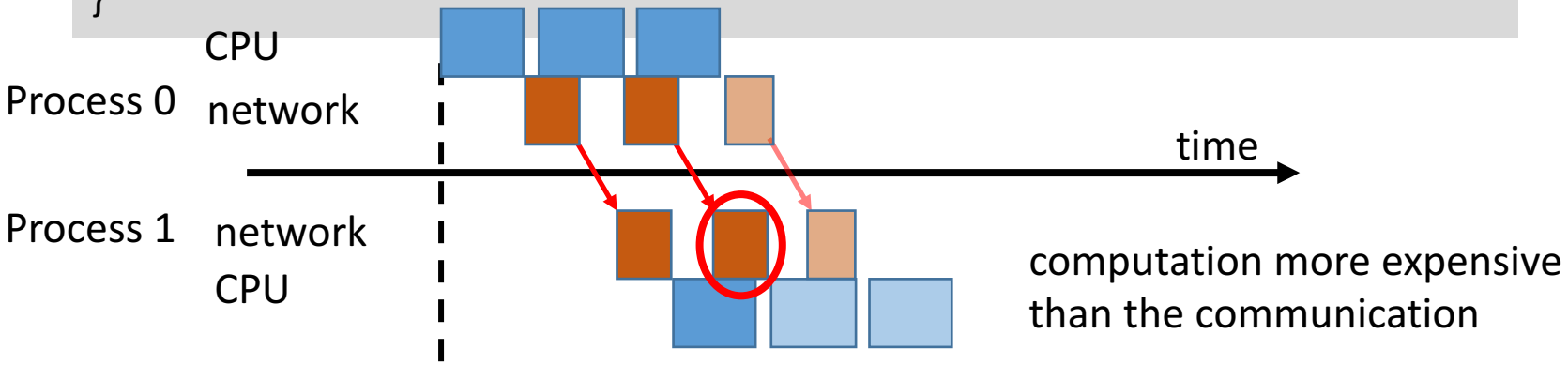
```
MPI_Request req = MPI_REQUEST_NULL;
if( 0 == rank ) {
   for( int b = 0; b < (size / BSIZE); b++ ) {
      MPI_wait( req, &status);  /* complete previous step */
      for( int i = b * BSIZE; i < ((b+1) * BSIZE); i++ )
         buf[i] = compute(buf, size, i);
      MPI_Isend(&buf[b * BSIZE], BSIZE,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

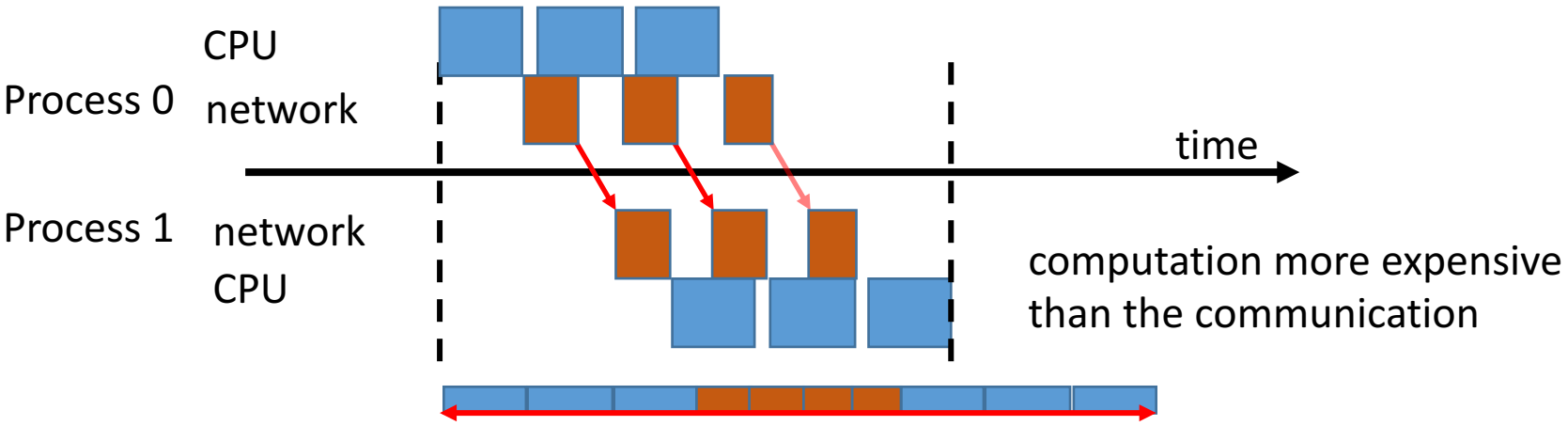
Software Pipelining - Implementation

```
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);
   }
}
```



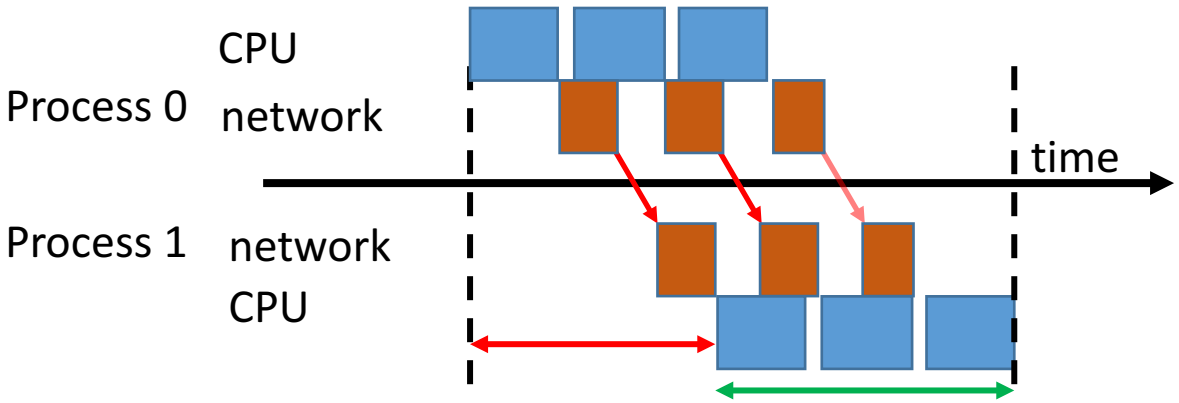
Software Pipelining - Implementation

```
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);
   }
}
```



Software pipelining - modelization

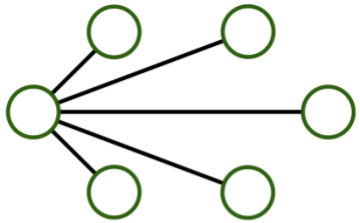
- No pipeline
  - $T = T_{comp}(s) + T_{comm}(s) + T_{startc}(s) + T'_{comp}(s)$
- Pipeline
  - $T = T_{comp}(bs) + T_{comm}(bs) + T_{startc}(bs) + nblocks * \max(T_{comp}(bs), T_{comm}(bs), T_{startc}(bs), T'_{comp}(bs))$

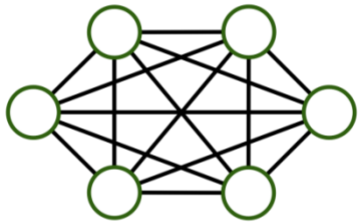


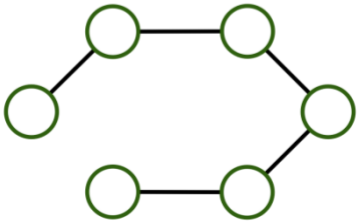
Communicators - Collectives

- 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

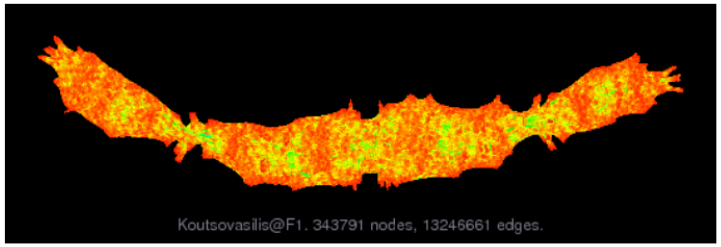
Nonblocking collectives

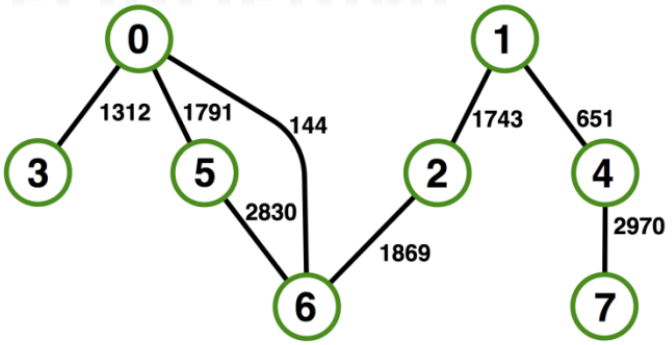
- Nonblocking variants of all collectives
  - MPI_Ibcast(, MPI_Request *req);
- Semantics:
  - Function returns no matter what
  - No guaranteed progress (quality of implementation)
  - Usual completion calls (wait, test) + mixing
  - Out-of order completion
- Restrictions:
  - No tags, in-order matching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

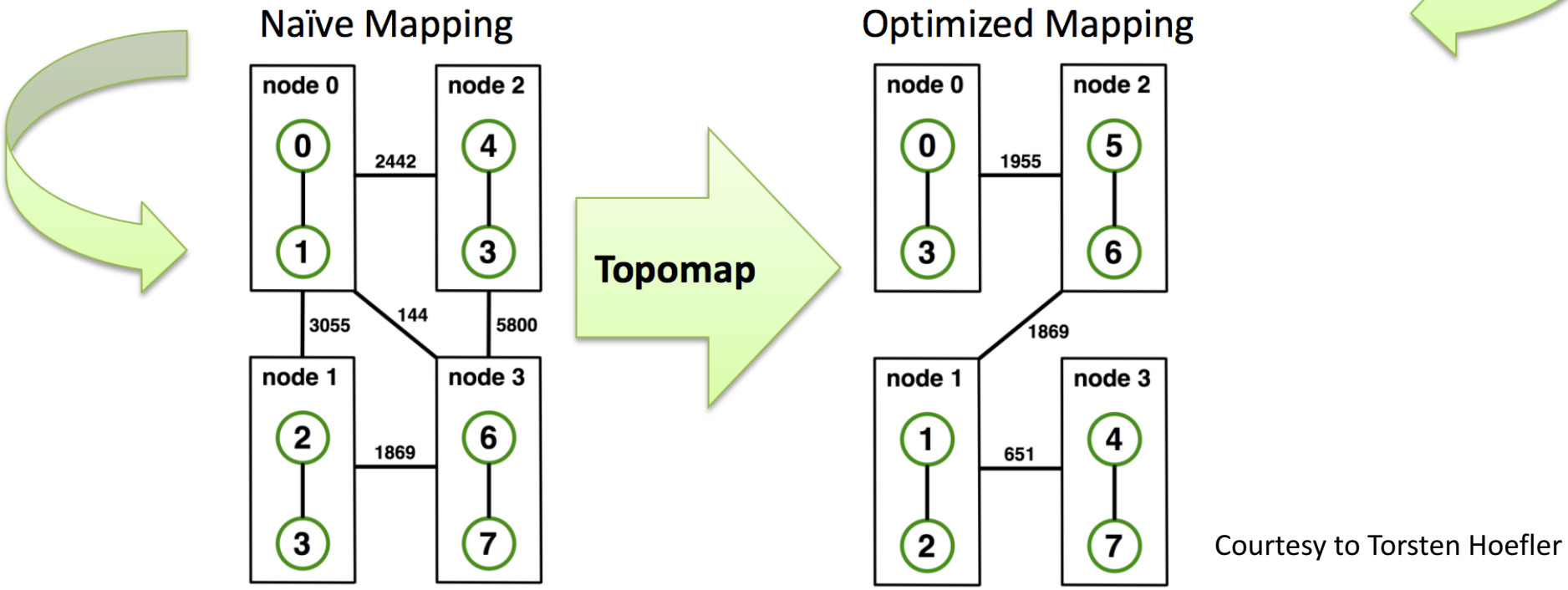
Nonblocking collectives

- 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







Courtesy to Torsten Hoefler

- 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

```
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
  - Not scalable

```
MPI_Graph_create(MPI_Comm comm_old, int nnodes,
                 const int *index, const int *edges, int reorder,
                 MPI_Comm *comm_graph)
```

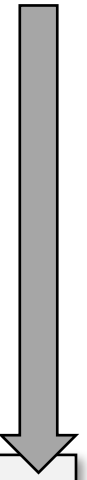
Distributed graph creation

- 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

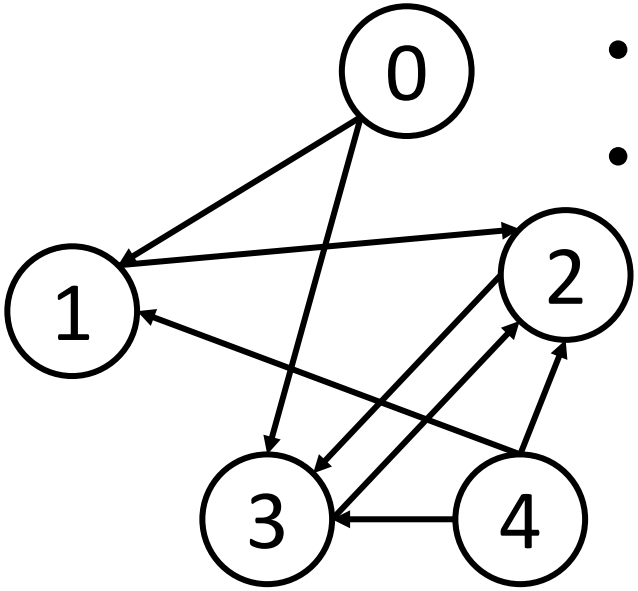
```
MPI_Dist_graph_create_adjacent(MPI_Comm old_comm
        int indegree, const int sources[], const int sourceweights[],
        int outdegree, const int destinations[], const int destweights[],
        MPI_Info info, int reorder, MPI_Comm *comm_dist_graph)
```

- 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

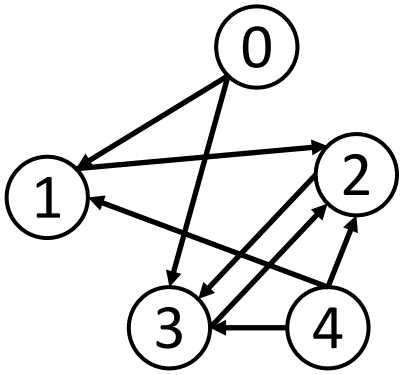
	P0	P1	P2	P3	P4
indegree	{0}	{2}	{3}	{3}	{0}
sources	{}	{0, 4}	{1, 3, 4}	{0, 2, 4}	{}
outdegree	{2}	{1}	{1}	{1}	{3}
destinations	{1, 3}	{2}	{3}	{2}	{1, 2, 3}

- 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.

```
MPI_Dist_graph_neighbors_count(MPI_Comm comm,
                int *indegree, int *outdegree, int *weighted)
MPI_Dist_graph_neighbors(MPI_Comm comm,
                int maxindegree, int sources[], int sourceweights[],
                int maxoutdegree, int destinations[],int destweights[])
```



	P0	P1	P2	P3	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}

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 (!)

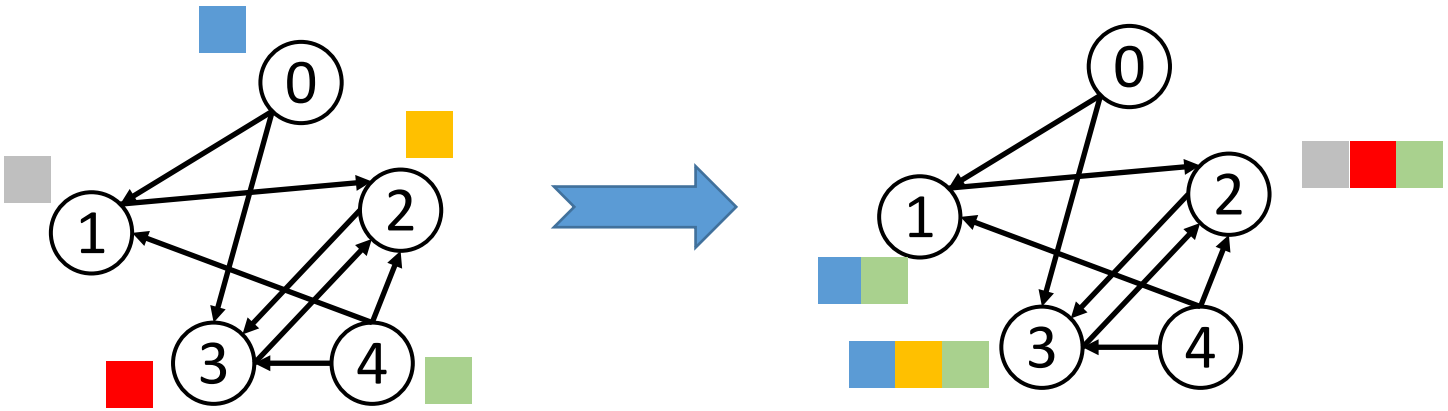
MPI_Neighbor_allgather

- 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)
```



	P0	P1	P2	P3	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)

```
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

```
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