MPI for Scalable Computing

https://anl.box.com/v/2019-ATPESC-MPI

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The MPI Part of ATPESC

- We assume everyone already has some MPI experience
- We will focus more on understanding MPI concepts than on coding details
- Emphasis will be on issues affecting scalability and performance
- There will be code walkthroughs and hands-on exercises

Outline

- Morning
  - Introduction to MPI and this tutorial
  - Performance issues in MPI programs
  - Avoiding unnecessary synchronization
  - Minimizing data motion
    - using MPI datatypes
  - Topics in collective communication
  - One-sided communication (or remote memory access)
  - Hands-on exercises

- Afternoon
  - One-sided communication contd.
  - Hybrid programming
    - MPI + threads/shared-memory/accelerators
  - Process topologies and neighborhood collectives
  - Hands-on exercises

- After dinner
  - Hands-on exercises contd.

What is MPI?

- MPI is a message-passing library interface standard.
  - Specification, not implementation
  - Library, not a language
  - Classical message-passing programming model
- MPI-1 was defined (1994) by a broadly-based group of parallel computer vendors, computer scientists, and applications developers.
  - 2-year intensive process
- Implementations appeared quickly and now MPI is taken for granted as vendor-supported software on any parallel machine.
- Free, portable implementations exist for clusters and other environments (MPICH, Open MPI)

Timeline of the MPI Standard

- MPI-1 (1994), presented at SC'93
  - Basic point-to-point communication, collectives, datatypes, etc
- MPI-2 (1997)
  - Added parallel I/O, Remote Memory Access (one-sided operations), dynamic processes, thread support, C++ bindings, …
- ---- Unchanged for 10 years ----
- MPI-2.1 (2008)
  - Minor clarifications and bug fixes to MPI-2
- MPI-2.2 (2009)
  - Small updates and additions to MPI 2.1
- MPI-3.0 (2012)
  - Major new features and additions to MPI (nonblocking collectives, neighborhood collectives, improved RMA, tools interface, Fortran 2008 bindings, etc.)
- MPI-3.1 (2015)
  - Small updates to MPI 3.0

Status of MPI-3.1 Implementations

	MPICH	MVAPICH	Open MPI	Cray	Tianhe	Intel		IBM			HPE	Fujitsu	MS	MPC	NEC	Sunway	RIKEN	AMPI
						IMPI	MPICH-OFI	BG/Q (legacy) [1]	PE (legacy) [2]	Spectrum								
NBC	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Nbr. Coll.	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✗	✓	✓	✓	✓	✓
RMA	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	(*)	✓	✓	✓	✓	Q2 ‘18
Shr. mem	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	Q1 ‘18
MPI_T	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	*	✓	✓	✓	✓	Q2 ‘18
Comm-create group	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	*	✓	✓	✓	✓	✓
F08 Bindings	✓	✓	✓	✓	✓	✓	✓	✓	✗	✓	✓	✗	✗	✓	✓	✓	✓	Q2 ‘18
New Dtypes	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Large Counts	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
MProbe	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	Q1 ‘18
NBC I/O	✓	✓	✓	✓	✗	✓	✓	✗	✗	✓	✓	✗	✗	*	✓	✗	✓	Q3 ‘18

Release dates are estimates; subject to change at any time

“✗” indicates no publicly announced plan to support that feature

Platform-specific restrictions might apply to the supported features

[1] Open Source but unsupported

[2] No MPI_T variables exposed

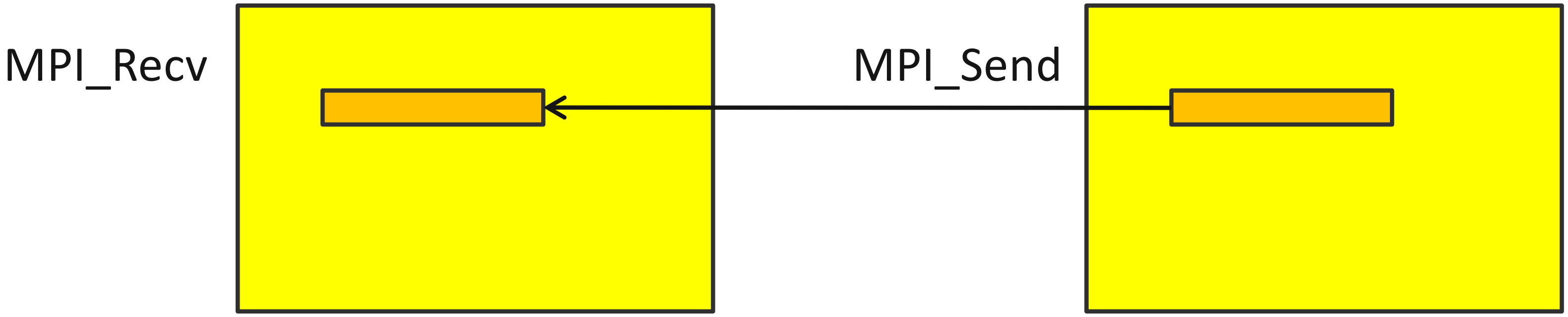
* Under development

(*) Partly done

Important considerations while using MPI

- All parallelism is explicit: the programmer is responsible for correctly identifying parallelism and implementing parallel algorithms using MPI constructs

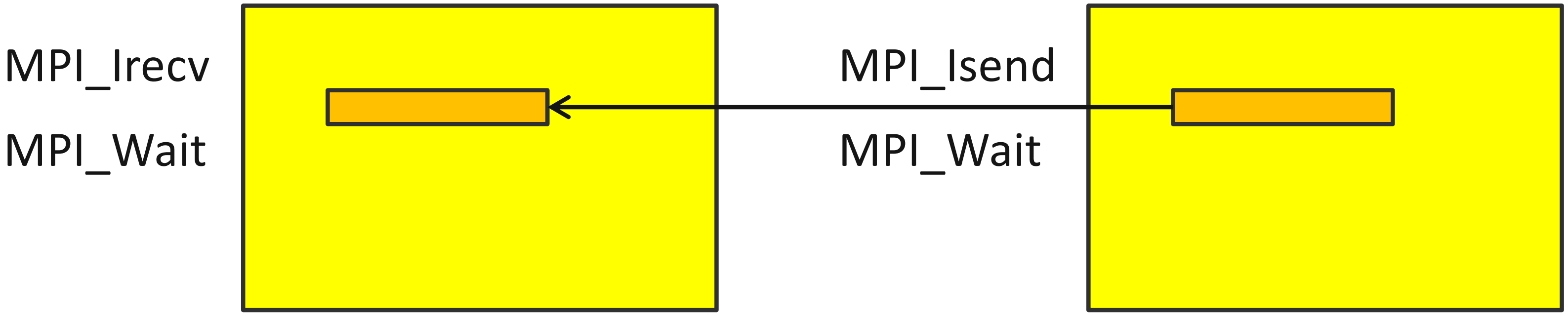
Basic MPI Communication



MPI_Recv

MPI_Send

OR



MPI_Irecv

MPI_Wait

MPI_Isend

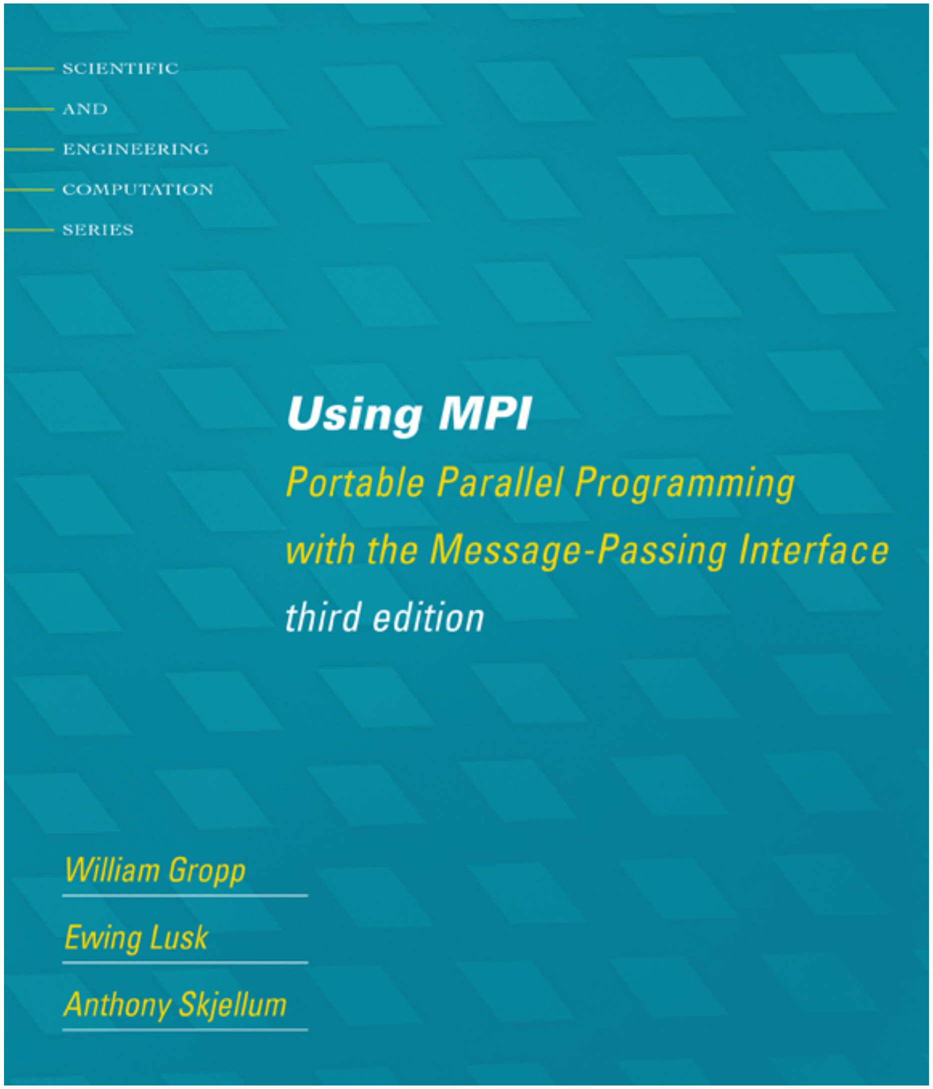
MPI_Wait

Web Pointers

- MPI Standard : http://www.mpi-forum.org/docs/docs.html
- MPI Forum : http://www.mpi-forum.org/

- MPI implementations:
  - MPICH : http://www.mpich.org
  - MVAPICH : http://mvapich.cse.ohio-state.edu/
  - Intel MPI: http://software.intel.com/en-us/intel-mpi-library/
  - Microsoft MPI: https://msdn.microsoft.com/en-us/library/bb524831%28v=vs.85%29.aspx
  - Open MPI : http://www.open-mpi.org/
  - IBM MPI, Cray MPI, HP MPI, TH MPI, …
- Several MPI tutorials can be found on the web

Tutorial Books on MPI (November 2014)



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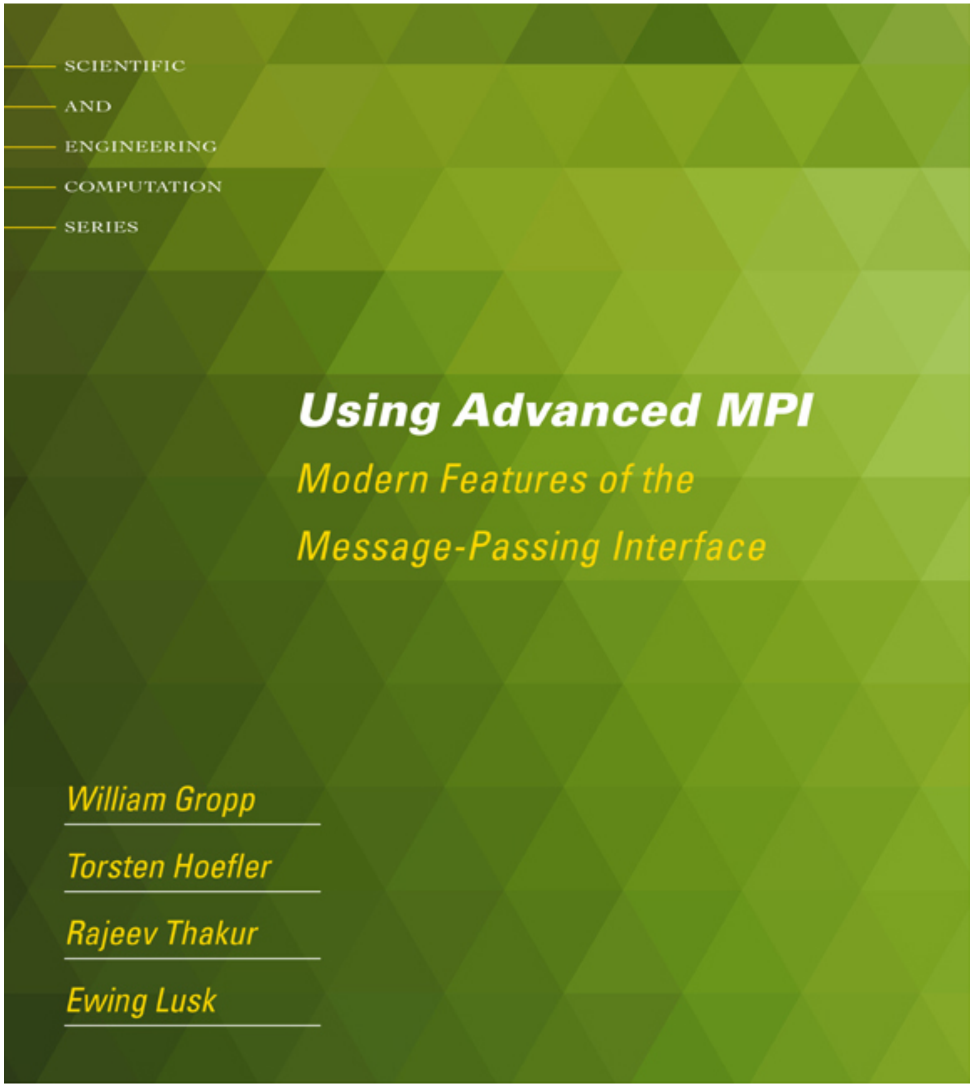
Using MPI

Portable Parallel Programming with the Message-Passing Interface

third edition

William Gropp
Ewing Lusk
Anthony Skjellum

Basic MPI



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COMPUTATION
SERIES

Using Advanced MPI

Modern Features of the Message-Passing Interface

William Gropp
Torsten Hoefler
Rajeev Thakur
Ewing Lusk

Advanced MPI, including MPI-2 and MPI-3

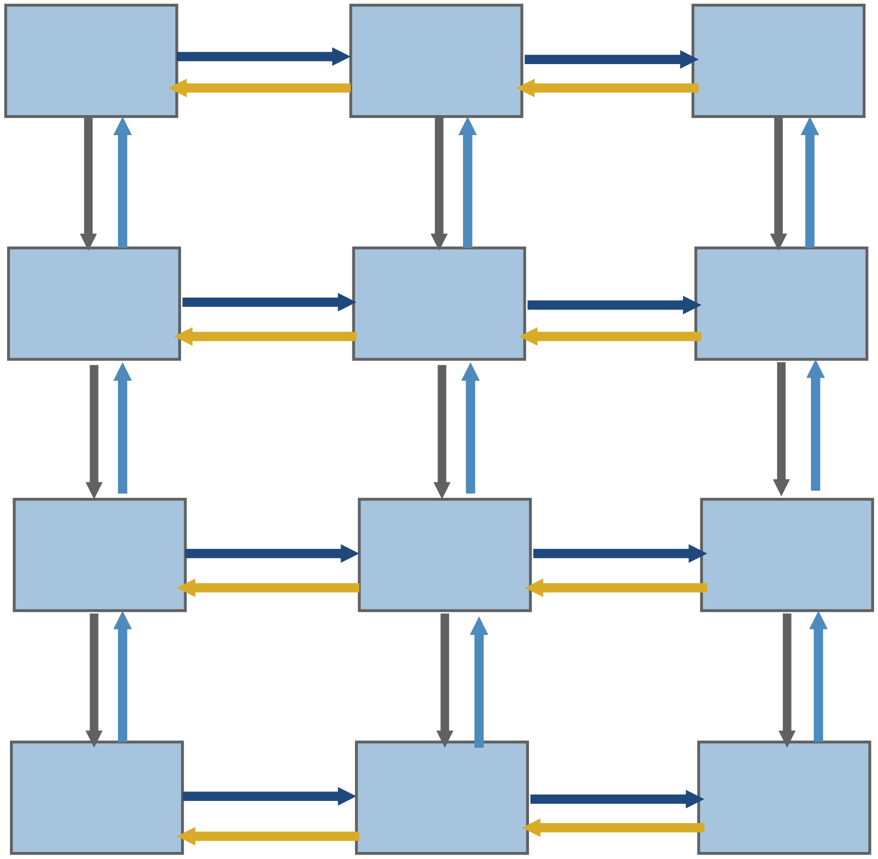
Costs of Unintended Synchronization

Unexpected Hot Spots

- Even simple operations can give surprising performance behavior.
- Examples arise even in common grid exchange patterns
- Message passing illustrates problems present even in shared memory
  - Blocking operations may cause unavoidable stalls

Mesh Exchange

- Exchange data on a mesh



Sample Code

```
Do i=1,n_neighbors
  Call MPI_Send(edge(1,i), len, MPI_REAL,&
                   nbr(i), tag,comm, ierr)
Enddo
Do i=1,n_neighbors
  Call MPI_Recv(edge(1,i), len, MPI_REAL,&
               nbr(i), tag, comm, status, ierr)
Enddo
```

Deadlocks!

- All of the sends may block, waiting for a matching receive (will for large enough messages)
- The variation of

  ```
  if (has down nbr) then
     Call MPI_Send( … down … )
  endif
  if (has up nbr) then
     Call MPI_Recv( … up … )
  endif
  …
  ```

  sequentializes (all except the bottom process blocks)

Sequentialization

Start	Start	Start	Start	Start	Start	Send	Recv
Send	Send	Send	Send	Send	Send		
					Send	Recv	
				Send	Recv		
			Send	Recv			
		Send	Recv				
	Send	Recv					
Send	Recv						

Fix 1: Use Irecv

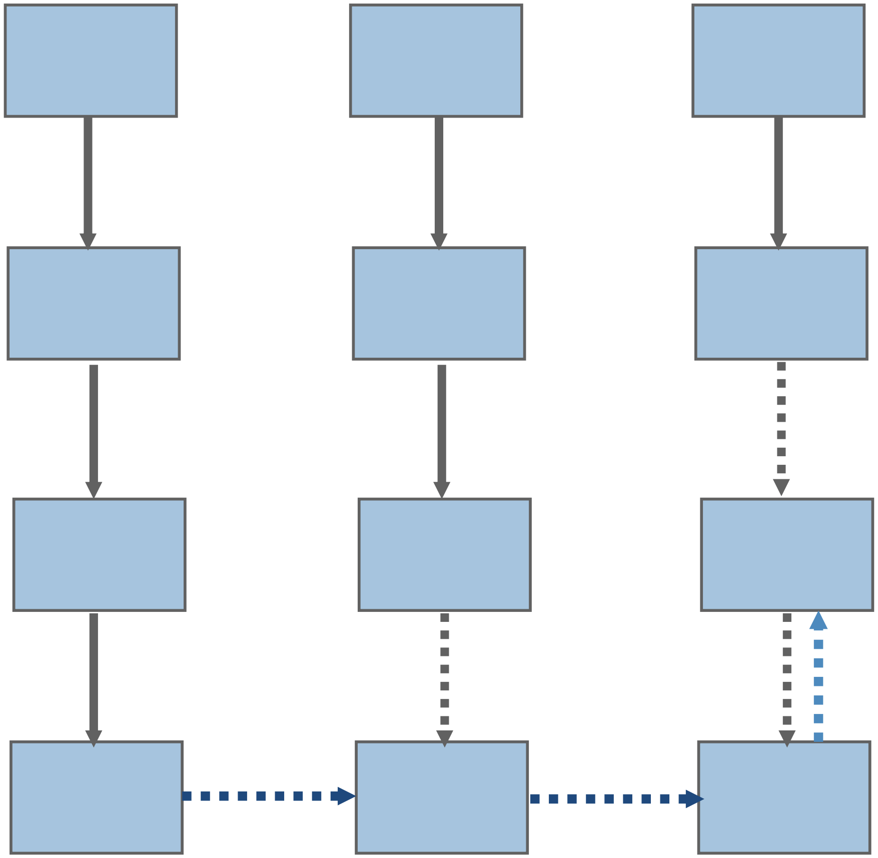
-
  ```
  Do i=1,n_neighbors
    Call MPI_Irecv(inedge(1,i), len, MPI_REAL, nbr(i), tag,&
                          comm, requests(i), ierr)
  Enddo
  Do i=1,n_neighbors
    Call MPI_Send(edge(1,i), len, MPI_REAL, nbr(i), tag,&
                          comm, ierr)
  Enddo
  Call MPI_Waitall(n_neighbors, requests, statuses, ierr)
  ```
- Does not perform well in practice. Why?

Understanding the Behavior: Timing Model

- Sends interleave
- Sends block (data larger than buffering will allow)
- Sends control timing
- Receives do not interfere with Sends
- Exchange can be done in 4 steps (down, right, up, left)

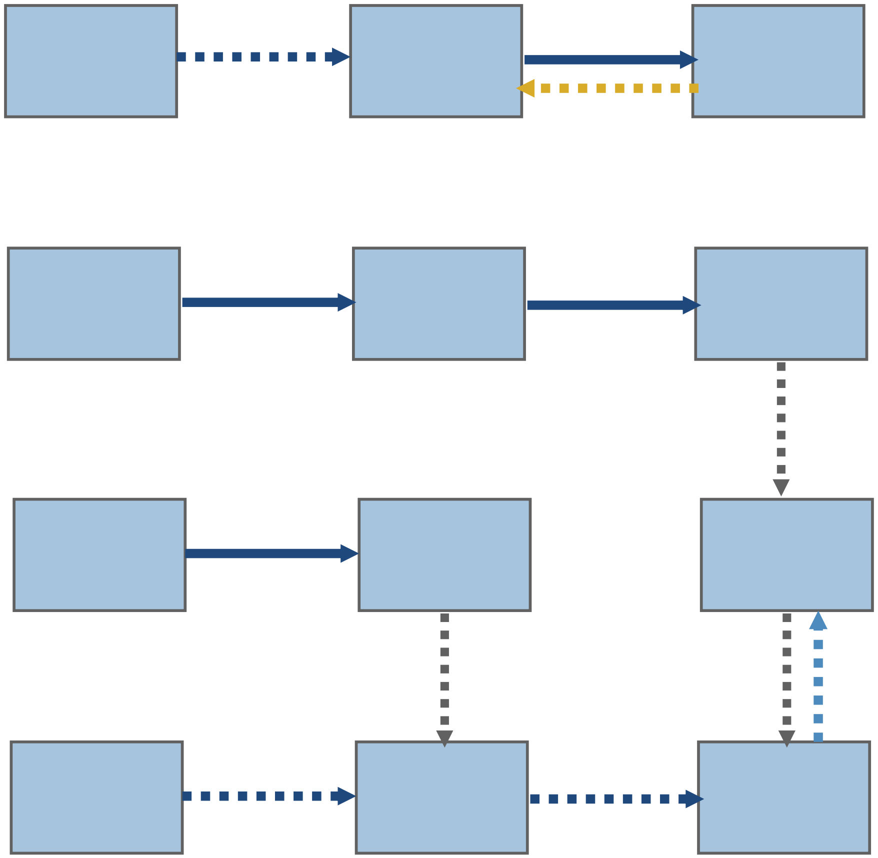
Mesh Exchange - Step 1

- Exchange data on a mesh



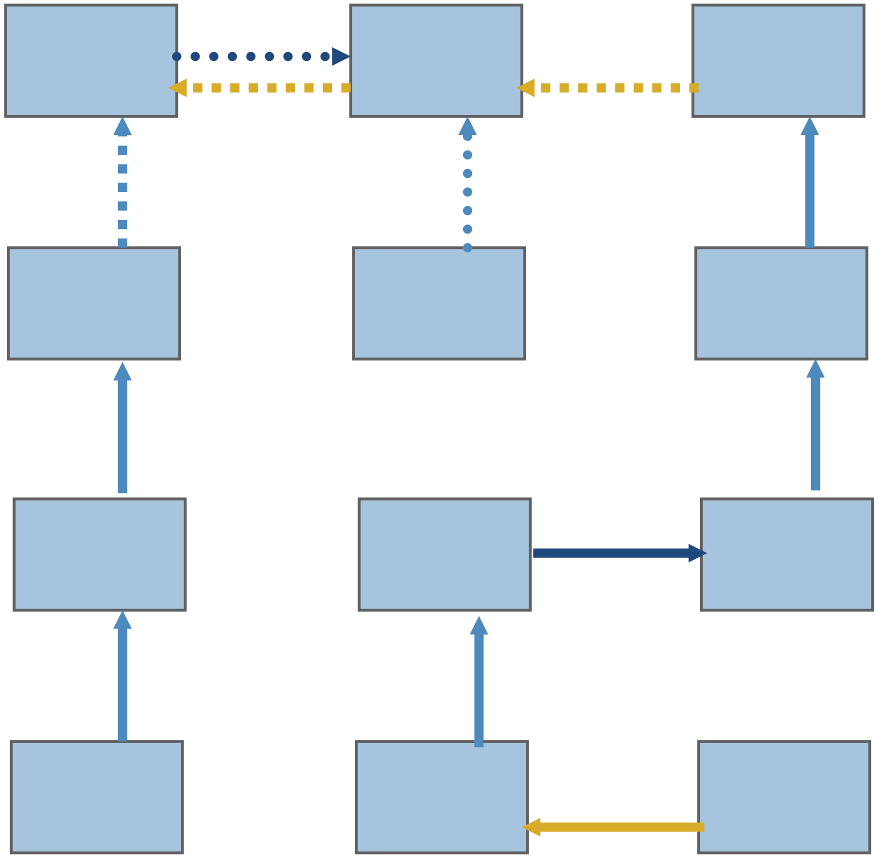
Mesh Exchange - Step 2

- Exchange data on a mesh



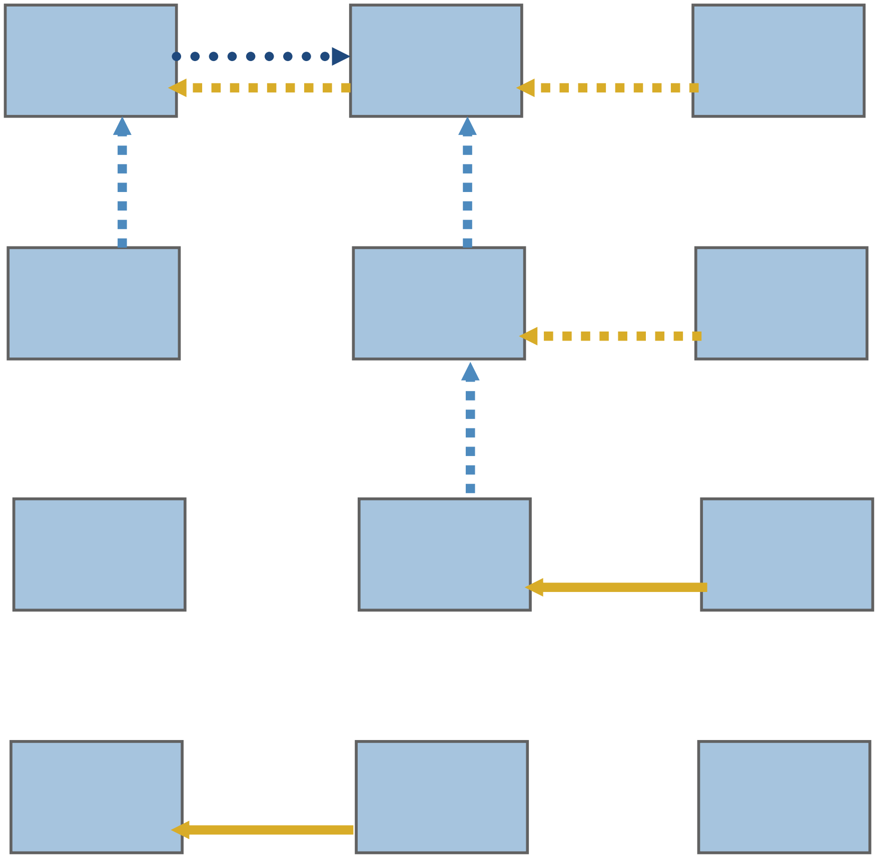
Mesh Exchange - Step 3

- Exchange data on a mesh



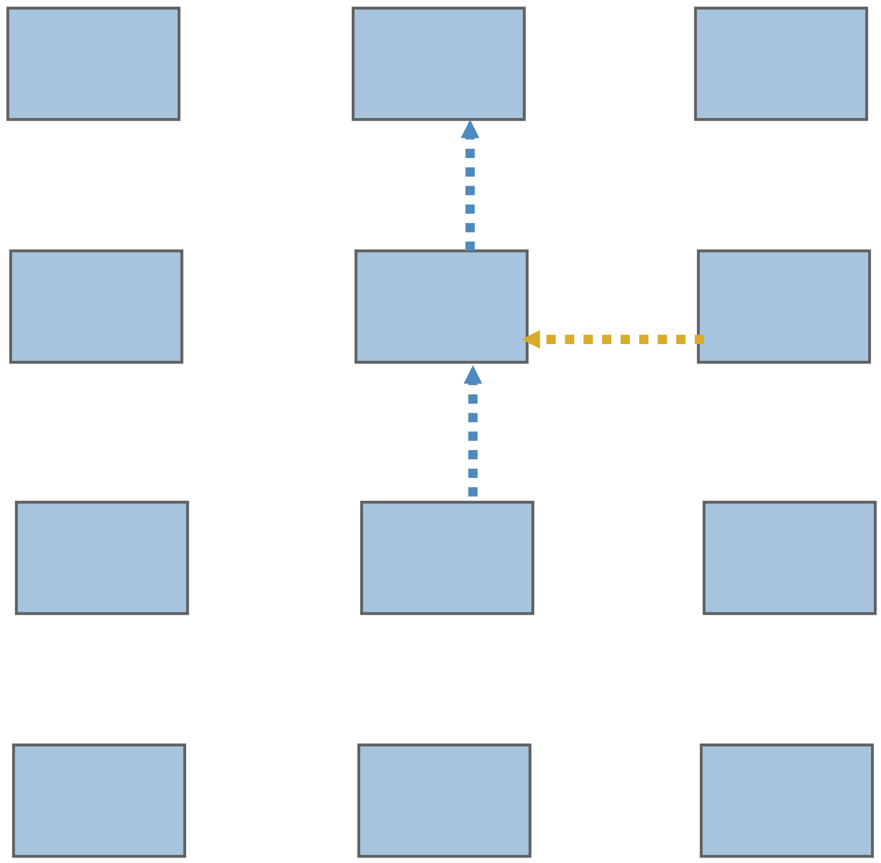
Mesh Exchange - Step 4

- Exchange data on a mesh



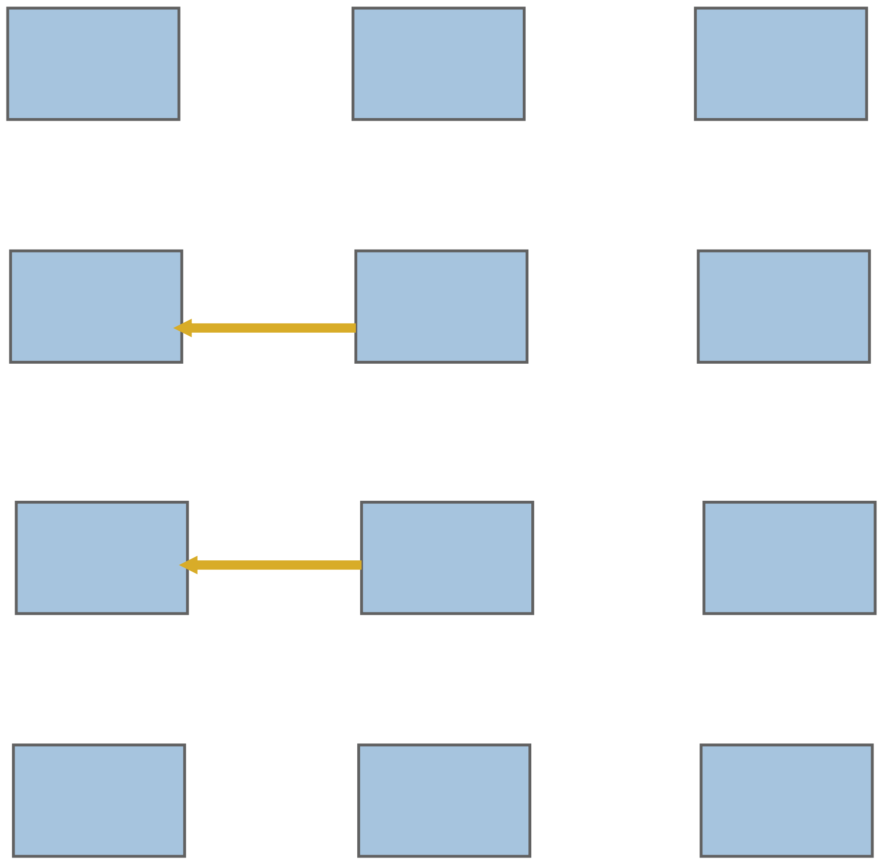
Mesh Exchange - Step 5

- Exchange data on a mesh

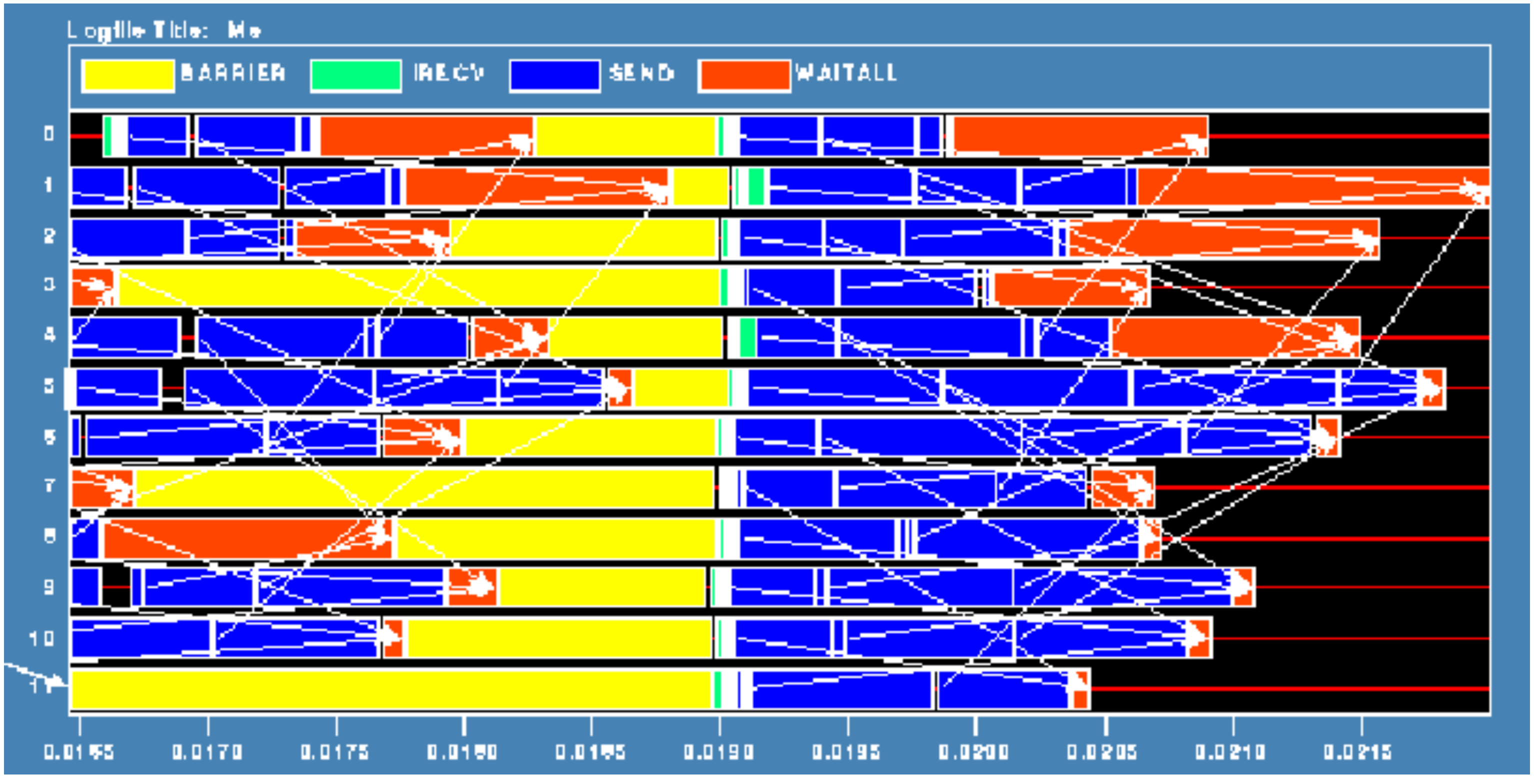


Mesh Exchange - Step 6

- Exchange data on a mesh

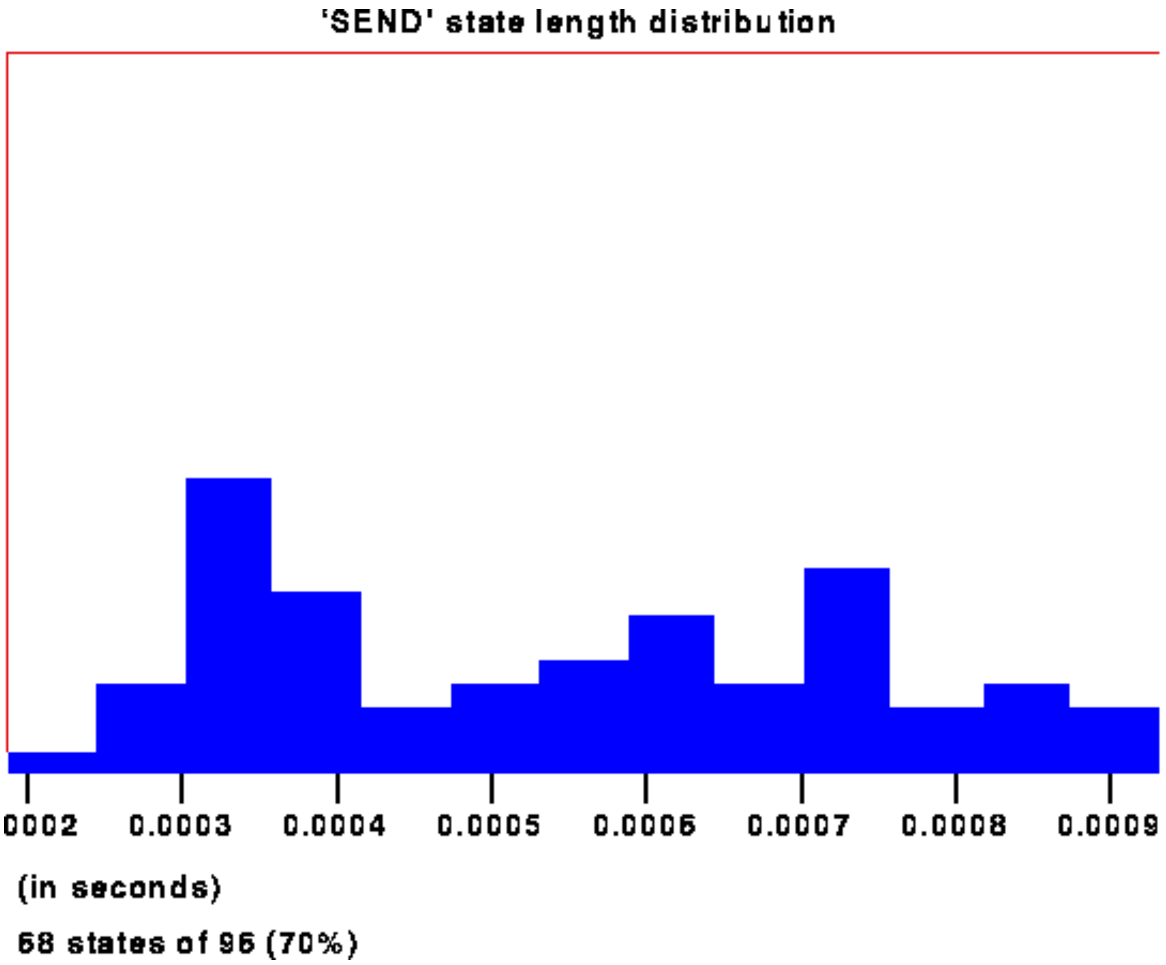


Timeline



- Note that process 1 finishes last, as predicted

Distribution of Sends



Why Six Steps?

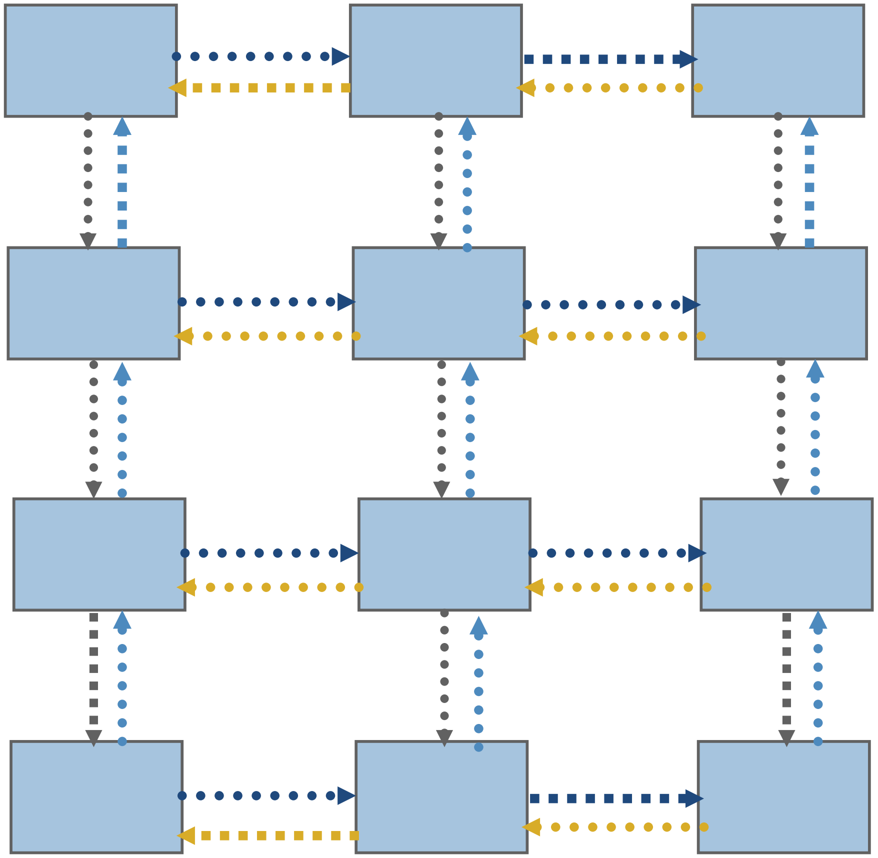
- Ordering of Sends introduces delays when there is contention at the receiver
- Takes roughly twice as long as it should
- Bandwidth is being wasted
- Same thing would happen if using memcpy and shared memory

Fix 2: Use Isend and Irecv

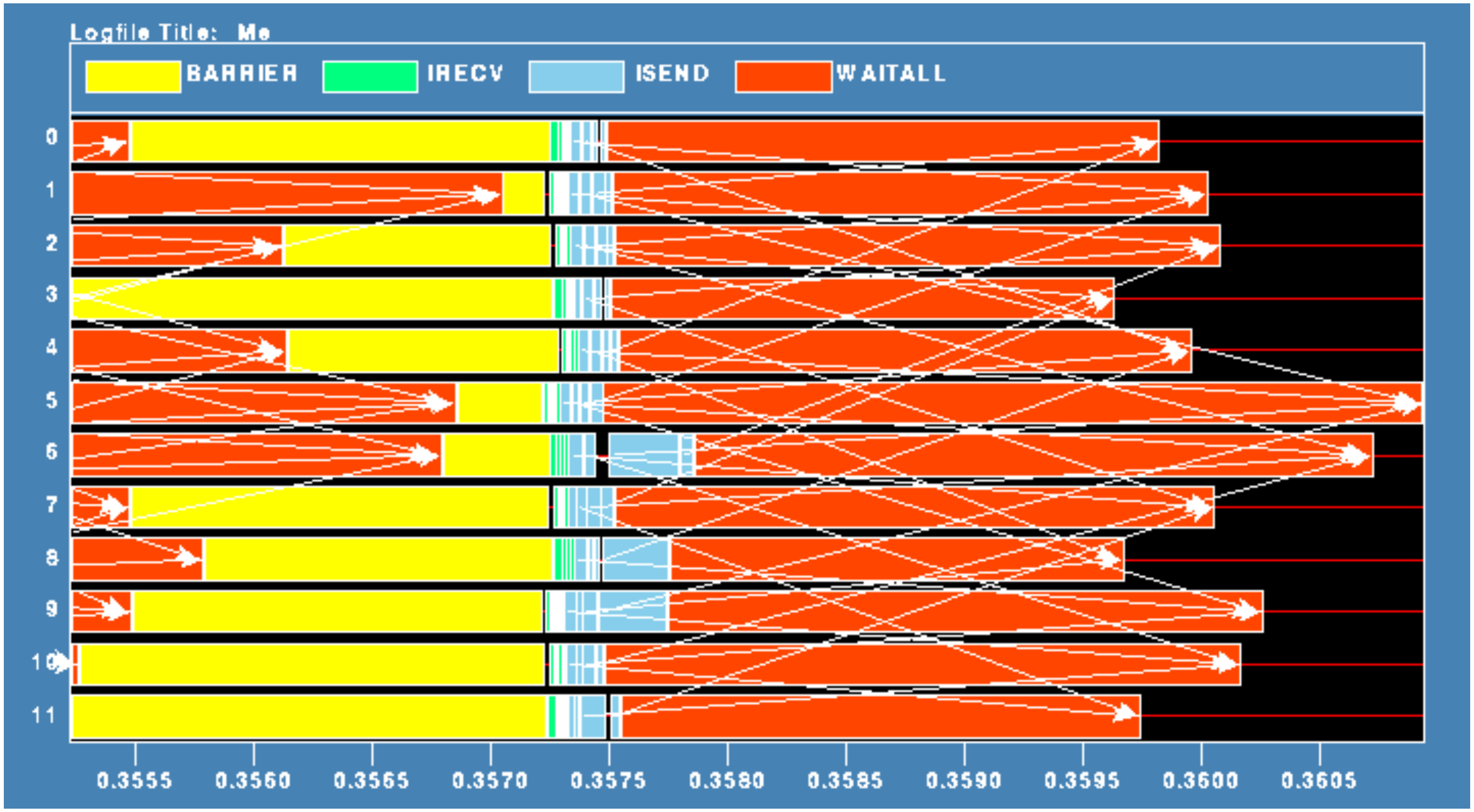
```
Do i=1,n_neighbors
  Call MPI_Irecv(inedge(1,i),len,MPI_REAL,nbr(i),tag,&
                 comm, requests(i),ierr)
Enddo
Do i=1,n_neighbors
  Call MPI_Isend(edge(1,i), len, MPI_REAL, nbr(i), tag,&
                 comm, requests(n_neighbors+i), ierr)
Enddo
Call MPI_Waitall(2*n_neighbors, requests, statuses, ierr)
```

Mesh Exchange - Steps 1-4

- Four interleaved steps



Timeline with Isend-Irecv



Note processes 5 and 6 are the only interior processes; these perform more communication than the other processes

Lesson: Defer Synchronization

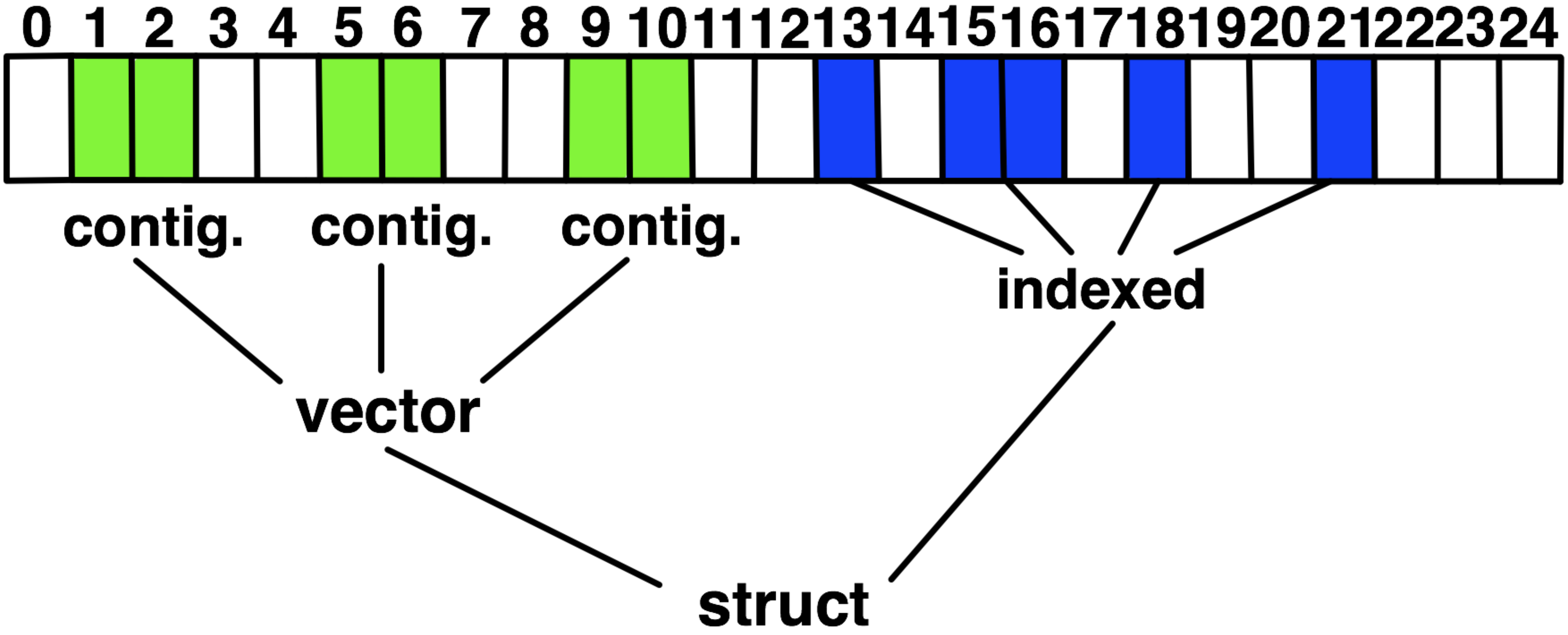
- Send-receive accomplishes two things:
  - Data transfer
  - Synchronization
- In many cases, there is more synchronization than required
- Consider the use of nonblocking operations and MPI_Waitall to defer synchronization
  - Effectiveness depends on how data is moved by the MPI implementation
  - E.g., If large messages are moved by blocking RMA operations "under the covers," the implementation can't adapt to contention at the target processes, and you may see no benefit.
  - This is more likely with larger messages

Datatypes

Introduction to Datatypes in MPI

- Datatypes allow users to serialize **arbitrary** data layouts into a message stream
  - Networks provide serial channels
  - Same for block devices and I/O
- Several constructors allow arbitrary layouts
  - Recursive specification possible
  - *Declarative* specification of data-layout
    - “what” and not “how”, leaves optimization to implementation (*many unexplored* possibilities!)
  - Choosing the right constructors is not always simple

Derived Datatype Example



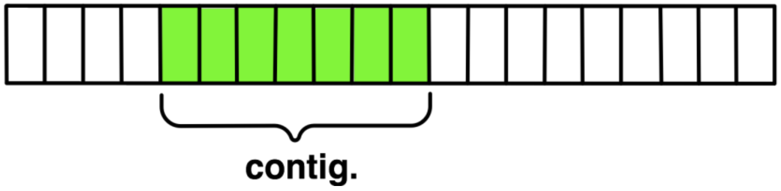
MPI’s Intrinsic Datatypes

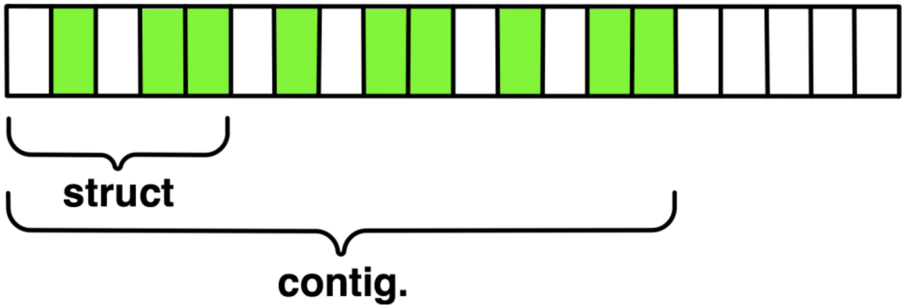
- Why intrinsic types?
  - Heterogeneity, nice to send a Boolean from C to Fortran
  - Conversion rules are complex, not discussed here
  - Length matches to language types
    - No sizeof(int) mess
- Users should generally use intrinsic types as basic types for communication and type construction!
  - MPI_BYTE should only be used for data that are raw bytes
- MPI-2.2 added some missing C types
  - E.g., unsigned long long

MPI_Type_contiguous

MPI_Type_contiguous(int count, MPI_Datatype oldtype, MPI_Datatype *newtype)

- Contiguous array of oldtype
- Should not be used as last type (can be replaced by count)

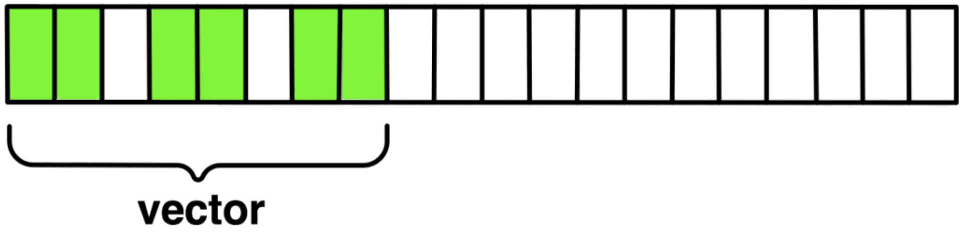


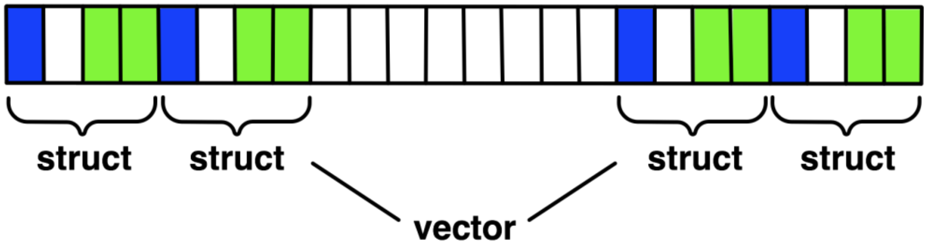


MPI_Type_vector

MPI_Type_vector(int count, int blocklength, int stride,
MPI_Datatype oldtype, MPI_Datatype *newtype)

- Specify strided blocks of data of oldtype
- Very useful for Cartesian arrays

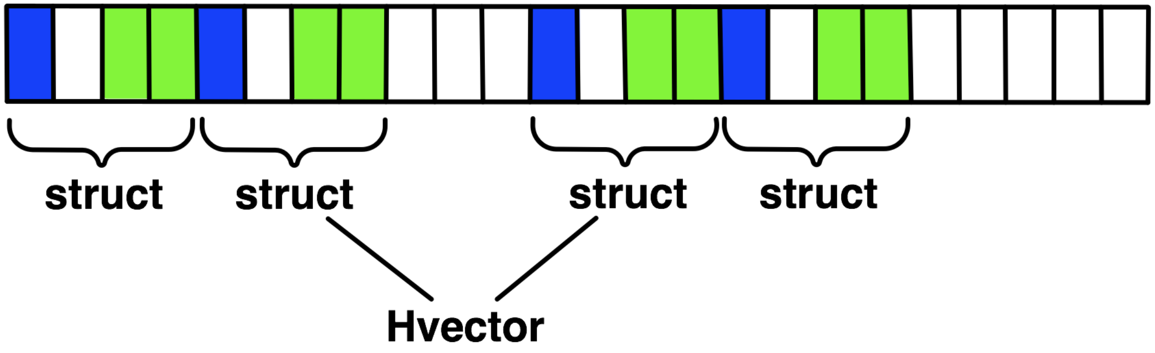




MPI_Type_create_hvector

MPI_Type_create_hvector(int count, int blocklength, MPI_Aint stride, MPI_Datatype oldtype, MPI_Datatype *newtype)

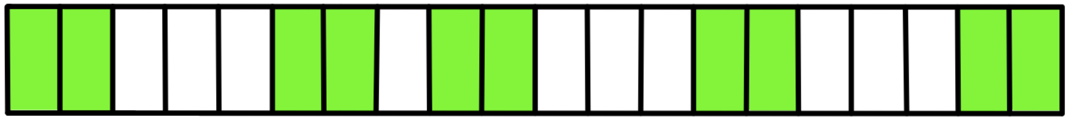
- Create non-unit strided vectors
- Useful for composition, e.g., vector of structs



MPI_Type_create_indexed_block

```
MPI_Type_create_indexed_block(int count, int blocklength,
int *array_of_displacements, MPI_Datatype oldtype,
MPI_Datatype *newtype)
```

- Like MPI_Type_indexed but blocklength is the same

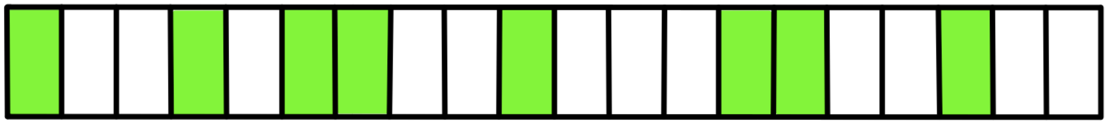


  - blen=2
  - displs={0,5,9,13,18}

MPI_Type_indexed

```
MPI_Type_indexed(int count, int *array_of_blocklengths,
int *array_of_displacements, MPI_Datatype oldtype,
MPI_Datatype *newtype)
```

- Pulling irregular subsets of data from a single array (cf. vector collectives)
  - Dynamic codes with index lists, expensive though!

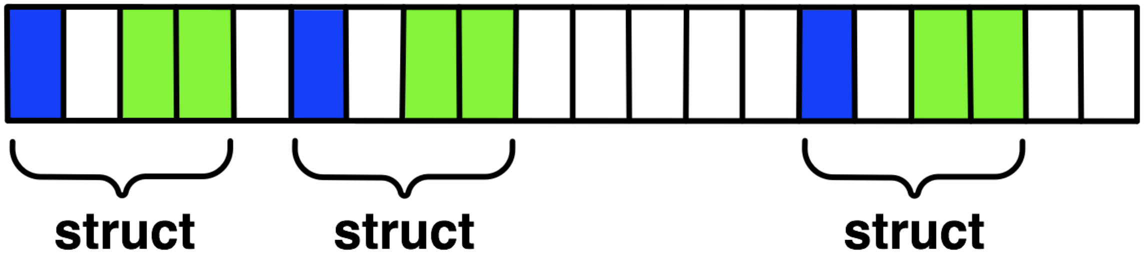


  - blen={1,1,2,1,2,1}
  - displs={0,3,5,9,13,17}

MPI_Type_create_hindexed

```
MPI_Type_create_hindexed(int count, int *arr_of_blocklengths,
MPI_Aint *arr_of_displacements, MPI_Datatype oldtype,
MPI_Datatype *newtype)
```

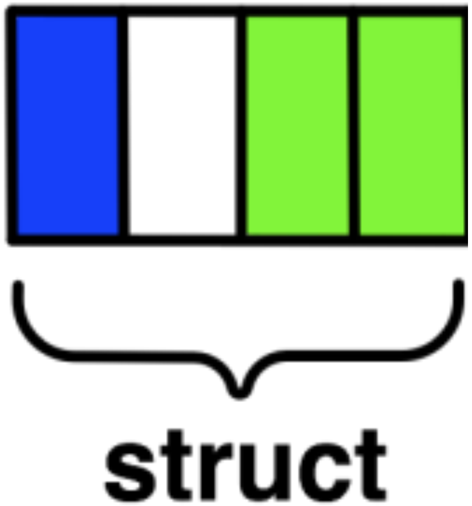
- Indexed with non-unit displacements, e.g., pulling types out of different arrays



MPI_Type_create_struct

MPI_Type_create_struct(int count, int array_of_blocklengths[], MPI_Aint array_of_displacements[], MPI_Datatype array_of_types[], MPI_Datatype *newtype)

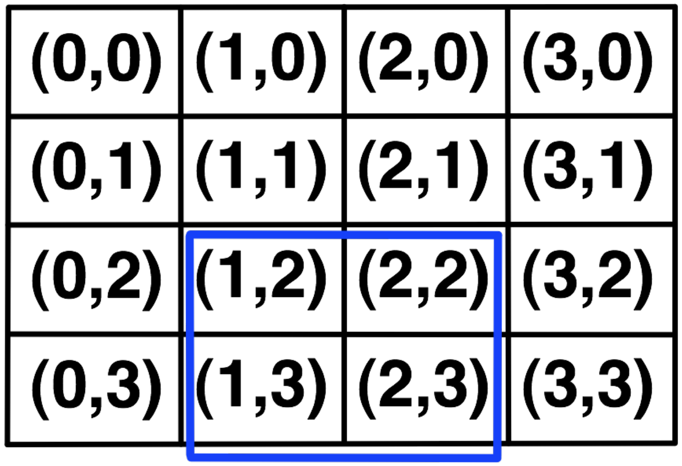
- Most general constructor, allows different types and arbitrary arrays (also most costly)



MPI_Type_create_subarray

```
MPI_Type_create_subarray(int ndims, int array_of_sizes[],
int array_of_subsizes[], int array_of_starts[], int order,
MPI_Datatype oldtype, MPI_Datatype *newtype)
```

- Specify subarray of n-dimensional array (sizes) by start (starts) and size (subsize)

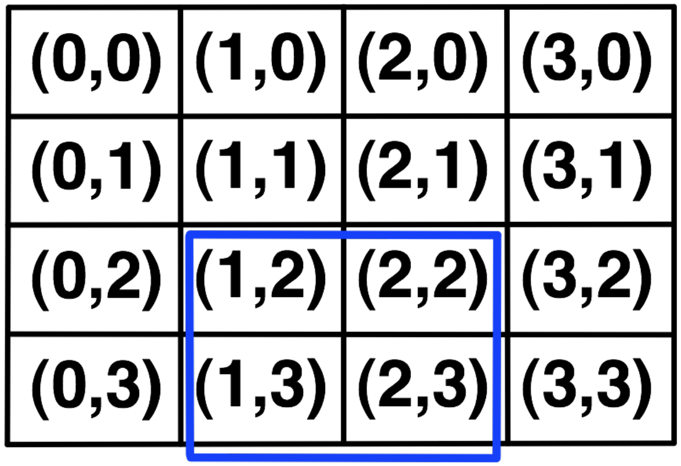


(0,0)	(1,0)	(2,0)	(3,0)
(0,1)	(1,1)	(2,1)	(3,1)
(0,2)	(1,2)	(2,2)	(3,2)
(0,3)	(1,3)	(2,3)	(3,3)

MPI_Type_create_darray

```
MPI_Type_create_darray(int size, int rank, int ndims,
int array_of_gsizes[], int array_of_distribs[], int
array_of_dargs[], int array_of_psizes[], int order,
MPI_Datatype oldtype, MPI_Datatype *newtype)
```

- Create distributed array, supports block, cyclic and no distribution for each dimension
  - Very useful for I/O



(0,0)	(1,0)	(2,0)	(3,0)
(0,1)	(1,1)	(2,1)	(3,1)
(0,2)	(1,2)	(2,2)	(3,2)
(0,3)	(1,3)	(2,3)	(3,3)

Commit, Free, and Dup

- Types must be committed before use
  - Only the ones that are used explicitly in a call!
  - MPI_Type_commit may perform time-consuming optimizations (but few implementations currently exploit this feature)
- MPI_Type_free
  - Free MPI resources of datatypes
  - Does not affect types built from it
- MPI_Type_dup
  - Duplicates a type
  - Library abstraction (composability)

Datatype Performance in Practice

- Datatypes *can* provide performance benefits, particularly for certain regular patterns
  - However, many implementations do not optimize datatype operations
  - If performance is critical, you will need to test
    - Even manual packing/unpacking can be slow if not properly optimized by the compiler – make sure to check optimization reports or if the compiler doesn’t provide good reports, inspect the assembly code
- For parallel I/O, datatypes *do* provide large performance benefits in many cases

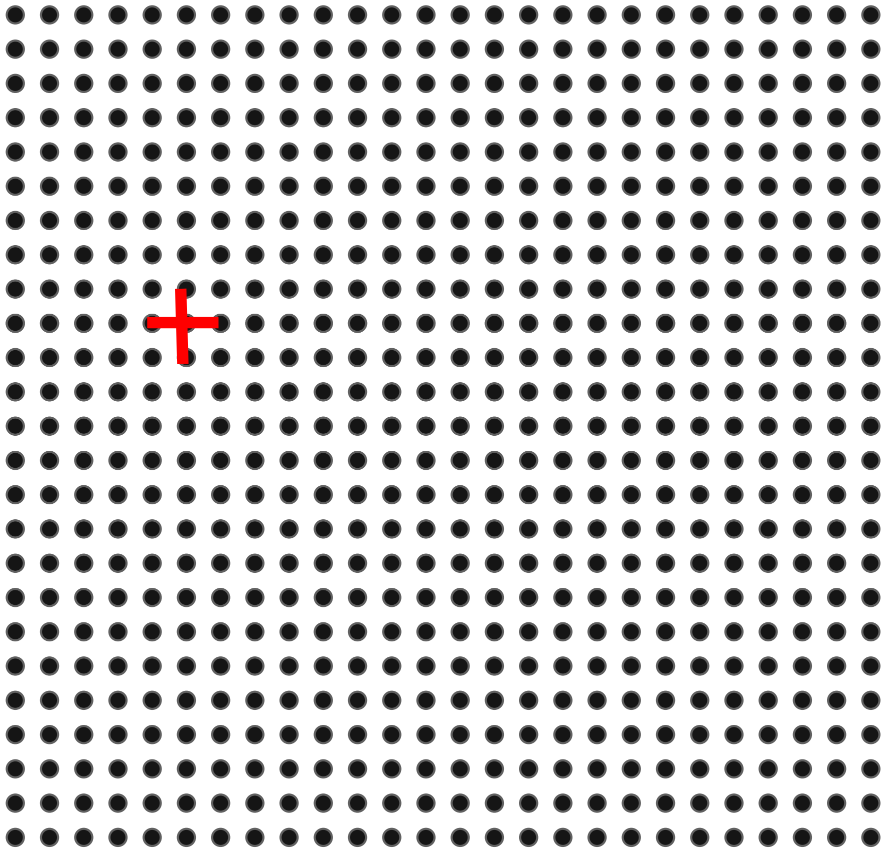
Example Code: Regular Mesh Algorithms

- Many scientific applications involve the solution of partial differential equations (PDEs)
- Many algorithms for approximating the solution of PDEs rely on forming a set of difference equations
  - Finite difference, finite elements, finite volume
- The exact form of the differential equations depends on the particular method
  - From the point of view of parallel programming for these algorithms, the operations are the same
- Five-point stencil is a popular approximation solution

```
https://anl.app.box.com/v/2019-ATPESC-MPI
On ALCF: /projects/ATPESC2019/MPI_tutorial
```

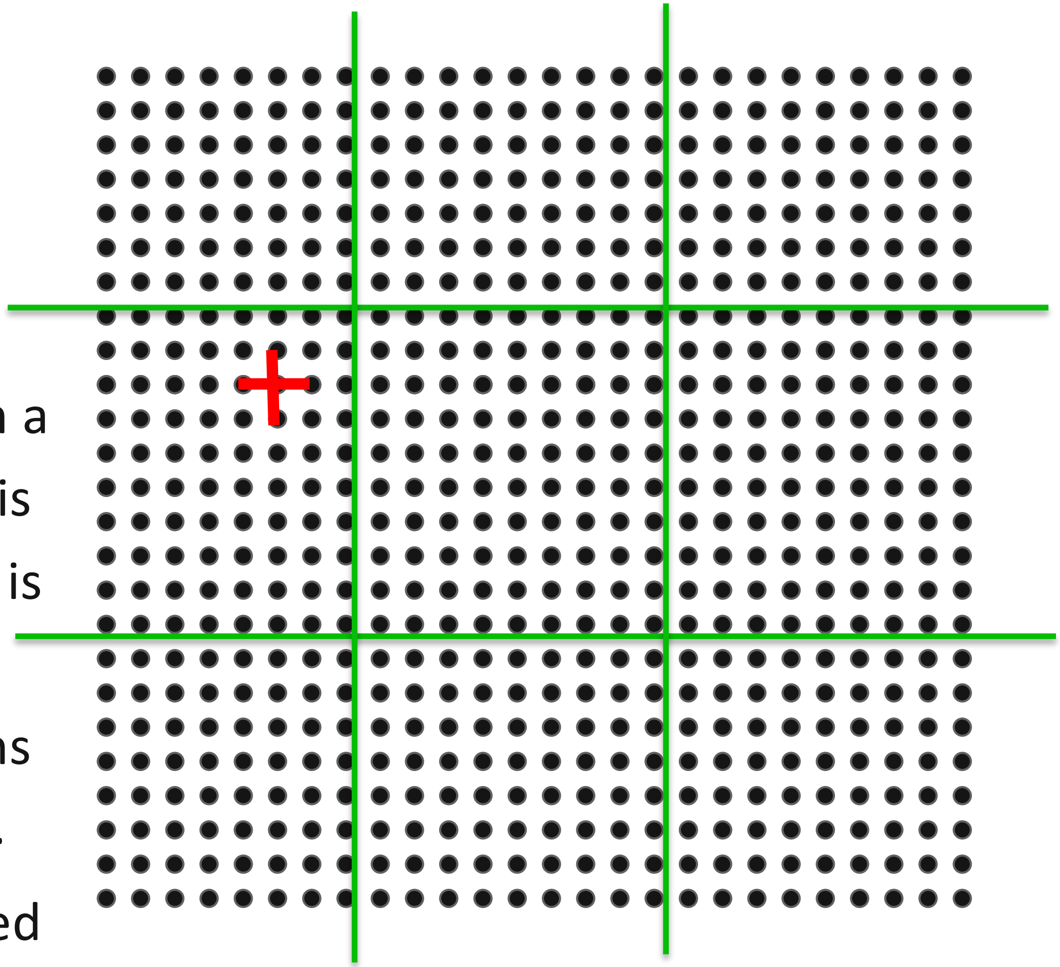
The Global Data Structure

- Each circle is a mesh point
- Difference equation evaluated at each point involves the four neighbors
- The red “plus” is called the method’s stencil
- Good numerical algorithms form a matrix equation Au=f; solving this requires computing Bv, where B is a matrix derived from A. These evaluations involve computations with the neighbors on the mesh.



The Global Data Structure

- Each circle is a mesh point
- Difference equation evaluated at each point involves the four neighbors
- The red “plus” is called the method’s stencil
- Good numerical algorithms form a matrix equation Au=f; solving this requires computing Bv, where B is a matrix derived from A. These evaluations involve computations with the neighbors on the mesh.
- Decompose mesh into equal sized (work) pieces



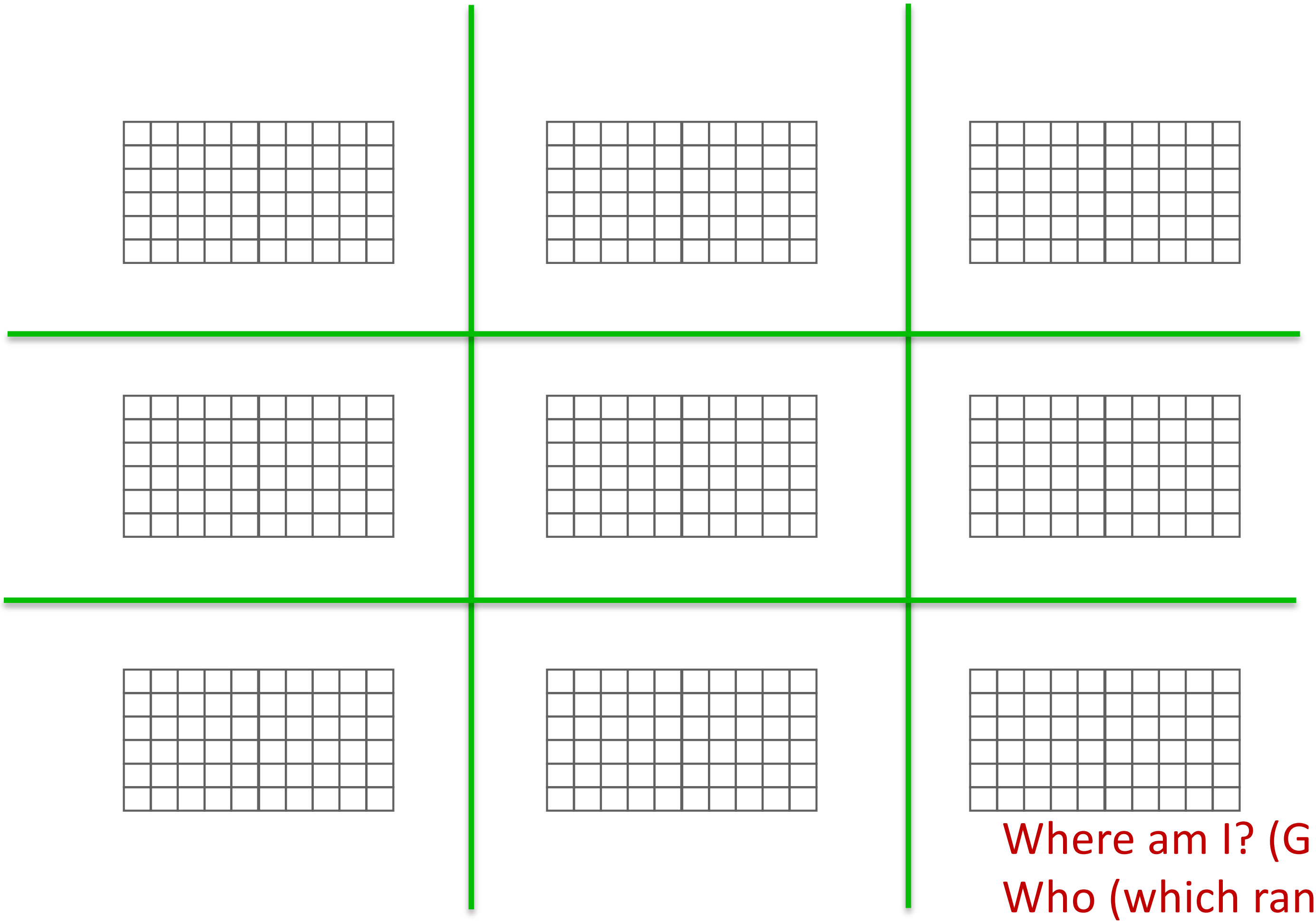
Step 1: Domain Decompositioin

Parameters for domain decomposition:

N = Size of the edge of the global problem domain (assuming square)

PX, PY = Number of processes in X and Y dimension

N % PX == 0, N % PY == 0

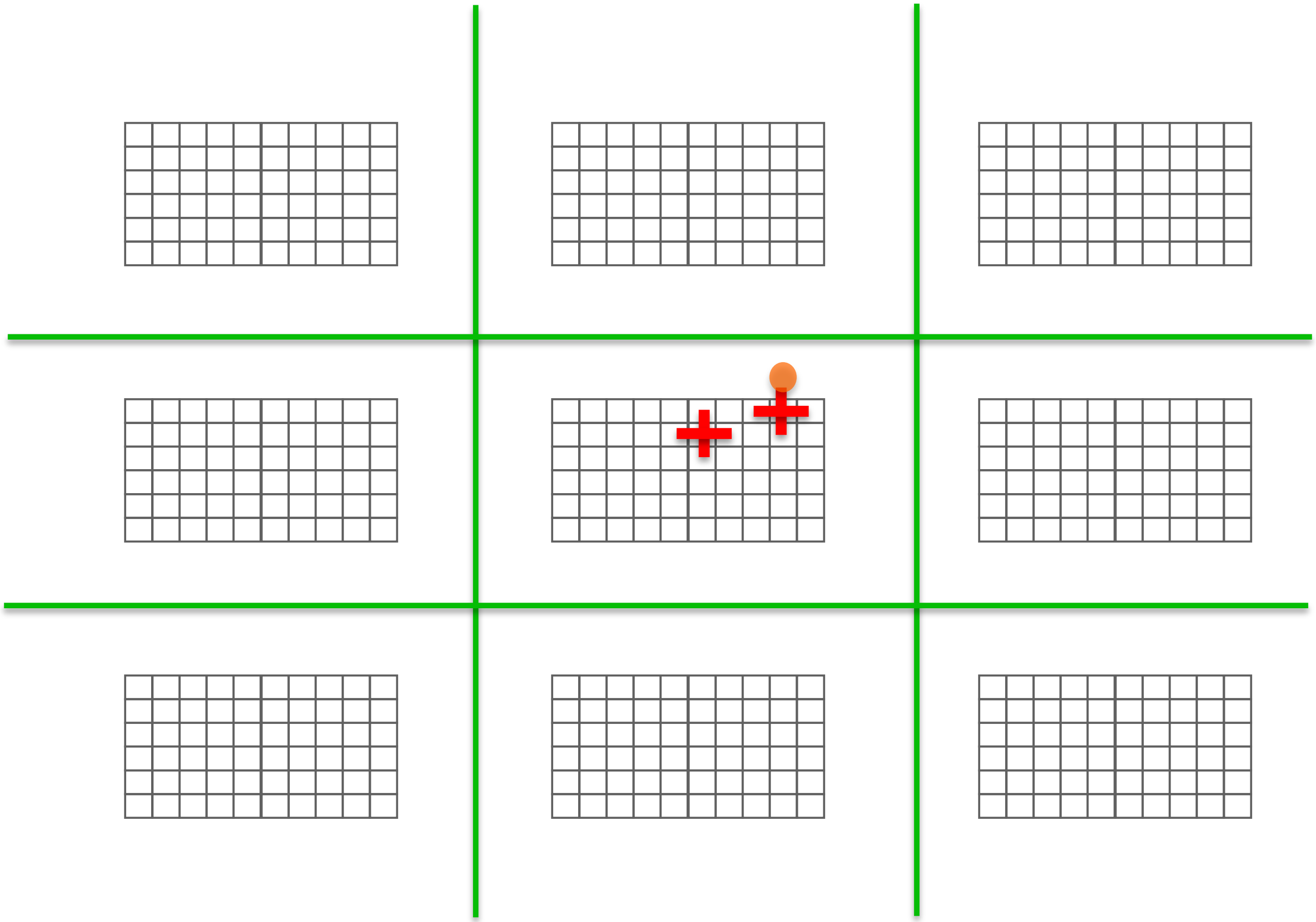


Where am I? (Global offset)

Who (which ranks) are my neigbhors?

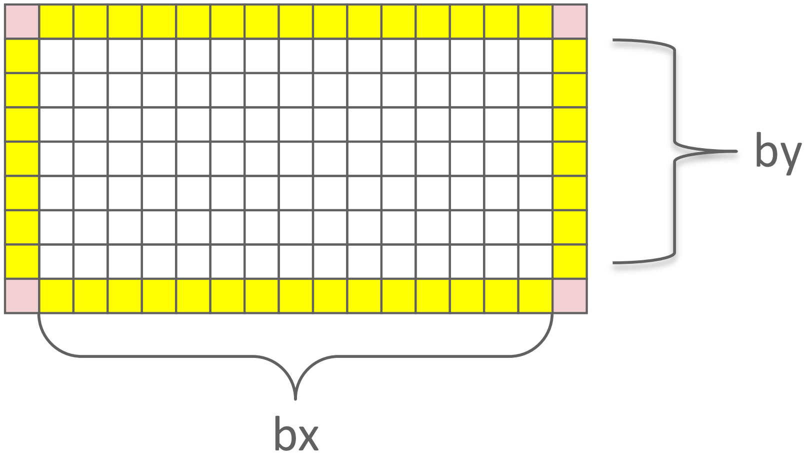
Use MPI_PROC_NULL for boundary

Necessary Data Transfers



Step 2: The Local Data Structure

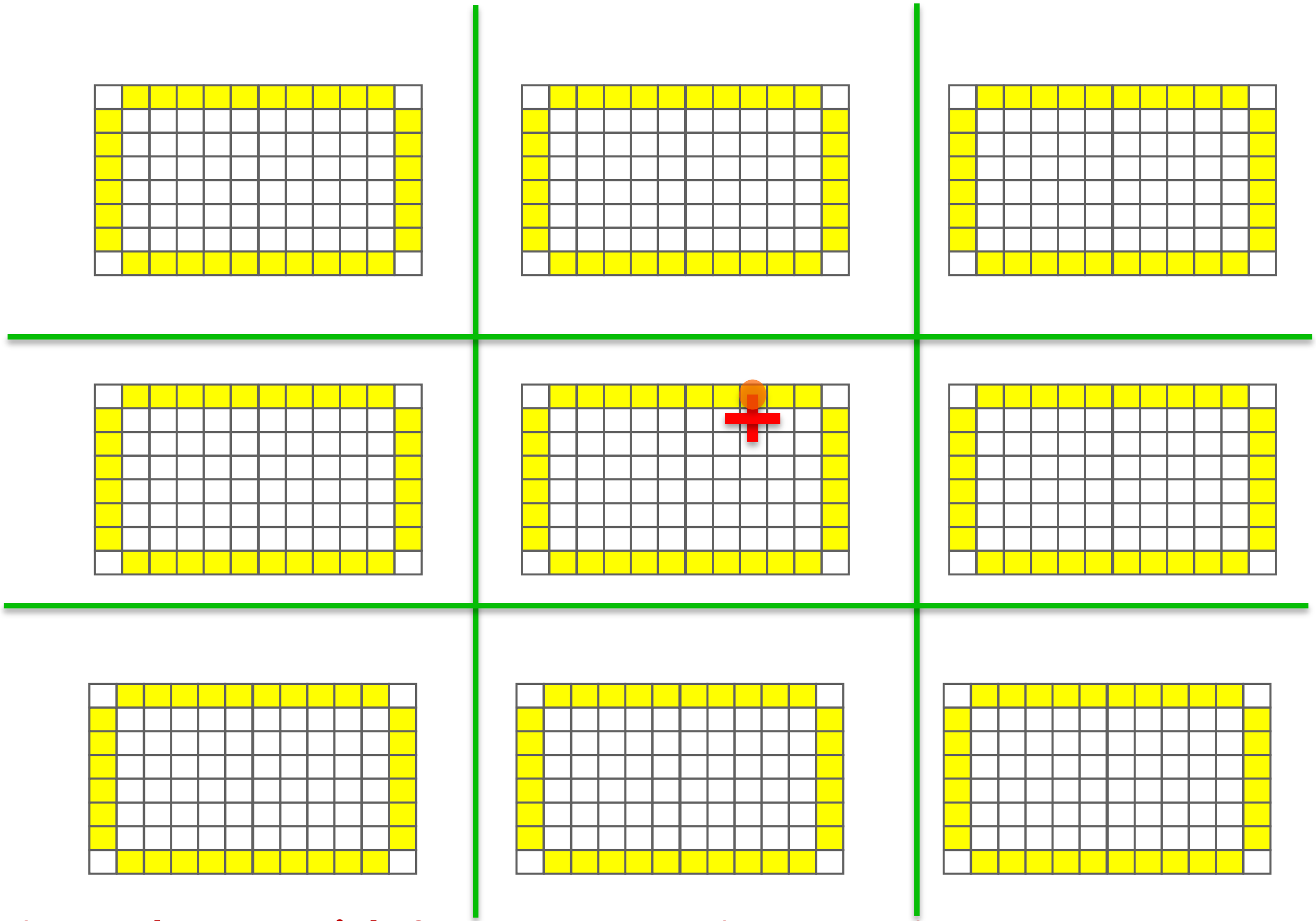
- Each process has its local “patch” of the global array
  - “bx” and “by” are the sizes of the local array
  - Always allocate a halo around the patch
  - Array allocated of size (bx+2)x(by+2)
- Each process also have send/recv buffers for each neighbor



Check the **`alloc_bufs`** function to see how buffers are allocated

Calculation

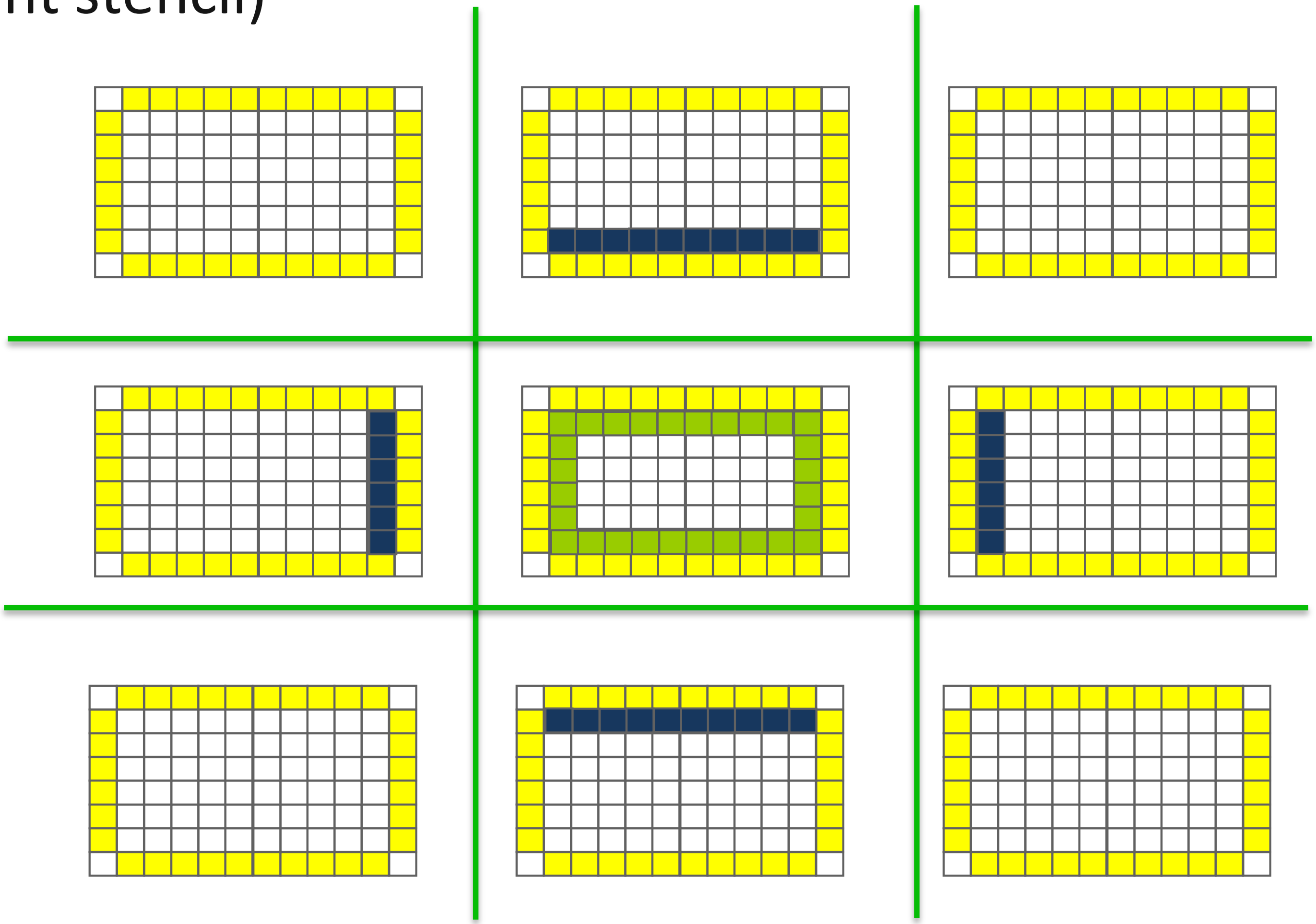
- Two buffers alternating
  - aold for current value
  - anew for newly value in this iteration (will become aold in next iter)



Check the **`update_grid`** function to see how it is done

Step 3: Data Transfers with MPI_Isend/MPI_Irecv

- Provide access to remote data through a halo exchange (5 point stencil)



Note the differences in send/recv buffers, the requirement of data packing.

Step 3: Data Transfers with MPI_Isend/MPI_Irecv (cont'd)

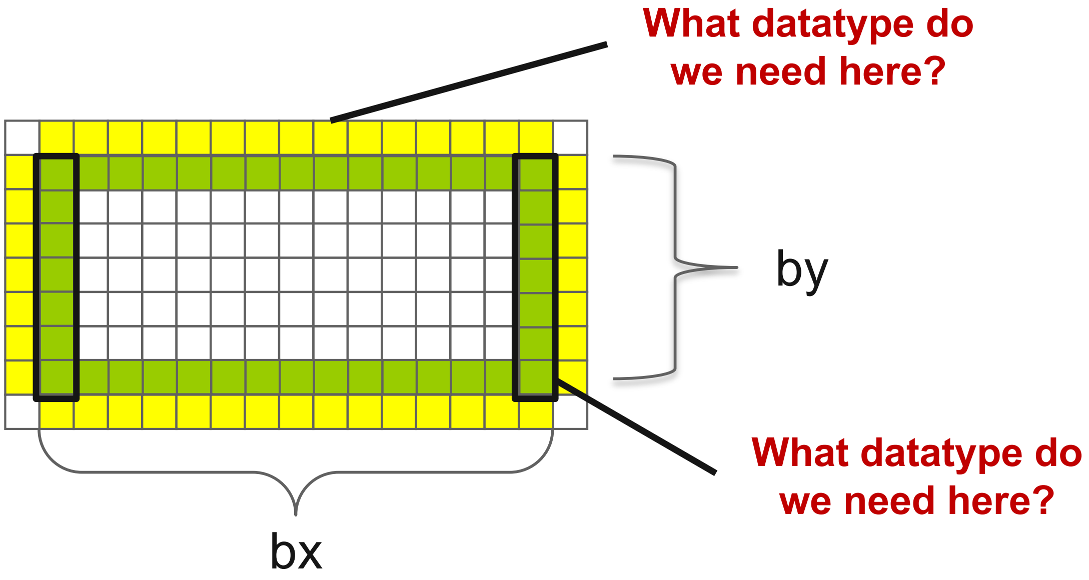
- Data exchange with neighbors using corresponding send/recv buffers
- How to complete the communication? (MPI_Wait? MPI_Waitall?)
- Does order matters?

Step 4: Calculating Total Heat

- Using MPI_Allreduce to calculate total heat

Exercise: Stencil with Derived Datatypes (1)

- In the basic version of the stencil code
  - Used nonblocking communication 👍
  - Used manual packing/unpacking of data 👎
- Let’s try to use derived datatypes
  - Specify the locations of the data instead of manually packing/unpacking



What datatype do we need here?

What datatype do we need here?

Exercise: Stencil with Derived Datatypes (2)

- Nonblocking sends and receives
- Data location specified by MPI datatypes
- Manual packing of data no longer required
- *Start from nonblocking_p2p/stencil.c*
- *Solution in derived_datatype/stencil.c*

Collectives and Nonblocking Collectives

Introduction to Collective Operations in MPI

- Collective operations are called by all processes in a communicator.
- **`MPI_BCAST`** distributes data from one process (the root) to all others in a communicator.
- **`MPI_REDUCE`** combines data from all processes in the communicator and returns it to one process.
- In many numerical algorithms, **`SEND/RECV`** can be replaced by **`BCAST/REDUCE`**, improving both simplicity and efficiency.

MPI Collective Communication

- Communication and computation is coordinated among a group of processes in a communicator
- Tags are not used; different communicators deliver similar functionality
- Non-blocking collective operations in MPI-3
- Three classes of operations: synchronization, data movement, collective computation

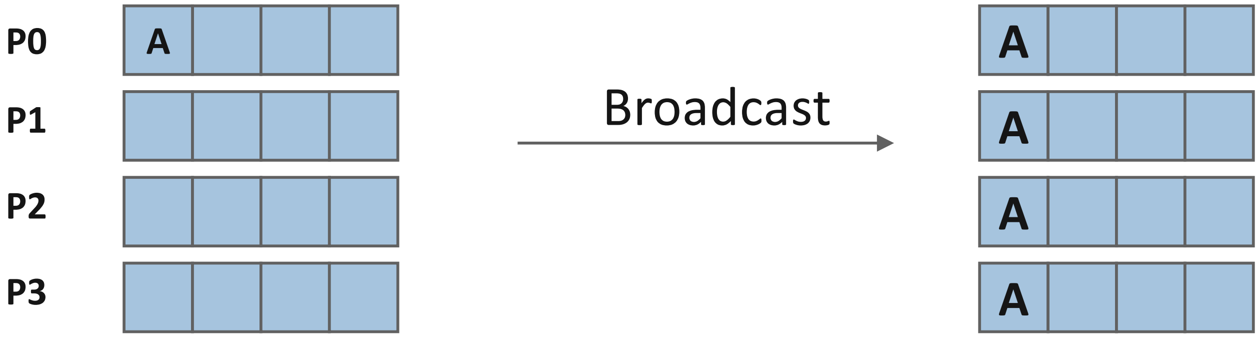
Synchronization

- **`MPI_BARRIER(comm)`**
  - Blocks until all processes in the group of communicator **`comm`** call it
  - A process cannot get out of the barrier until all other processes have reached barrier

- Note that a barrier is rarely, if ever, necessary in an MPI program
- Adding barriers "just to be sure" is a bad practice and causes unnecessary synchronization. Remove unnecessary barriers from your code.

- One legitimate use of a barrier is before the first call to MPI_Wtime to start a timing measurement. This causes each process to start at *approximately* the same time.
- Avoid using barriers other than for this.

Collective Data Movement


P0

P1

P2

P3

A

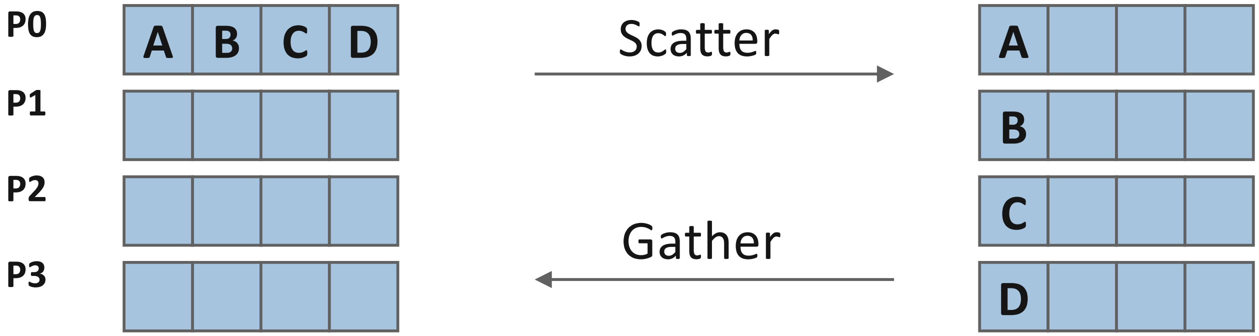
Broadcast

A

A

A

A


P0

P1

P2

P3

A B C D

Scatter

Gather

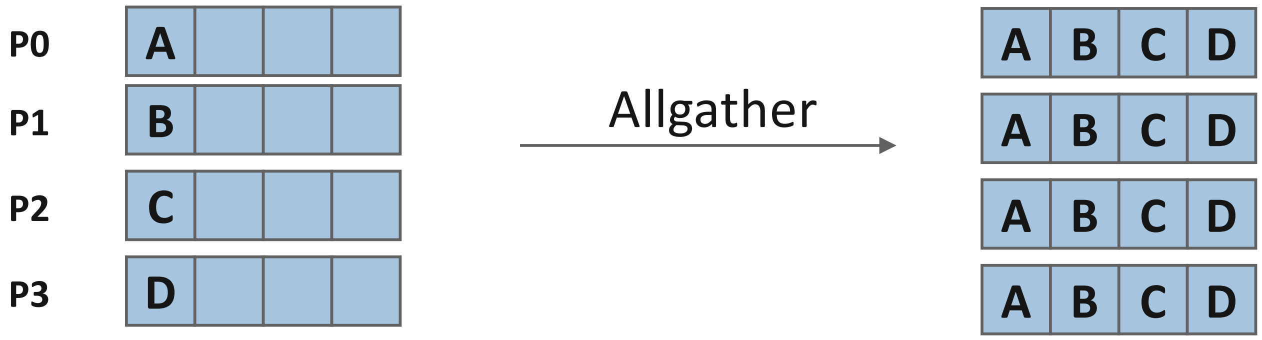
A

B

C

D

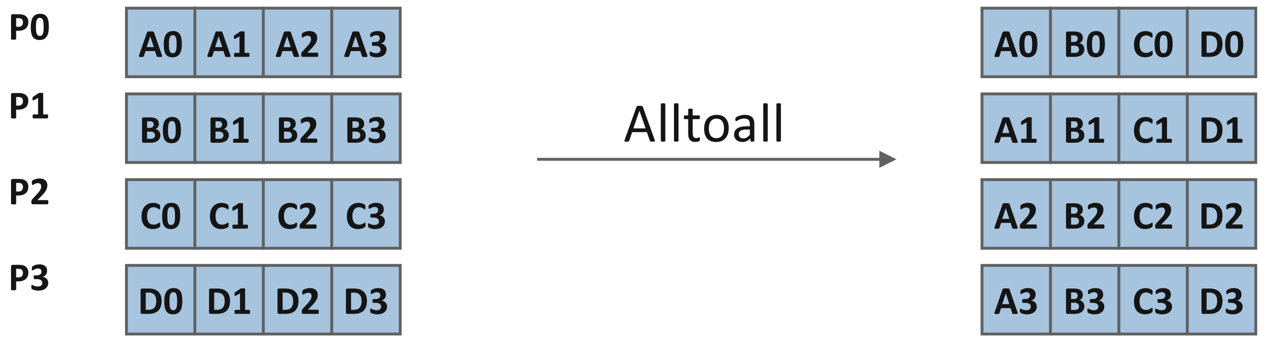
More Collective Data Movement



P0	A			
P1	B			
P2	C			
P3	D			

Allgather

A	B	C	D
A	B	C	D
A	B	C	D
A	B	C	D

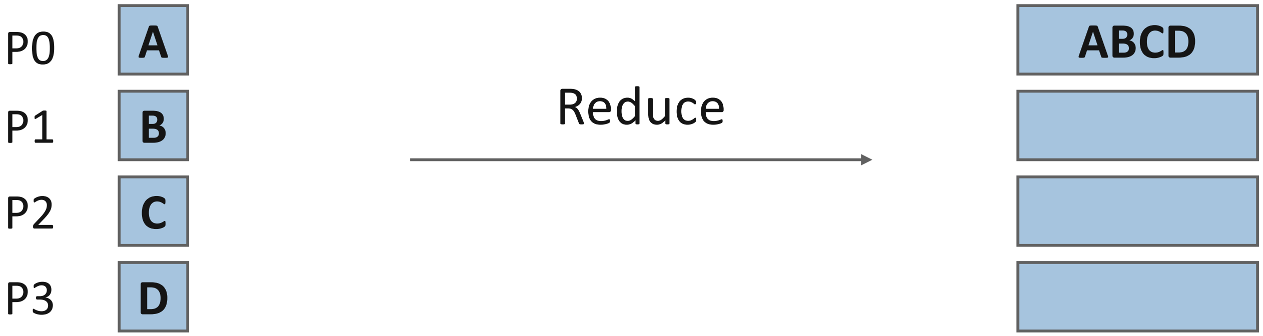


P0	A0	A1	A2	A3
P1	B0	B1	B2	B3
P2	C0	C1	C2	C3
P3	D0	D1	D2	D3

Alltoall

A0	B0	C0	D0
A1	B1	C1	D1
A2	B2	C2	D2
A3	B3	C3	D3

Collective Computation



P0 A

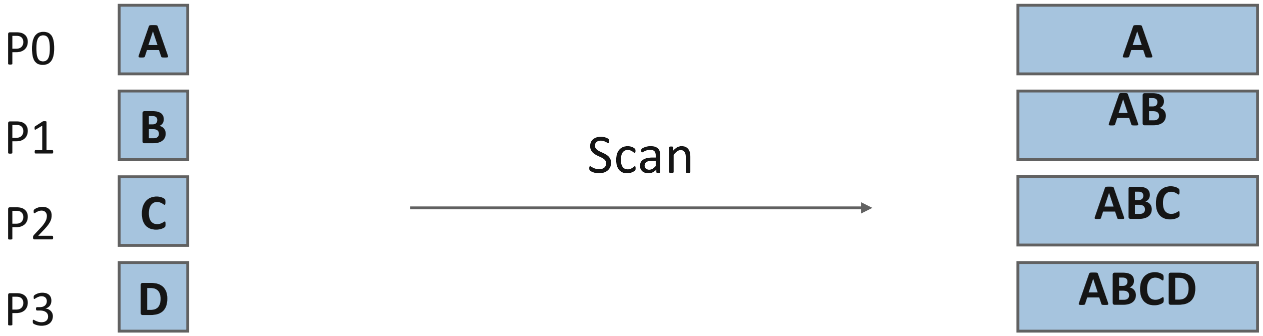
P1 B

P2 C

P3 D

Reduce

ABCD



P0 A

P1 B

P2 C

P3 D

Scan

A

AB

ABC

ABCD

MPI Collective Routines

- Many Routines, including: **MPI_ALLGATHER, MPI_ALLGATHERV, MPI_ALLREDUCE, MPI_ALLTOALL, MPI_ALLTOALLV, MPI_BCAST, MPI_EXSCAN, MPI_GATHER, MPI_GATHERV, MPI_REDUCE, MPI_REDUCE_SCATTER, MPI_SCAN, MPI_SCATTER, MPI_SCATTERV**
- "**All**" versions deliver results to all participating processes
- "**V**" versions (stands for vector) allow the chunks to have different sizes
- "**W**" versions for ALLTOALL allow the chunks to have different sizes in bytes, rather than units of datatypes
- **MPI_ALLREDUCE**, **MPI_REDUCE**, **MPI_REDUCE_SCATTER**, M**PI_REDUCE_SCATTER_BLOCK**, **MPI_EXSCAN**, and **MPI_SCAN** take both built-in and user-defined combiner functions

MPI Built-in Collective Computation Operations

MPI_MAX	Maximum
MPI_MIN	Minimum
MPI_PROD	Product
MPI_SUM	Sum
MPI_LAND	Logical and
MPI_LOR	Logical or
MPI_LXOR	Logical exclusive or
MPI_BAND	Bitwise and
MPI_BOR	Bitwise or
MPI_BXOR	Bitwise exclusive or
MPI_MAXLOC	Maximum and location
MPI_MINLOC	Minimum and location
MPI_REPLACE, MPI_NO_OP	Replace and no operation (RMA)

Defining your own Collective Operations

- Create your own collective computations with:

```
MPI_OP_CREATE(user_fn, commutes, &op);
MPI_OP_FREE(&op);

user_fn(invec, inoutvec, len, datatype);
```

- The user function should perform:

```
inoutvec[i]  =  invec[i]  op  inoutvec[i];
```

  for i from 0 to len-1

- The user function can be non-commutative, but must be associative

Nonblocking Collectives

Nonblocking Collective Communication

- Nonblocking communication
  - Deadlock avoidance
  - Overlapping communication/computation
- Collective communication
  - Collection of pre-defined optimized routines
- Nonblocking collective communication
  - Combines both advantages
  - System noise/imbalance resiliency
  - Semantic advantages

Nonblocking Communication

- Semantics are simple:
  - Function returns no matter what
  - No progress guarantee!
- E.g., MPI_Isend(<send-args>, MPI_Request *req);
- Nonblocking tests:
  - Test, Testany, Testall, Testsome
- Blocking wait:
  - Wait, Waitany, Waitall, Waitsome

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

A Non-Blocking Barrier?

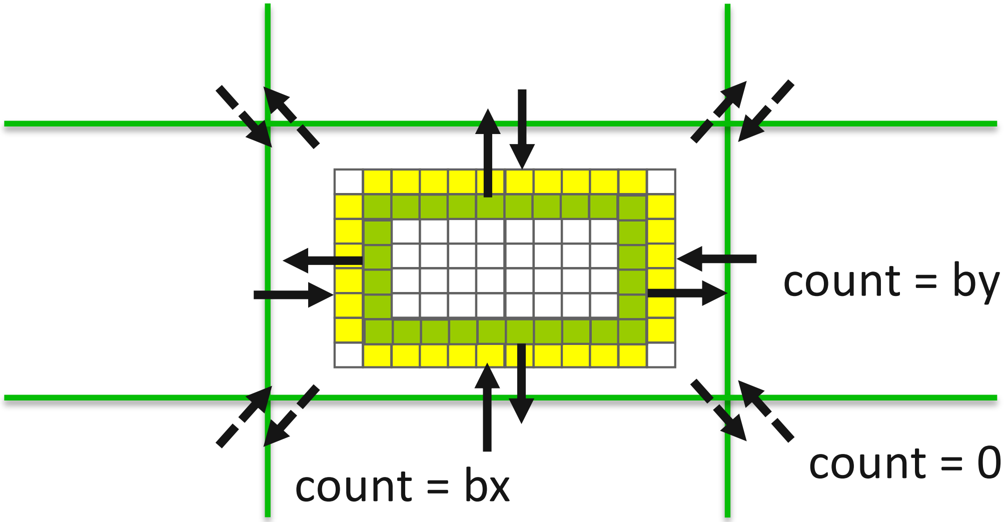
- What can that be good for? Well, quite a bit!
- Semantics:
  - MPI_Ibarrier() – calling process entered the barrier, **no** synchronization happens
  - Synchronization **may** happen asynchronously
  - MPI_Test/Wait() – synchronization happens **if** necessary
- Uses:
  - Overlap barrier latency (small benefit)
  - Use the split semantics! Processes **notify** non-collectively but **synchronize** collectively!

Nonblocking And Collective Summary

- Nonblocking communication
  - Overlap and relax synchronization
- Collective communication
  - Specialized pre-optimized routines
  - Performance portability
  - Hopefully transparent performance
- They can be composed
  - E.g., software pipelining

Exercise: Stencil using Alltoallv

- In the basic version of the stencil code
  - Used nonblocking send/receive for each direction
- Let’s try to use single alltoallv collective call
- *Start from nonblocking_p2p/stencil.c*
- *Solution available in blocking_coll/stencil_alltoallv.c*



Exercise: Stencil with Derived Datatypes and Collectives

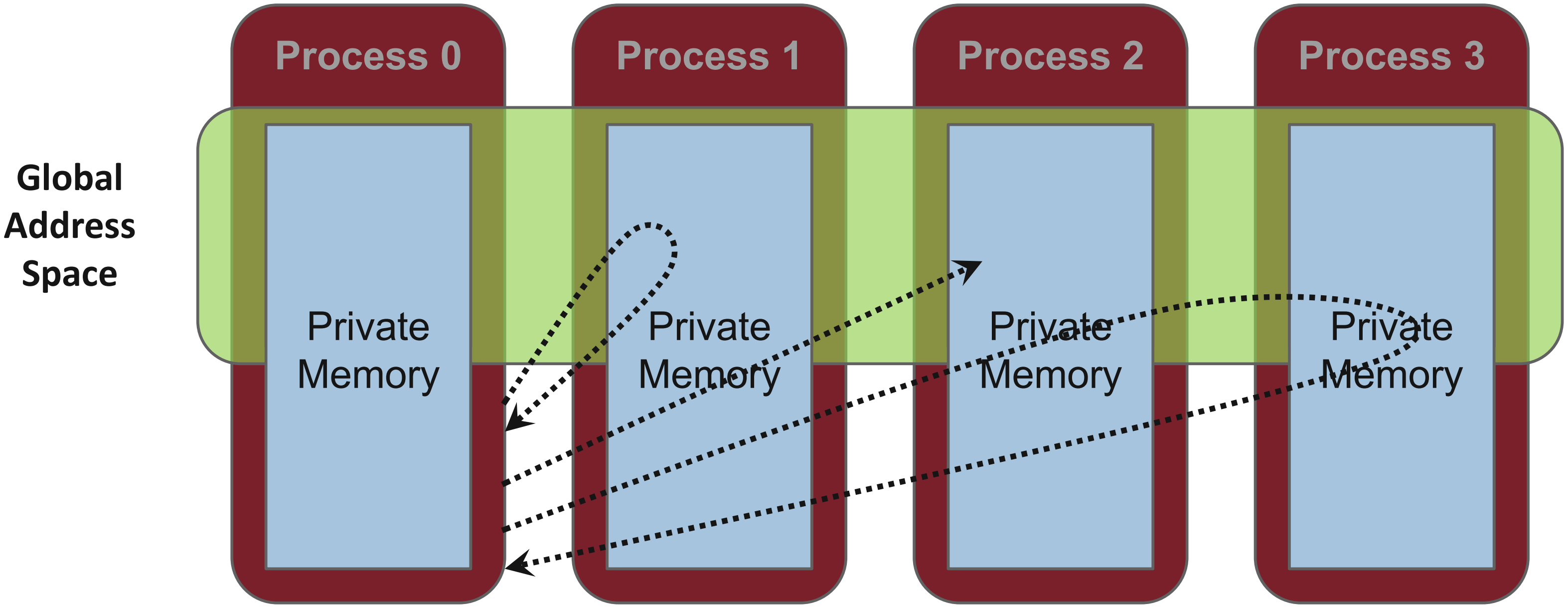
- Simplify collective version of stencil
  - Alltoallv: defines a set of counts and displacements with the same datatype (see *blocking_coll/stencil_alltoallv.c*)
  - Alltoallw: defines a set of counts, displacements, and datatypes
- Data location specified by MPI datatypes
- Manual packing of data no longer required
- *Start from blocking_coll/stencil_alltoallv.c*
- *Solution in derived_datatype/stencil_alltoallw.c*

Advanced Topics: One-sided Communication

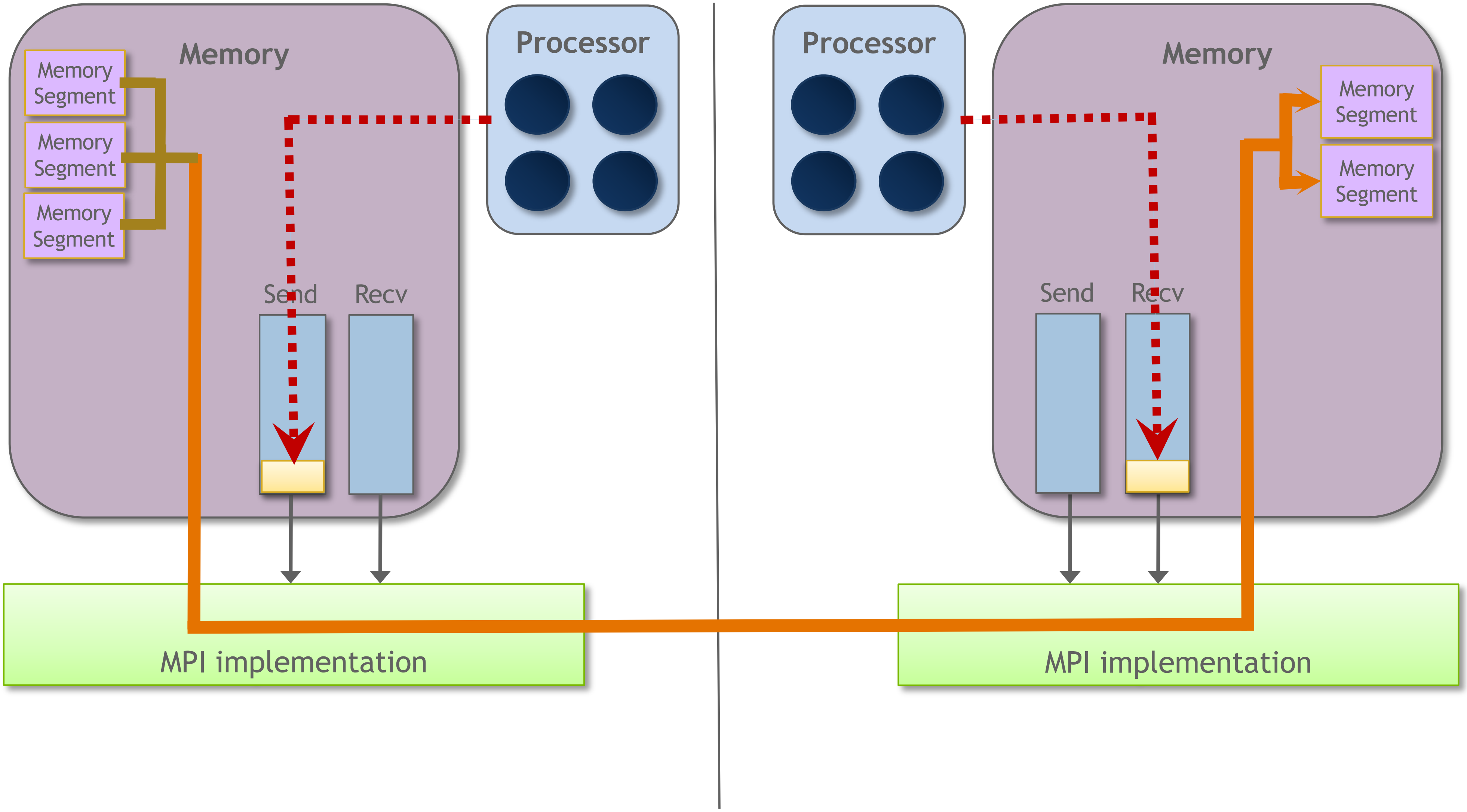
https://anl.box.com/v/2019-ATPESC-MPI

One-sided Communication

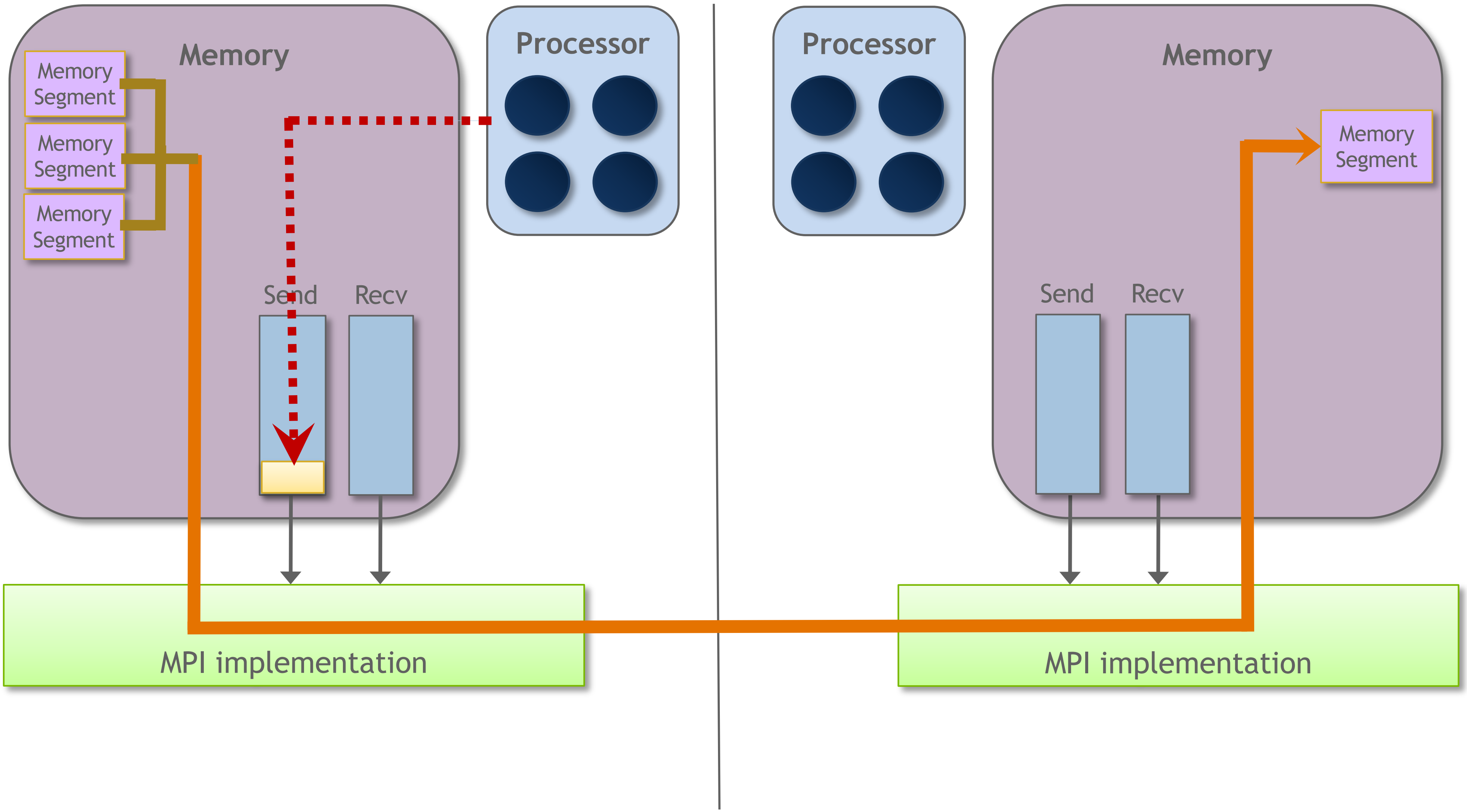
- The basic idea of one-sided communication models is to decouple data movement with process synchronization
  - Should be able to move data without requiring that the remote process synchronize
  - Each process exposes a part of its memory to other processes
  - Other processes can directly read from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



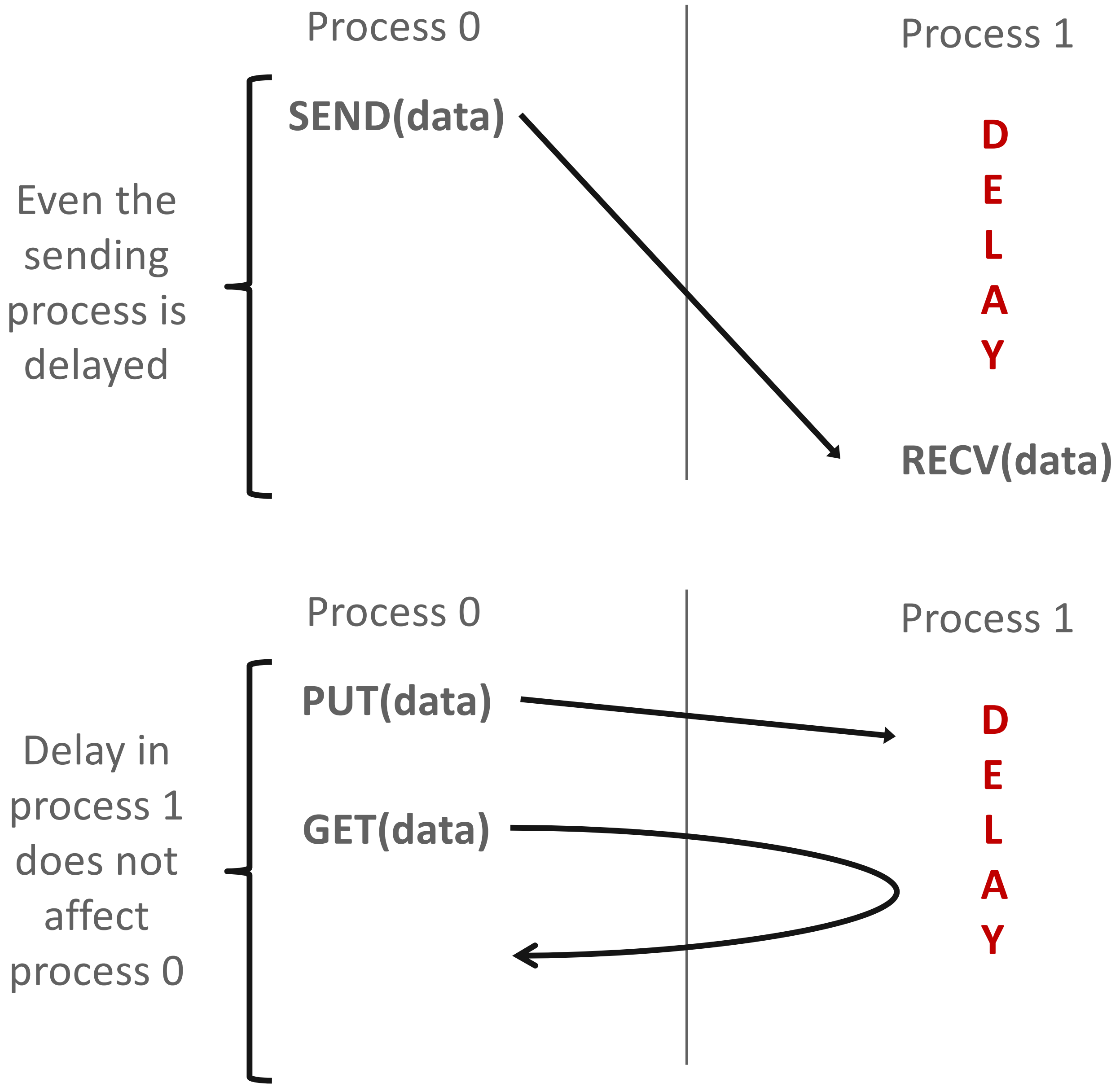
Two-sided Communication Example



One-sided Communication Example



Comparing One-sided and Two-sided Programming



Process 0

Process 1

SEND(data)

D E L A Y

RECV(data)

Even the sending process is delayed

Process 0

Process 1

PUT(data)

GET(data)

D E L A Y

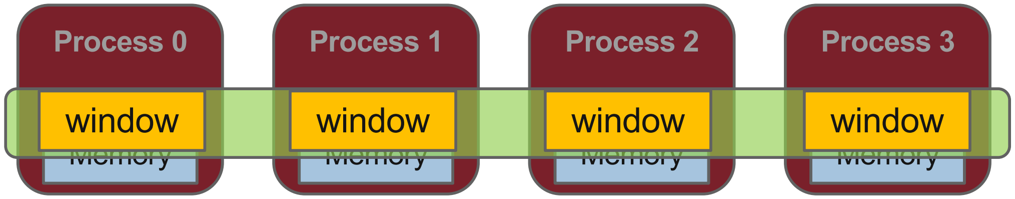
Delay in process 1 does not affect process 0

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 Public Memory

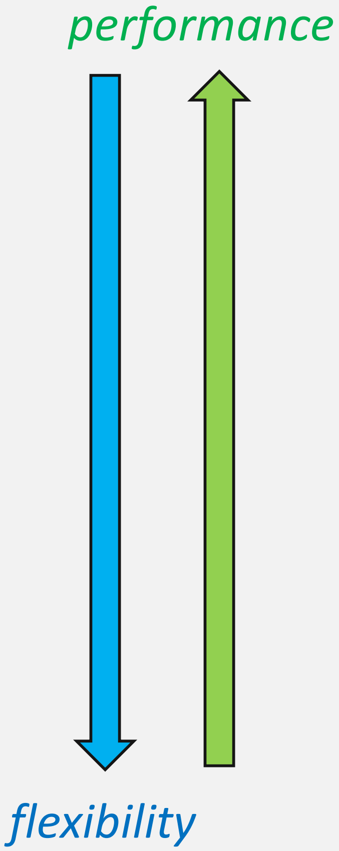
- Any memory used by a process is, by default, only locally accessible
  - X = malloc(100);



- 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_ALLOCATE`
    - You want to create a buffer and directly make it remotely accessible
  - `MPI_WIN_CREATE`
    - You already have an allocated buffer that you would like to make 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_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);

    MPI_Finalize(); return 0;
}
```

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_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;
}
```

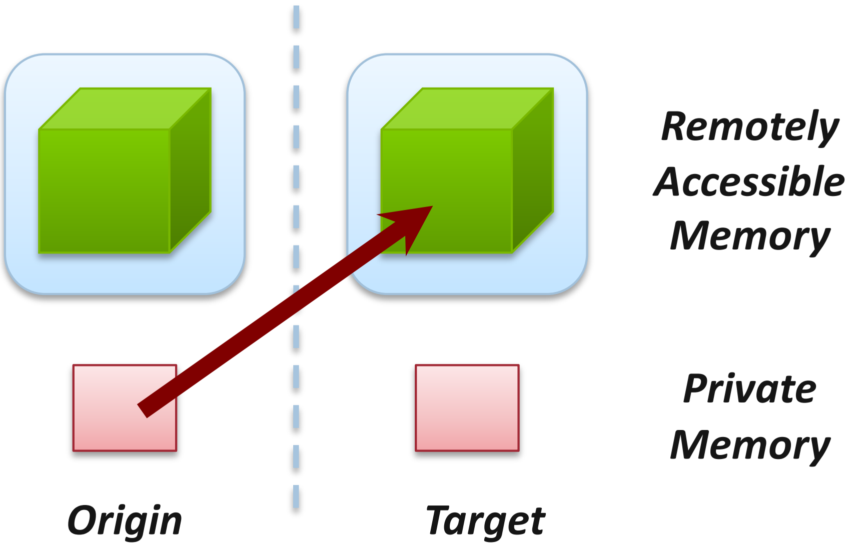
Data movement

- 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(const 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)
```

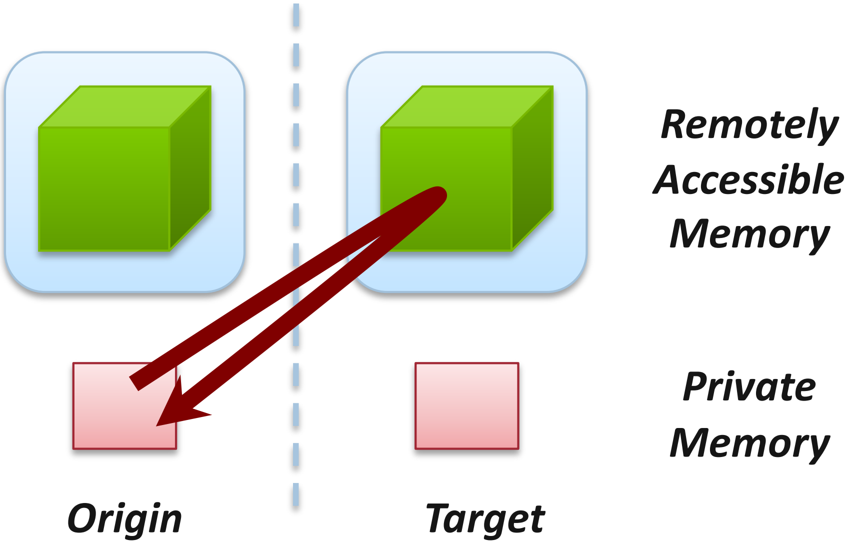
- Move data from origin, to target
- Separate data description triples for **origin** and **target**



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**



Remotely Accessible Memory

Private Memory

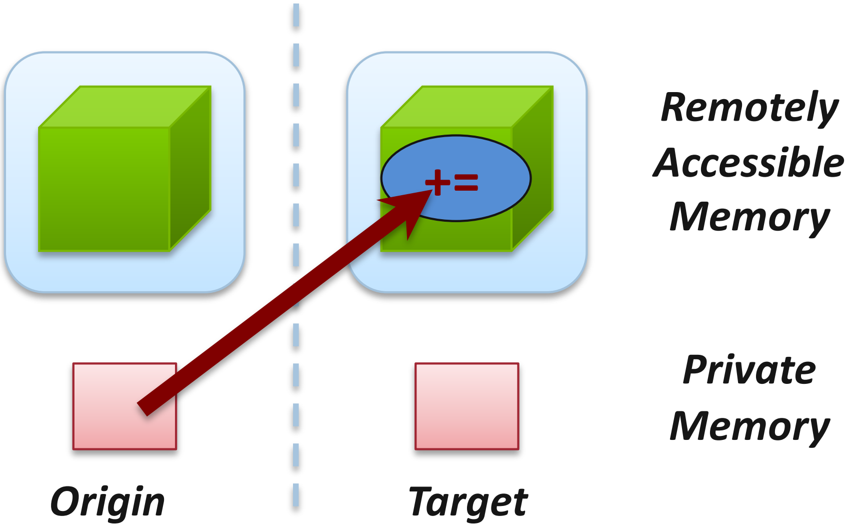
Origin

Target

Atomic Data Aggregation: *Accumulate*

```
MPI_Accumulate(const 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)
```

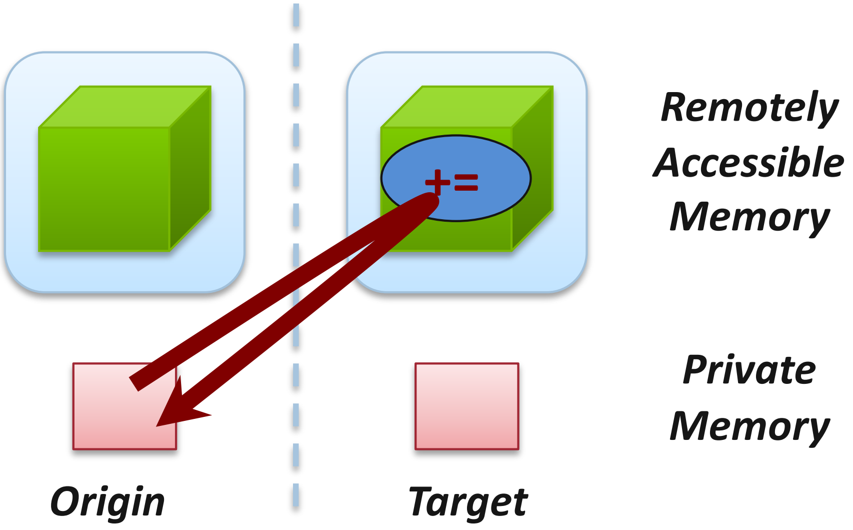
- Atomic update operation, similar to a put
  - Reduces origin and target data into target buffer using op argument as combiner
  - Op = MPI_SUM, MPI_PROD, MPI_OR, MPI_REPLACE, MPI_NO_OP, …
  - Predefined ops only, no user-defined operations
- Different data layouts between target/origin OK
  - Basic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



Atomic Data Aggregation: *Get Accumulate*

```
MPI_Get_accumulate(const 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 in result buf
- 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(const void *origin_addr, void *result_addr,
        MPI_Datatype dtype, int target_rank,
        MPI_Aint target_disp, MPI_Op op, MPI_Win win)
```

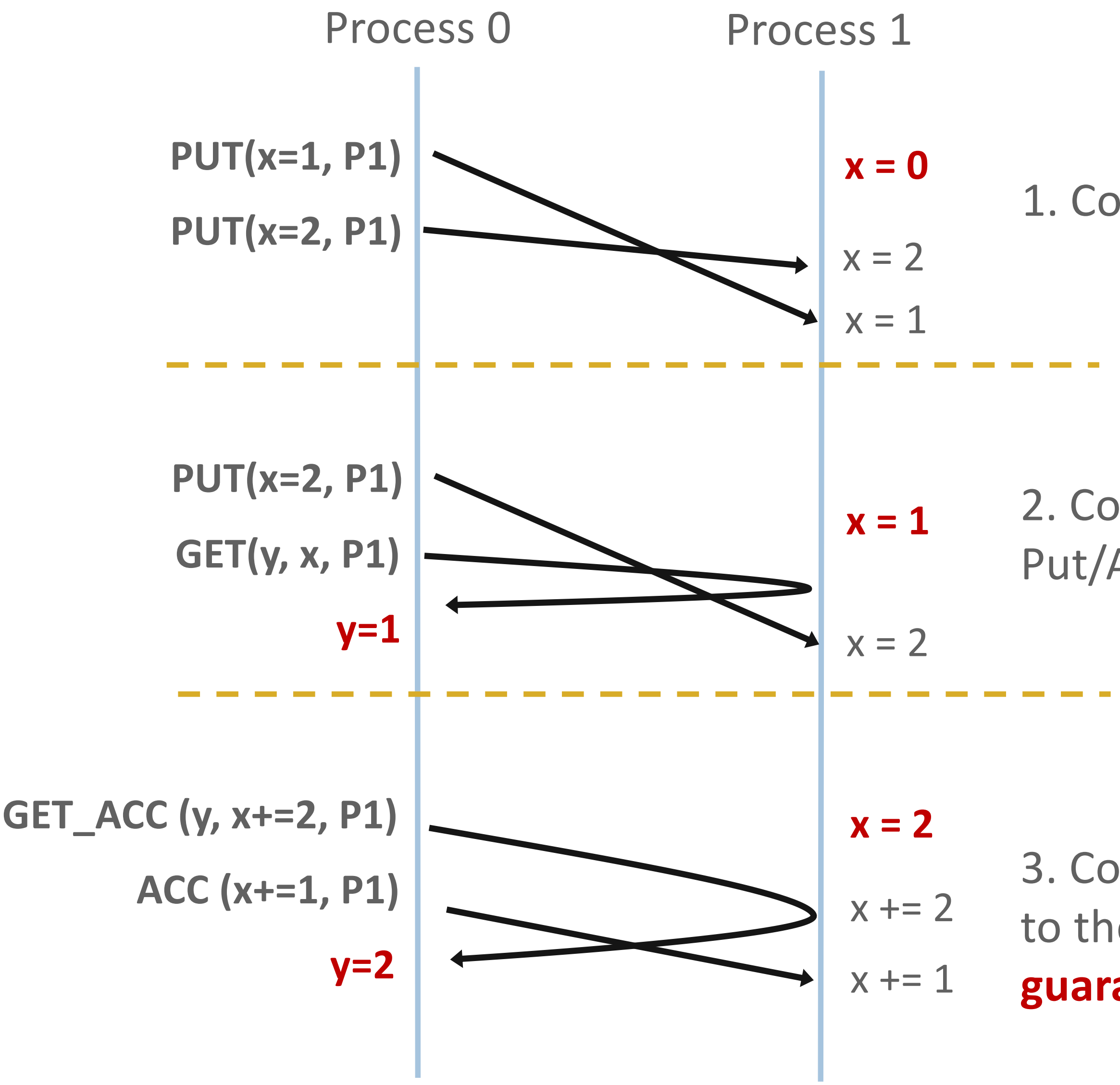
```
MPI_Compare_and_swap(const void *origin_addr,
        const void *compare_addr, void *result_addr,
        MPI_Datatype dtype, int target_rank,
        MPI_Aint target_disp, MPI_Win win)
```

- 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



1. Concurrent Puts: **undefined**

2. Concurrent Get and Put/Accumulates: **undefined**

3. Concurrent Accumulate operations to the same location : **ordering is guaranteed**

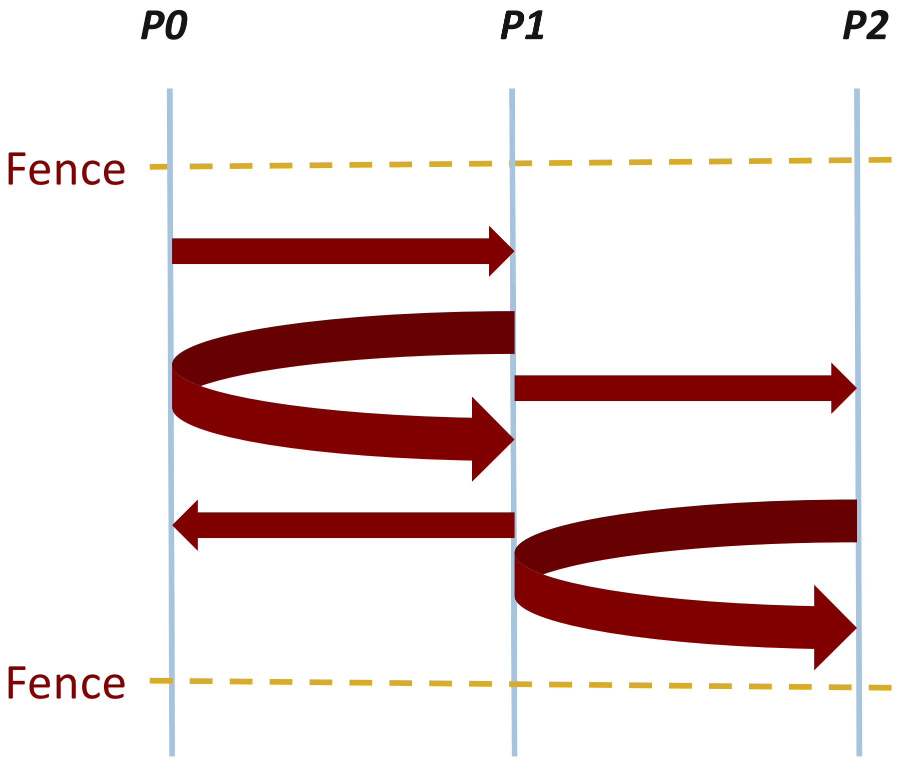
RMA Synchronization Models

- 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; rarely used now)
  - 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

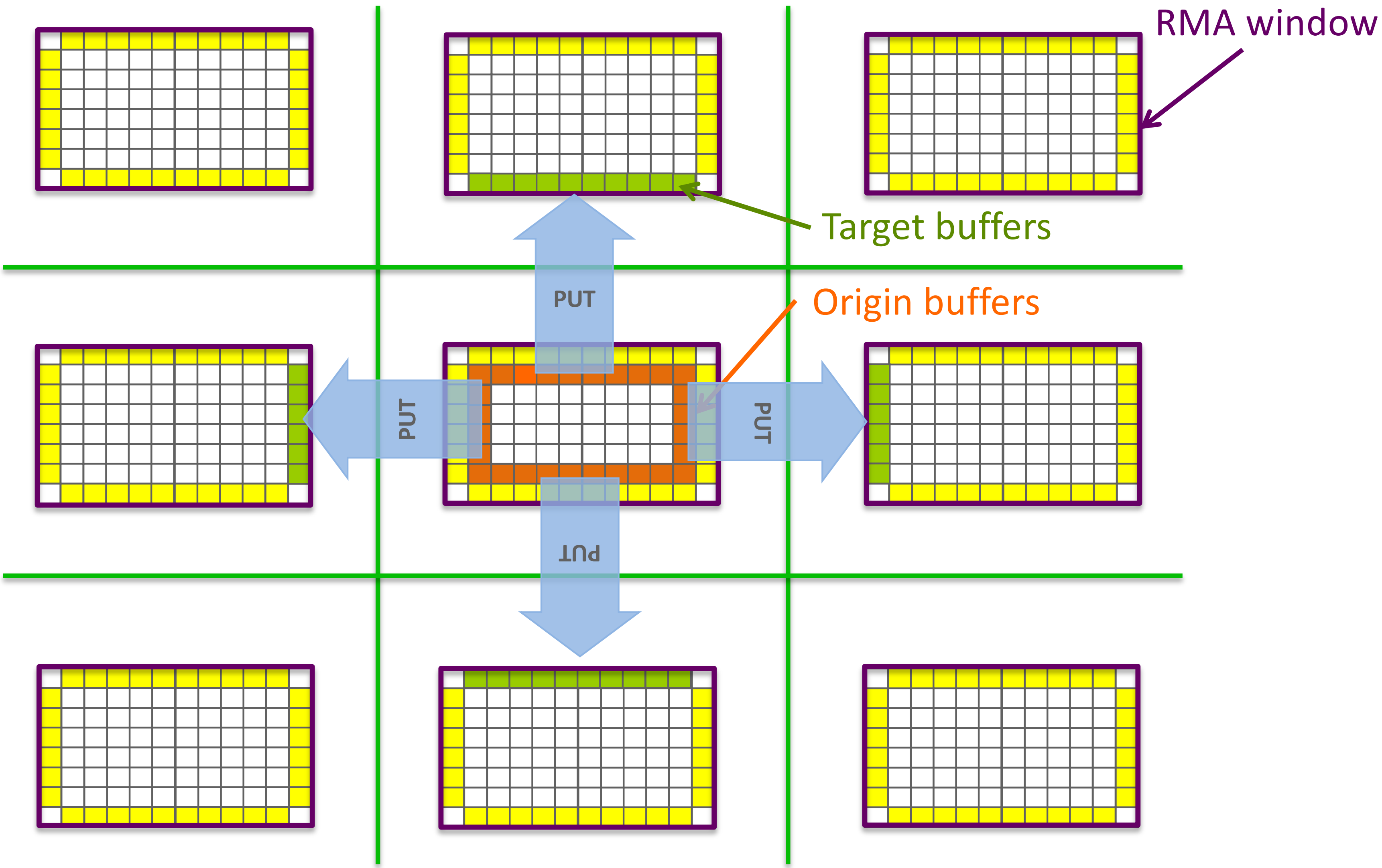
Fence: Active Target Synchronization

```
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



Implementing Stencil Computation with RMA Fence



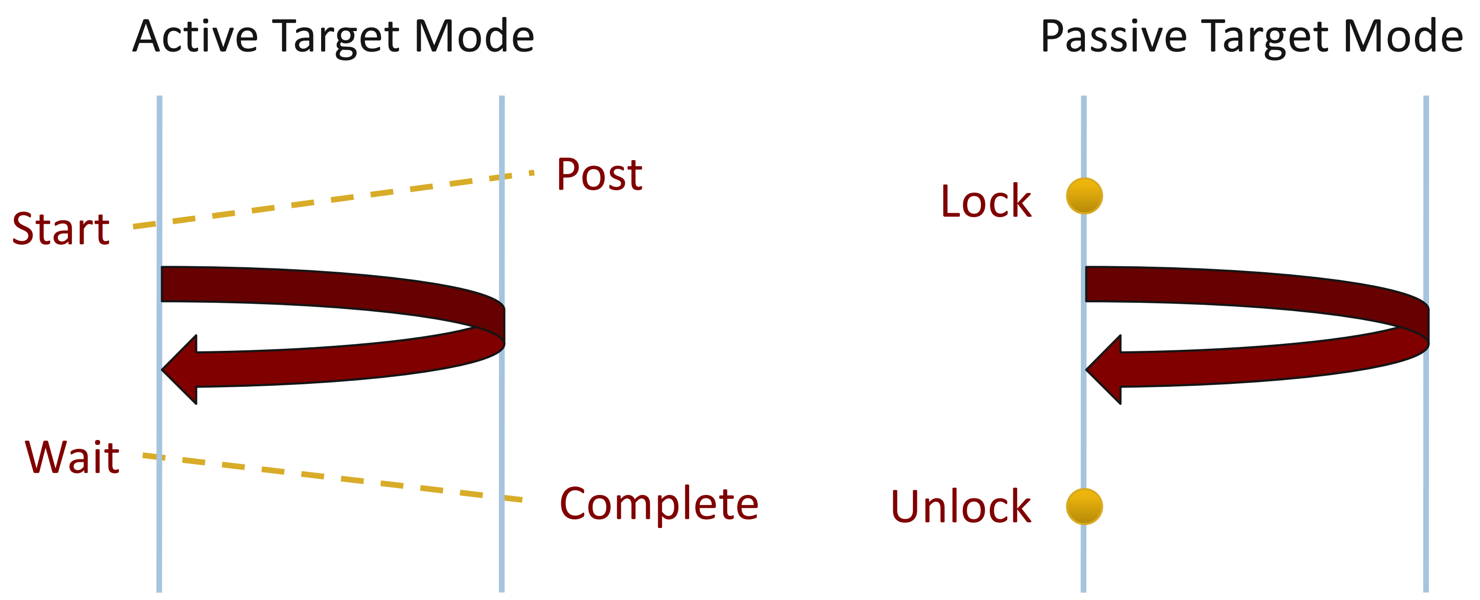
Exercise: Stencil with RMA Fence

- In the derived datatype version of the stencil code
  - Used nonblocking communication
  - Used derived datatypes
- Let’s try to use RMA fence
  - Move data with PUT instead of send/recv
- *Start from derived_datatype/stencil.c*
- *Solution available in rma/stencil_fence_put.c*

Exercise: Stencil with RMA Fence (GET model)

- In the derived datatype version of the stencil code
  - Used nonblocking communication
  - Used derived datatypes
- Let’s try to use RMA fence
  - Move data with GET instead of send/recv
- *Start from rma/stencil_fence_put.c*
- *Solution available in rma/stencil_fence_get.c*

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)
```

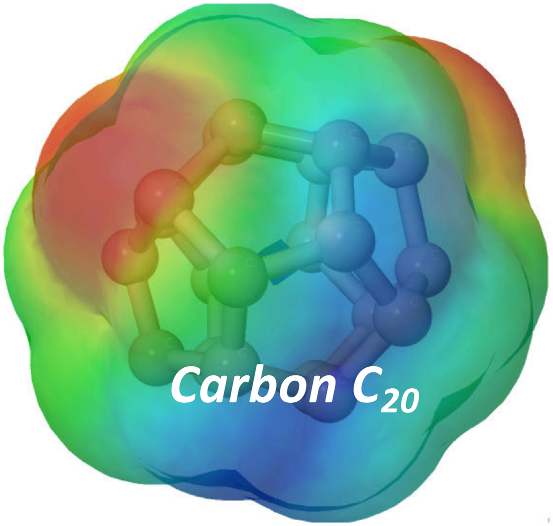
```
MPI_Win_unlock_all(MPI_Win win)
```

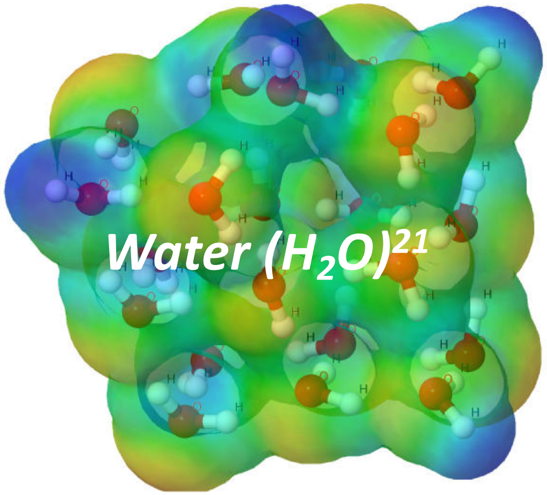
```
MPI_Win_flush_all/flush_local_all(MPI_Win win)
```

- 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

NWChem [1]

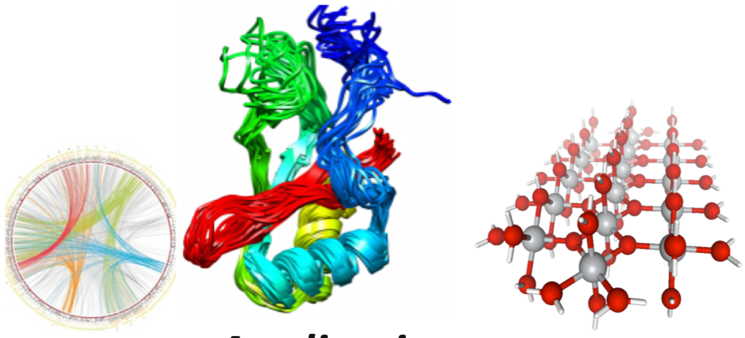
- High performance computational chemistry application suite
- Quantum level simulation of molecular systems
  - Very expensive in computation and data movement, so is used for small systems
  - Larger systems use molecular level simulations
- Composed of many simulation capabilities
  - Molecular Electronic Structure
  - Quantum Mechanics/Molecular Mechanics
  - Pseudo potential Plane-Wave Electronic Structure
  - Molecular Dynamics
- Very large code base
  - 4M LOC; Total investment of ~200M $ to date



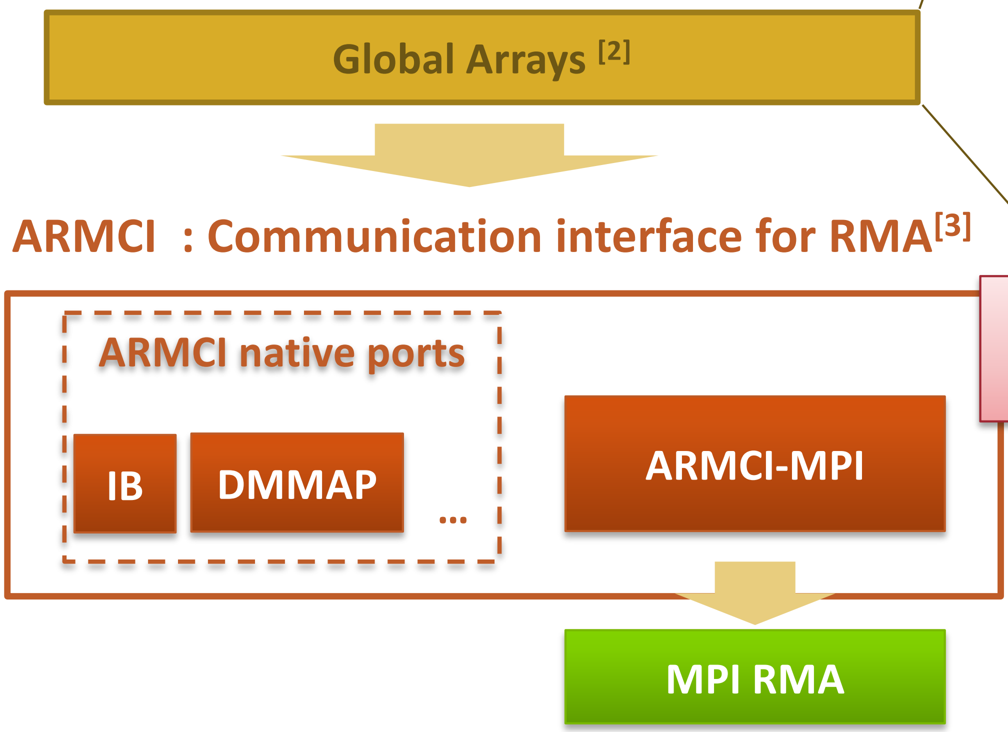


[1] M. Valiev, E.J. Bylaska, N. Govind, K. Kowalski, T.P. Straatsma, H.J.J. van Dam, D. Wang, J. Nieplocha, E. Apra, T.L. Windus, W.A. de Jong, "NWChem: a comprehensive and scalable open-source solution for large scale molecular simulations" Comput. Phys. Commun. 181, 1477 (2010)

NWChem Communication Runtime



Applications



Global Arrays [2]

ARMCI : Communication interface for RMA[3]

ARMCI native ports

IB

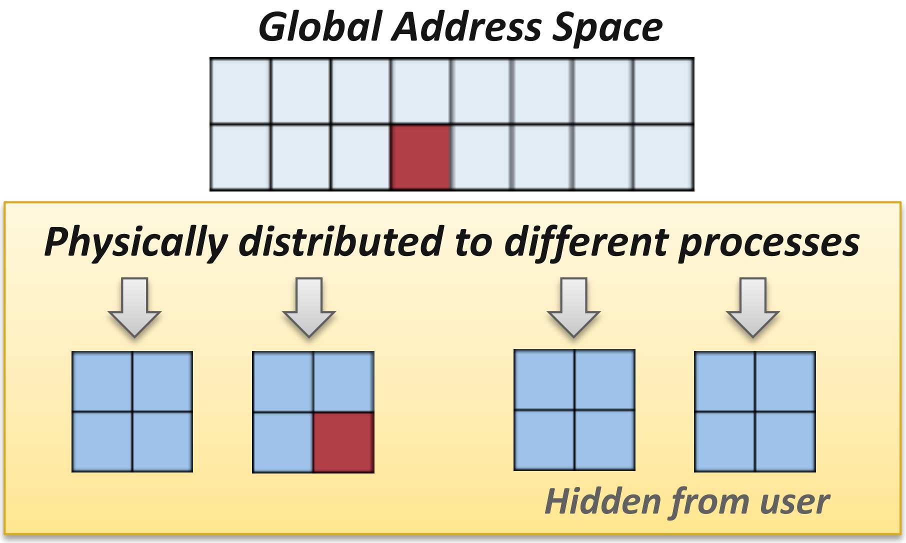
DMMAP

…

ARMCI-MPI

MPI RMA

Abstractions for distributed arrays



Global Address Space

Physically distributed to different processes

Hidden from user

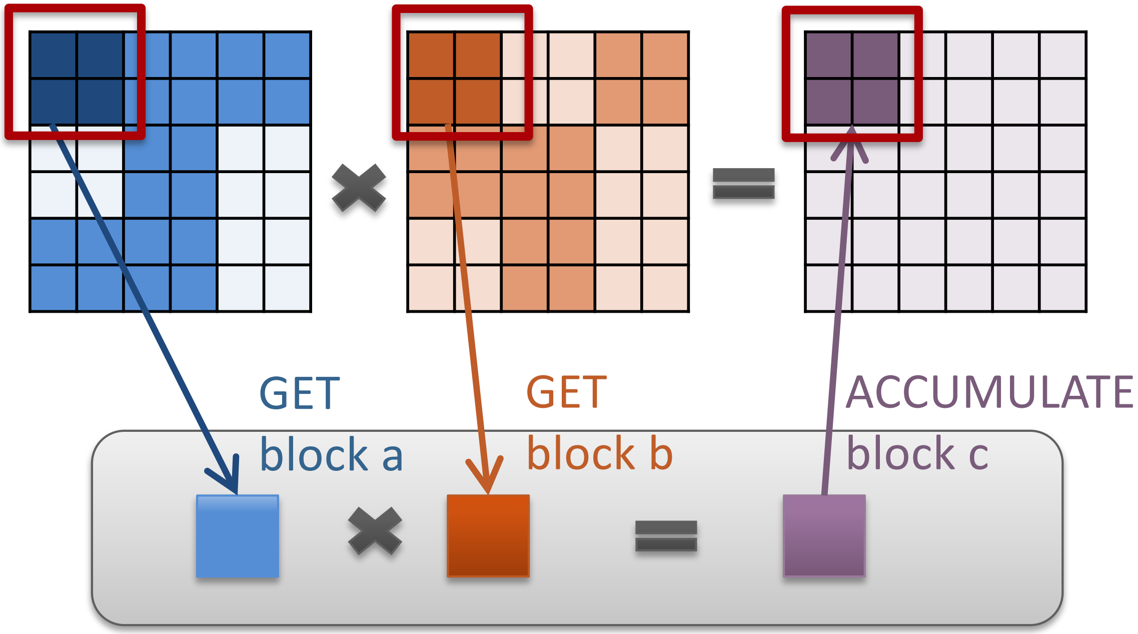
Irregularly access large amount of remote memory regions

[2] http://hpc.pnl.gov/globalarrays
[3] http://hpc.pnl.gov/armci

Get-Compute-Update

- Typical Get-Compute-Update mode in GA programming

All of the blocks are non-contiguous data



Perform DGEMM in local buffer

Pseudo code

```
for i in I blocks:
  for j in J blocks:
     for k in K blocks:
        GET block a from A
        GET block b from B
        c += a * b   /*computing*/
      end do
      ACC block c to C
      NXTASK
  end do
end do
```

Mock figure showing 2D DGEMM with block-sparse computations. In reality, NWChem uses 6D tensors.

Which synchronization mode should I use, when?

- RMA communication often has low overheads versus send/recv
  - Two-sided: Matching, queuing, buffering, unexpected receives, etc…
  - One-sided: No matching, no buffering, always ready to receive (but must separately sync the communication)
  - Direct use of RDMA provided by high-speed interconnects (e.g. InfiniBand)
    - Good two-sided implementations will also use RDMA, but must first match messages
- 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

Exercise: Stencil with RMA Lock_all/Unlock_all (PUT model)

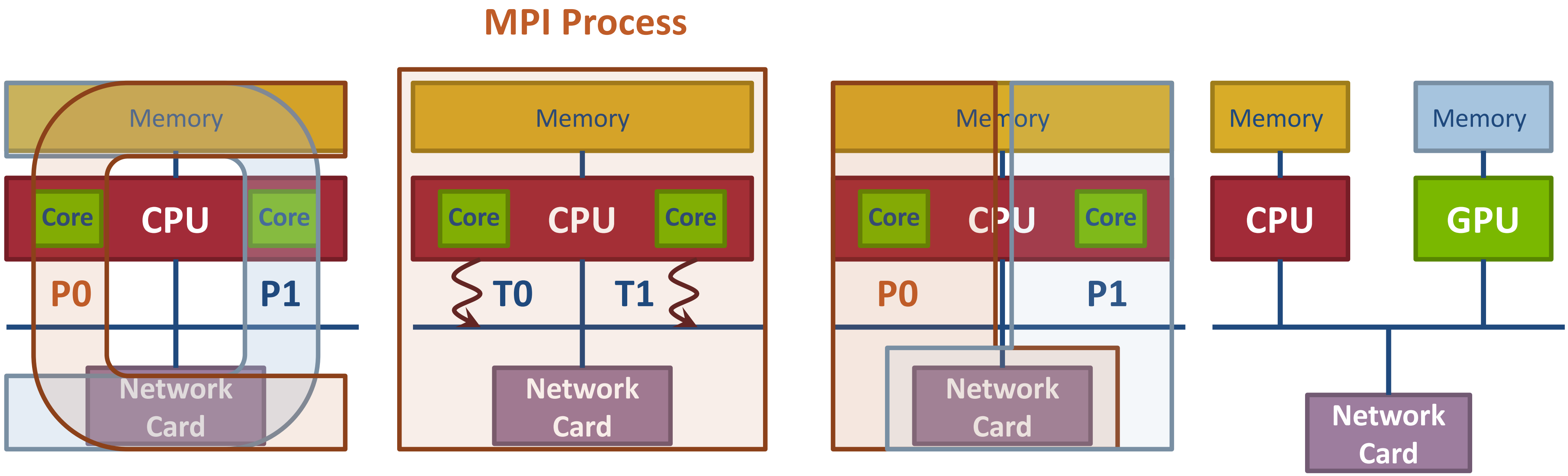
- In the fence and PSCW versions of the stencil code, RMA synchronization involves the target processes
- Let’s try to use RMA Lock_all/Flush_all/Unlock_all
  - Only the origin processes call RMA synchronization
  - Still need **Barrier** for process synchronization (e.g., ensure neighbors have completed data update to my local window)
  - Need **Win_sync** for memory synchronization
- *Start from rma/stencil_fence_put.c*
- *Solution available in rma/stencil_lock_put.c*

Advanced Topics: Hybrid Programming with Threads, Shared Memory, and Accelerators

https://anl.box.com/v/2019-ATPESC-MPI

Hybrid MPI + X : Most Popular Forms

MPI + X



MPI + 0

MPI + Threads

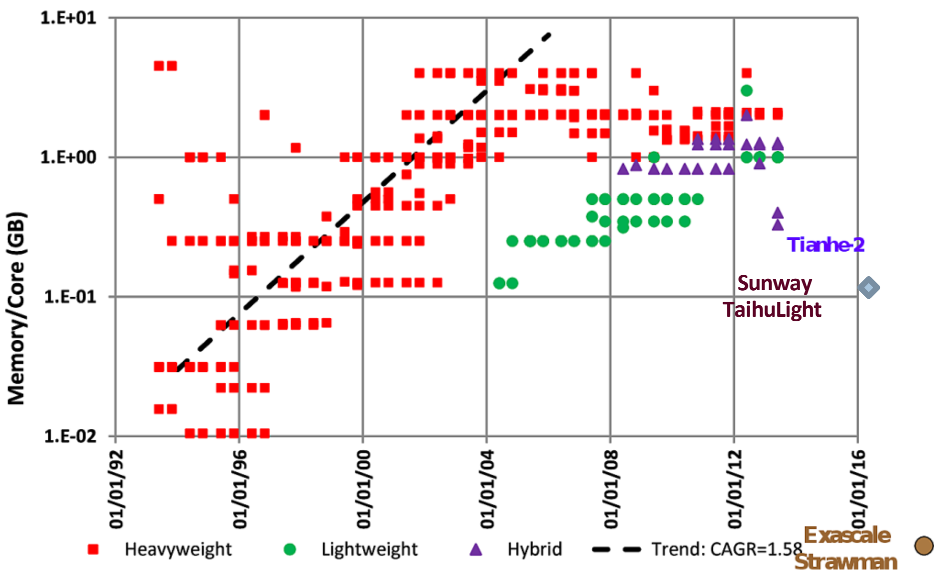
MPI + Shared Memory

MPI + ACC

MPI + Threads

Why Hybrid MPI+X? Towards Strong Scaling (1/3)

- Strong scaling applications is increasing in importance
  - Hardware limitations: not all resources scale at the same rate as cores (e.g., memory capacity, network resources)
  - Desire to solve the same problem faster on a bigger machine
    - Nek5000, HACC, LAMMPS



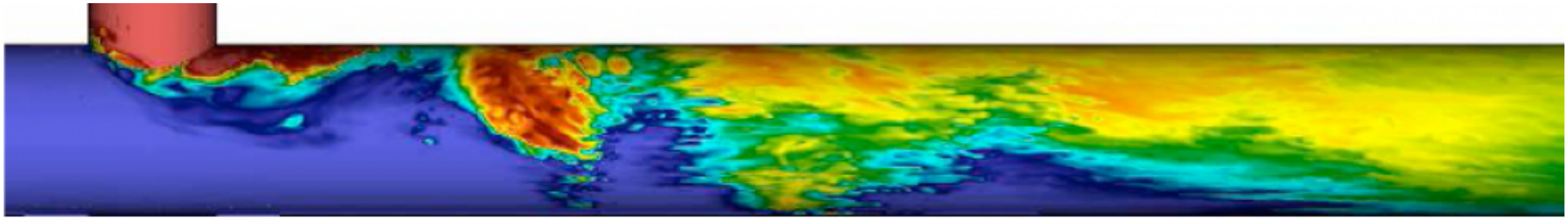
Evolution of the memory capacity per core in the Top500 list (Peter Kogge. PIM & memory: The need for a revolution in architecture.)

- Strong scaling pure MPI applications is getting harder
  - On-node communication is costly compared to load/stores
  - O(Px) communication patterns (e.g., All-to-all) costly

Why Hybrid MPI+X? Towards Strong Scaling (2/3)

- MPI+X benefits (X= {threads,MPI shared-memory, etc.})
  - Less memory hungry (MPI runtime consumption, O(P) data structures, etc.)
  - Load/stores to access memory instead of message passing
  - P is reduced by constant C (#cores/process) for O(Px) communication patterns
- Example 1: the Nek5000 team is working at the strong scaling limit

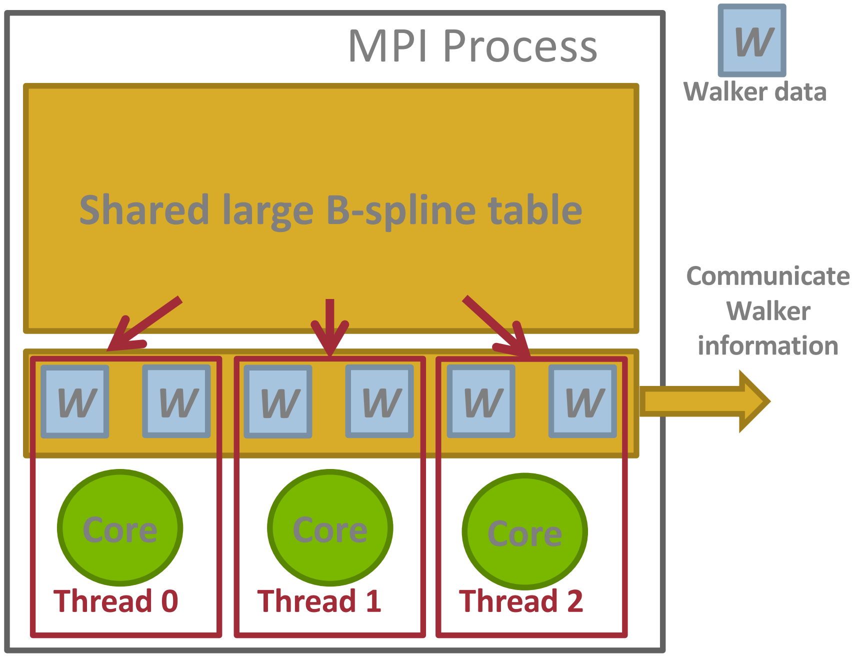
Nek5000



Why Hybrid MPI+X? Towards Strong Scaling (3/3)

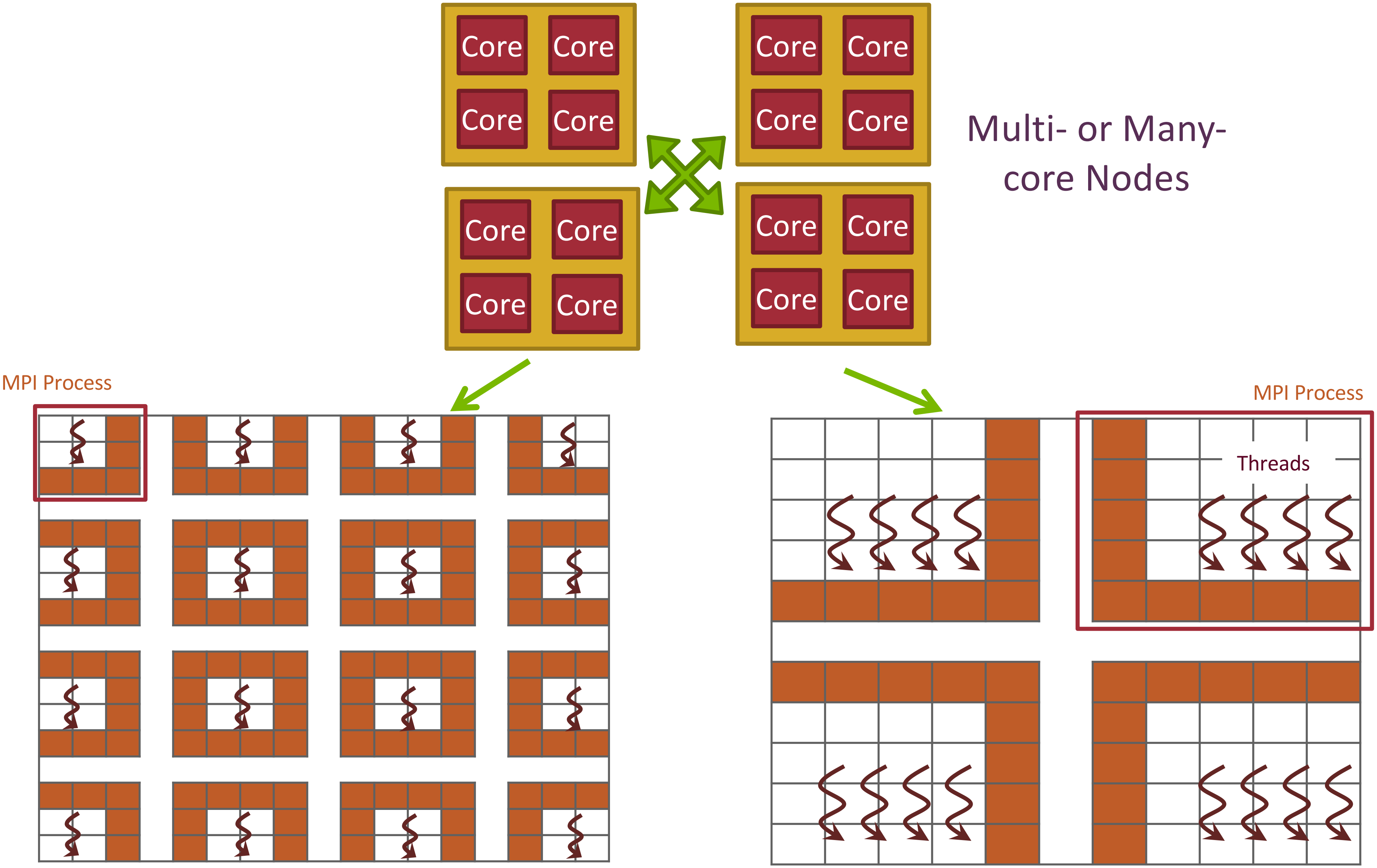
- Example 2: Quantum Monte Carlo Simulation (QCMPACK)
  - Size of the physical system to simulate is bound by memory capacity [1]
  - Memory space dominated by large interpolation tables (typically several GB of storage)
  - Threads are used to share those tables
  - Memory for communication buffers must be kept low to be allow simulation of larger and highly detailed simulations.

QMCPACK



[1] Kim, Jeongnim, et al. "Hybrid algorithms in quantum Monte Carlo." Journal of Physics, 2012.

MPI + Threads: How To? (1/3)



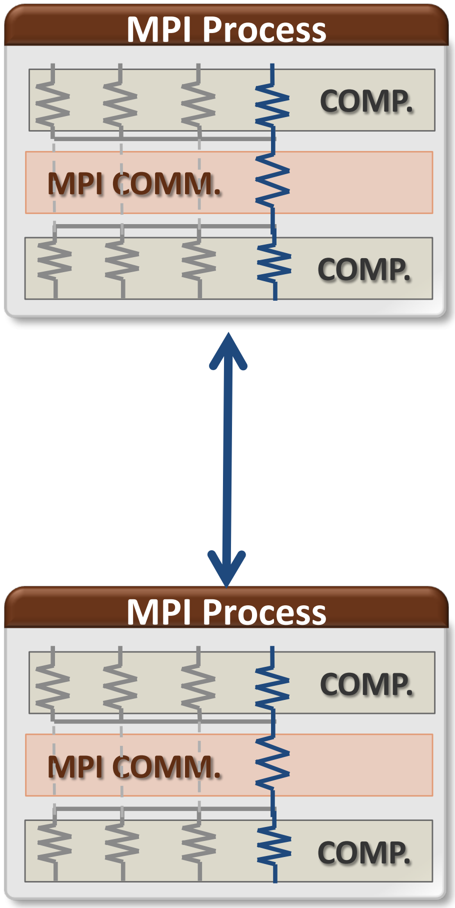
Multi- or Many-core Nodes

MPI only

MPI + Threads

MPI + Threads: How To? (2/3)

- MPI describes parallelism between *processes* (with separate address spaces)
- *Thread* parallelism provides a shared-memory model within a process
- OpenMP and Pthreads are common models
  - OpenMP provides convenient features for loop-level parallelism. Threads are created and managed by the compiler, based on user directives.
  - Pthreads provide more complex and dynamic approaches. Threads are created and managed explicitly by the user.



MPI + Threads: How To? (3/3)

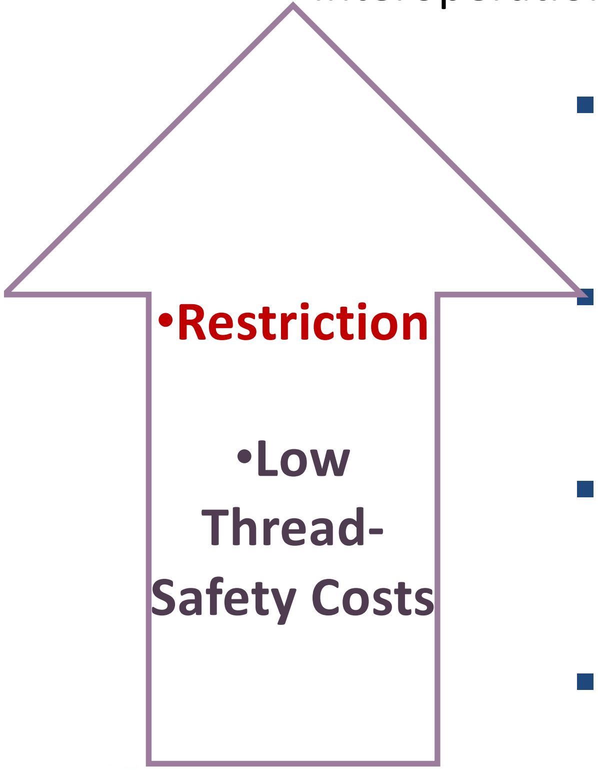
MPI + Threads

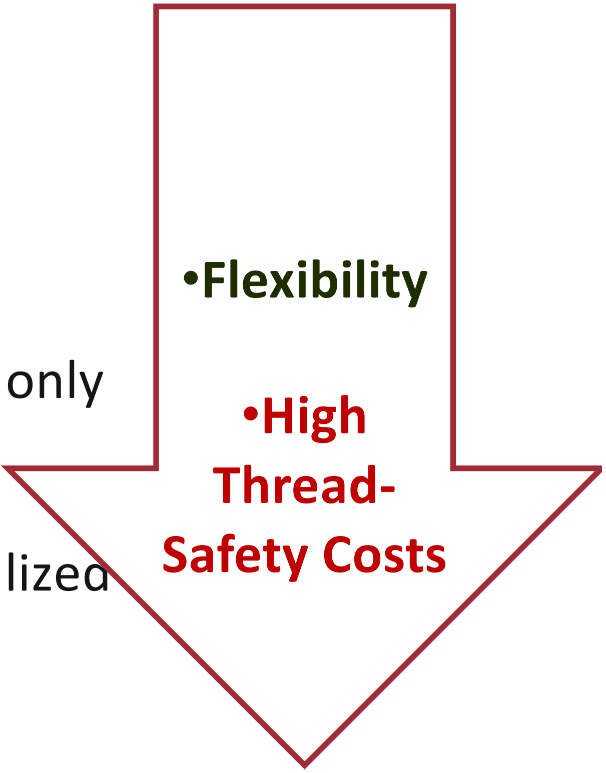
↓

Interoperability

Interoperation or thread levels:

- MPI_THREAD_SINGLE
  - No additional threads
- MPI_THREAD_FUNNELED
  - Master thread communication only
- MPI_THREAD_SERIALIZED
  - Threaded communication serialized
- MPI_THREAD_MULTIPLE
  - No restrictions





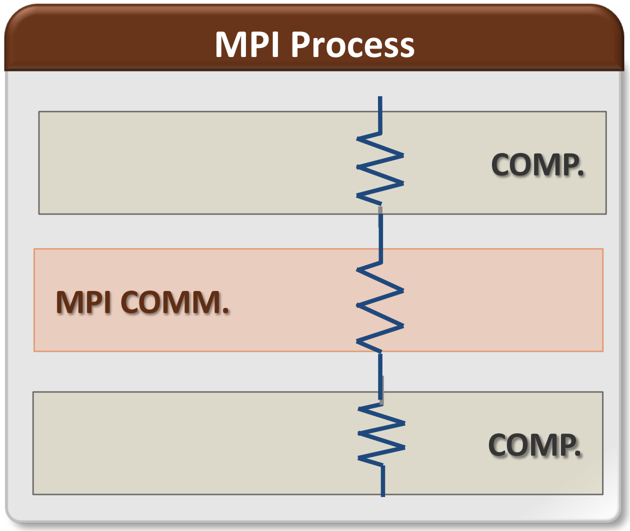
MPI’s Four Levels of Thread Safety

- MPI defines four levels of thread safety -- these are commitments the application makes to the MPI
- Thread levels are in increasing order
  - If an application works in FUNNELED mode, it can work in SERIALIZED
- MPI defines an alternative to MPI_Init
  - **MPI_Init_thread**(int argc, char **argv, int requested, int *provided): *Application specifies level it needs; MPI implementation returns level it supports*

MPI_THREAD_SINGLE

- There are no additional user threads in the system
  - E.g., there are no OpenMP parallel regions

```
int buf[100];
int main(int argc, char ** argv)
{
    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);

    for (i = 0; i < 100; i++)
        compute(buf[i]);

    /* Do MPI stuff */

    MPI_Finalize();

    return 0;
}
```

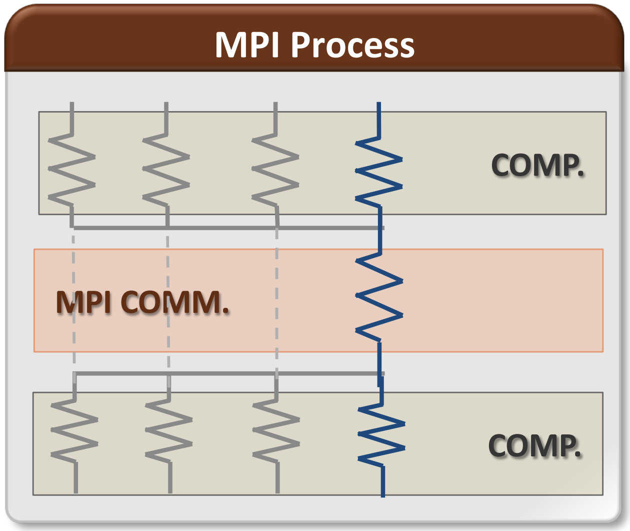


MPI_THREAD_FUNNELED

- All MPI calls are made by the **master** thread
  - Outside the OpenMP parallel regions
  - In OpenMP master regions

```
int buf[100];
int main(int argc, char ** argv)
{
   int provided;

   MPI_Init_thread(&argc, &argv,
       MPI_THREAD_FUNNELED, &provided);
   if (provided < MPI_THREAD_FUNNELED)
       MPI_Abort(MPI_COMM_WORLD,1);

   for (i = 0; i < 100; i++)
       pthread_create(…,func,(void*)i);
   for (i = 0; i < 100; i++)
       pthread_join(…);

   /* Do MPI stuff */

   MPI_Finalize();
   return 0;
}
```

```
void* func(void* arg) {
    int i = (int)arg;
   compute(buf[i]);
   return 0;
}
```

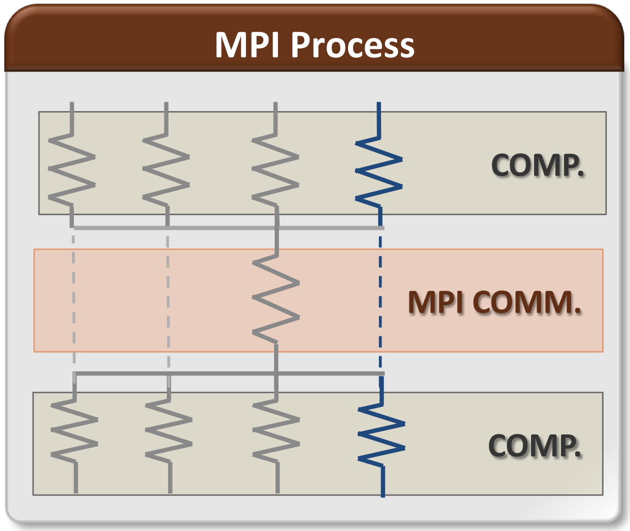


MPI_THREAD_SERIALIZED

- Only **one** thread can make MPI calls at a time
  - Protected by OpenMP critical regions

```
int buf[100];
int main(int argc, char ** argv)
{
   int provided;
   pthread_mutex_t mutex;

   MPI_Init_thread(&argc, &argv,
      MPI_THREAD_SERIALIZED, &provided);
   if (provided < MPI_THREAD_SERIALIZED)
      MPI_Abort(MPI_COMM_WORLD,1);

   for (i = 0; i < 100; i++)
       pthread_create(…,func,(void*)i);
   for (i = 0; i < 100; i++)
       pthread_join(…);

   MPI_Finalize();
   return 0;
}
```

```
void* func(void* arg) {
    int i = (int)arg;
    compute(buf[i]);
    pthread_mutex_lock(&mutex);
    /* Do MPI stuff */
    pthread_mutex_unlock(&mutex);
    return 0;
}
```

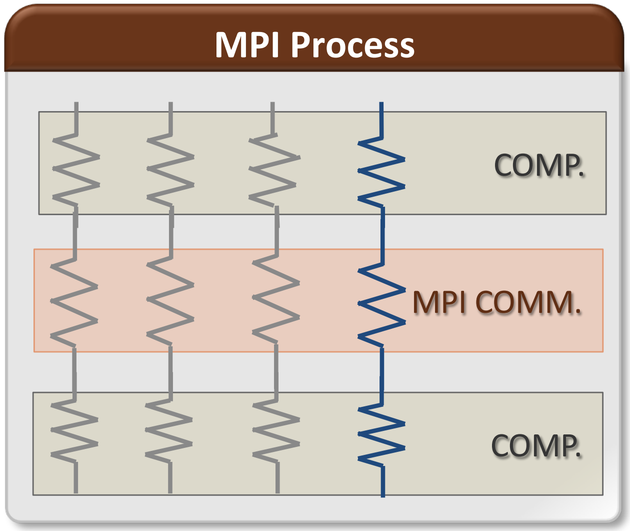


MPI_THREAD_MULTIPLE

- **Any** thread can make MPI calls any time (restrictions apply)

```
int buf[100];
int main(int argc, char ** argv)
{
   int provided;

   MPI_Init_thread(&argc, &argv,
   MPI_THREAD_MULTIPLE, &provided);
   if (provided < MPI_THREAD_SERIALIZED)
   MPI_Abort(MPI_COMM_WORLD,1);

   for (i = 0; i < 100; i++)
        pthread_create(…,func,(void*)i);

   MPI_Finalize();
   return 0;
}
```

```
void* func(void* arg) {
   int i = (int)arg;
   compute(buf[i]);

   /* Do MPI stuff */
   …
   return 0;
}
```



Threads and MPI

- An implementation is not required to support levels higher than MPI_THREAD_SINGLE; that is, an implementation is not required to be thread safe
- A fully thread-safe implementation will support MPI_THREAD_MULTIPLE
- A program that calls MPI_Init (instead of MPI_Init_thread) should assume that only MPI_THREAD_SINGLE is supported
- *A threaded MPI program that does not call MPI_Init_thread is an incorrect program (common user error we see)*
  - But rarely causes problems except for when MPI_THREAD_MULTIPLE required

MPI Semantics and MPI_THREAD_MULTIPLE

- ***Ordering:*** When multiple threads make MPI calls concurrently, the outcome will be as if the calls executed sequentially in some (any) order
  - Ordering is maintained within each thread
  - User must ensure that collective operations on the same communicator, window, or file handle are correctly ordered among threads
    - E.g., cannot call a broadcast on one thread and a reduce on another thread on the same communicator
  - It is the user's responsibility to prevent races when threads in the same application post conflicting MPI calls
    - E.g., accessing an info object from one thread and freeing it from another thread
- ***Progress:*** Blocking MPI calls will block only the calling thread and will not prevent other threads from running or executing MPI functions

Ordering in MPI_THREAD_MULTIPLE: Incorrect Example with Collectives

	Process 0	***Process 1***
Thread 0	MPI_Bcast(comm)	MPI_Bcast(comm)
Thread 1	MPI_Barrier(comm)	MPI_Barrier(comm)

Ordering in MPI_THREAD_MULTIPLE: Incorrect Example with Collectives

Process 0		*Process 1*	
Thread 1	Thread 2	Thread 1	Thread 2
MPI_Bcast(comm)			MPI_Barrier(comm)
	MPI_Barrier(comm)	MPI_Bcast(comm)	

- P0 and P1 can have different orderings of Bcast and Barrier
- Here the user must use some kind of synchronization to ensure that either thread 1 or thread 2 gets scheduled first on both processes
- Otherwise a broadcast may get matched with a barrier on the same communicator, which is not allowed in MPI

Ordering in MPI_THREAD_MULTIPLE: Incorrect Example with Object Management

Process 0

Thread 1	Thread 2
	MPI_Comm_free(comm)
MPI_Bcast(comm)	

- The user has to make sure that one thread is not using an object while another thread is freeing it
  - This is essentially an ordering issue; the object might get freed before it is used

Blocking Calls in MPI_THREAD_MULTIPLE: Correct Example

	Process 0	***Process 1***
Thread 1	MPI_Recv(src=1)	MPI_Recv(src=0)
Thread 2	MPI_Send(dst=1)	MPI_Send(dst=0)

- An implementation must ensure that the above example never deadlocks for any ordering of thread execution
- That means the implementation cannot simply acquire a thread lock and block within an MPI function. It must release the lock to allow other threads to make progress.

The Current Situation

- All MPI implementations support MPI_THREAD_SINGLE
- They probably support MPI_THREAD_FUNNELED even if they don't admit it.
  - Does require thread-safety for some system routines (e.g. malloc)
  - On most systems `-pthread` will guarantee it (OpenMP implies `-pthread`)
- Many (but not all) implementations support THREAD_MULTIPLE
  - Hard to implement efficiently though (thread synchronization issues)
- Bulk-synchronous OpenMP programs (loops parallelized with OpenMP, communication between loops) only need FUNNELED
  - So don't need "fully thread-safe" MPI for many hybrid programs
  - But watch out for Amdahl's Law!

Hybrid Programming: Correctness Requirements

- Hybrid programming with MPI+threads does not do much to reduce the complexity of thread programming
  - Your application still has to be a correct multi-threaded application
  - On top of that, you also need to make sure you are correctly following MPI semantics
- Many commercial debuggers offer support for debugging hybrid MPI+threads applications (mostly for MPI+Pthreads and MPI+OpenMP)

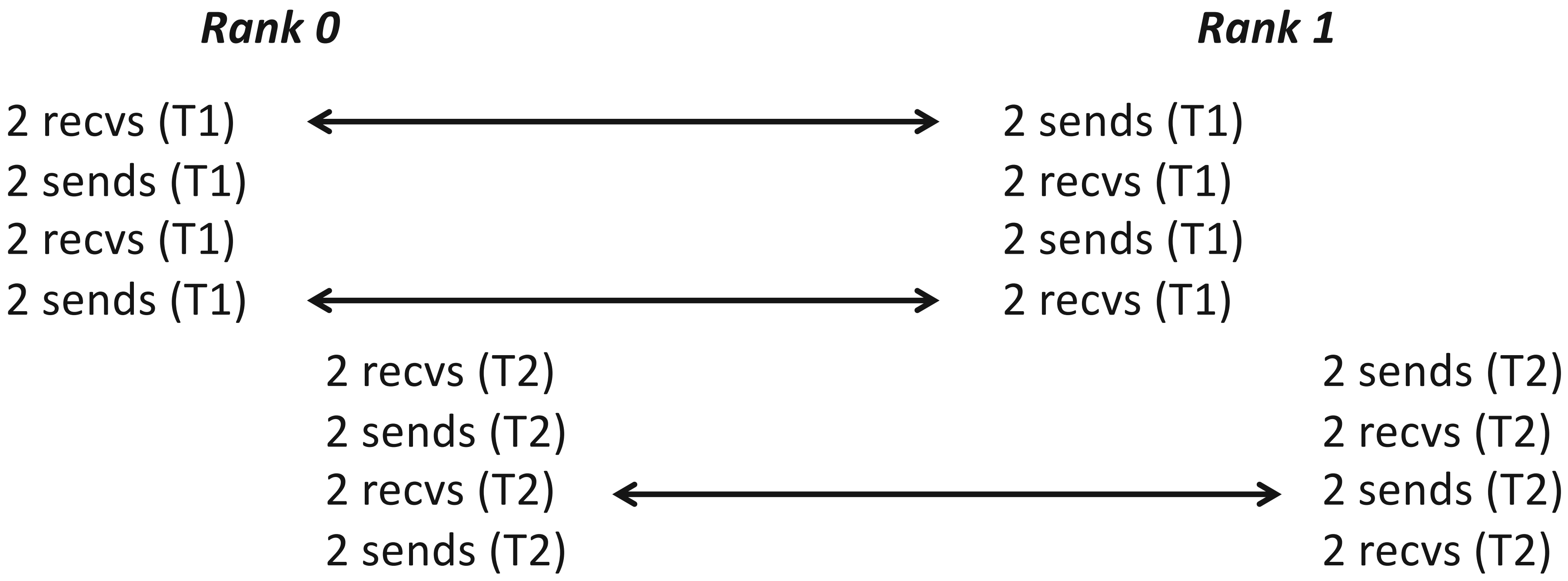
An Example we encountered

- We received a bug report about a very simple multithreaded MPI program that hangs
- Run with 2 processes
- Each process has 2 threads
- Both threads communicate with threads on the other process as shown in the next slide
- We spent several hours trying to debug MPICH before discovering that the bug is actually in the user’s program ☹

2 Proceses, 2 Threads (Each Thread Executes this Code)

```
if (rank == 1) {
   MPI_Send(NULL, 0, MPI_CHAR, 0, 0, MPI_COMM_WORLD);
   MPI_Send(NULL, 0, MPI_CHAR, 0, 0, MPI_COMM_WORLD);
   MPI_Recv(NULL, 0, MPI_CHAR, 0, 0, MPI_COMM_WORLD, &stat);
   MPI_Recv(NULL, 0, MPI_CHAR, 0, 0, MPI_COMM_WORLD, &stat);

   MPI_Send(NULL, 0, MPI_CHAR, 0, 0, MPI_COMM_WORLD);
   MPI_Send(NULL, 0, MPI_CHAR, 0, 0, MPI_COMM_WORLD);
   MPI_Recv(NULL, 0, MPI_CHAR, 0, 0, MPI_COMM_WORLD, &stat);
   MPI_Recv(NULL, 0, MPI_CHAR, 0, 0, MPI_COMM_WORLD, &stat);
} else {  /* rank == 0 */
   MPI_Recv(NULL, 0, MPI_CHAR, 1, 0, MPI_COMM_WORLD, &stat);
   MPI_Recv(NULL, 0, MPI_CHAR, 1, 0, MPI_COMM_WORLD, &stat);
   MPI_Send(NULL, 0, MPI_CHAR, 1, 0, MPI_COMM_WORLD);
   MPI_Send(NULL, 0, MPI_CHAR, 1, 0, MPI_COMM_WORLD);

   MPI_Recv(NULL, 0, MPI_CHAR, 1, 0, MPI_COMM_WORLD, &stat);
   MPI_Recv(NULL, 0, MPI_CHAR, 1, 0, MPI_COMM_WORLD, &stat);
   MPI_Send(NULL, 0, MPI_CHAR, 1, 0, MPI_COMM_WORLD);
   MPI_Send(NULL, 0, MPI_CHAR, 1, 0, MPI_COMM_WORLD);
}
```

Intended Ordering of Operations



Rank 0

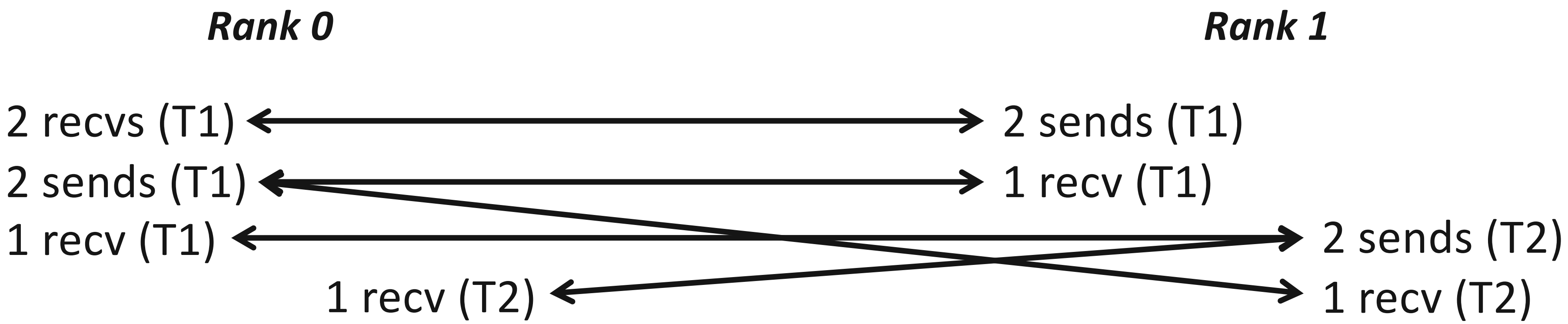
2 recvs (T1)
2 sends (T1)
2 recvs (T1)
2 sends (T1)
2 recvs (T2)
2 sends (T2)
2 recvs (T2)
2 sends (T2)

Rank 1

2 sends (T1)
2 recvs (T1)
2 sends (T1)
2 recvs (T1)
2 sends (T2)
2 recvs (T2)
2 sends (T2)
2 recvs (T2)

- Every send matches a receive on the other rank

Possible Ordering of Operations in Practice



Rank 0

Rank 1

2 recvs (T1)

2 sends (T1)

1 recv (T1)

1 recv (T2)

2 sends (T1)

1 recv (T1)

2 sends (T2)

1 recv (T2)

---

1 recv (T1)
1 recv (T2)
1 recv (T1)
1 recv (T2)

---

2 sends (T1)

2 sends (T2)
2 recvs (T2)
2 sends (T2)

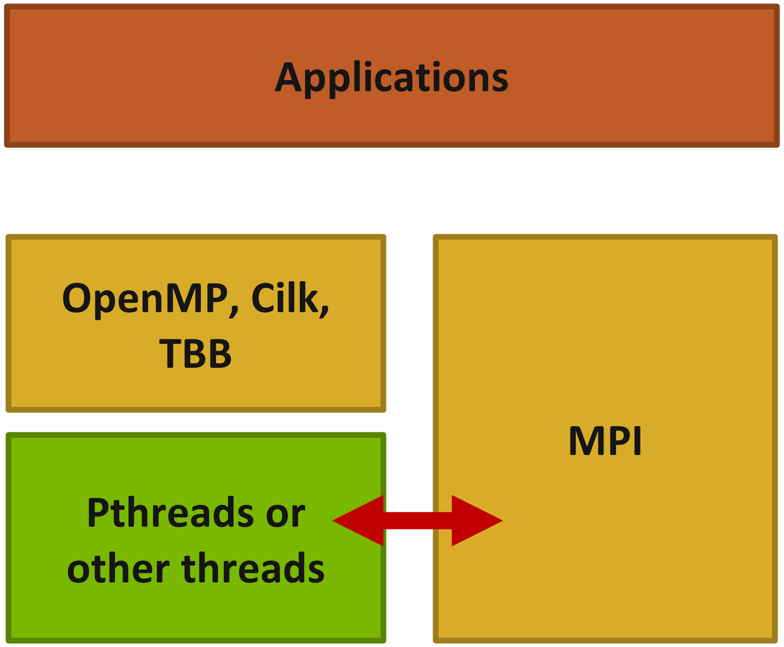
2 sends (T1)
2 recvs (T1)

2 sends (T2)
2 recvs (T2)

- Because the MPI operations can be issued in an arbitrary order across threads, all threads could block in a RECV call

MPI+OpenMP correctness semantics

- MPI only specifies interoperability with threads, not with OpenMP (or any other high-level programming model using threads)
  - OpenMP iterations need to be carefully mapped to which thread executes them (some schedules in OpenMP make this harder)
- For OpenMP tasks, the general model to use is that an OpenMP thread can execute one or more OpenMP tasks
  - An MPI blocking call should be assumed to block the entire OpenMP thread, so other tasks might not get executed



OpenMP threads: MPI blocking Calls (1/2)

```
int main(int argc, char ** argv)
{
    MPI_Init_thread(NULL, NULL, MPI_THREAD_MULTIPLE, &provided);

#pragma omp parallel for
    for (i = 0; i < 100; i++) {
        if (i % 2 == 0)
            MPI_Send(.., to_myself, ..);
        else
            MPI_Recv(.., from_myself, ..);
    }

    MPI_Finalize();

    return 0;
}
```

Iteration to OpenMP thread mapping needs to explicitly be handled by the user; otherwise, OpenMP threads might all issue the same operation and deadlock

OpenMP threads: MPI blocking Calls (2/2)

```
int main(int argc, char ** argv)
{
    MPI_Init_thread(NULL, NULL, MPI_THREAD_MULTIPLE, &provided);

#pragma omp parallel
{
    assert(omp_get_num_threads() > 1)
    #pragma omp for schedule(static, 1)
    for (i = 0; i < 100; i++) {
        if (i % 2 == 0)
            MPI_Send(.., to_myself, ..);
        else
            MPI_Recv(.., from_myself, ..);
    }
}
    MPI_Finalize();

    return 0;
}
```

Either explicit/careful mapping of iterations to threads, or using nonblocking versions of send/recv would solve this problem

OpenMP tasks: MPI blocking Calls (1/5)

```
int main(int argc, char ** argv)
{
    MPI_Init_thread(NULL, NULL, MPI_THREAD_MULTIPLE, &provided);

#pragma omp parallel
{
   #pragma omp for
   for (i = 0; i < 100; i++) {
      #pragma omp task
      {
        if (i % 2 == 0)
          MPI_Send(.., to_myself, ..);
        else
          MPI_Recv(.., from_myself, ..);
      }
   }
}
    MPI_Finalize();
    return 0;
}
```

This can lead to deadlocks. No ordering or progress guarantees in OpenMP task scheduling should be assumed; a blocked task blocks it's thread and tasks can be executed in any order.

OpenMP tasks: MPI blocking Calls (2/5)

```
int main(int argc, char ** argv)
{
    MPI_Init_thread(NULL, NULL, MPI_THREAD_MULTIPLE, &provided);

#pragma omp parallel
{
   #pragma omp taskloop
   for (i = 0; i < 100; i++) {
      if (i % 2 == 0)
        MPI_Send(.., to_myself, ..);
      else
        MPI_Recv(.., from_myself, ..)
   }
}
    MPI_Finalize();
    return 0;
}
```

Same problem as before.

OpenMP tasks: MPI blocking Calls (3/5)

```
int main(int argc, char ** argv)
{
    MPI_Init_thread(NULL, NULL, MPI_THREAD_MULTIPLE, &provided);

#pragma omp parallel
{
   #pragma omp taskloop
   for (i = 0; i < 100; i++) {
      MPI_Request req;
      if (i % 2 == 0)
         MPI_Isend(.., to_myself, .., &req);
      else
         MPI_Irecv(.., from_myself, .., &req);
      MPI_Wait(&req, ..);
   }
}
    MPI_Finalize();
    return 0;
}
```

Using nonblocking operations but with MPI_Wait inside the task region does not solve the problem

OpenMP tasks: MPI blocking Calls (4/5)

```
int main(int argc, char ** argv)
{
    MPI_Init_thread(NULL, NULL, MPI_THREAD_MULTIPLE, &provided);

#pragma omp parallel
{
   #pragma omp taskloop
   for (i = 0; i < 100; i++) {
           MPI_Request req; int done = 0;
        if (i % 2 == 0)
           MPI_Isend(.., to_myself, .., &req);
        else
           MPI_Irecv(.., from_myself, .., &req);
        While (!done) {
           #pragma omp taskyield
           MPI_Test(&req, &done, ..);
        }
      }
   }
}
    MPI_Finalize();
    return 0;
}
```

Still incorrect; taskyield does not guarantee a task switch

OpenMP tasks: MPI blocking Calls (5/5)

```
int main(int argc, char ** argv)
{
    MPI_Init_thread(NULL, NULL, MPI_THREAD_MULTIPLE, &provided);
    MPI_Request req[100];

#pragma omp parallel
{
   #pragma omp taskloop
   for (i = 0; i < 100; i++) {
      if (i % 2 == 0)
         MPI_Isend(.., to_myself, .., &req[i]);
      else
         MPI_Irecv(.., from_myself, .., &req[i]);
   }
}
    MPI_Waitall(100, req, ..);
    MPI_Finalize();
    return 0;
}
```

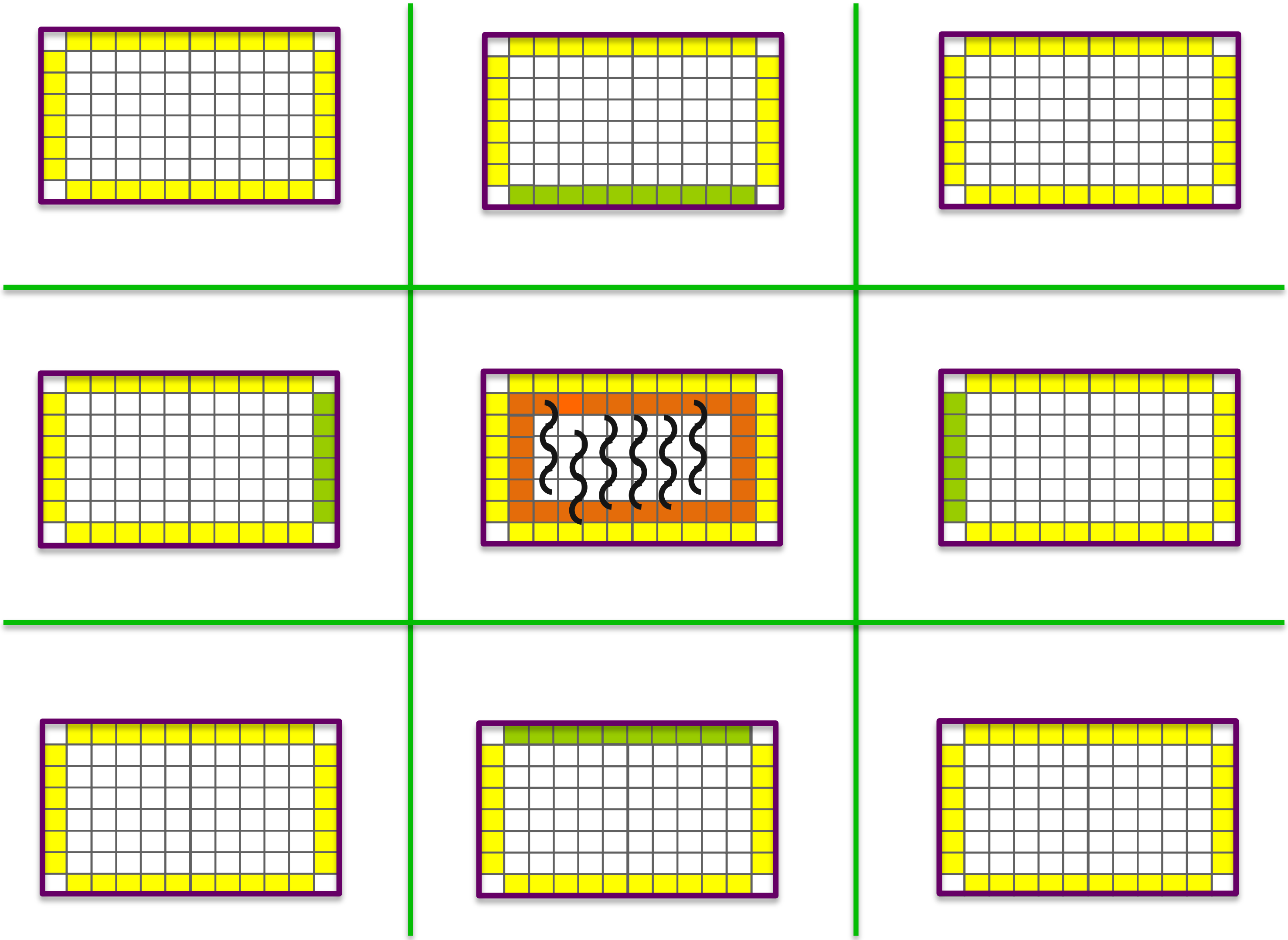
Correct example. Each task is nonblocking.

Ordering in MPI_THREAD_MULTIPLE: Incorrect Example with RMA

```
int main(int argc, char ** argv)
{
    /* Initialize MPI and RMA window */

#pragma omp parallel for
    for (i = 0; i < 100; i++) {
        target = rand();
        MPI_Win_lock(MPI_LOCK_EXCLUSIVE, target, 0, win);
        MPI_Put(..., win);
        MPI_Win_unlock(target, win);
    }

    /* Free MPI and RMA window */

    return 0;
}
```

Different threads can lock the same process causing multiple locks to the same target before the first lock is unlocked

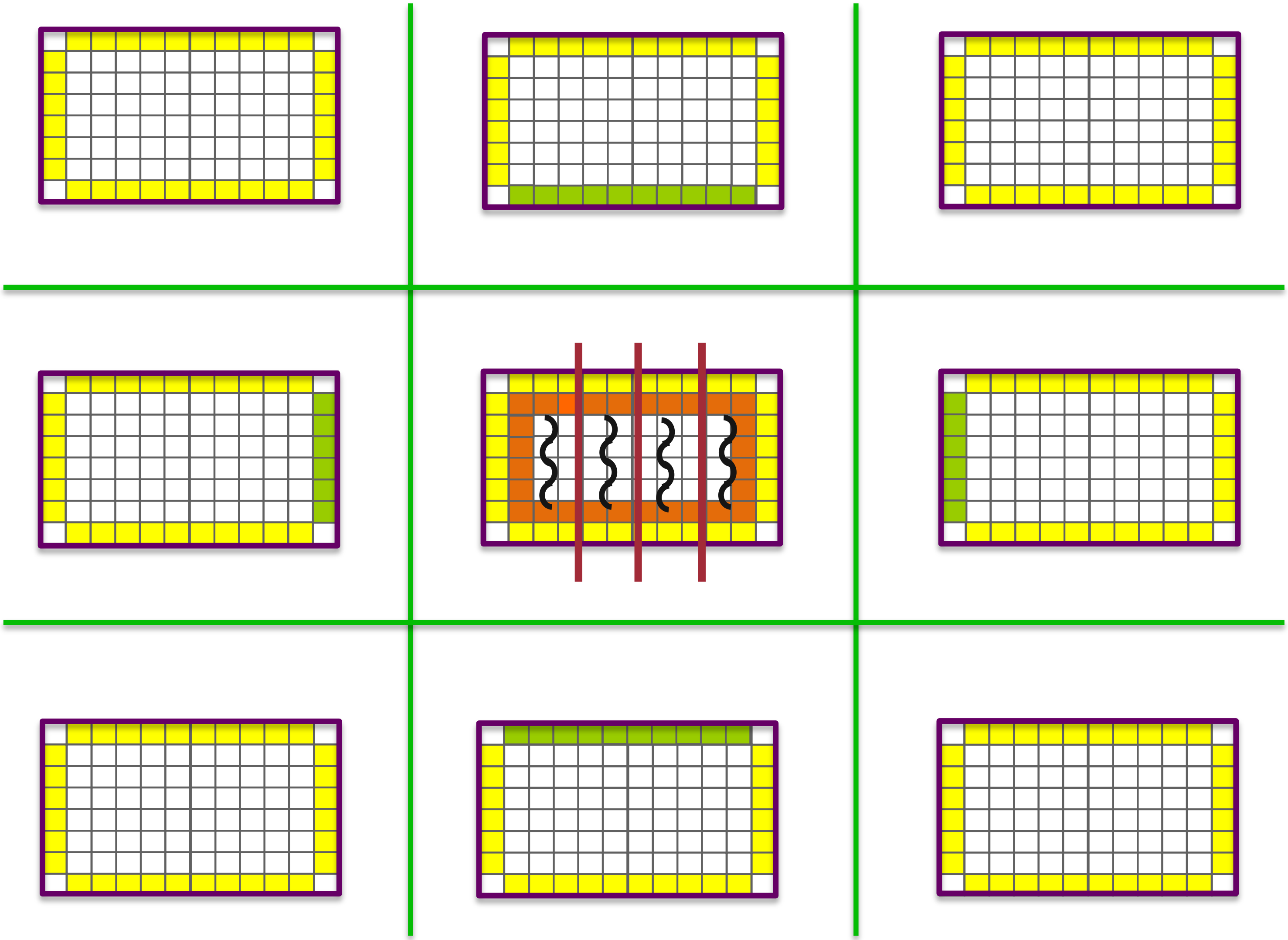
Exercise 1: Stencil in Funneled mode (1/2)



Exercise 1: Stencil in Funneled mode (2/2)

- Parallelize computation (OpenMP parallel for)
- Main thread does all communication
- *Start from derived_datatype/stencil.c*
- *Solution available in threads/stencil_funneled.c*

Exercise 2: Stencil in Multiple mode (1/2)



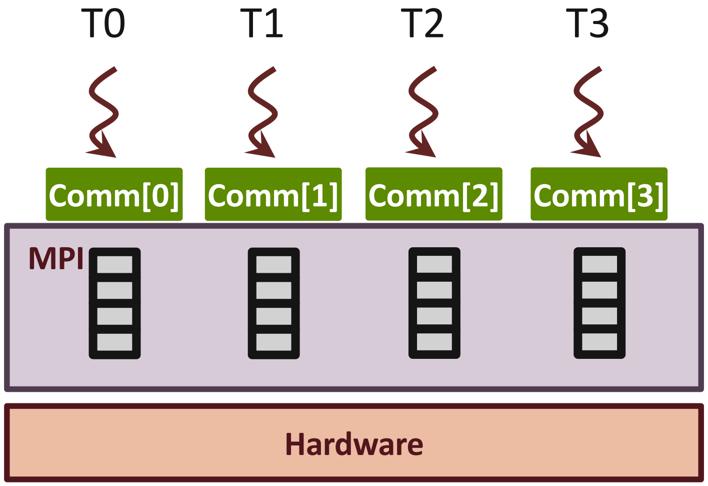
Exercise 2: Stencil in Multiple mode (2/2)

- Divide the process memory among OpenMP threads
- Each thread responsible for communication and computation
- *Start from threads/stencil_funneled.c*
- *Solution available in threads/stencil_multiple.c*

Recommendation: Maximize independence between threads with communicators

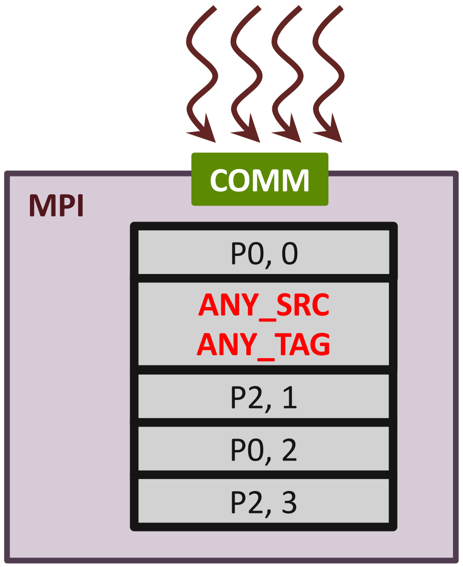
- Each thread accesses a **different communicator**
  - Each communicator may be associated with isolated resource in an MPI implementation

```
MPI_Comm *comms;
int nthreads = omp_get_num_threads();
comms = malloc(sizeof(MPI_Comm) * nthreads);

for (i = 0; i < nthreads; i++)
    MPI_Comm_dup(MPI_COMM_WORLD, &comms[i]);

#pragma omp parallel
{
   int tid = omp_get_thread_num();
   #pragma omp taskloop
   for (i = 0; i < 100; i++)
         MPI_Isend(.., comm[tid], &req[i]);}
}
MPI_Waitall(100, req, ..);
```



Recommendation: Maximize independence between threads with ranks or tags (1/2)

- Threads have to match all receive messages in sequential (e.g., a single receive-queue) if a **wildcard receive** may be posted
  - Ensure ordering of message matching
- **Let MPI know if you do not use wildcard receive**
  - Info hints **no_any_source, no_any_tag** (accepted for inclusion in MPI-4)
  - MPI can get rid of the single receive-queue for the communicator

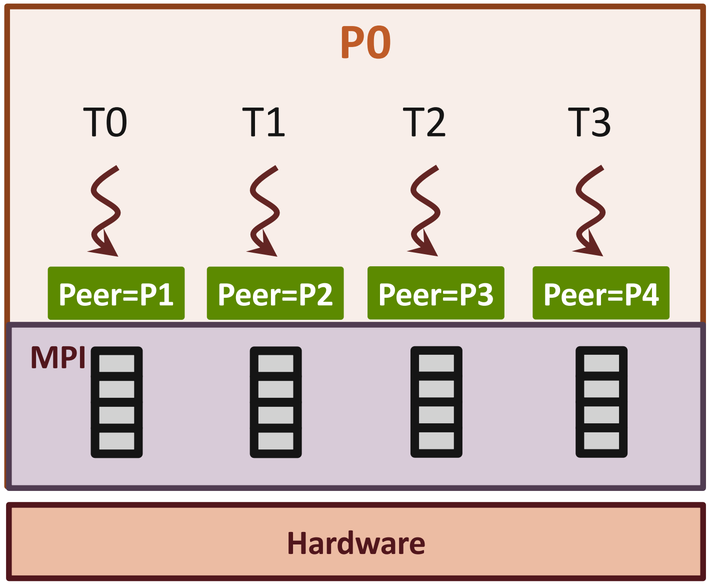


```
MPI_Info info;
info = MPI_Info_create();
MPI_Info_set(info, "no_any_source",
     "true");
MPI_Comm_set_info(comm, info);
MPI_Info_free(&info);
/* Communicate without
    MPI_ANY_SOURCE */
```

Recommendation: Maximize independence between threads with ranks or tags (2/2)

- Each thread communicates with **different peer_rank or tag**
  - MPI may assign isolated resource for different set of [peer_rank + tag]

```
#pragma omp parallel
{
   int tid = omp_get_thread_num();
   #pragma omp taskloop
   for (i = 0; i < 100; i++)
         MPI_Isend(.., peer_ranks[tid], tid,
                  comm, &req[i]);}
}
MPI_Waitall(100, req, ..);
```



Exercise 3: Stencil with Independent Communicators

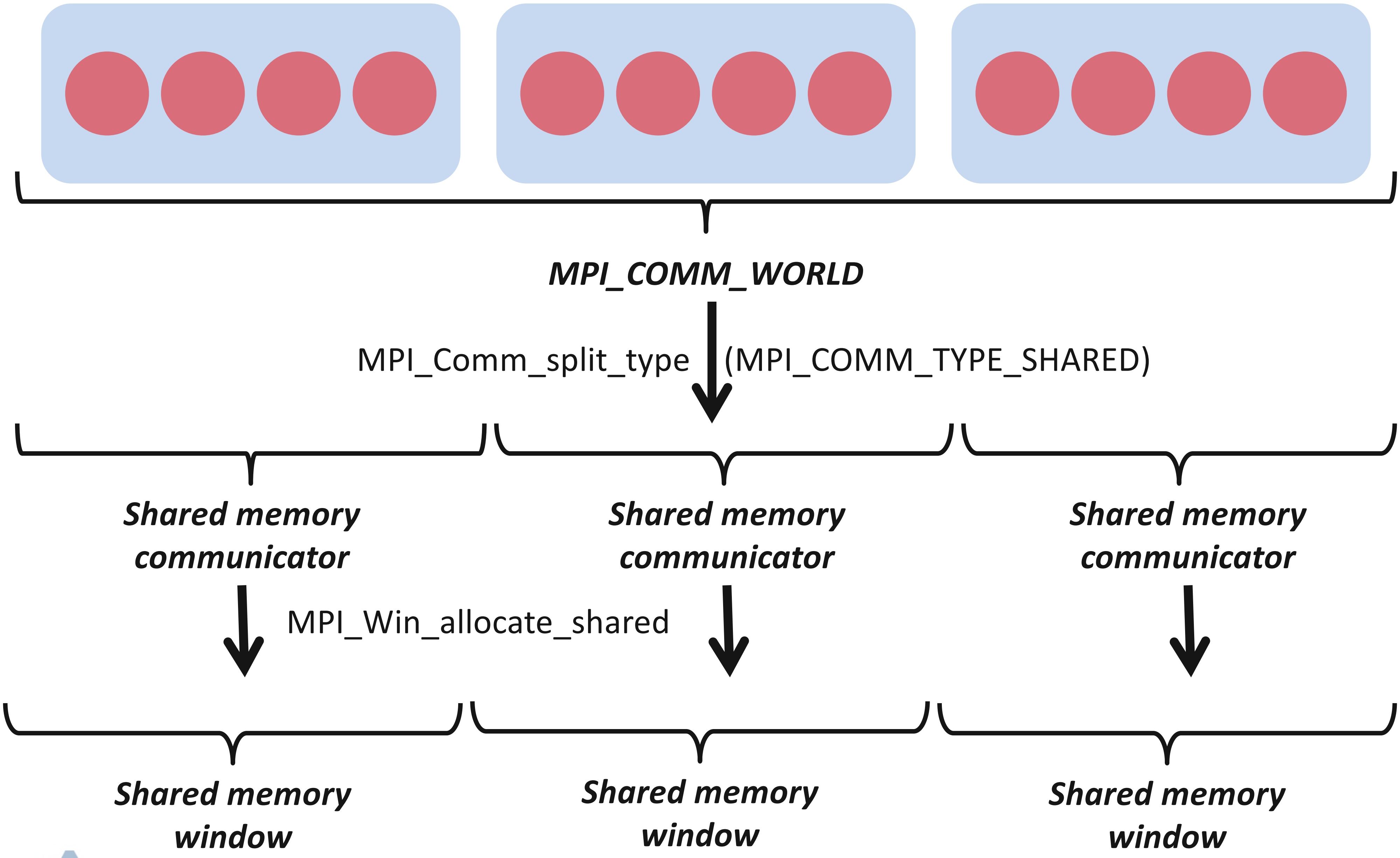
- Divide the process memory among OpenMP threads
- Each thread responsible for communication and computation
- Each thread uses a different communicator
- *Start from threads/stencil_multiple.c*
- *Solution available in threads/stencil_multiple_ncomms.c*

MPI + Shared-Memory

Hybrid Programming with Shared Memory

- MPI-3 allows different processes to allocate shared memory through MPI
  - MPI_Win_allocate_shared
- Uses many of the concepts of one-sided communication
- Applications can do hybrid programming using MPI or load/store accesses on the shared memory window
- Other MPI functions can be used to synchronize access to shared memory regions
- Can be simpler to program than threads
  - Because memory locality is clear (needed for performance) and data sharing is explicit

Creating Shared Memory Regions in MPI



MPI_COMM_WORLD

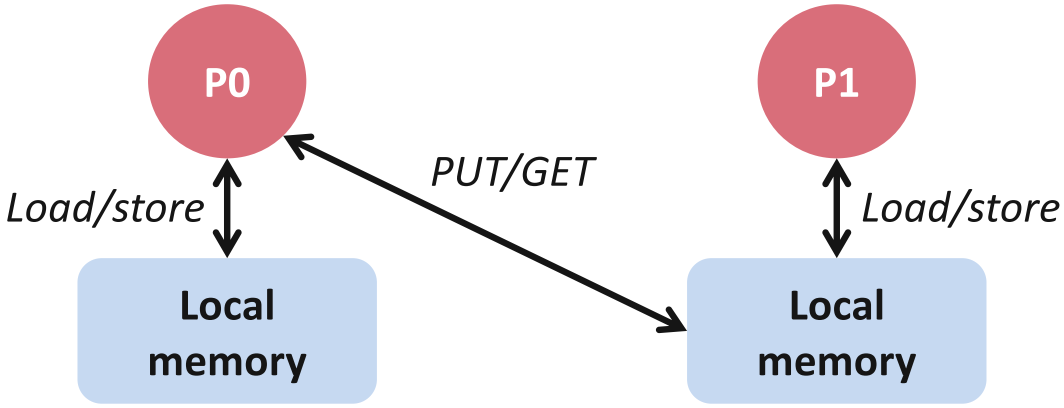
MPI_Comm_split_type (MPI_COMM_TYPE_SHARED)

Shared memory communicator ***Shared memory communicator*** ***Shared memory communicator***

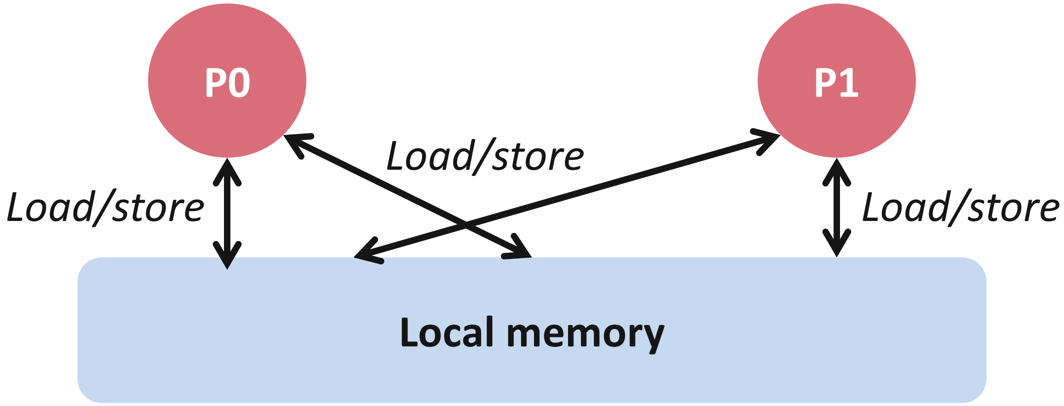
MPI_Win_allocate_shared

Shared memory window ***Shared memory window*** ***Shared memory window***

Regular RMA windows vs. Shared memory windows



Traditional RMA windows



Shared memory windows

- Shared memory windows allow application processes to directly perform load/store accesses on all of the window memory
  - E.g., x[100] = 10
- All of the existing RMA functions can also be used on such memory for more advanced semantics such as atomic operations
- Can be very useful when processes want to use threads only to get access to all of the memory on the node
  - You can create a shared memory window and put your shared data

MPI_COMM_SPLIT_TYPE

```
MPI_Comm_split_type(MPI_Comm comm, int split_type,
                    int key, MPI_Info info, MPI_Comm *newcomm)
```

- Create a communicator where processes “share a property”
  - Properties are defined by the “split_type”
  - In MPI 3.1, only split_type is MPI_COMM_TYPE_SHARED
- Arguments:
  - comm   - input communicator (handle)
  - Split_type - property of the partitioning (integer)
  - Key   - Rank assignment ordering (nonnegative integer)
  - info   - info argument (handle)
  - newcomm- output communicator (handle)

MPI_WIN_ALLOCATE_SHARED

```
MPI_Win_allocate_shared(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
  - Data exposed in a window can be accessed with RMA ops or load/store
- 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)

Shared Arrays with Shared memory windows

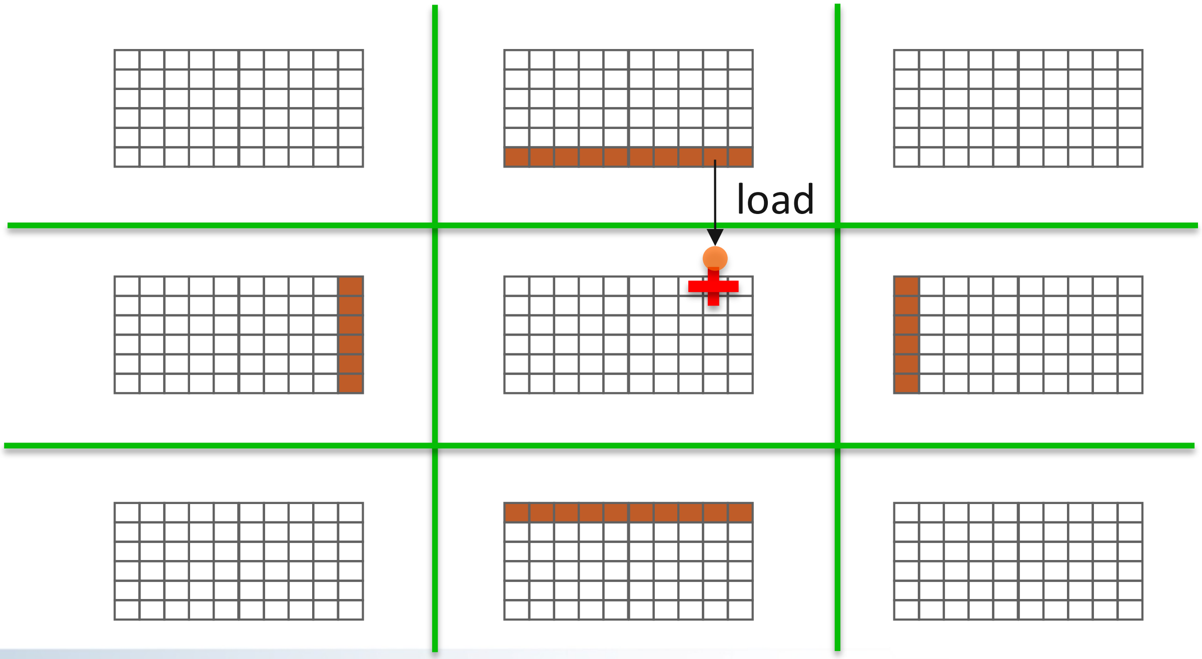
```
int main(int argc, char ** argv)
{
    int buf[100];

    MPI_Init(&argc, &argv);
    MPI_Comm_split_type(..., MPI_COMM_TYPE_SHARED, .., &comm);
    MPI_Win_allocate_shared(comm, ..., &win);

    MPI_Win_lockall(win);

    /* copy data to local part of shared memory */
    MPI_Win_sync(win);

    /* use shared memory */

    MPI_Win_unlock_all(win);

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

Memory allocation and placement

- Shared memory allocation does not need to be uniform across processes
  - Processes can allocate a different amount of memory (even zero)
- The MPI standard does not specify where the memory would be placed (e.g., which physical memory it will be pinned to)
  - Implementations can choose their own strategies, though it is expected that an implementation will try to place shared memory allocated by a process "close to it"
- The total allocated shared memory on a communicator is contiguous by default
  - Users can pass an info hint called "noncontig" that will allow the MPI implementation to align memory allocations from each process to appropriate boundaries to assist with placement

Exercise: Stencil with Shared Memory

- Message passing model requires ghost-cells to be explicitly communicated to neighbor processes
- In the shared-memory model, there is no communication. Neighbors directly access your data.
- *Start from rma/stencil_lock_put.c*
- *Solution available in shared_mem/stencil.c*



What should you use: Threads or Process Shared Memory

- It depends on the application, target machine, and MPI implementation
- When should I use process shared memory?
  - The only resource that needs sharing is memory
  - Few allocated objects need sharing (easy to place them in a public shared region)
- When should I use threads?
  - More than memory resources need sharing (e.g., TLB)
  - Many application objects require sharing
  - Application computation structure can be easily parallelized with high-level OpenMP loops

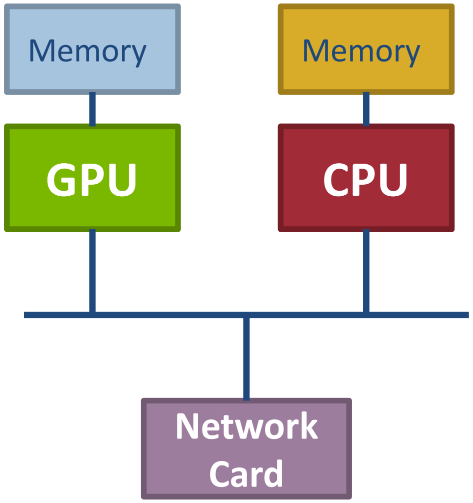
Shortcomings: Restricted Allocation Methods

- In MPI-3 shared memory, memory allocation is restrictive
  - Allocation has to be done using the MPI call
  - Cannot use the plethora of other memory allocation libraries out there, e.g., cannot allocate aligned memory (important for vectorization)
- With threads, most of those other memory allocation techniques are directly usable

MPI + Accelerators

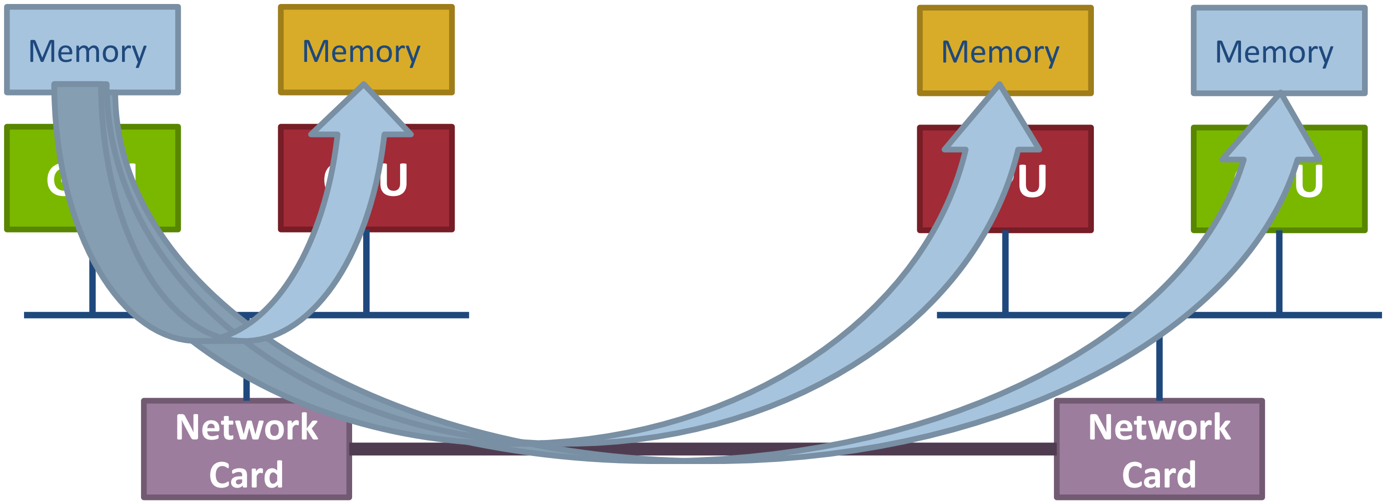
Accelerators in Parallel Computing

- General purpose, highly parallel processors
  - High FLOPs/Watt
  - Unit of execution *Kernel*
  - Separate physical memory subsystems
  - Programming Models: OpenAcc, CUDA, OpenCL, …
- Clusters with accelerators are becoming common
- New programmability and performance challenges for programming models and runtime systems



MPI + Accelerator Programming Examples

How to move data between GPUs with MPI?



Real answer: It depends on what GPU library, what hardware and what MPI implementation you are using

Simple answer: For modern GPUs, “just like you would with a non-GPU machine”

CUDA Awareness in MPI

- The MPI standard does not explicitly require GPU support
  - Each MPI implementation can choose whether or not it wants to support GPUs
- Current status: Many, but not all, MPI implementations support CUDA
  - Already supported by MVAPICH, Open MPI, Spectrum MPI
- You can use GPUs even with MPI implementations that do not support CUDA, but data movement will need to be explicit
  - MPI does not understand data residing on GPUs
- With CUDA-aware MPI implementations, some things are automatically handled by the MPI library

Non-CUDA-aware MPI implementations: Programmability Limitations (1/2)

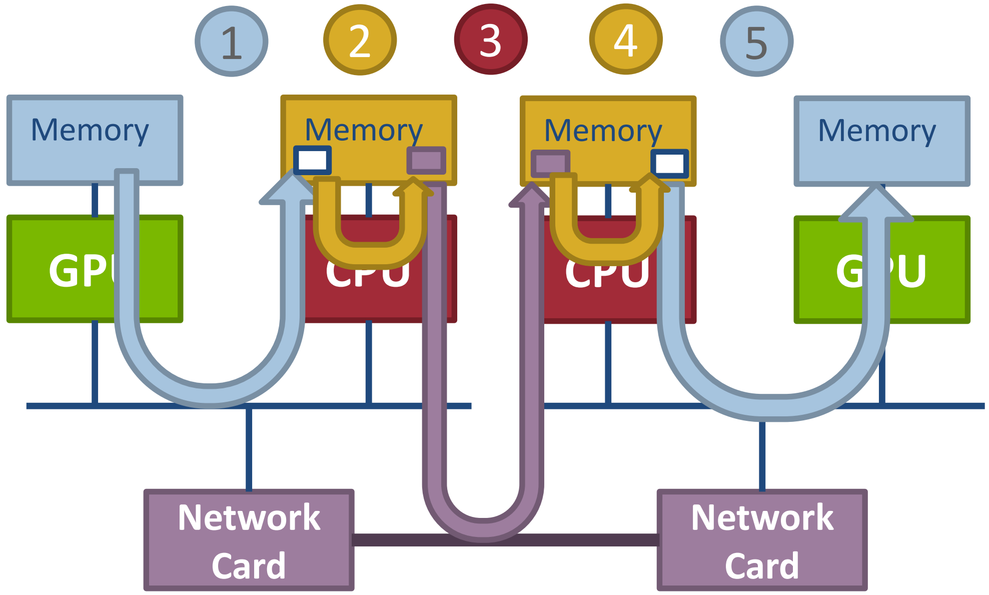
CUDA

```
double *dev_buf, *host_buf;
cudaMalloc(&dev_buf, size);
cudaMallocHost(&host_buf, size);

if(my_rank == sender) {
    computation_on_GPU(dev_buf);
    cudaMemcpy(host_buf, dev_buf, size, …);
    MPI_Isend(host_buf, size, …);
} else {
    MPI_Recv(host_buf, size, …);
    cudaMemcpy(dev_buf, host_buf, size, …);
    computation_on_GPU(dev_buf);
}
```

OpenACC

```
double *buf;
buf = (double*)malloc(size * sizeof(double));
#pragma acc enter data create(buf[0:size])

if(my_rank == sender) {
    computation_on_GPU(buf);
    #pragma acc update host (buf[0:size])
    MPI_Isend(buf, size, …);
} else {
    MPI_Recv(buf, size, …);
    #pragma acc update device (buf[0:size])
    computation_on_GPU(buf);
}
```

Non-CUDA-aware MPI implementations: Programmability Limitations (2/2)



```
computation_on_GPU(dev_buf);
cudaMemcpy(host_buf, dev_buf, size, …);
MPI_Isend(host_buf, size, …);

MPI_Recv(host_buf, size, …);
cudaMemcpy(dev_buf, host_buf, size, …);
computation_on_GPU(dev_buf);
```

CUDA

```
computation_on_GPU(buf);
#pragma acc update host (buf[0:size])
MPI_Isend(buf, size, …);

MPI_Recv(buf, size, …);
#pragma acc update device (buf[0:size])
computation_on_GPU(buf);
```

OpenACC

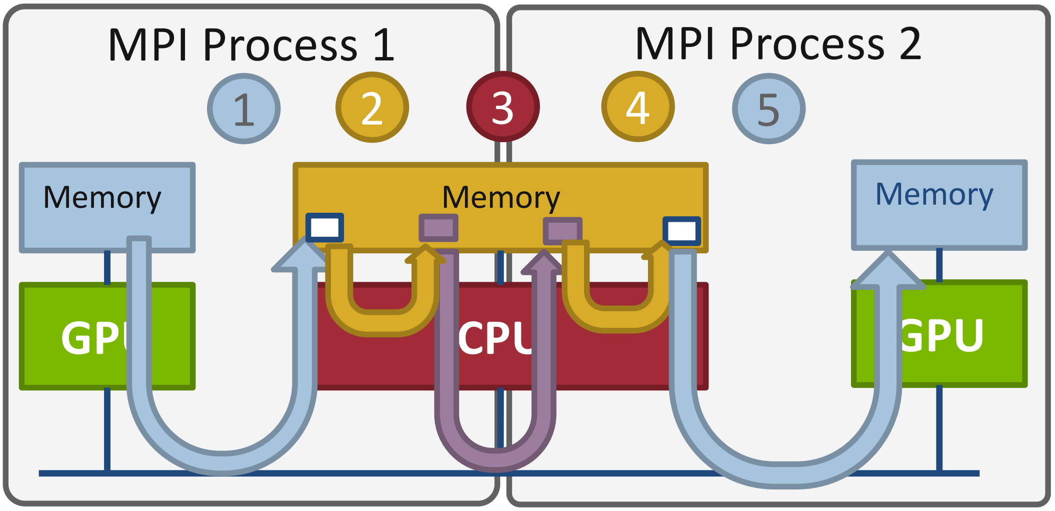
MPI assumes host memory

The user ensures that host memory is synchronized

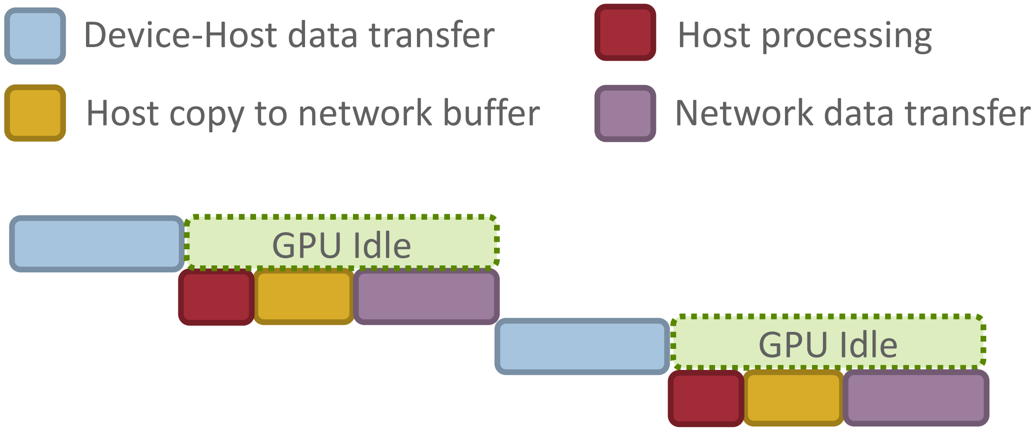
Using cudaMemcpyAsync before MPI_Isend would be incorrect

Non-CUDA-aware MPI implementations: Performance Limitations

- Inefficient intranode GPU-GPU data transfer between MPI processes
  - Several DMA and memory copies on the critical path
- Inefficient bulk-synchronous transfer model
  - The CPU cannot trigger the MPI data transfer until the GPU completed the device-host data transfer
- Inefficient GPU resource utilization
  - The GPU could potentially be idle while the host handles MPI communication



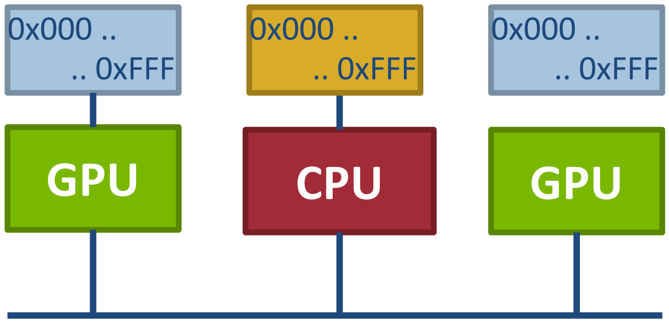
Inefficient intra-node GPU data transfer



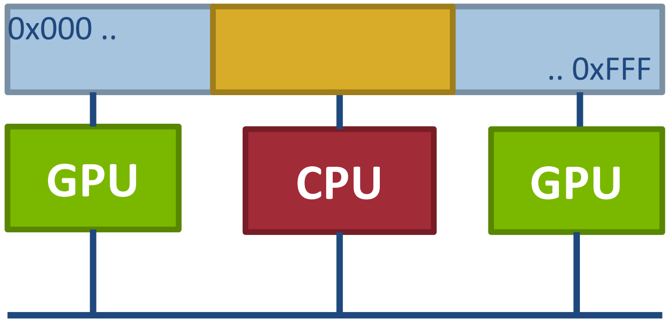
Inefficient bulk-synchronous and GPU-wasteful data transfer model

CUDA-aware MPI implementation requirements

- CUDA-awareness in MPI requires the Unified Virtual Address (UVA) feature of GPUs, at the very least
  - Introduced in CUDA-4.0
  - Host memory and all GPUs share the same virtual address space
  - The user can query the location of the data allocation given a pointer in the unified address space with **cuPointerGetAttribute()**
- GPU Direct 1.0, GPU Direct 2.0 and GPU Direct RDMA are not required for correctness, but improve performance
  - Needs to be supported by the GPU and the network
  - ***This is the state-of-the-art for modern NVIDIA GPUs and Mellanox InfiniBand, but might not be supported by other GPUs or other networks***



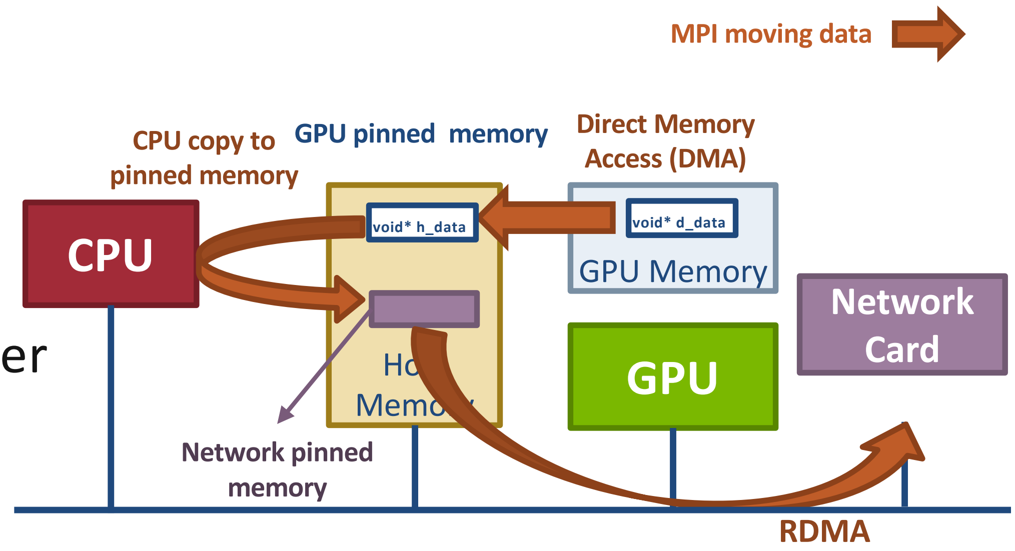
Non-UVA: Separate virtual address spaces for the host and devices



UVA: Single virtual address space for the host and all devices

CUDA-aware MPI implementations: Programmability

- User can pass device pointer to MPI
- MPI implementation can query for the owner (host or device) of the data
- If the data is on the device, **the MPI implementation can handle** data transfer from GPU to the network



Example of MPI moving data from the GPU device to the network

CUDA

```
computation_on_GPU(dev_buf);
MPI_Isend(dev_buf, size, …);


MPI_Recv(dev_buf, size, …);
computation_on_GPU(dev_buf);
```

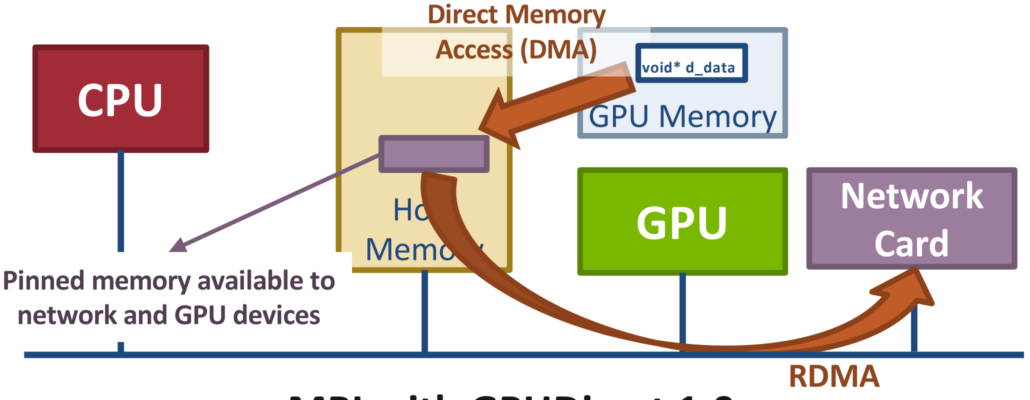
OpenACC

```
computation_on_GPU(buf);
#pragma acc host_data use_device (buf)
MPI_Isend(buf, size, …);

 #pragma acc host_data use_device (buf)
MPI_Recv(buf, size, …);
computation_on_GPU(buf);
```

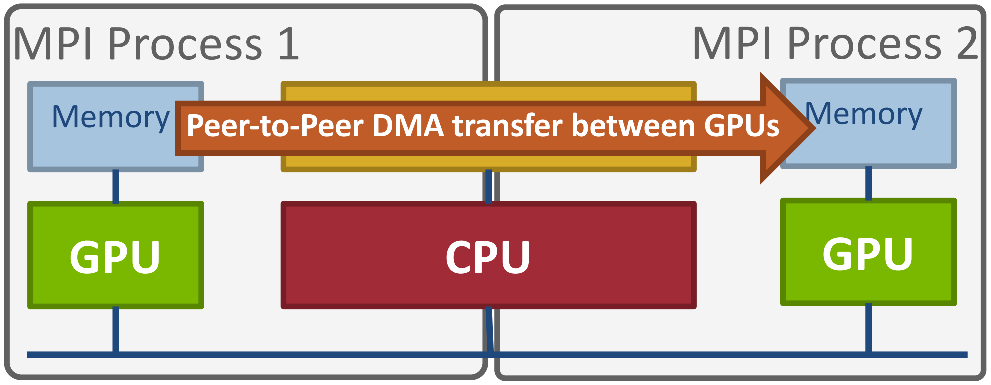
MPI can transparently figure out the physical location of the data

CUDA-aware MPI implementations: Performance (2/3)

- GPUDirect 1.0 (Q2’ 2010)
  - Avoid unnecessary system memory copies copying data directly to/from pinned CUDA host memory
  - RDMA can use directly the CUDA pinned memory
  - Required kernel driver updates
- GPUDirect 2.0 (Peer-to-Peer, 2011)
  - GPU peer-to-peer data transfers are possible
  - MPI can directly move data between GPU devices



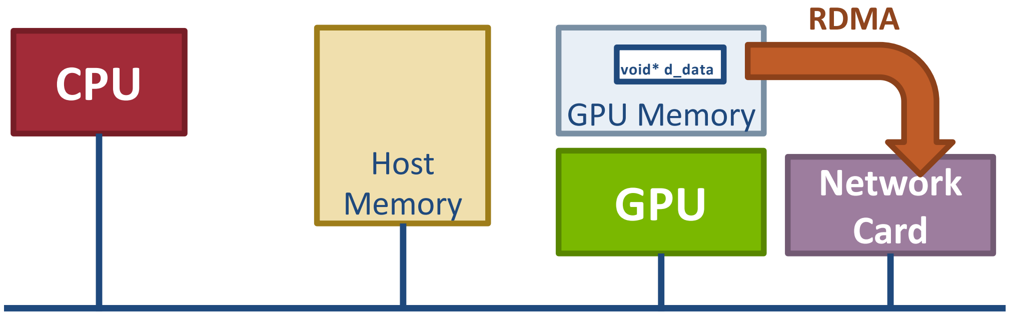
MPI with GPUDirect 1.0



MPI with GPUDirect 2.0

CUDA-aware MPI implementations: Performance (3/3)

- GPUDirect RDMA
  - CUDA >= 5, 2013
  - Technology introduced in Kepler-class GPUs and CUDA-5
  - GPU memory is directly accessible to third-party devices, including network interfaces
  - RDMA operations to/from the device memory are possible and completely bypass the host memory



MPI with GPUDirect RDMA

Section Summary

- Programming with accelerators is becoming increasingly important
- MPI is playing its role in enabling the usage of accelerators across distributed memory nodes
- The situation with MPI + GPU support is improving in both MPI implementations and in GPU hardware/software capabilities

Process Topologies and Neighborhood Collectives

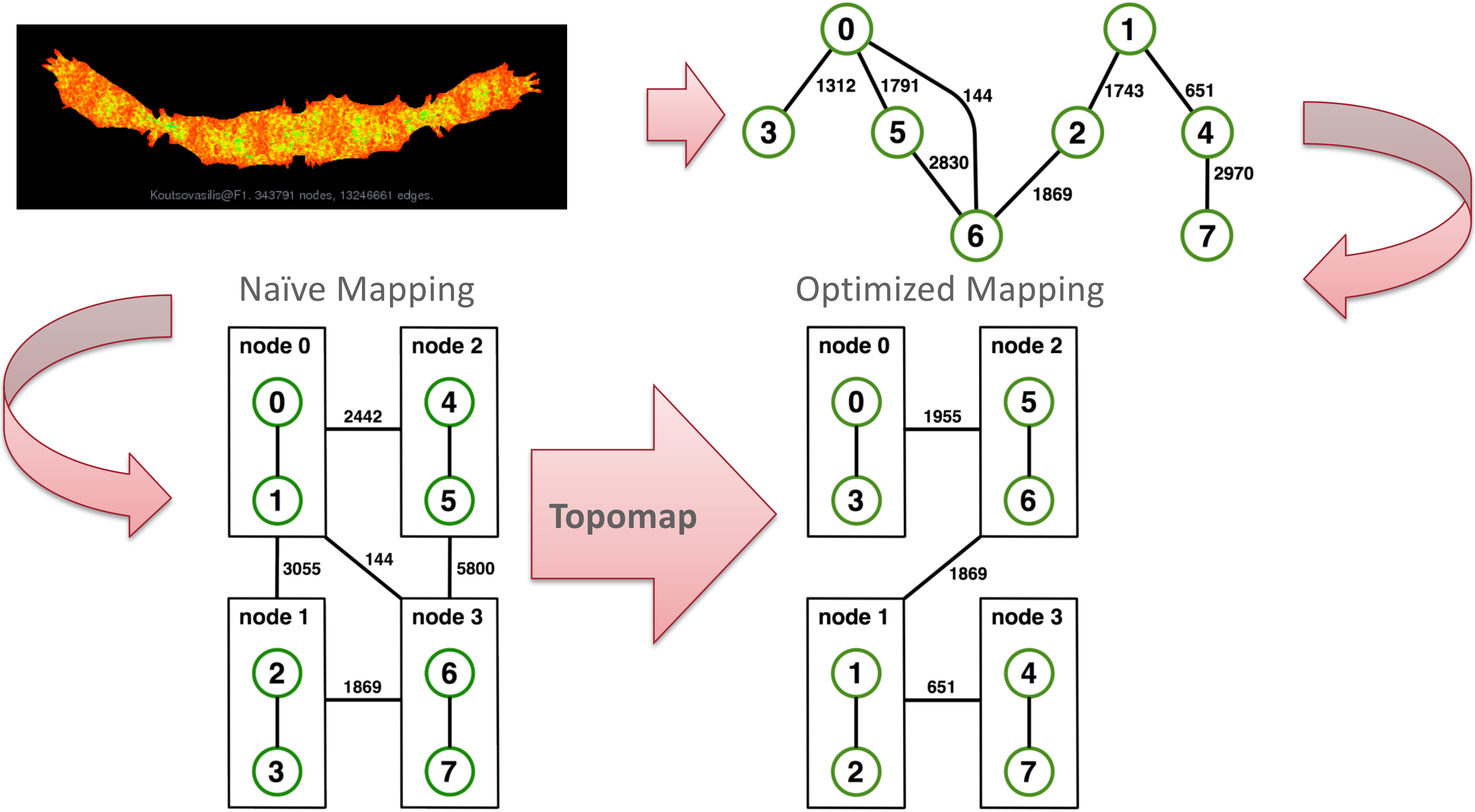
Topology Mapping Basics

- First type: Allocation mapping (when job is submitted)
  - Up-front specification of communication pattern
  - Batch system picks good set of nodes for given topology
- Properties:
  - Not widely supported by current batch systems
  - Either predefined allocation (BG/P), random allocation, or “global bandwidth maximization”
  - Also problematic to specify communication pattern upfront, not always possible (or static)

Topology Mapping Basics contd.

- Rank reordering
  - Change numbering in a given allocation to reduce congestion or dilation
  - Sometimes automatic (early IBM SP machines)
- Properties
  - Always possible, but effect may be limited (e.g., in a bad allocation)
  - Portable way: MPI process topologies
    - Network topology is not exposed
  - Manual data shuffling after remapping step

On-Node Reordering


Koutsovasilis@F1. 343791 nodes, 13246661 edges.

Naïve Mapping

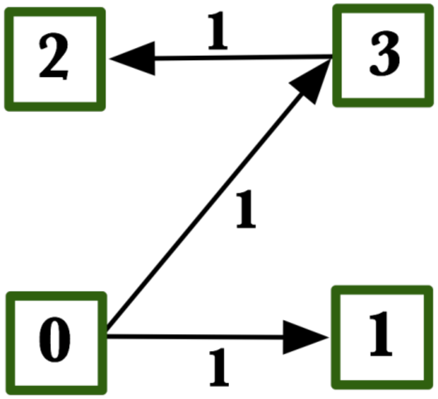
Topomap

Optimized Mapping

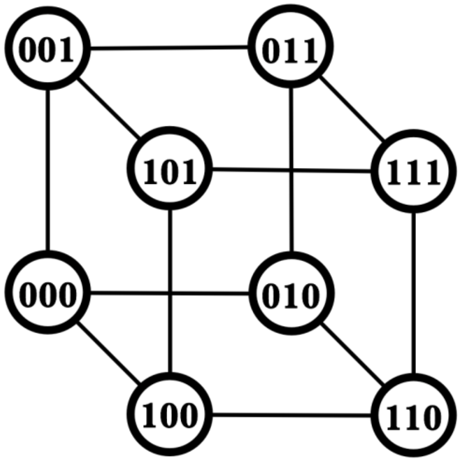
Gottschling and Hoefler: Productive Parallel Linear Algebra Programming with Unstructured Topology Adaption, 12th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing, 2012

Off-Node (Network) Reordering

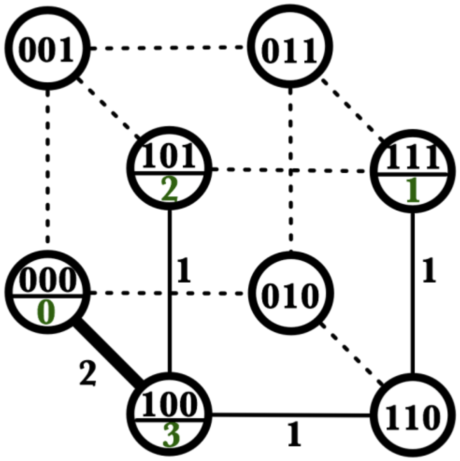
Application Topology



Network Topology

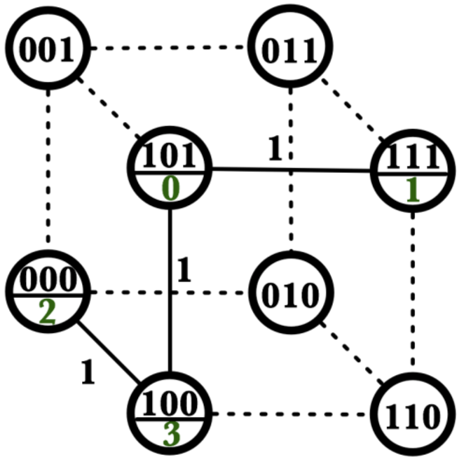


Naïve Mapping



Topomap

Optimal Mapping



MPI Topology Intro

- Convenience functions (in MPI-1)
  - Create a graph and query it, nothing else
  - Useful especially for Cartesian topologies
    - Query neighbors in n-dimensional space
  - Graph topology: each rank specifies full graph ☹
- Scalable Graph topology (MPI-2.2)
  - Graph topology: each rank specifies its neighbors **or** an arbitrary subset of the graph
- Neighborhood collectives (MPI-3.0)
  - Adding communication functions defined on graph topologies (neighborhood of distance one)

MPI Topology Realities

- Cartesian Topologies
  - MPI_Dims_create is required to provide a “square” decomposition
    - May not match underlying physical network
    - Even if it did, hard to define unless physical network is mesh or torus
  - MPI_Cart_create is supposed to provide a “good” remapping (if requested)
    - But implementations are poor and may just return the original mapping
- Graph Topologies
  - The general process mapping problem is very hard
  - Many implementations are poor
  - Some research work has developed tools to create better mappings
    - You can use them with MPI_Comm_dup to create a “well ordered” communicator
- Neighborhood collectives
  - MPI-3 introduced these; permit collective communication with just the neighbors as defined by the MPI process topology
  - Offers opportunities for the MPI implementation to optimize

MPI_Dims_create

```
MPI_Dims_create(int nnodes, int ndims, int *dims)
```

- Create dims array for Cart_create with nnodes and ndims
  - Dimensions are as close as possible (well, in theory)
- Non-zero entries in dims will not be changed
  - nnodes must be multiple of all non-zeroes in dims

MPI_Dims_create Example

```
int p;
int dims[3] = {0,0,0};
MPI_Comm_size(MPI_COMM_WORLD, &p);
MPI_Dims_create(p, 3, dims);

int periods[3] = {1,1,1};
MPI_Comm topocomm;
MPI_Cart_create(comm, 3, dims, periods, 0, &topocomm);
```

- Makes life a little bit easier
  - Some problems may be better with a non-square layout though

MPI_Cart_create

```
MPI_Cart_create(MPI_Comm comm_old, int ndims,
        const int *dims, const int *periods, int reorder,
        MPI_Comm *comm_cart)
```

- Specify ndims-dimensional topology
  - Optionally periodic in each dimension (Torus)
- Some processes may return MPI_COMM_NULL
  - Product of dims must be ≤ P
- Reorder argument allows for topology mapping
  - Each calling process may have a new rank in the created communicator
  - Data has to be remapped manually

MPI_Cart_create Example

```
int dims[3] = {5,5,5};
int periods[3] = {1,1,1};
MPI_Comm topocomm;
MPI_Cart_create(comm, 3, dims, periods, 0, &topocomm);
```

- But we’re starting MPI processes with a one-dimensional argument (-p X)
  - User has to determine size of each dimension
  - Often as “square” as possible, MPI can help!

Cartesian Query Functions

- Library support and convenience!
- MPI_Cartdim_get()
  - Gets dimensions of a Cartesian communicator
- MPI_Cart_get()
  - Gets size of dimensions
- MPI_Cart_rank()
  - Translate coordinates to rank
- MPI_Cart_coords()
  - Translate rank to coordinates

Cartesian Communication Helpers

```
MPI_Cart_shift(MPI_Comm comm, int direction, int disp,
int *rank_source, int *rank_dest)
```

- Shift in one dimension
  - Dimensions are numbered from 0 to ndims-1
  - Displacement indicates neighbor distance (-1, 1, …)
  - May return MPI_PROC_NULL
- Very convenient, all you need for nearest neighbor communication

Neighborhood Collectives

MPI_Neighbor_allgather

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

- Sends the same message to all neighbors
- Receives indegree distinct messages
- Similar to MPI_Gather
  - The all prefix expresses that each process is a “root” of his neighborhood
- Also a vector “v” version for full flexibility

MPI_Neighbor_alltoall

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

- Sends outdegree distinct messages
- Received indegree distinct messages
- Similar to MPI_Alltoall
  - Neighborhood specifies full communication relationship
- Vector and w versions for full flexibility

Nonblocking Neighborhood Collectives

```
MPI_Ineighbor_allgather(…, MPI_Request *req);
MPI_Ineighbor_alltoall(…, MPI_Request *req);
```

- Very similar to nonblocking collectives
- Collective invocation
- Matching in-order (no tags)
  - No wild tricks with neighborhoods! In order matching per communicator!

Section Summary

- MPI does not expose information about the network topology (would be very complex)
- Topology functions allow users to specify application communication patterns/topology
  - Convenience functions (e.g., Cartesian)
  - Storing neighborhood relations (Graph)
- Neighborhood collectives allow user virtual topologies to be exploited in collective communication

Concluding Remarks

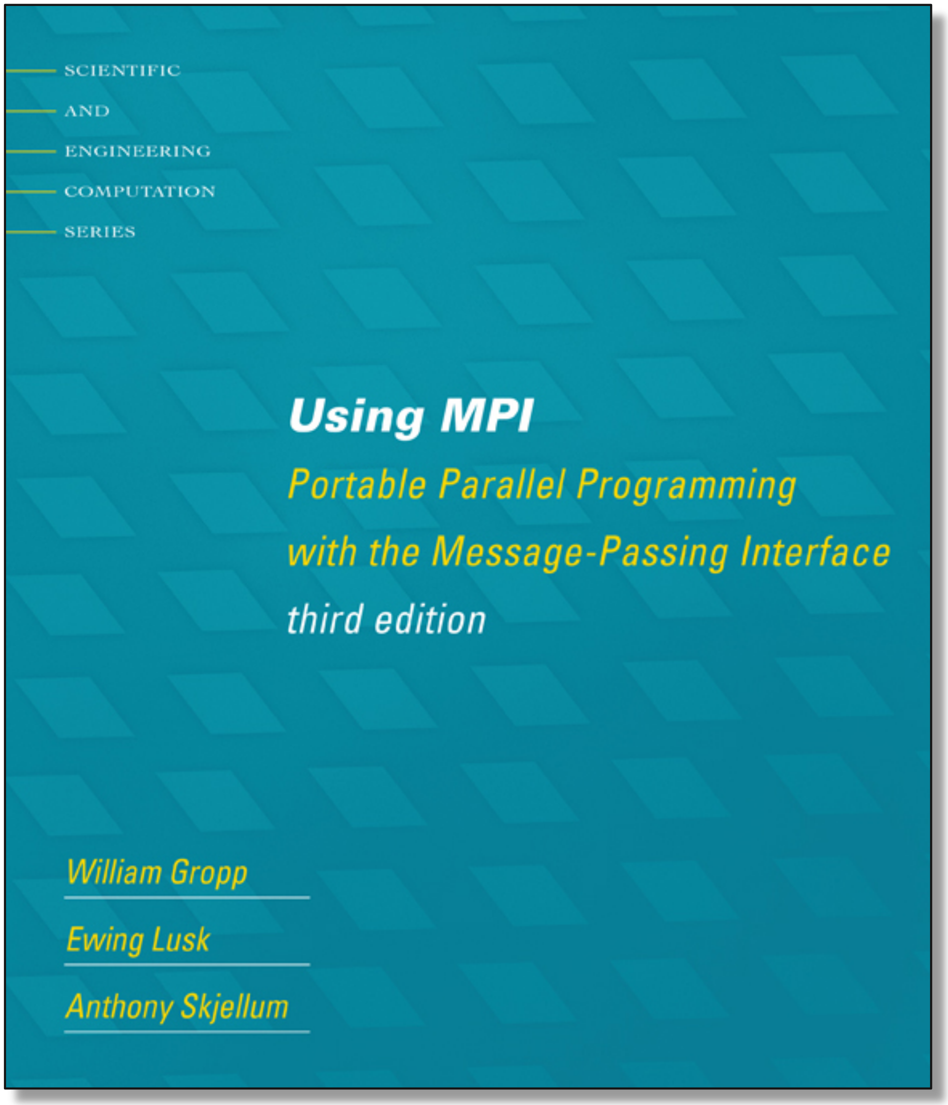
- Parallelism is critical today, given that that is the only way to achieve performance improvement with the modern hardware
- MPI is an industry standard model for parallel programming
  - A large number of implementations of MPI exist (both commercial and public domain)
  - Virtually every system in the world supports MPI
- Gives user explicit control on data management
- Widely used by many scientific applications with great success

Web Pointers

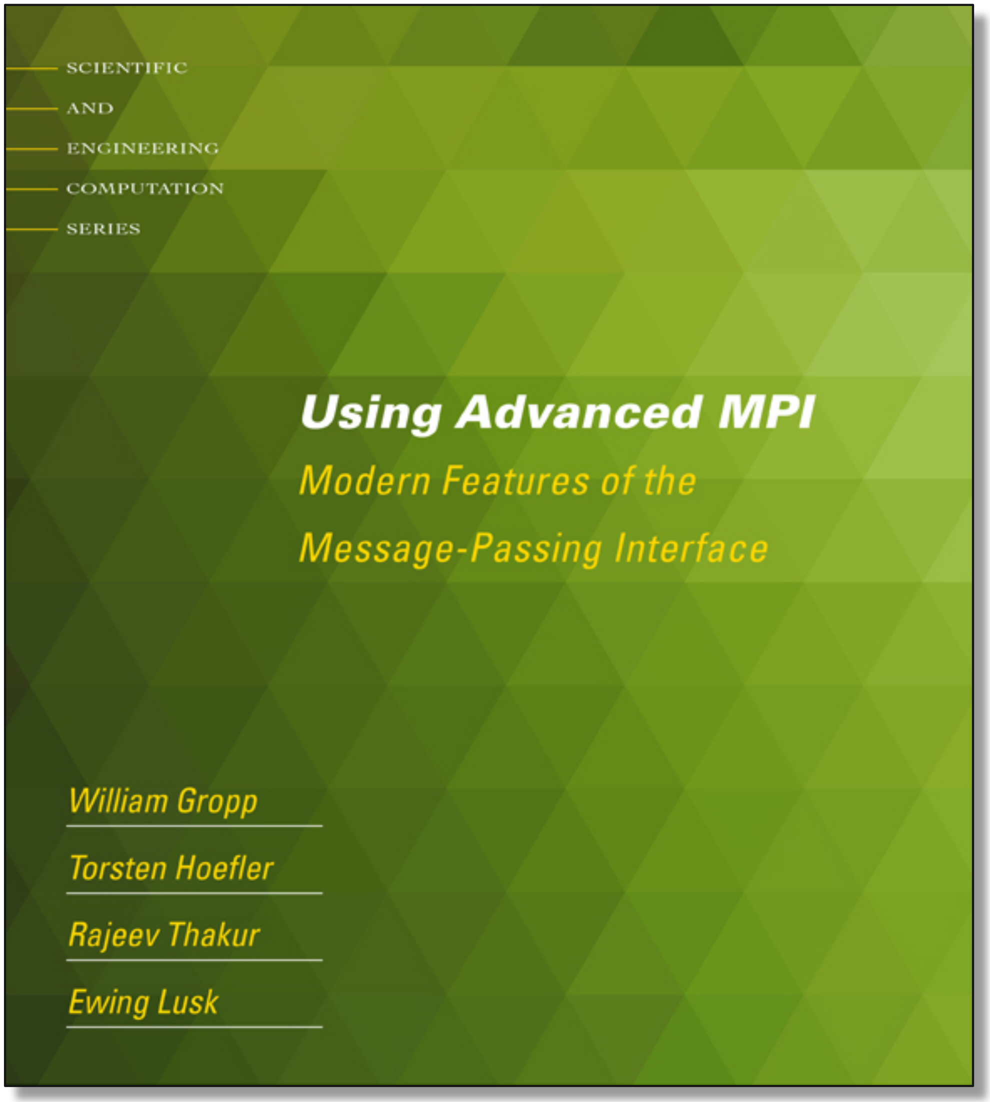
- MPI standard : http://www.mpi-forum.org/docs/docs.html
- MPI Forum : http://www.mpi-forum.org/

- MPI implementations:
  - MPICH : http://www.mpich.org
  - MVAPICH : http://mvapich.cse.ohio-state.edu/
  - Intel MPI: http://software.intel.com/en-us/intel-mpi-library/
  - Microsoft MPI: www.microsoft.com/en-us/download/details.aspx?id=39961
  - Open MPI : http://www.open-mpi.org/
  - IBM MPI, Cray MPI, HP MPI, TH MPI, NEC MPI, Fujitsu MPI, …
- Several MPI tutorials can be found on the web

Tutorial Books on MPI



Basic MPI



Advanced MPI, including MPI-3