Advanced MPI Programming

Tutorial at SC16, November 2016

Latest slides and code examples are available at

www.mcs.anl.gov/~thakur/sc16-mpi-tutorial

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About the Speakers

- **Pavan Balaji**: Computer Scientist, Mathematics and Computer Science Division, Argonne National Laboratory
- **William Gropp**: Professor, University of Illinois, Urbana-Champaign; Acting Director, NCSA
- **Torsten Hoefler**: Assistant Professor, ETH Zurich
- **Rajeev Thakur**: Senior Computer Scientist, Argonne National Laboratory

- All four of us are deeply involved in MPI standardization (in the MPI Forum) and in MPI implementation

Outline

Morning

- Introduction
  - MPI-1, MPI-2, MPI-3
- Running example: 2D stencil code
  - Simple point-to-point version
- Derived datatypes
  - Use in 2D stencil code
- One-sided communication
  - Basics and new features in MPI-3
  - Use in 2D stencil code
  - Advanced topics
    - Global address space communication

Afternoon

- MPI and Threads
  - Thread safety specification in MPI
  - How it enables hybrid programming
  - Hybrid (MPI + shared memory) version of 2D stencil code
- Nonblocking collectives
  - Parallel FFT example
- Process topologies
  - 2D stencil example
- Neighborhood collectives
  - 2D stencil example
- Recent efforts of the MPI Forum
- Conclusions

MPI-1

- MPI is a message-passing library interface standard.
  - Specification, not implementation
  - Library, not a language
- MPI-1 supports the classical message-passing programming model: basic point-to-point communication, collectives, datatypes, etc
- 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)

MPI-2

- Same process of definition by MPI Forum
- MPI-2 is an extension of MPI
  - Extends the message-passing model
    - Parallel I/O
    - Remote memory operations (one-sided)
    - Dynamic process management
  - Adds other functionality
    - C++ and Fortran 90 bindings
      - similar to original C and Fortran-77 bindings
    - External interfaces
    - Language interoperability
    - MPI interaction with threads

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, …
- ---- Stable 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
- MPI-3.1 (2015)
  - Minor updates and fixes to MPI 3.0

Overview of New Features in MPI-3

- Major new features
  - Nonblocking collectives
  - Neighborhood collectives
  - Improved one-sided communication interface
  - Tools interface
  - Fortran 2008 bindings
- Other new features
  - Matching Probe and Recv for thread-safe probe and receive
  - Noncollective communicator creation function
  - “const” correct C bindings
  - Comm_split_type function
  - Nonblocking Comm_dup
  - Type_create_hindexed_block function
- C++ bindings removed
- Previously deprecated functions removed
- MPI 3.1 added nonblocking collective I/O functions

Status of MPI-3.1 Implementations

	MPICH	MVAPICH	Open MPI	Cray	Tianhe	Intel	IBM				SGI	Fujitsu	MS	MPC	NEC	Sunway	RIKEN
							BG/Q [1]	PE [2]	Spectrum	Platform							
NBC	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Nbr. Coll.	✓	✓	✓	✓	✓	✓	✓	✓	✓	✘	✓	✓	✘	✓	✓	✓	✓
RMA	✓	✓	✓	✓	✓	✓	✓	✓	✓	✘	✓	✓	✘	Q2’17	✓	✓	✓
Shr. mem	✓	✓	✓	✓	✓	✓	✓	✓	✓	✘	✓	✓	✓	*	✓	✓	✓
MPI_T	✓	✓	✓	✓	✓	✓	✓	✓	✓	✘	✓	✓	*	Q1’17	✓	✓	✓
Comm-create group	✓	✓	✓	✓	✓	✓	✓	✓	✓	✘	✓	✓	✘	*	✓	✓	✓
F08 Bindings	✓	✓	✓	✓	✓	✓	✓	✘	✓	✘	✓	✘	✘	Q1’17	✓	✓	✓
New Dtypes	✓	✓	✓	✓	✓	✓	✓	✓	✓	✘	✓	✓	✓	✓	✓	✓	✓
Large Counts	✓	✓	✓	✓	✓	✓	✓	✓	✓	✘	✓	✓	✓	Q1’17	✓	✓	✓
MProbe	✓	✓	✓	✓	✓	✓	✓	✓	✓	✘	✓	✓	✓	Q1’17	✓	✓	✓
NBC I/O	✓	Q4’16	✓	✓	✘	✓	✘	✘	✓	✘	✓	✘	✘	Q1’17	✓	✘	✓

Release dates are estimates and are subject to change at any time.

“✘” indicates no publicly announced plan to implement/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

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

New Tutorial Books on MPI

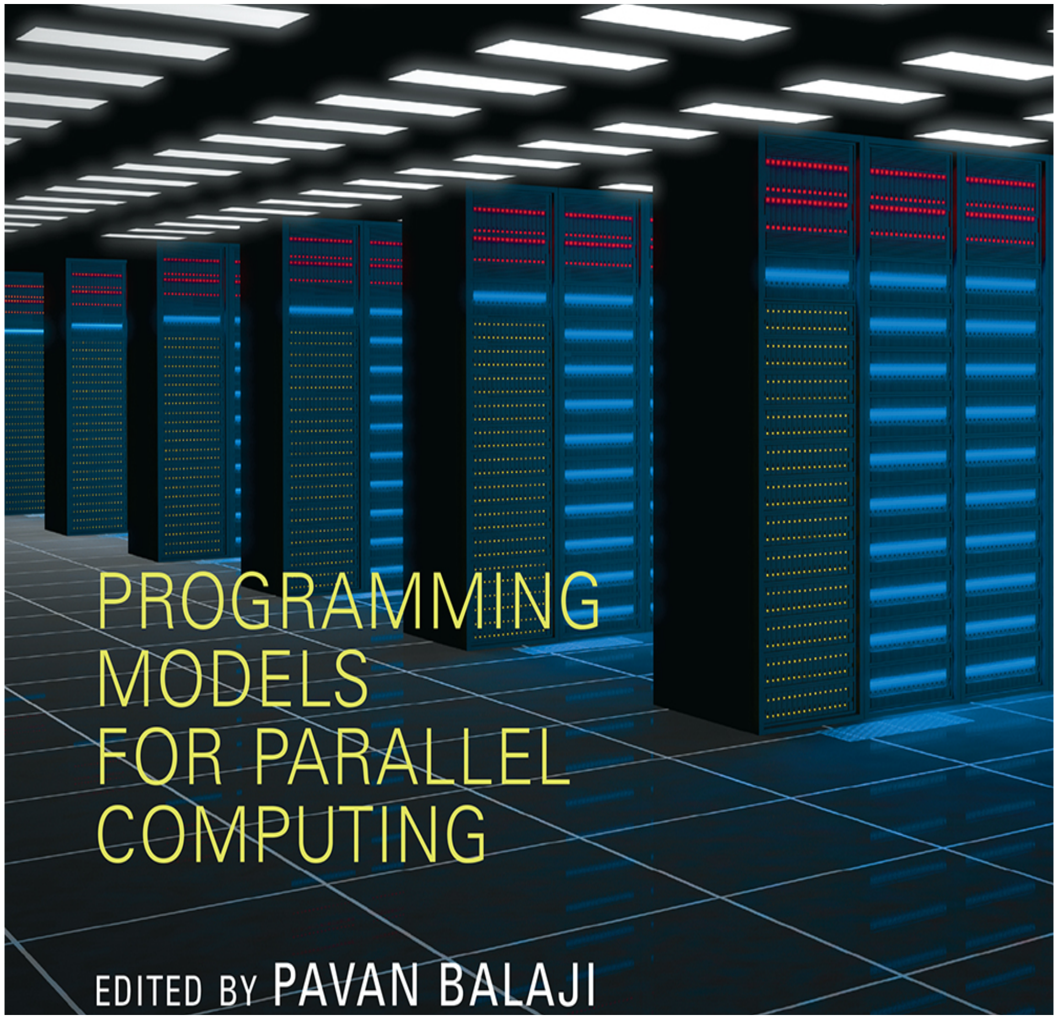
- For basic MPI
  - ***Using MPI, 3rd edition, 2014***, by William Gropp, Ewing Lusk, and Anthony Skjellum
  - https://mitpress.mit.edu/using-MPI-3ed

- For advanced MPI, including MPI-3
  - ***Using Advanced MPI, 2014,*** by William Gropp, Torsten Hoefler, Rajeev Thakur, and Ewing Lusk
  - https://mitpress.mit.edu/using-advanced-MPI

New Book on Parallel Programming Models

Edited by Pavan Balaji

- ***MPI:*** W. Gropp and R. Thakur
- ***GASNet:*** P. Hargrove
- ***OpenSHMEM:*** J. Kuehn and S. Poole
- ***UPC:*** K. Yelick and Y. Zheng
- ***Global Arrays:*** S. Krishnamoorthy, J. Daily, A. Vishnu, and B. Palmer
- ***Chapel:*** B. Chamberlain
- ***Charm++:*** L. Kale, N. Jain, and J. Lifflander
- ***ADLB:*** E. Lusk, R. Butler, and S. Pieper
- ***Scioto:*** J. Dinan
- ***SWIFT:*** T. Armstrong, J. M. Wozniak, M. Wilde, and I. Foster
- ***CnC:*** K. Knobe, M. Burke, and F. Schlimbach
- ***OpenMP:*** B. Chapman, D. Eachempati, and S. Chandrasekaran
- ***Cilk Plus:*** A. Robison and C. Leiserson
- ***Intel TBB:*** A. Kukanov
- ***CUDA:*** W. Hwu and D. Kirk
- ***OpenCL:*** T. Mattson



https://mitpress.mit.edu/models

Our Approach in this Tutorial

- Example driven
  - 2D stencil code used as a running example throughout the tutorial
  - Other examples used to illustrate specific features
- We will walk through actual code
- We assume familiarity with basic concepts of MPI-1

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 difference equations depends on the particular method
  - From the point of view of parallel programming for these algorithms, the operations are the same

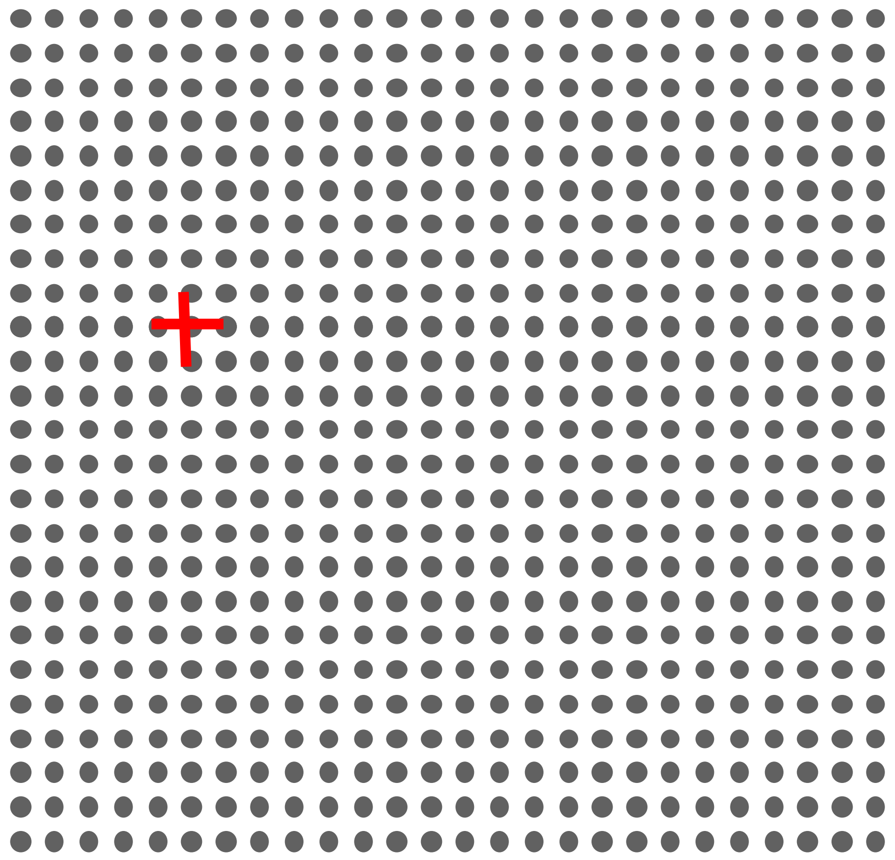
Poisson Problem

- To approximate the solution of the Poisson Problem $\nabla^2 u = f$ on the unit square, with u defined on the boundaries of the domain (Dirichlet boundary conditions), this simple 2nd order difference scheme is often used:
  - $(U(x+h,y) - 2U(x,y) + U(x-h,y)) / h^2 +$
    $(U(x,y+h) - 2U(x,y) + U(x,y-h)) / h^2 = f(x,y)$
    - Where the solution U is approximated on a discrete grid of points x=0, h, 2h, 3h, … , (1/h)h=1, y=0, h, 2h, 3h, … 1.
    - To simplify the notation, U(ih,jh) is denoted U_{ij}

- This is defined on a discrete mesh of points (x,y) = (ih,jh), for a mesh spacing “h”

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.



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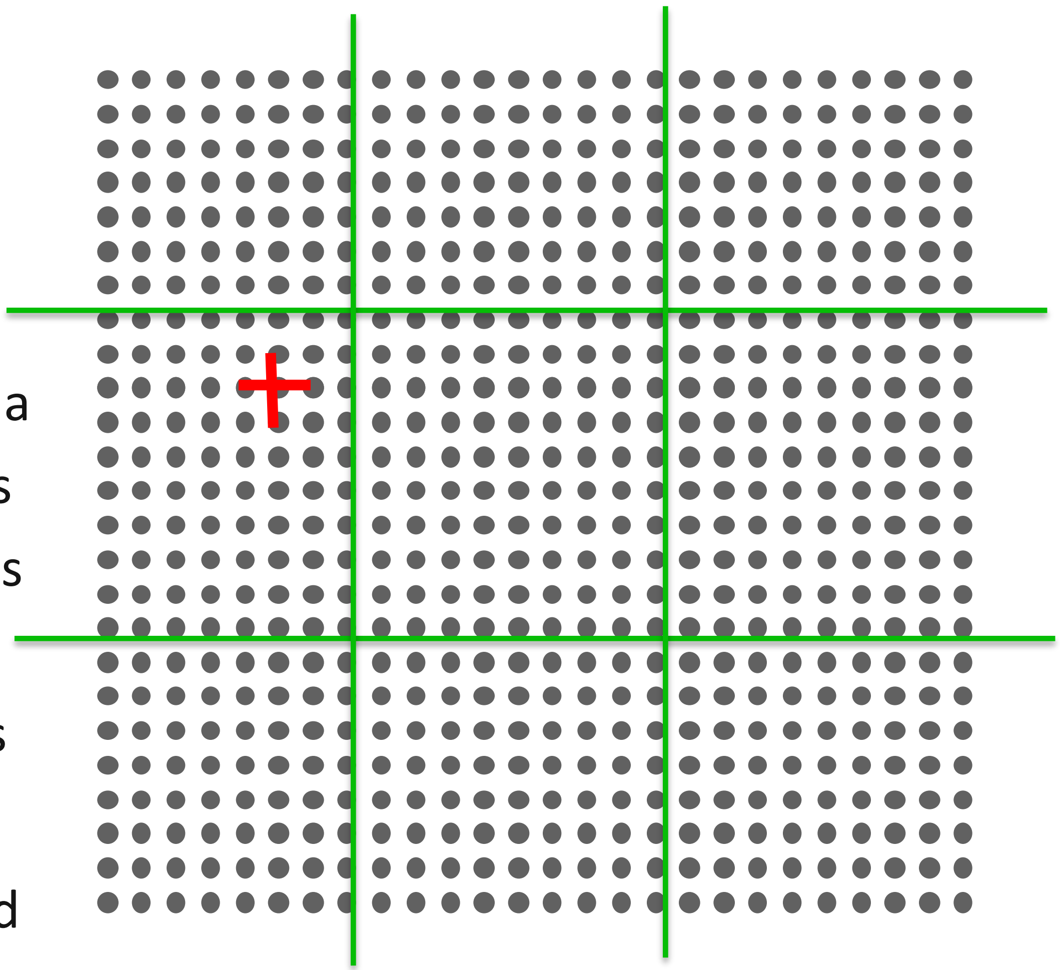
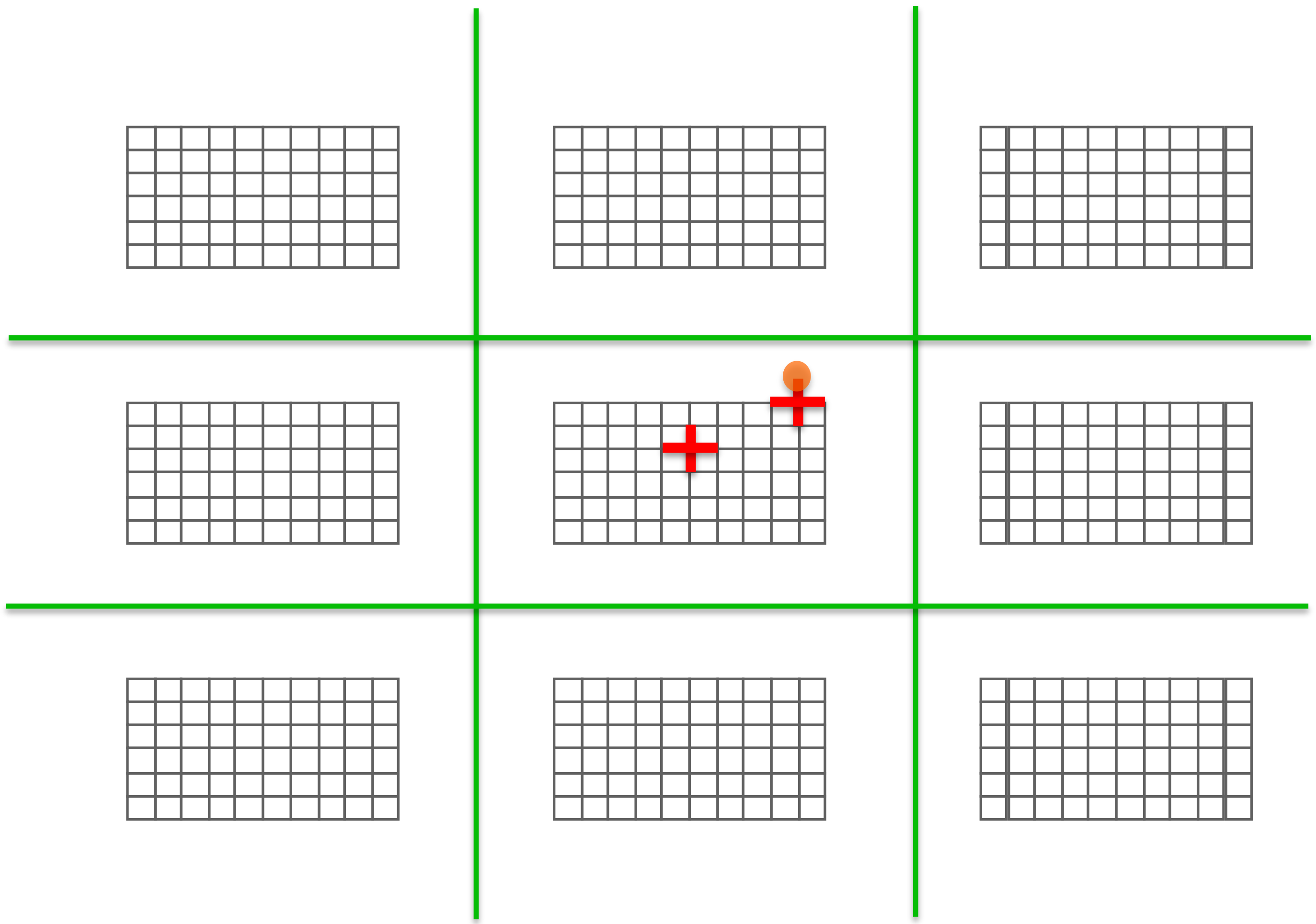
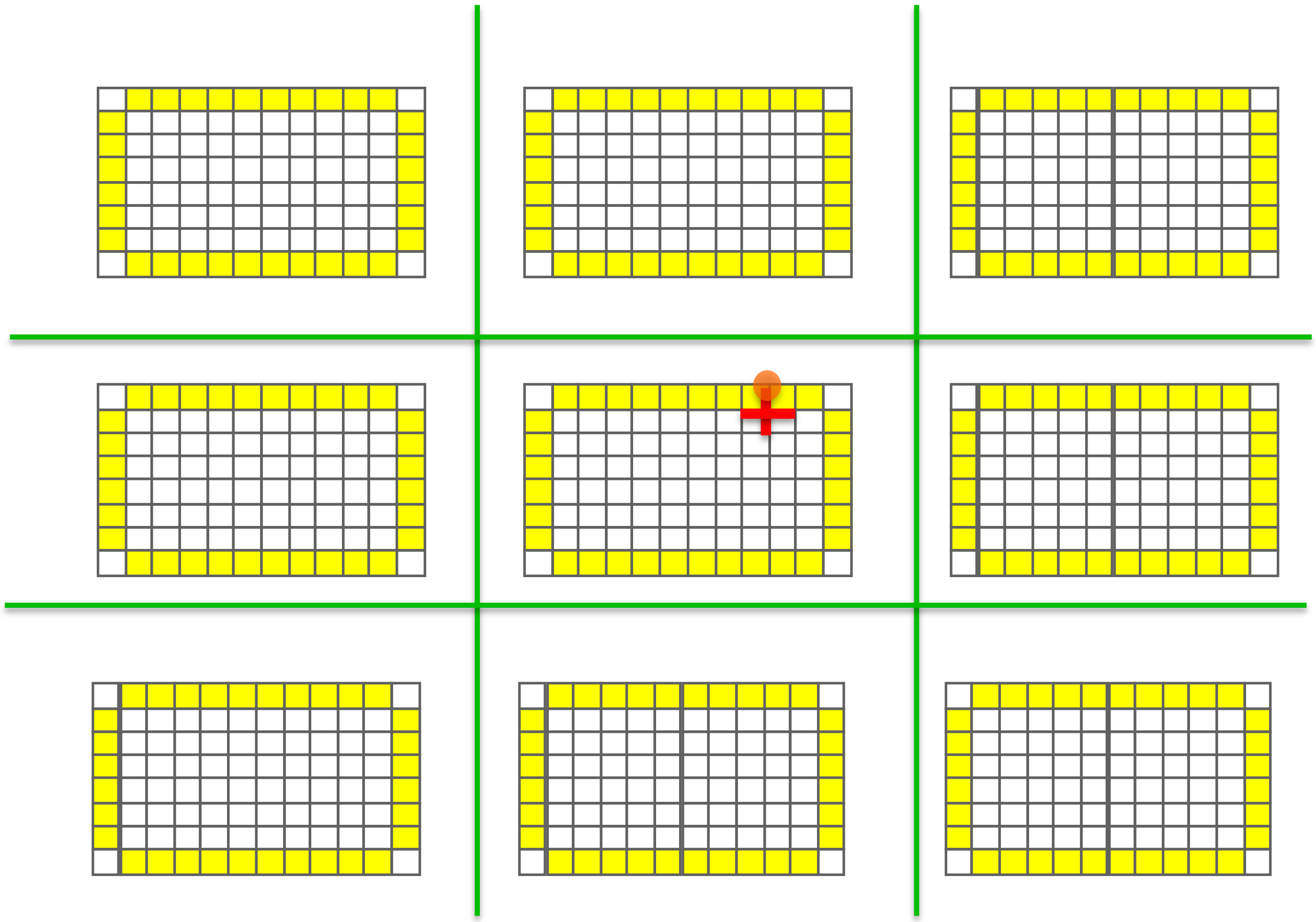
- Good numerical algorithms form a matrix equation Au=f; solving this requires computing Bv, where B is a matrix derived from A. These evaluations involve computations with the neighbors on the mesh.
- Decompose mesh into equal sized (work) pieces



Necessary Data Transfers

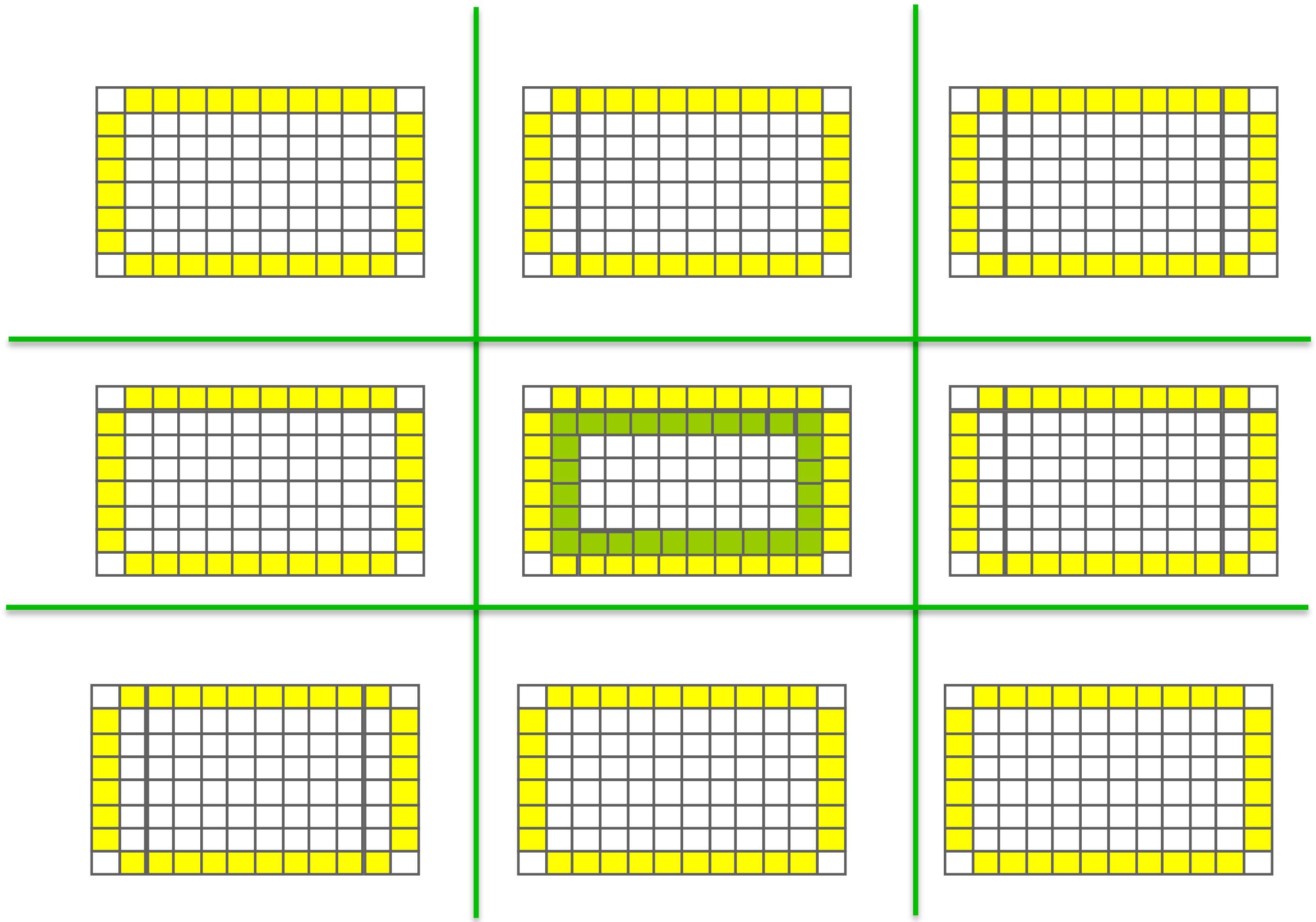


Necessary Data Transfers



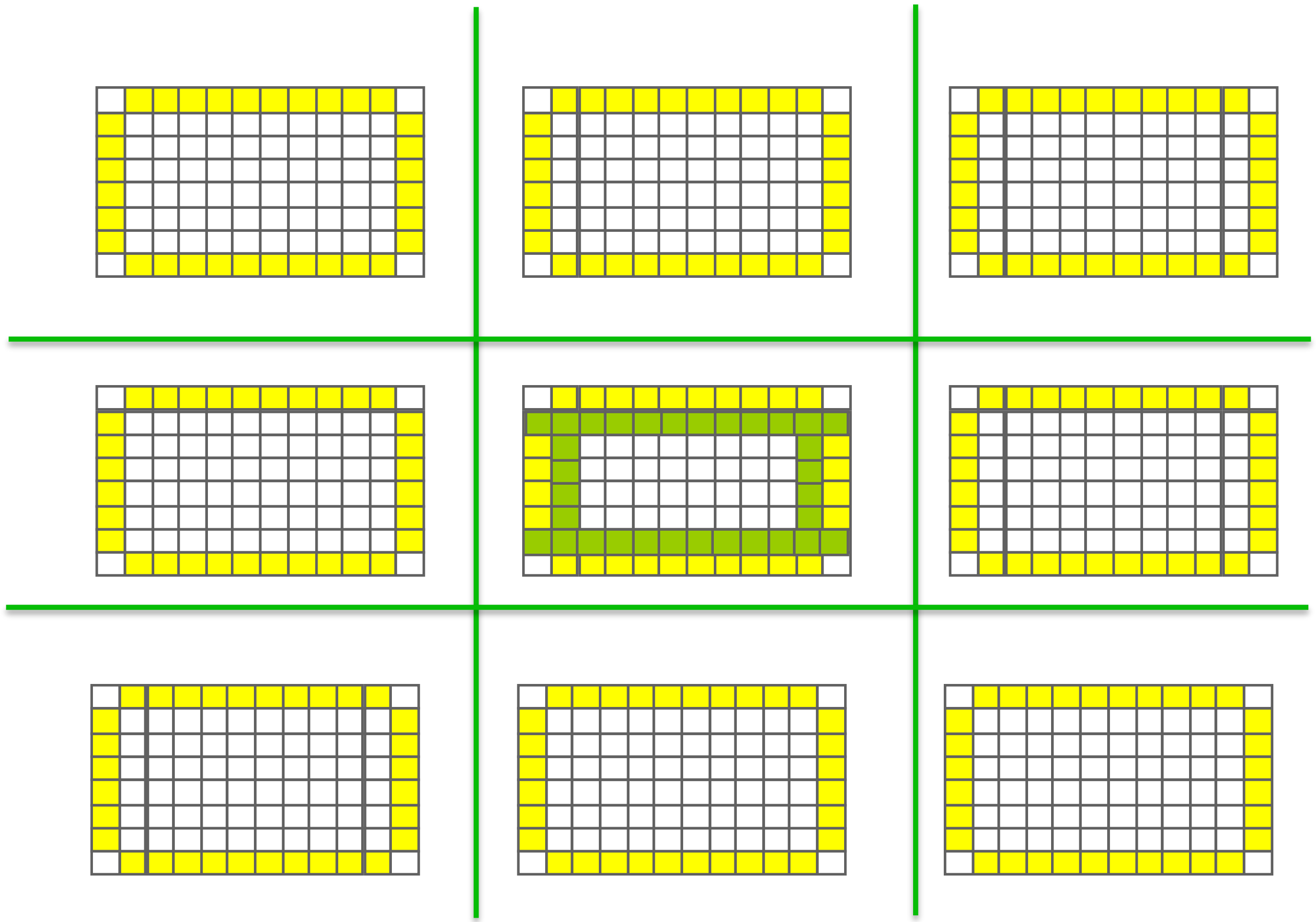
Necessary Data Transfers

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



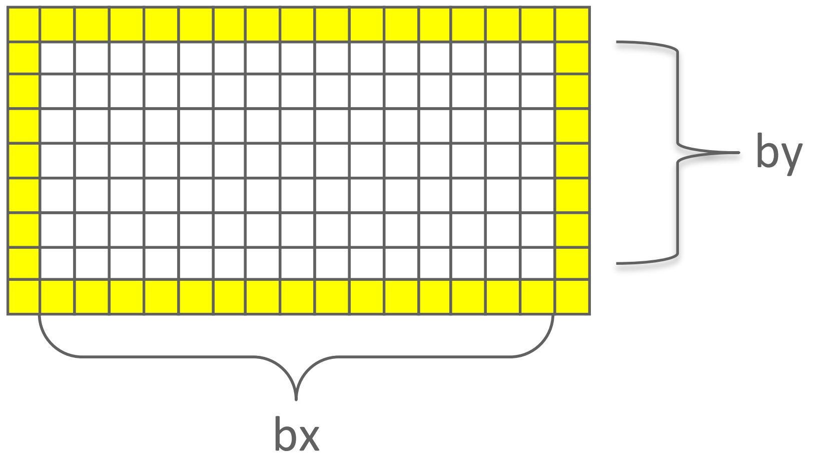
Necessary Data Transfers

- Provide access to remote data through a *halo* exchange (9 point with trick)



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)



2D Stencil Code Walkthrough

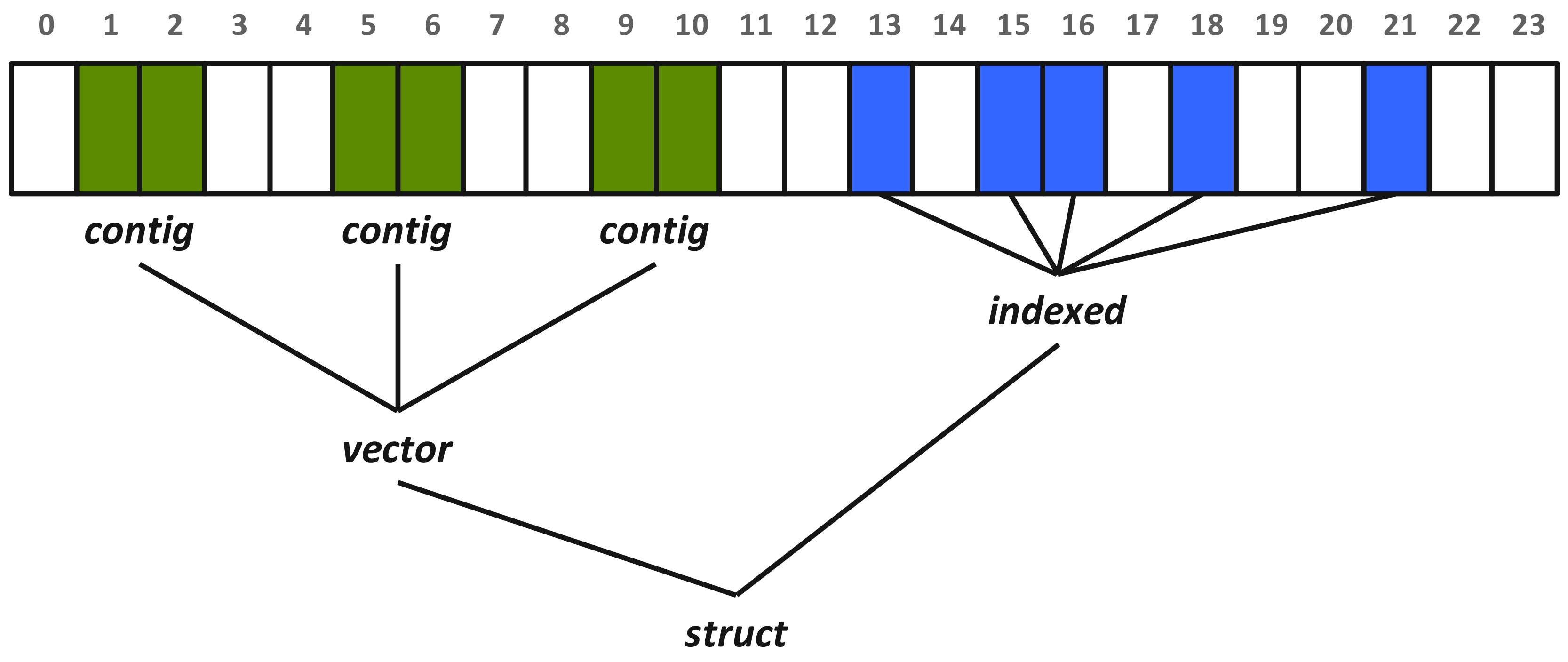
- Code can be downloaded from `www.mcs.anl.gov/~thakur/sc16-mpi-tutorial`

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



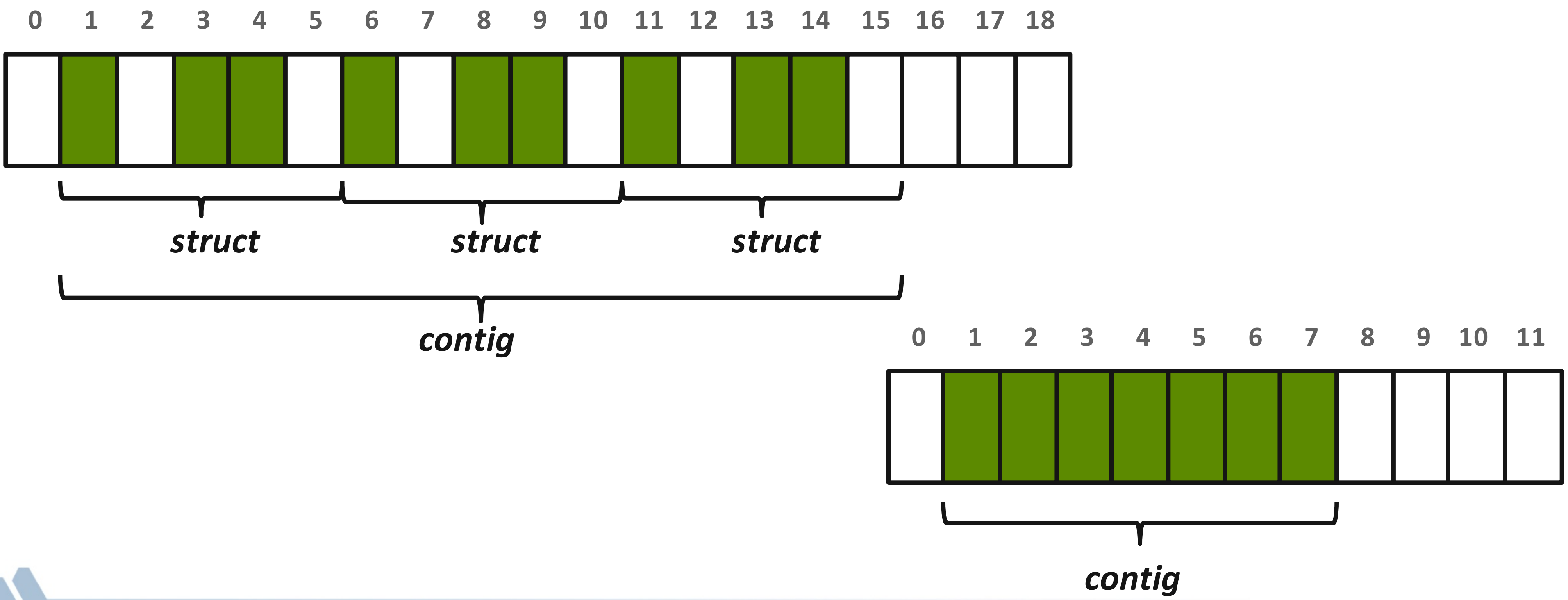
MPI's Intrinsic Datatypes

- 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-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)
```

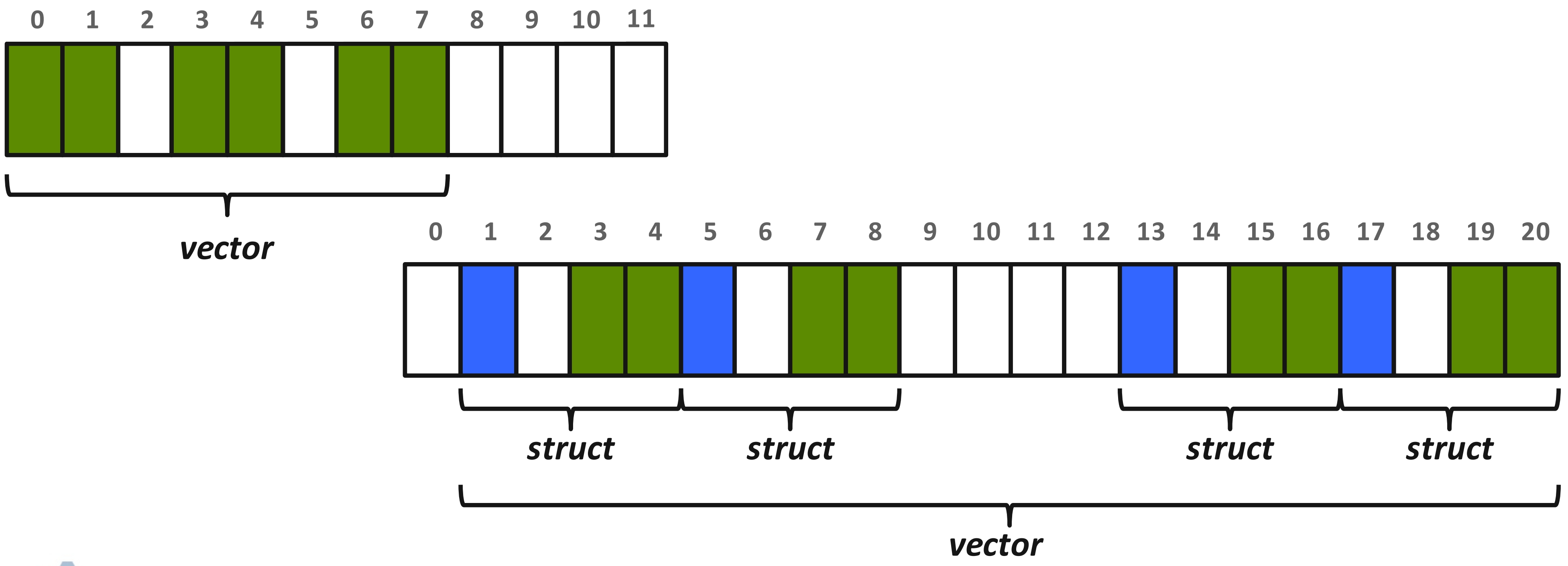
- Contiguous array of oldtype
- Should not be used as last type (can be replaced by count)



MPI_Type_vector

```
MPI_Type_vector(int count, int blocklen, int stride,
        MPI_Datatype oldtype, MPI_Datatype *newtype)
```

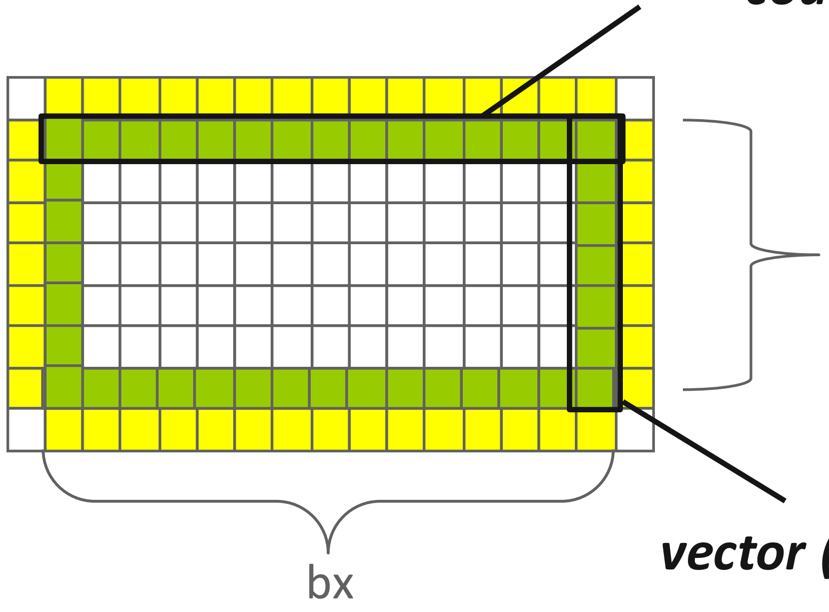
- Specify strided blocks of data of oldtype
- Very useful for Cartesian arrays



Use Datatype in Halo Exchange

contig (count=bx, MPI_DOUBLE, …) or

count with MPI_DOUBLE



vector (count=by, blocklen=1, stride=bx+2, MPI_DOUBLE, …)

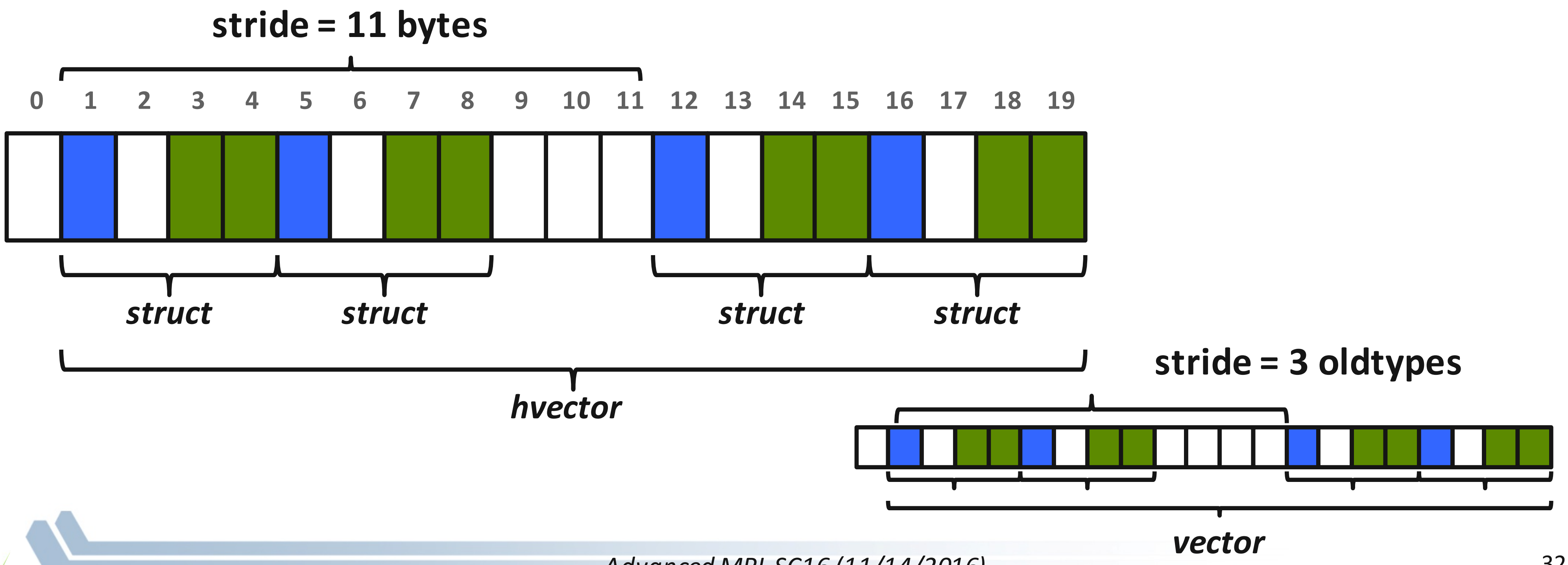
2D Stencil Code with Datatypes Walkthrough

- Code can be downloaded from
  `www.mcs.anl.gov/~thakur/sc16-mpi-tutorial`

MPI_Type_create_hvector

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

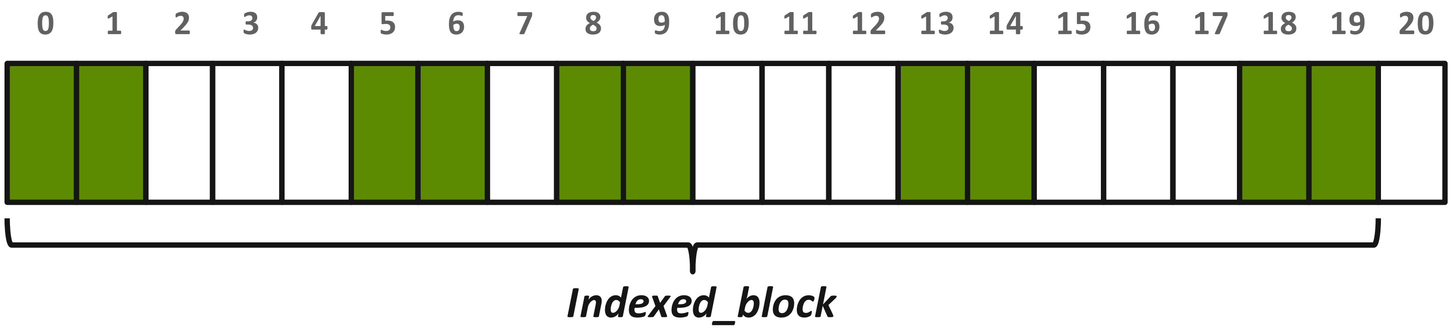
- Stride is specified in bytes instead of size of oldtype
- Useful for composition, e.g., vector of structs



MPI_Type_create_indexed_block

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

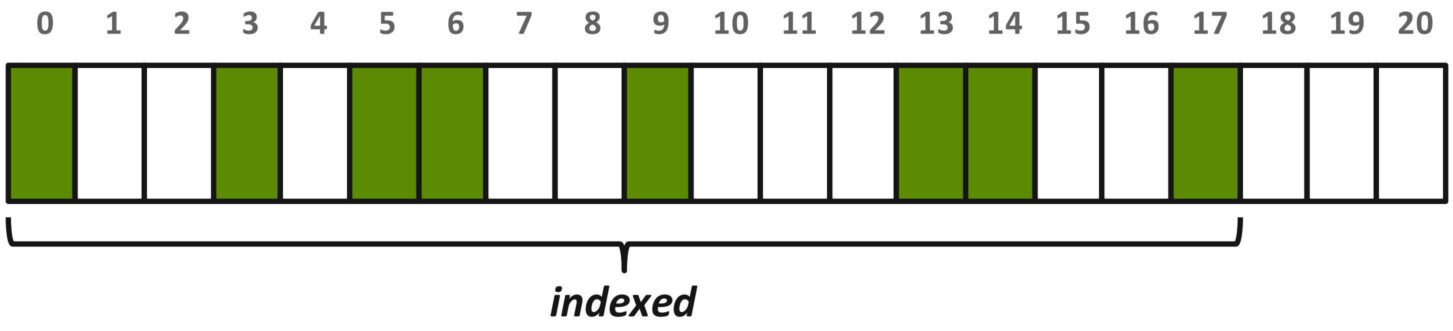
- Pulling irregular subsets of data from a single array
  - dynamic codes with index lists, expensive though!
  - blen=2
  - displs={0,5,8,13,18}



MPI_Type_indexed

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

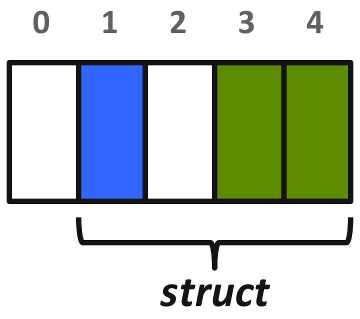
- Like indexed_block, but can have different block lengths
  - blen={1,1,2,1,2,1}
  - displs={0,3,5,9,13,17}



MPI_Type_create_struct

```
MPI_Type_create_struct(int  count,
          int *array_of_blocklens,
          MPI_Aint *array_of_displacements,
          MPI_Datatype *array_of_types,
          MPI_Datatype *newtype)
```

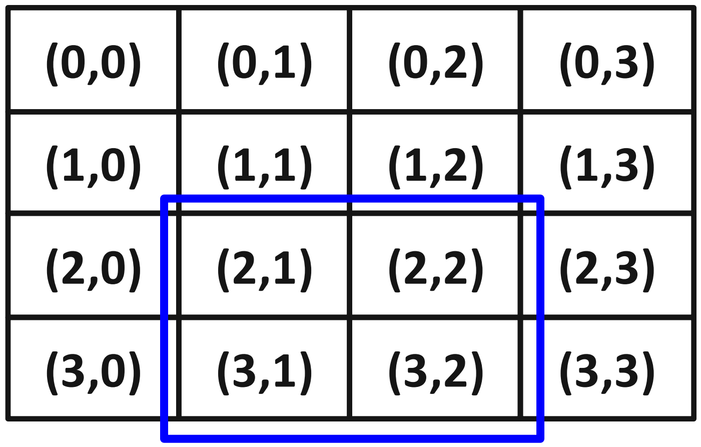
- Most general constructor, allows different types and arbitrary arrays (also most costly)



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)
```

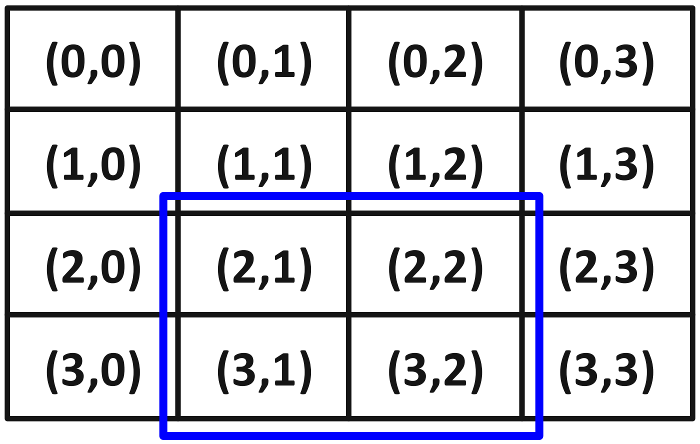
- Convenience function for creating datatypes for array segments
- Specify subarray of n-dimensional array (sizes) by start (starts) and size (subsize)



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



MPI_BOTTOM and MPI_Get_address

- MPI_BOTTOM is the absolute zero address
  - Portability (e.g., may be non-zero in globally shared memory)
- MPI_Get_address
  - Returns address relative to MPI_BOTTOM
  - Portability (do not use "&" operator in C!)
- Very important to
  - build struct datatypes
  - If data spans multiple arrays

```
int a = 4;
float b = 9.6;
MPI_Datatype struct;

MPI_Get_address(&a, &disps[0]);
MPI_Get_address(&b, &disps[1]);

MPI_Type_create_struct(count,
              blocklens[], disps,
              oldtypes[], &struct);
```

Commit, Free, and Dup

- Types must be committed before use
  - Only the ones that are used!
  - MPI_Type_commit may perform heavy optimizations (and will hopefully)
- MPI_Type_free
  - Free MPI resources of datatypes
  - Does not affect types built from it
- MPI_Type_dup
  - Duplicates a type
  - Library abstraction (composability)

Other Datatype Functions

- Pack/Unpack
  - Mainly for compatibility to legacy libraries
  - Avoid using it yourself
- Get_envelope/contents
  - Only for expert library developers
  - Libraries such as MPITypes[1] make this easier
- MPI_Type_create_resized
  - Change extent and size (dangerous but useful)

[1]http://www.mcs.anl.gov/mpitypes/

Datatype Selection Order

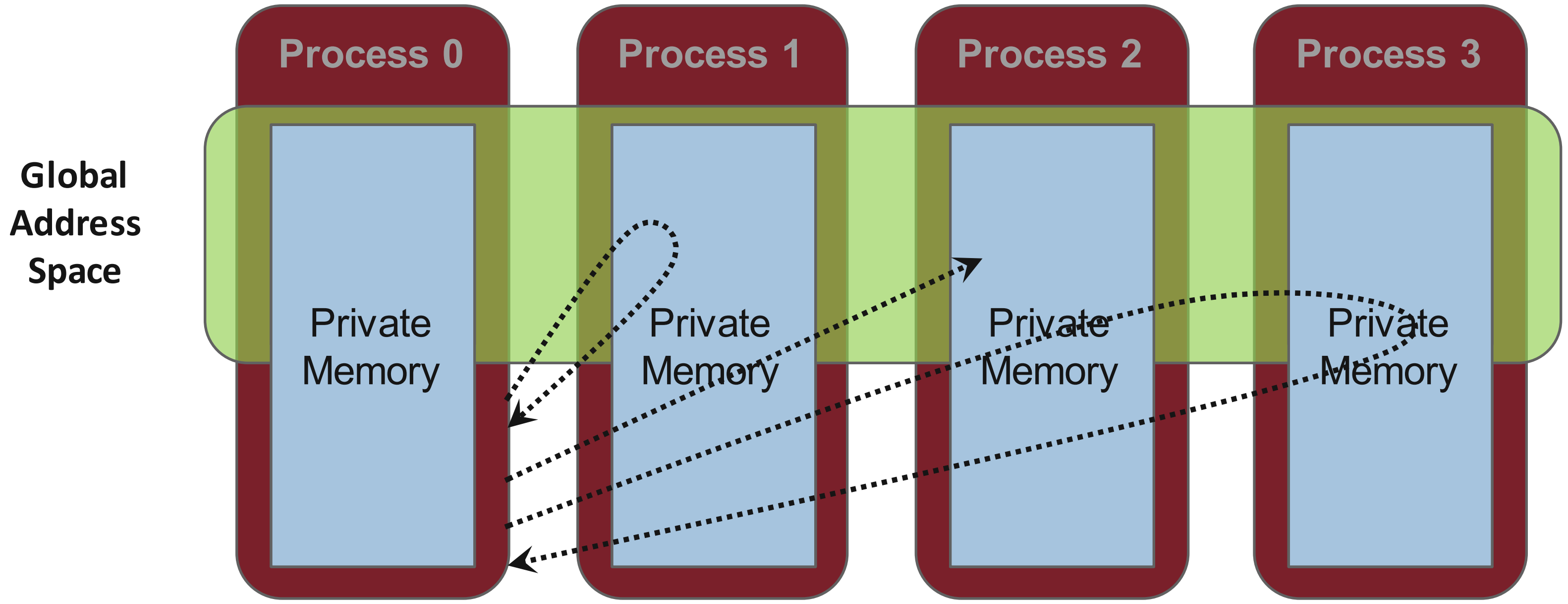
- Simple and effective performance model:
  - More parameters == slower
- **predefined < contig < vector < index_block < index < struct**
- Some (most) MPIs are inconsistent
  - But this rule is portable
- Advice to users:
  - Construct datatypes hierarchically bottom-up

W. Gropp et al.: Performance Expectations and Guidelines for MPI Derived Datatypes

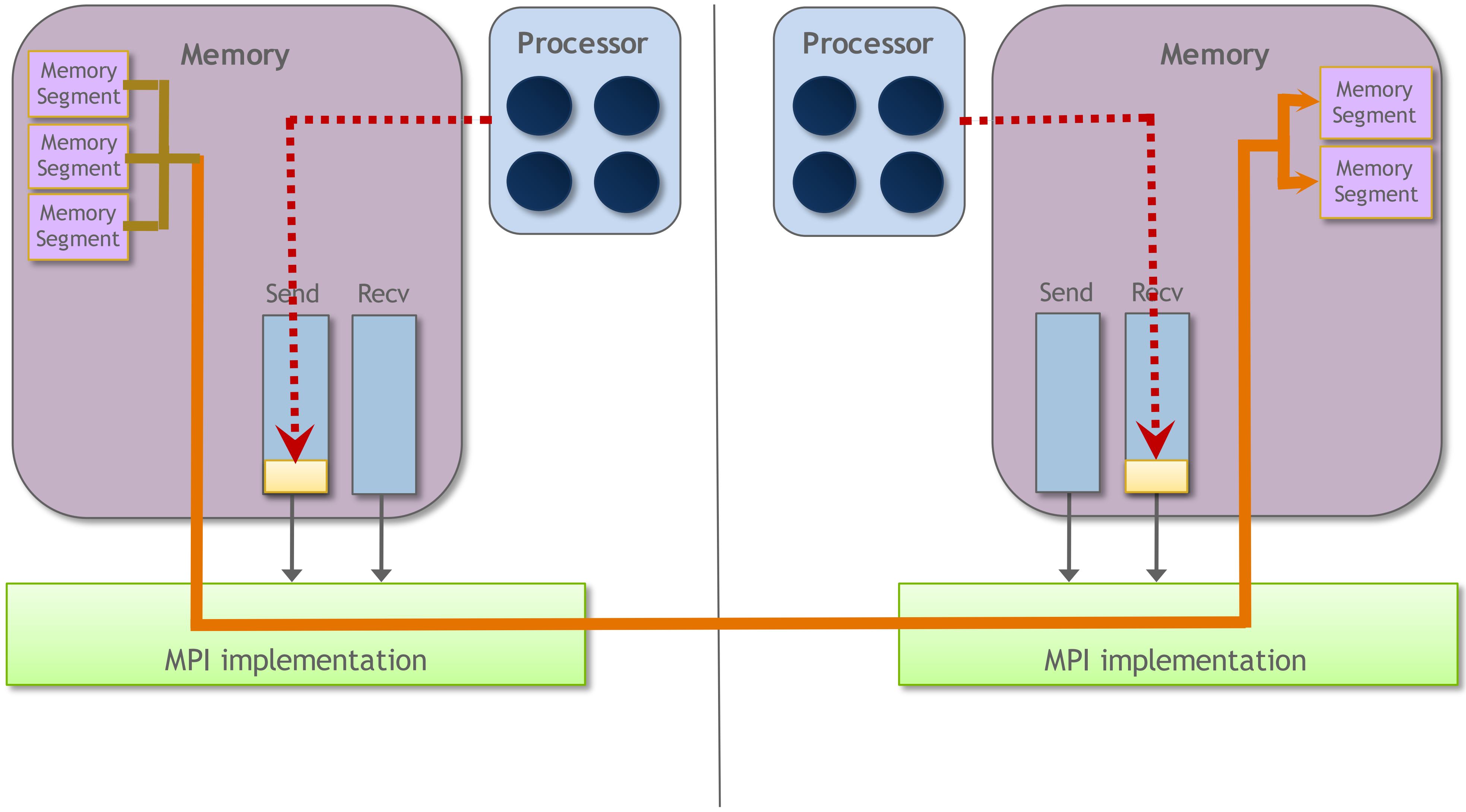
Advanced Topics: One-sided Communication

One-sided Communication

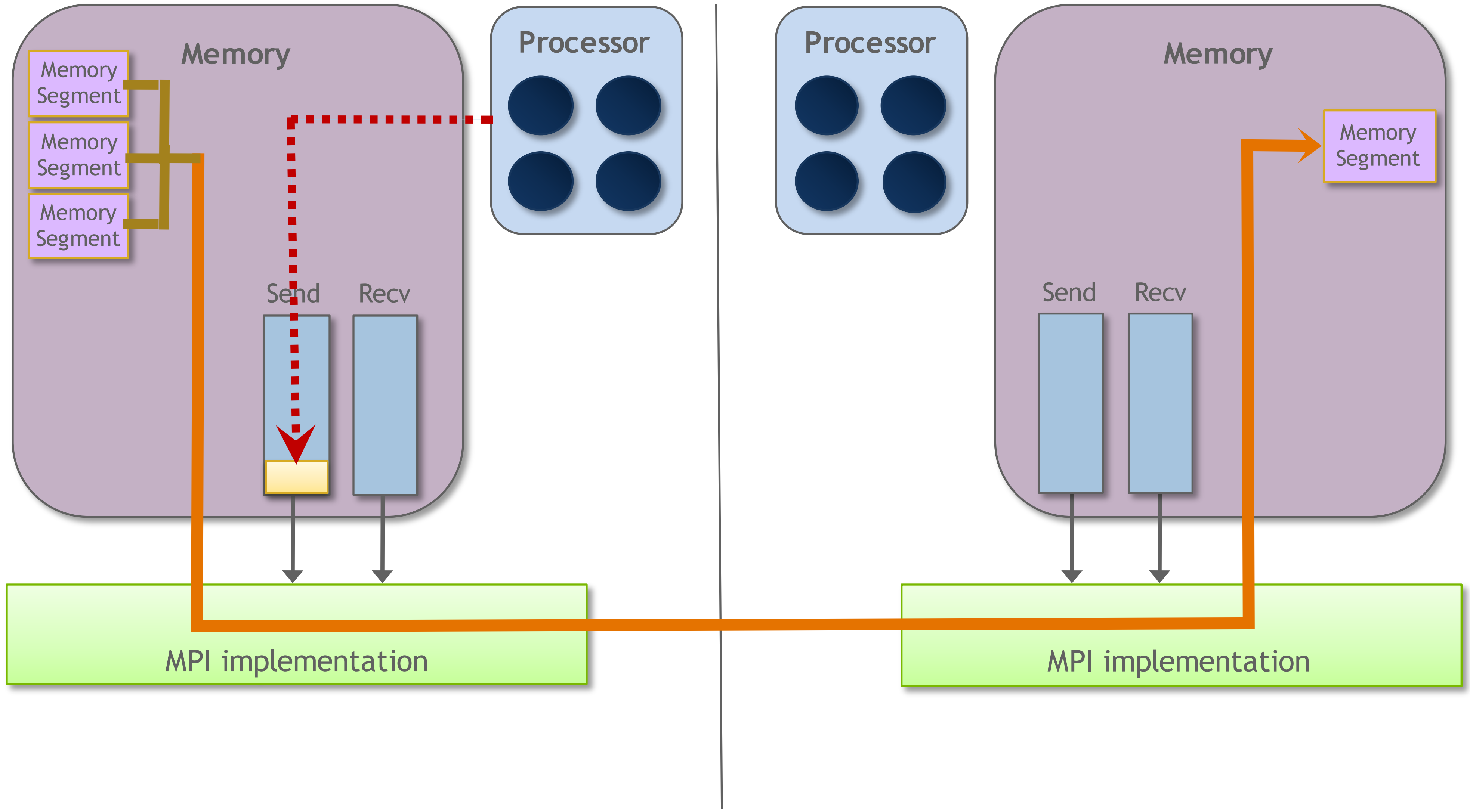
- The basic idea of one-sided communication models is to decouple data movement with process synchronization
  - Should be able to move data without requiring that the remote process synchronize
  - Each process exposes a part of its memory to other processes
  - Other processes can directly read from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



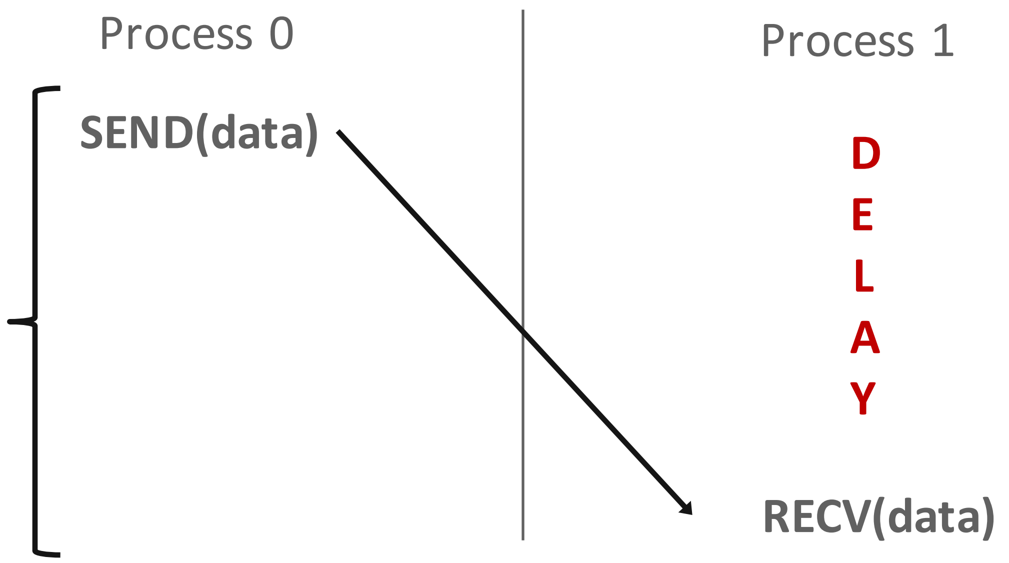
Two-sided Communication Example



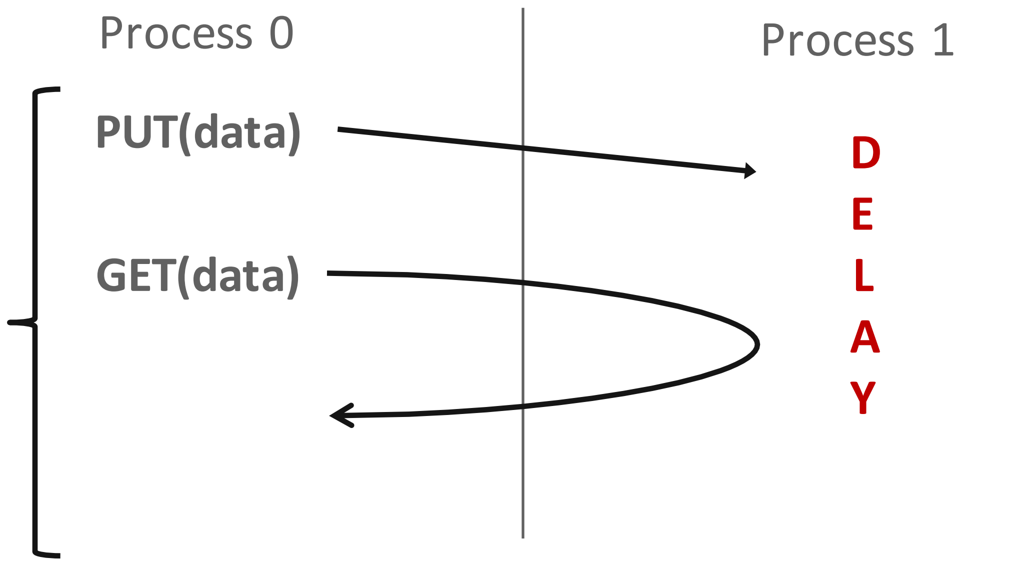
One-sided Communication Example



Comparing One-sided and Two-sided Programming



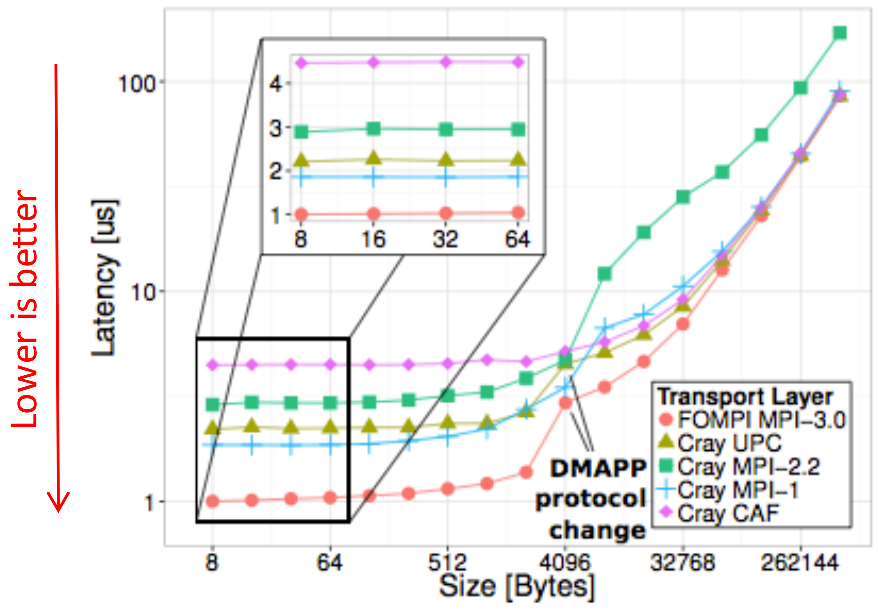
Even the sending process is delayed



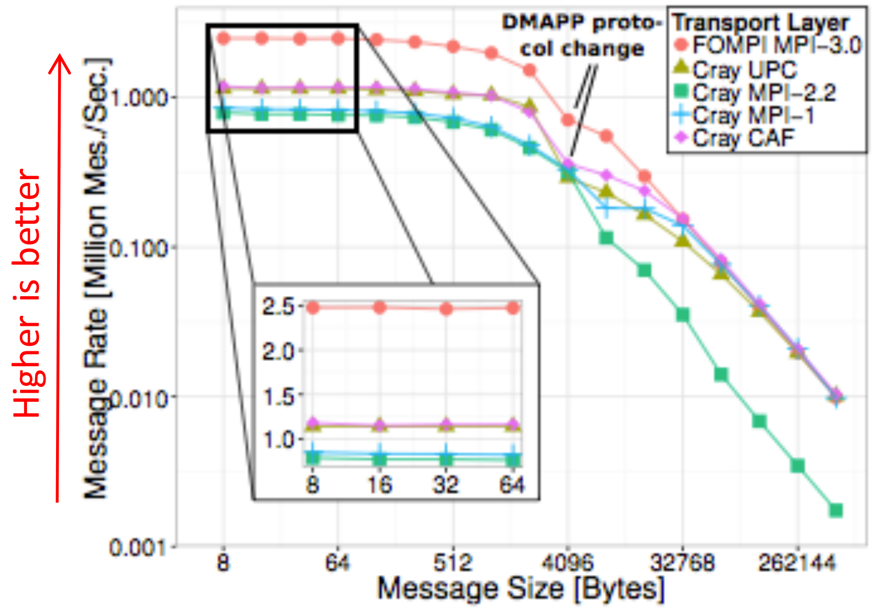
Delay in process 1 does not affect process 0

MPI RMA can be efficiently implemented

- "Enabling Highly-Scalable Remote Memory Access Programming with MPI-3 One Sided" by Robert Gerstenberger, Maciej Besta, Torsten Hoefler (SC13 Best Paper Award)
- They implemented complete MPI-3 RMA for Cray Gemini (XK5, XE6) and Aries (XC30) systems on top of lowest-level Cray APIs
- Achieved better latency, bandwidth, message rate, and application performance than Cray's MPI RMA, UPC, and Coarray Fortran

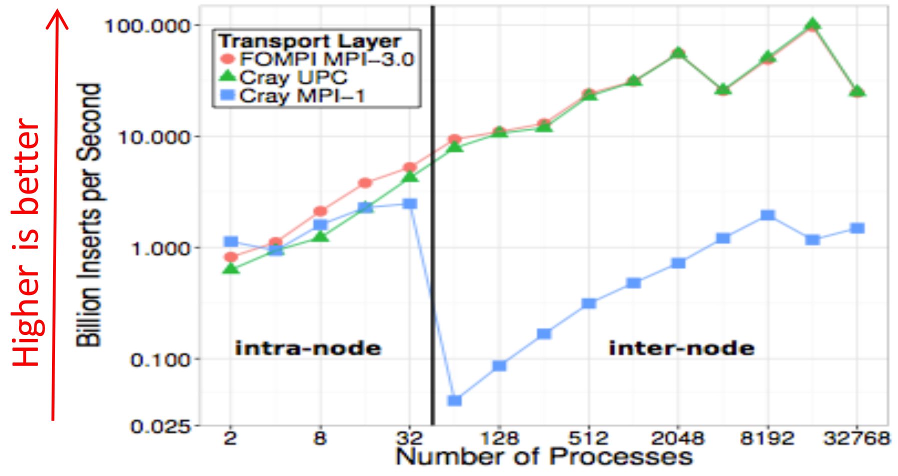


(a) Latency inter-node Put



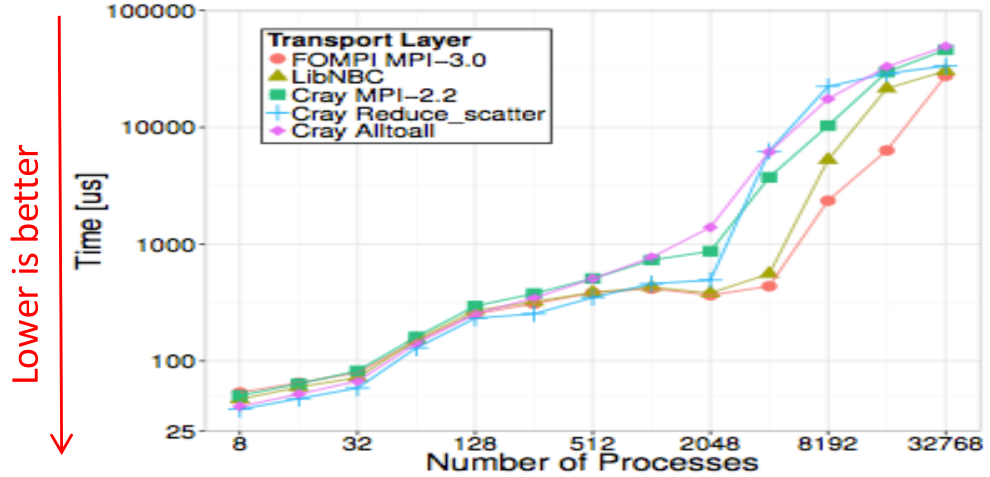
(b) Message Rate inter-node

Application Performance with Tuned MPI-3 RMA



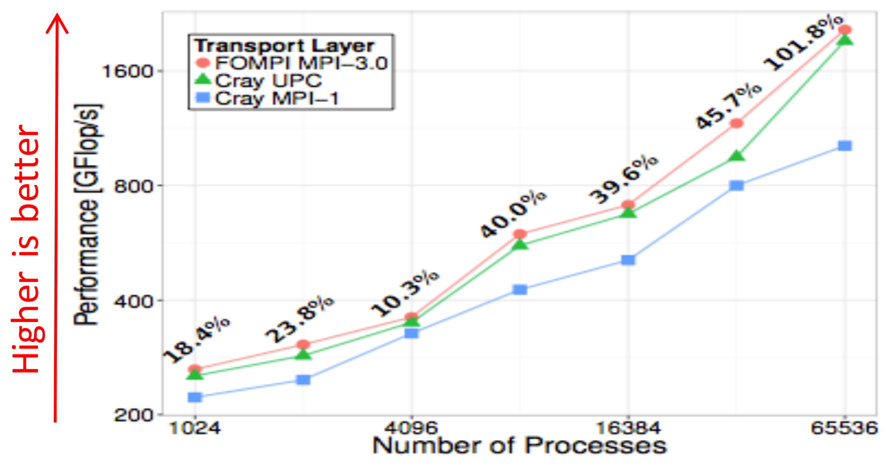
(a) Inserts per second for inserting 16k elements per process including synchronization.

Distributed Hash Table



(b) Time to perform one dynamic sparse data exchange (DSDE) with 6 random neighbors

Dynamic Sparse Data Exchange



(c) 3D FFT Performance. The annotations represent the improvement of FOMPI over MPI-1.

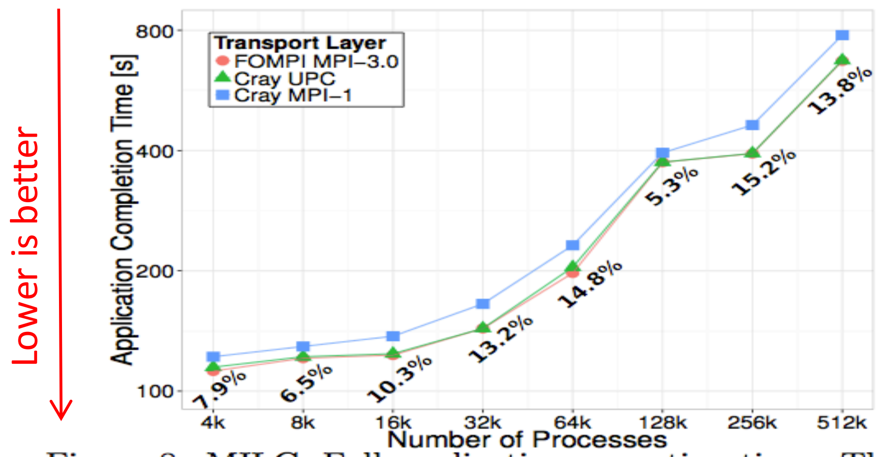


Figure 8: MILC: Full application execution time. The annotations represent the improvement of FOMPI and UPC over MPI-1.

3D FFT

MILC

Gerstenberger, Besta, Hoefler (SC13)

MPI RMA is Carefully and Precisely Specified

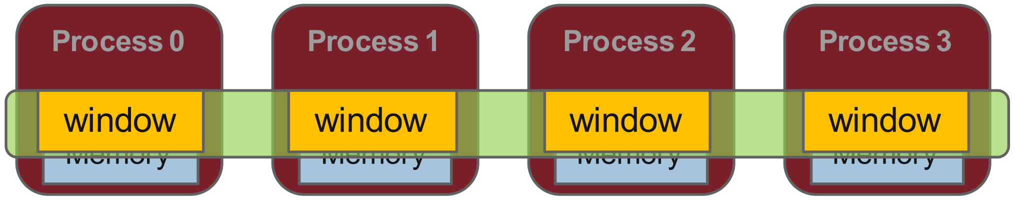
- To work on both cache-coherent and non-cache-coherent systems
  - Even though there aren’t many non-cache-coherent systems, it is designed with the future in mind
- There even exists a *formal model* for MPI-3 RMA that can be used by tools and compilers for optimization, verification, etc.
  - See “Remote Memory Access Programming in MPI-3” by Hoefler, Dinan, Thakur, Barrett, Balaji, Gropp, Underwood. ACM TOPC, July 2015.
  - http://htor.inf.ethz.ch/publications/index.php?pub=201

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;
}
```

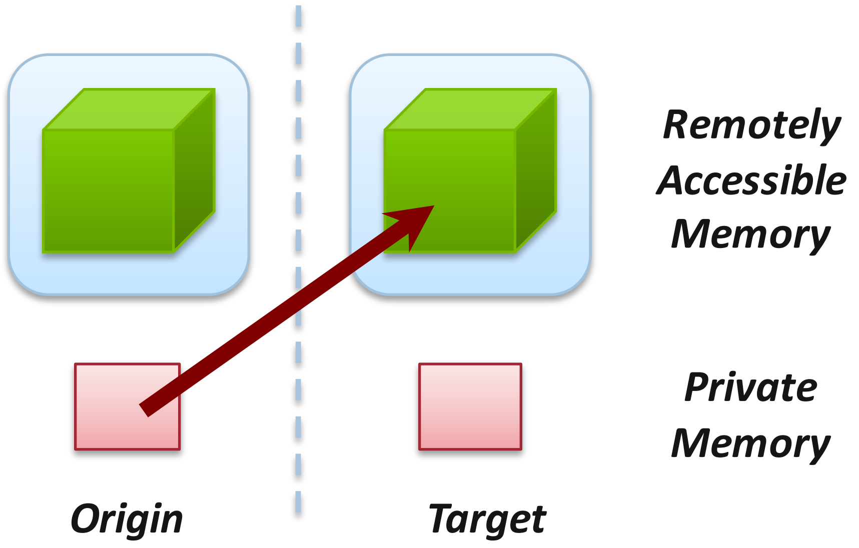
Data movement

- 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(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)
```

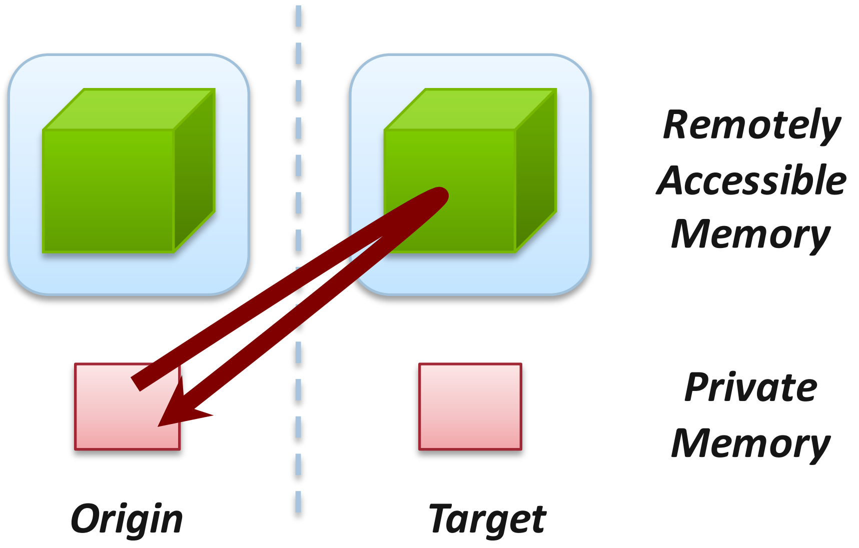
- Move data from origin, to target
- Separate data description triples for **origin** and **target**



Data movement: *Get*

```
MPI_Get(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)
```

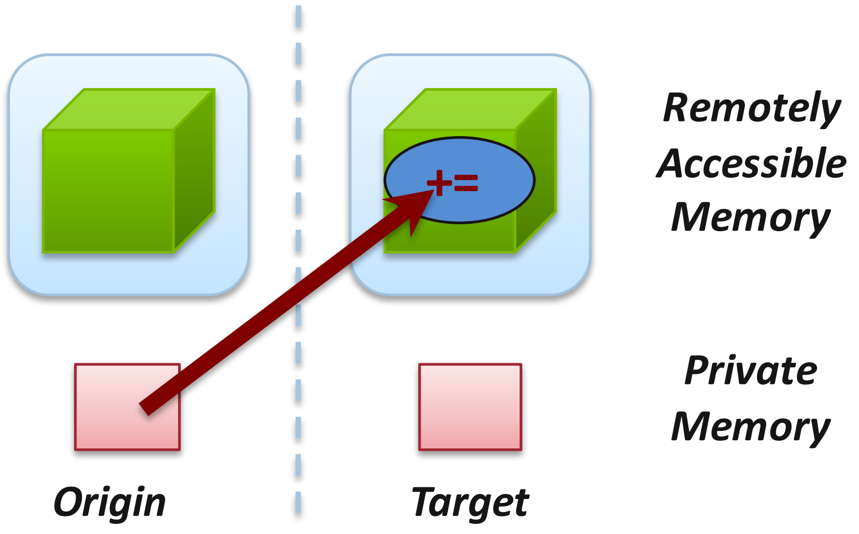
- Move data to origin, from target
- Separate data description triples for **origin** and **target**



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)
```

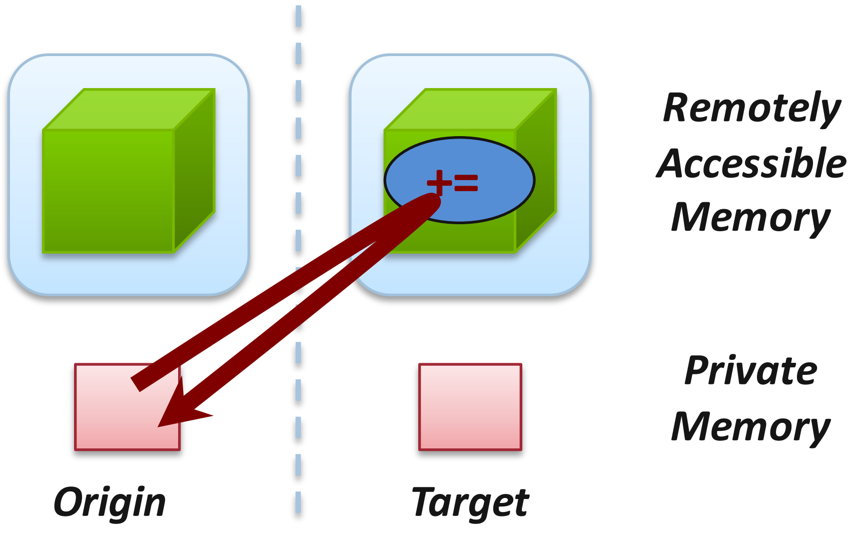
- Atomic update operation, similar to a put
  - Reduces origin and target data into target buffer using op argument as combiner
  - Op = MPI_SUM, MPI_PROD, MPI_OR, MPI_REPLACE, MPI_NO_OP, …
  - Predefined ops only, no user-defined operations
- Different data layouts between target/origin OK
  - Basic 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(void *origin_addr, void *result_addr,
        MPI_Datatype dtype, int target_rank,
        MPI_Aint target_disp, MPI_Op op, MPI_Win win)
```

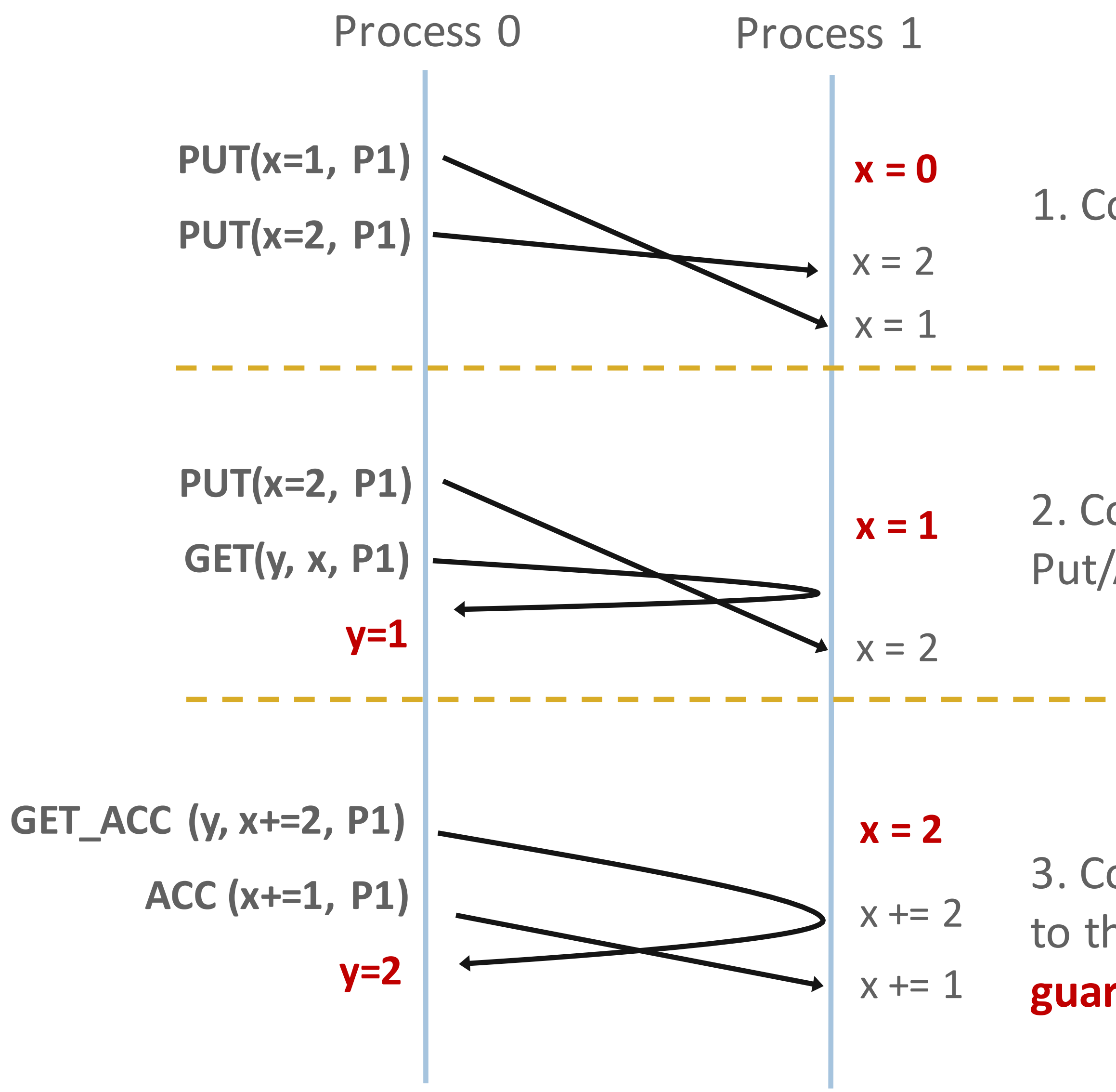
```
MPI_Compare_and_swap(void *origin_addr, void *compare_addr,
        void *result_addr, MPI_Datatype dtype, int target_rank,
        MPI_Aint target_disp, MPI_Win win)
```

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

Ordering of Operations in MPI RMA

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

Examples with operation ordering



1. Concurrent Puts: **undefined**

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

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

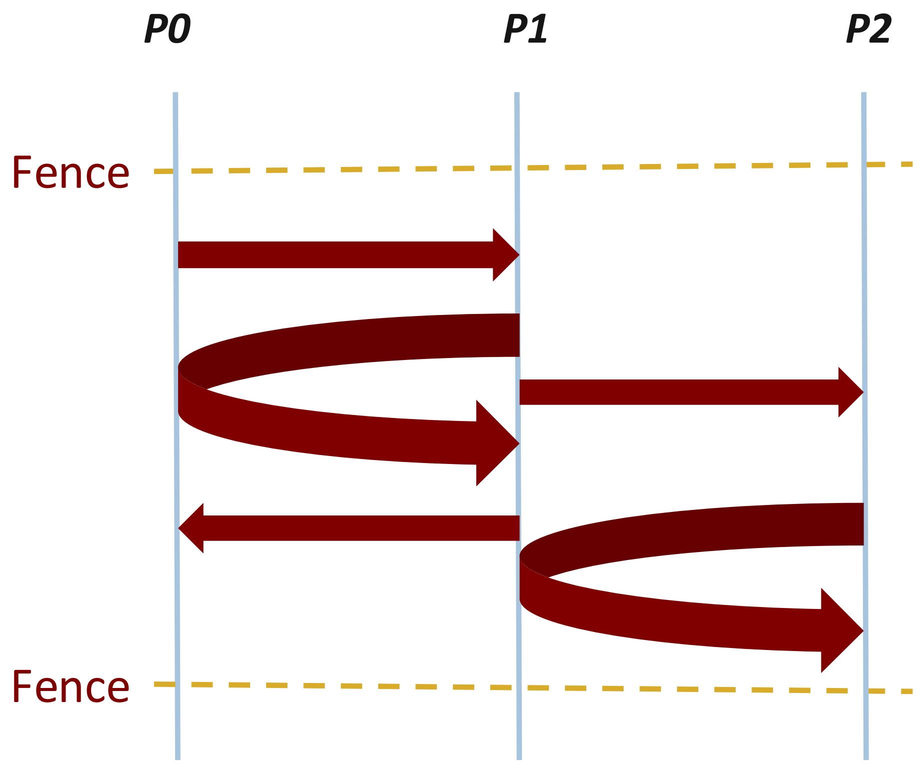
RMA Synchronization Models

- 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)
  - 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

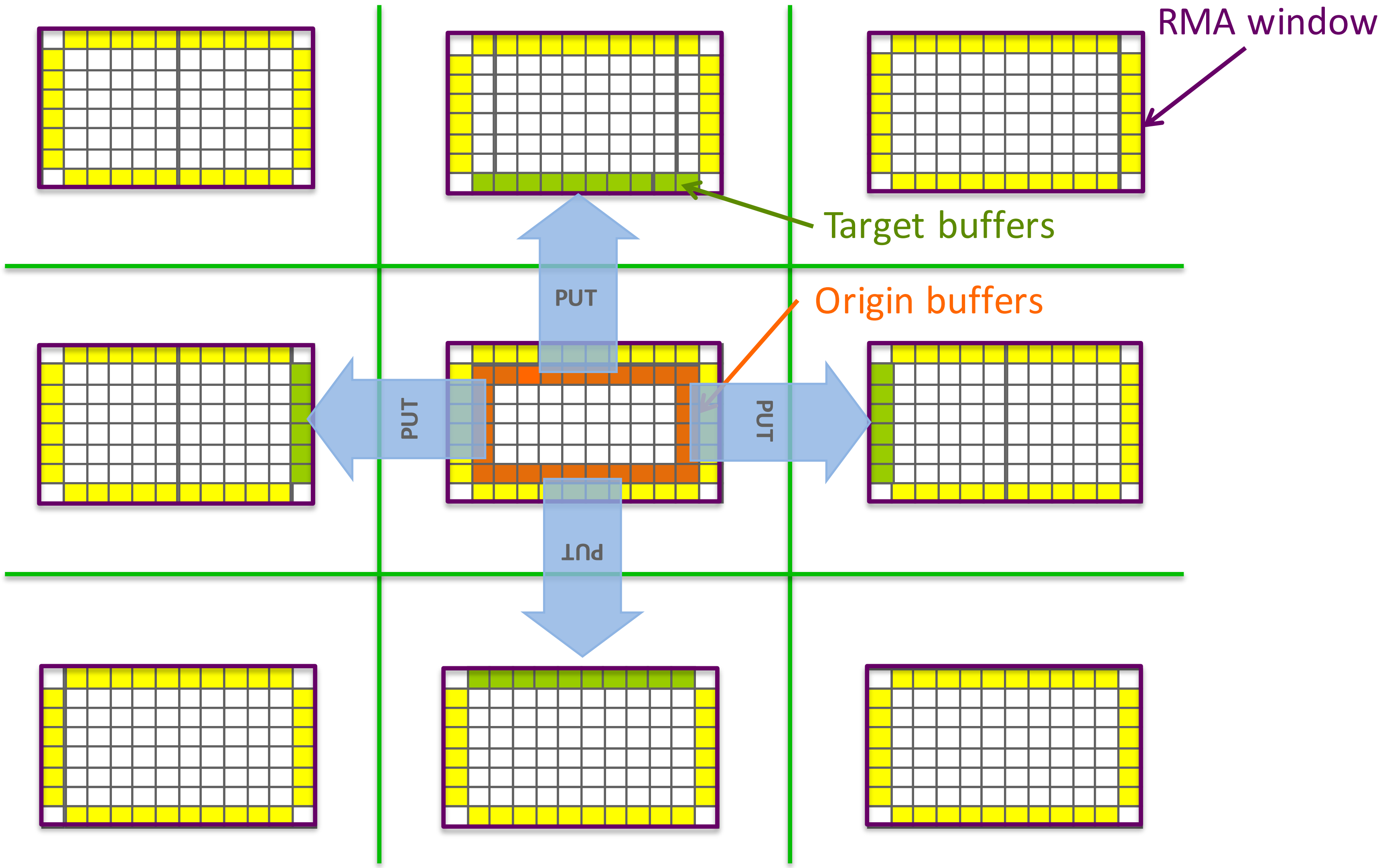
Fence: Active Target Synchronization

```
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



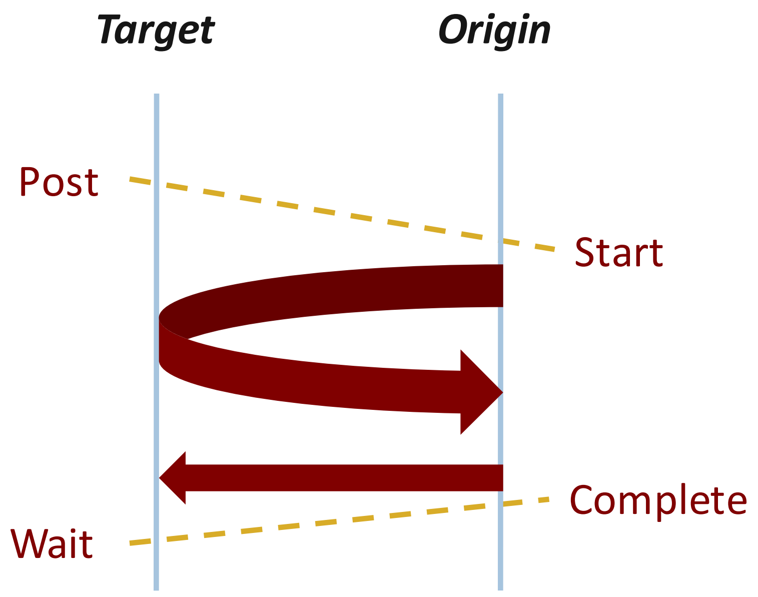
Code Example

- *stencil_mpi_ddt_rma.c*
- Use MPI_PUTs to move data, explicit receives are not needed
- Data location specified by MPI datatypes
- Manual packing of data no longer required

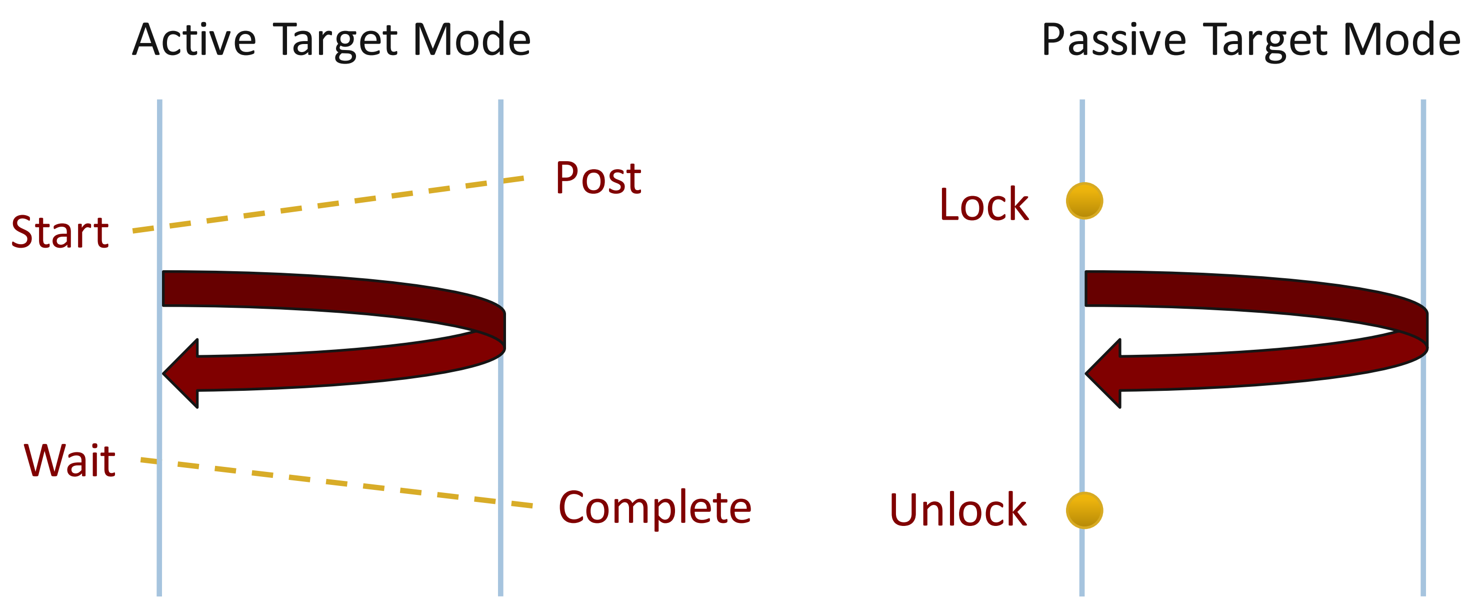
PSCW: Generalized Active Target Synchronization

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

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



Lock/Unlock: Passive Target Synchronization



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

Passive Target Synchronization

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

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

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

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

Advanced Passive Target Synchronization

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

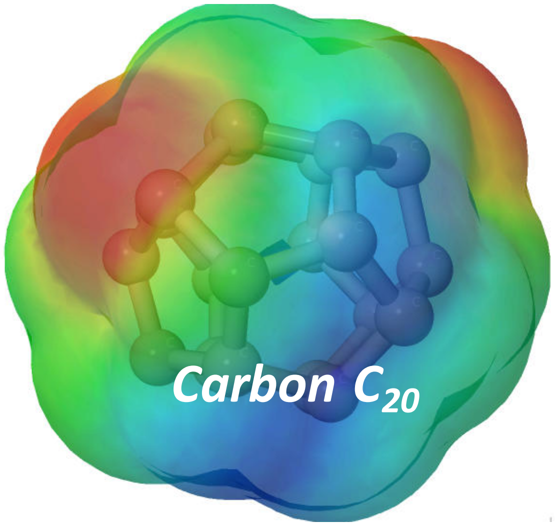
```
MPI_Win_unlock_all(MPI_Win win)
```

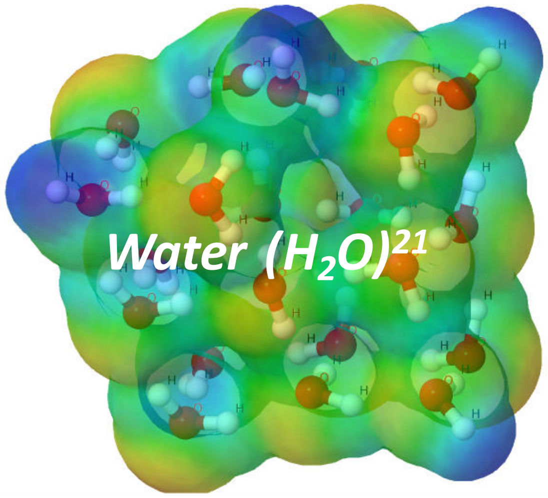
```
MPI_Win_flush_all/flush_local_all(MPI_Win win)
```

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

NWChem [1]

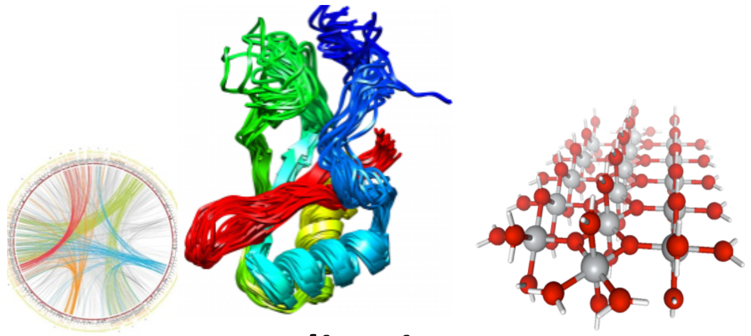
- High performance computational chemistry application suite
- Quantum level simulation of molecular systems
  - Very expensive in computation and data movement, so is used for small systems
  - Larger systems use molecular level simulations
- Composed of many simulation capabilities
  - Molecular Electronic 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



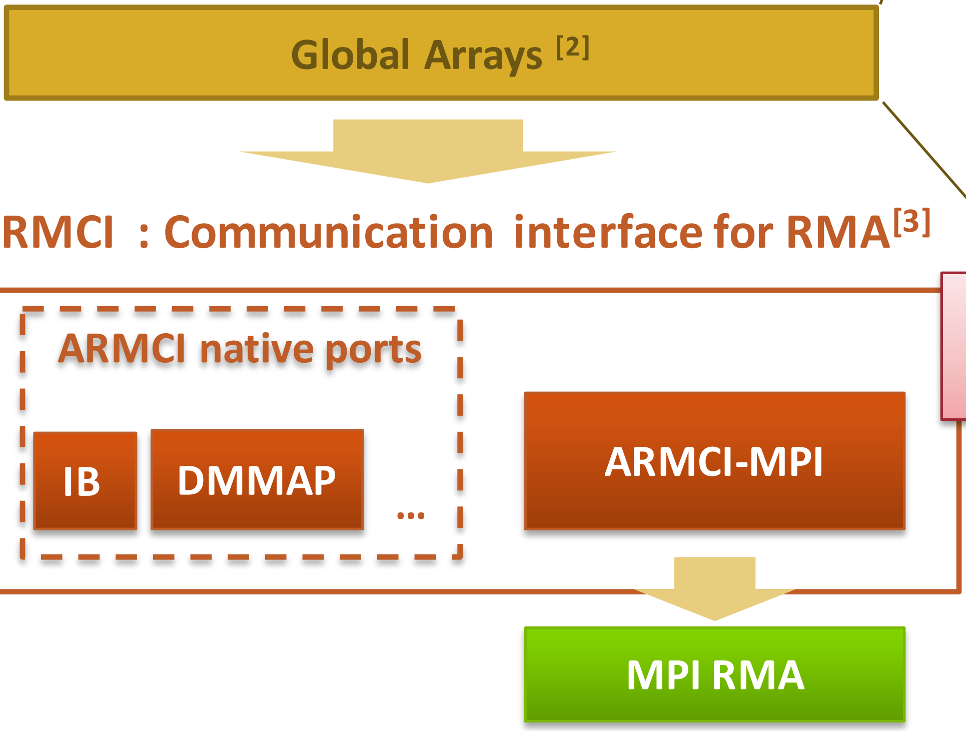


[1] M. Valiev, E.J. Bylaska, N. Govind, K. Kowalski, T.P. Straatsma, H.J.J. van Dam, D. Wang, J. Nieplocha, E. Apra, T.L. Windus, W.A. de Jong, "NWChem: a comprehensive and scalable open-source solution for large scale molecular simulations" Comput. Phys. Commun. 181, 1477 (2010)

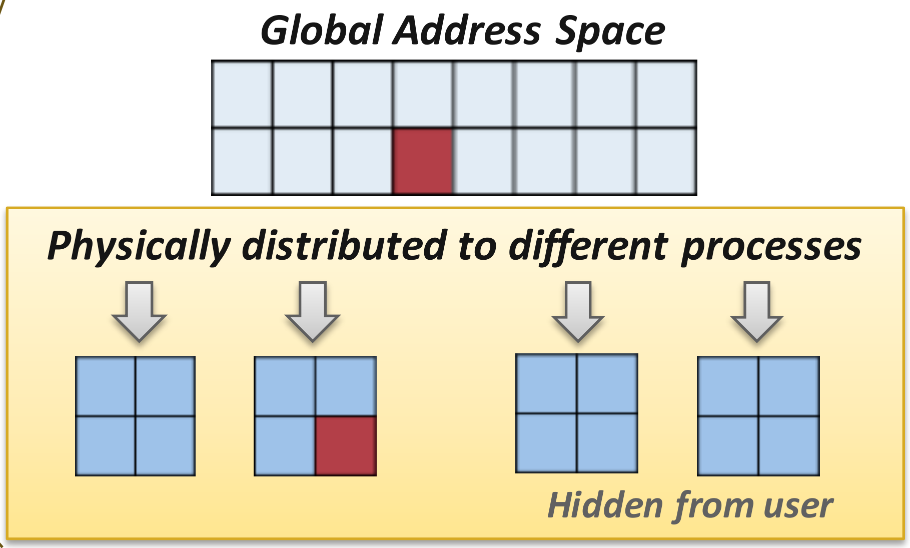
NWChem Communication Runtime



Applications



Abstractions for distributed arrays



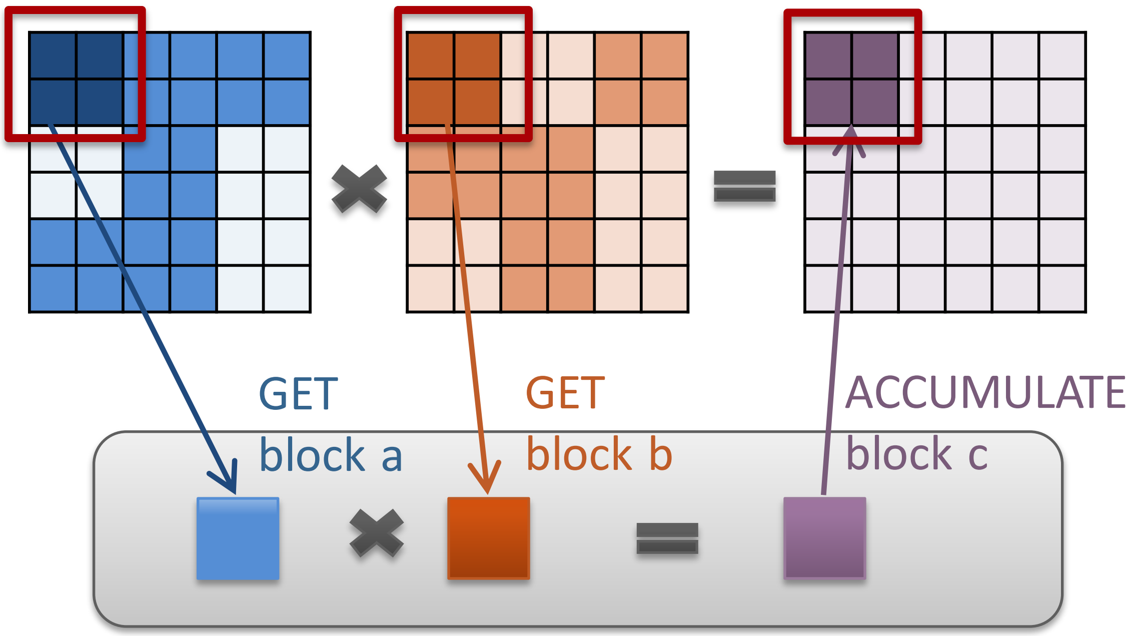
Irregularly access large amount of remote memory regions

[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.

Code Example

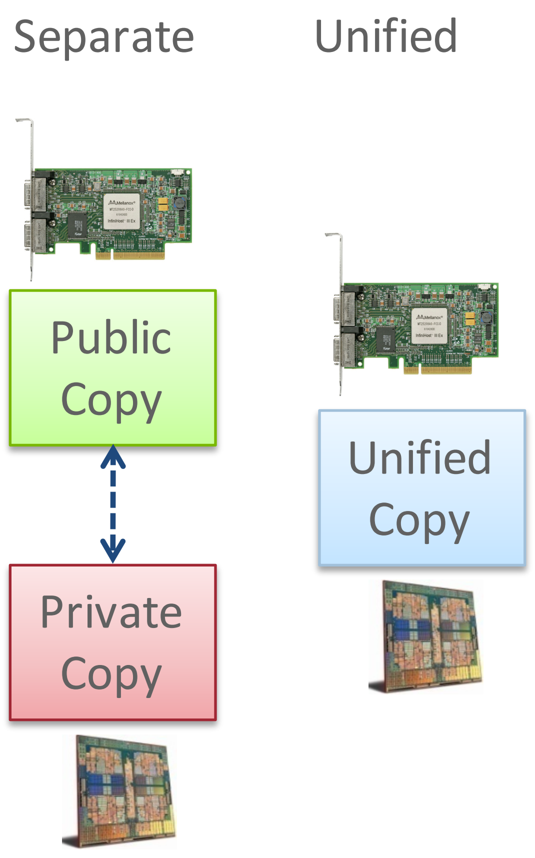
- ga_mpi_ddt_rma.c
- Only synchronization from origin processes, no synchronization from target processes

Which synchronization mode should I use, when?

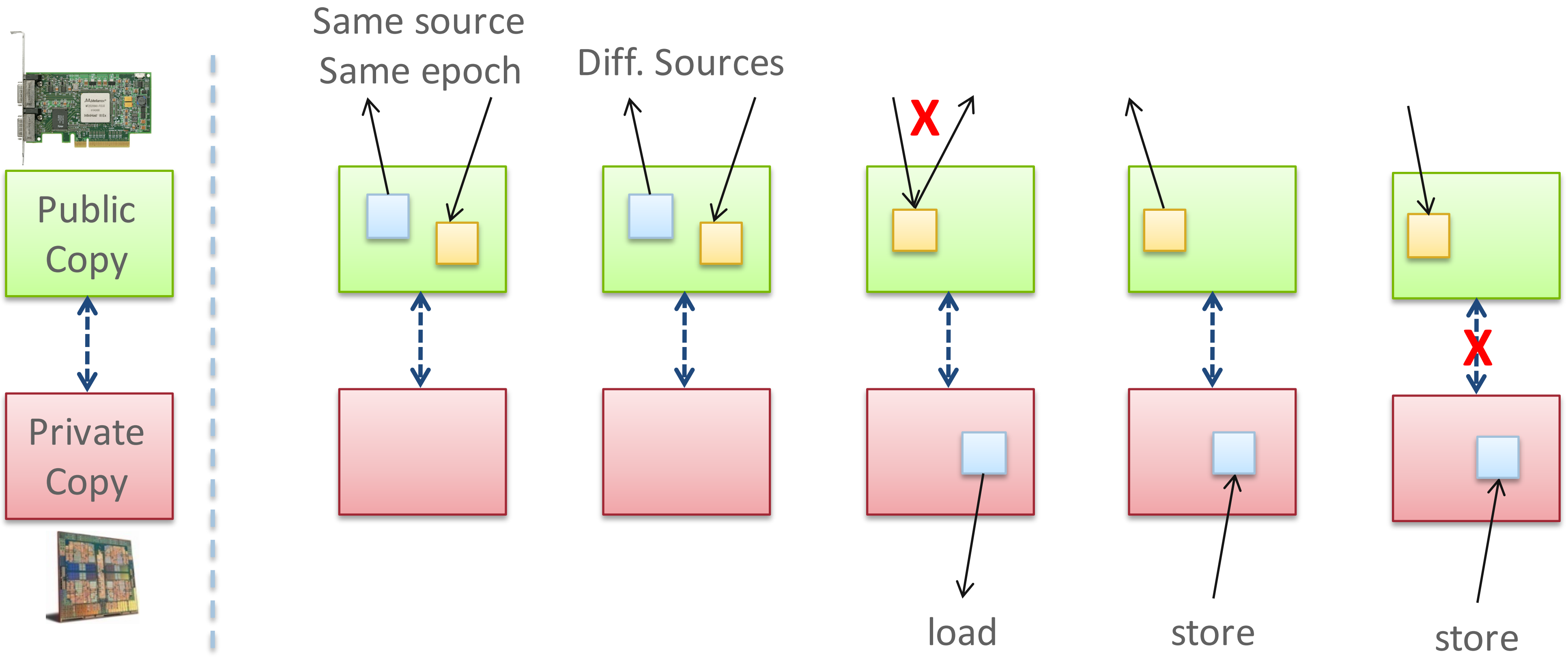
- RMA communication has low overheads versus send/recv
  - Two-sided: Matching, queuing, buffering, unexpected receives, etc…
  - One-sided: No matching, no buffering, always ready to receive
  - Utilize RDMA provided by high-speed interconnects (e.g. InfiniBand)
- Active mode: bulk synchronization
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

MPI RMA Memory Model

- MPI-3 provides two memory models: separate and unified
- MPI-2: Separate Model
  - Logical public and private copies
  - MPI provides software coherence between window copies
  - Extremely portable, to systems that don't provide hardware coherence
- MPI-3: New Unified Model
  - Single copy of the window
  - System must provide coherence
  - Superset of separate semantics
    - E.g. allows concurrent local/remote access
  - Provides access to full performance potential of hardware

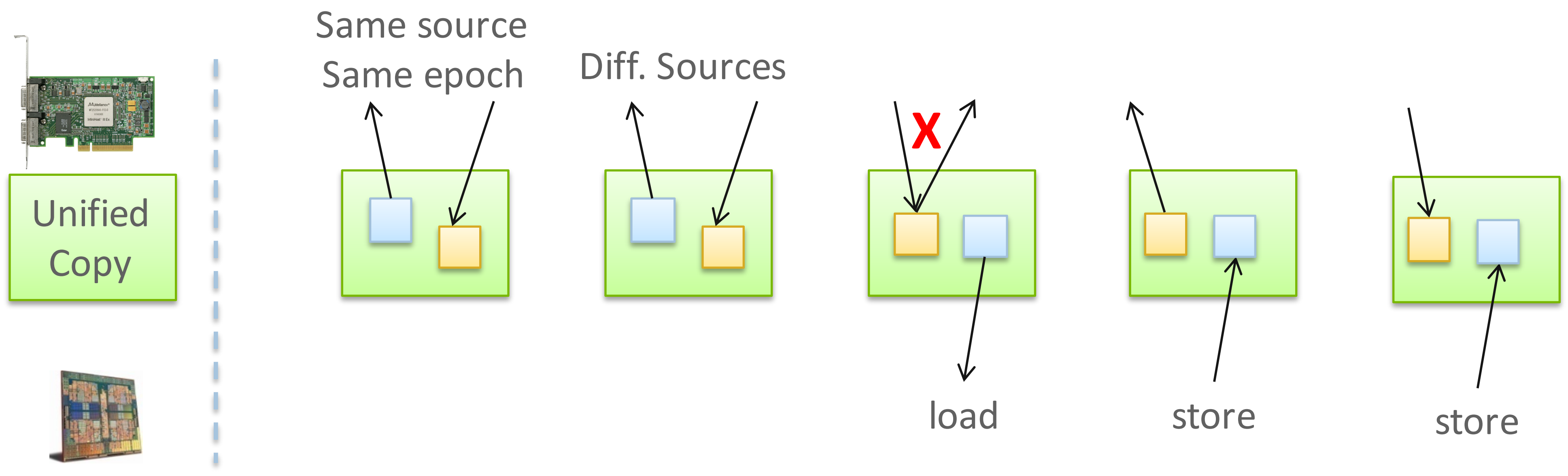


MPI RMA Memory Model (separate windows)



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

MPI RMA Memory Model (unified windows)



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

MPI RMA Operation Compatibility (Separate)

	Load	Store	Get	Put	Acc
Load	OVL+NOVL	OVL+NOVL	OVL+NOVL	NOVL	NOVL
Store	OVL+NOVL	OVL+NOVL	NOVL	X	X
Get	OVL+NOVL	NOVL	OVL+NOVL	NOVL	NOVL
Put	NOVL	X	NOVL	NOVL	NOVL
Acc	NOVL	X	NOVL	NOVL	OVL+NOVL

This matrix shows the compatibility of MPI-RMA operations when two or more processes access a window at the same target concurrently.

OVL	– Overlapping operations permitted
NOVL	– Nonoverlapping operations permitted
X	– Combining these operations is OK, but data might be garbage

MPI RMA Operation Compatibility (Unified)

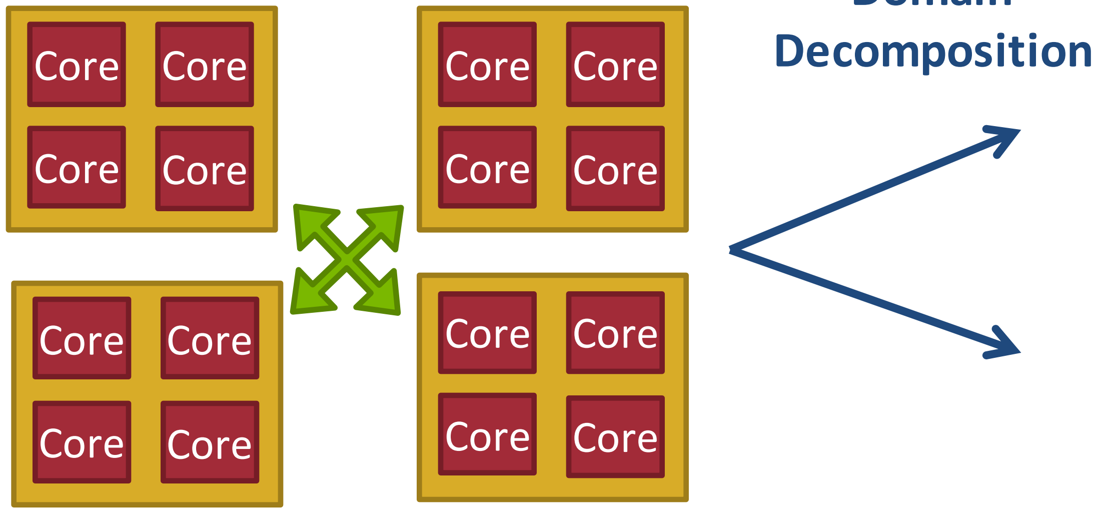
	Load	Store	Get	Put	Acc
Load	OVL+NOVL	OVL+NOVL	OVL+NOVL	NOVL	NOVL
Store	OVL+NOVL	OVL+NOVL	NOVL	NOVL	NOVL
Get	OVL+NOVL	NOVL	OVL+NOVL	NOVL	NOVL
Put	NOVL	NOVL	NOVL	NOVL	NOVL
Acc	NOVL	NOVL	NOVL	NOVL	OVL+NOVL

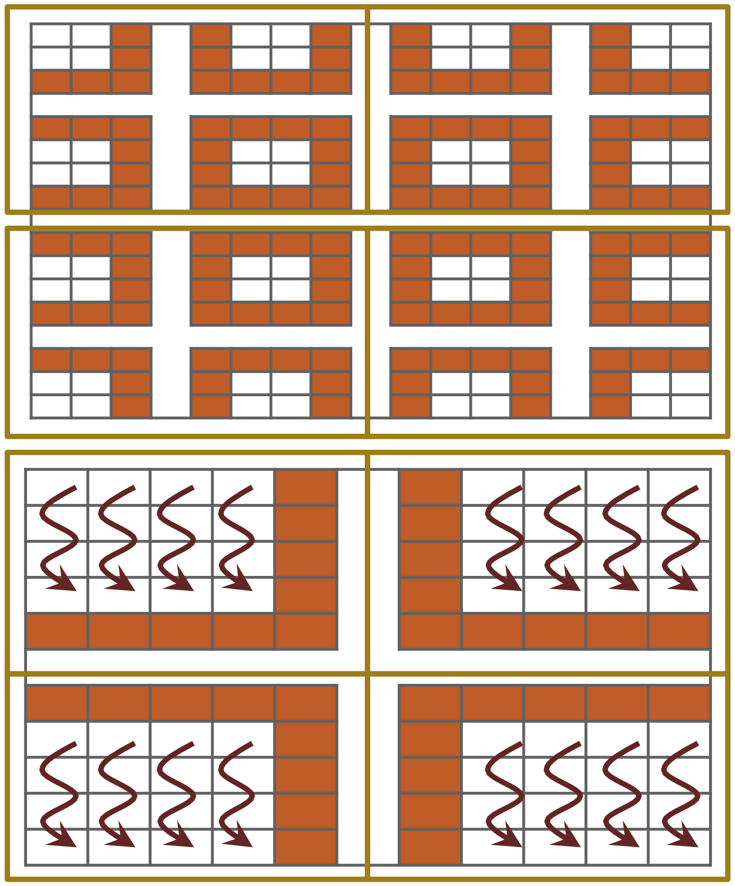
This matrix shows the compatibility of MPI-RMA operations when two or more processes access a window at the same target concurrently.

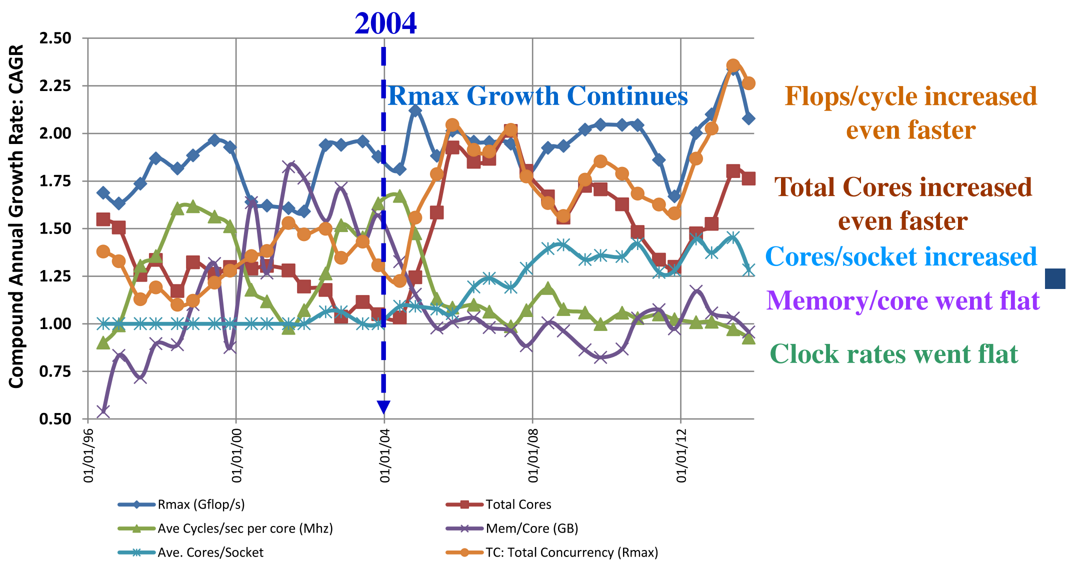
OVL	– Overlapping operations permitted
NOVL	– Nonoverlapping operations permitted

Hybrid Programming with Threads, Shared Memory, and GPUs

Why Hybrid MPI + X Programming?







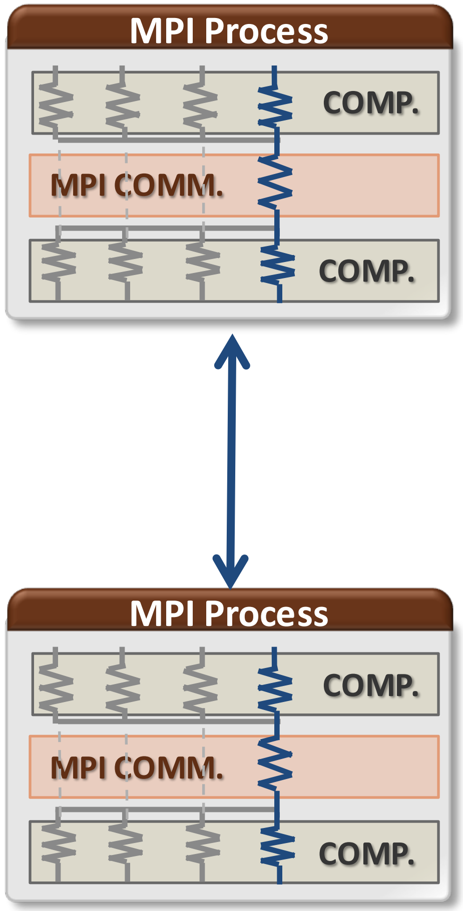
Growth of node resources in the Top500 systems. Peter Kogge: "Reading the Tea-Leaves: How Architecture Has Evolved at the High End". IPDPS 2014 Keynote

- Sharing promotes cooperation
  - Reduced memory consumption
  - Efficient use of shared resources: caches, TLB entries, network endpoints, etc.

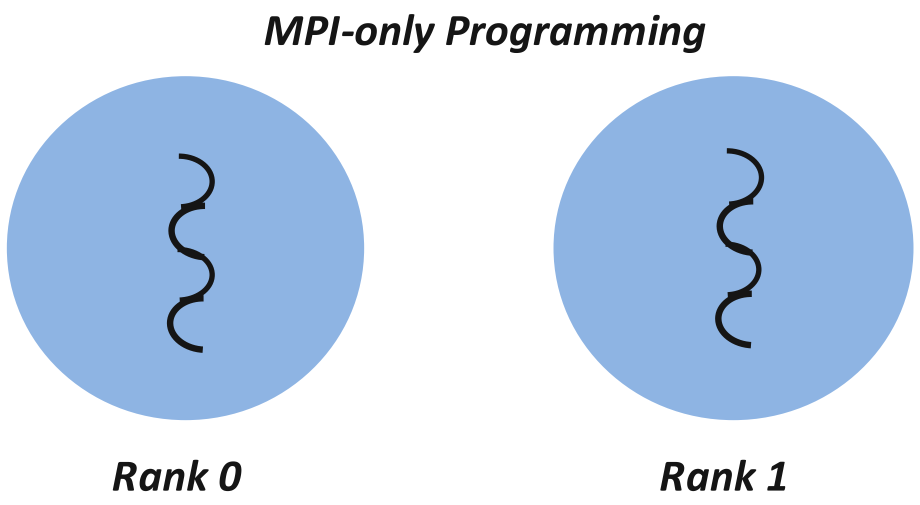
MPI + Threads

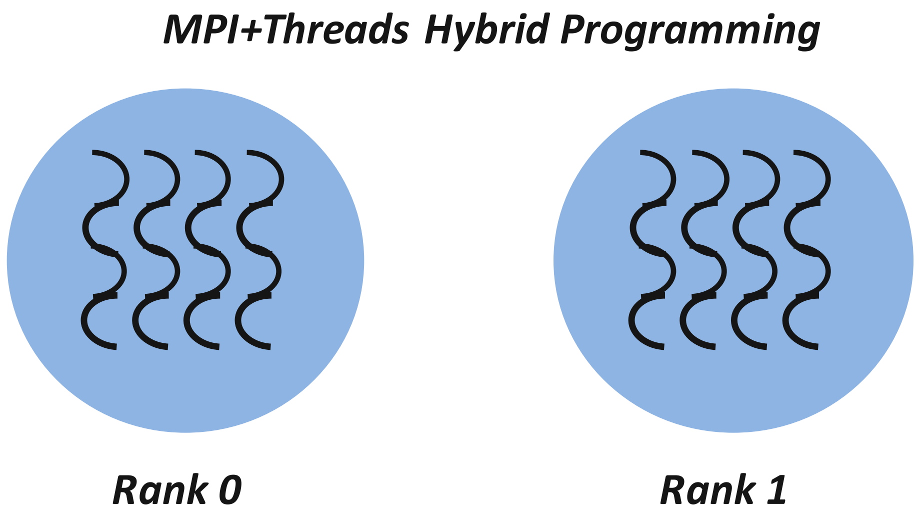
MPI and Threads

- 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.



Hybrid Programming with MPI+Threads





- In MPI-only programming, each MPI process has a single thread of execution
- In MPI+threads hybrid programming, there can be multiple threads executing simultaneously
  - All threads share all MPI objects (communicators, requests)
  - The MPI implementation might need to take precautions to make sure the state of the MPI stack is consistent

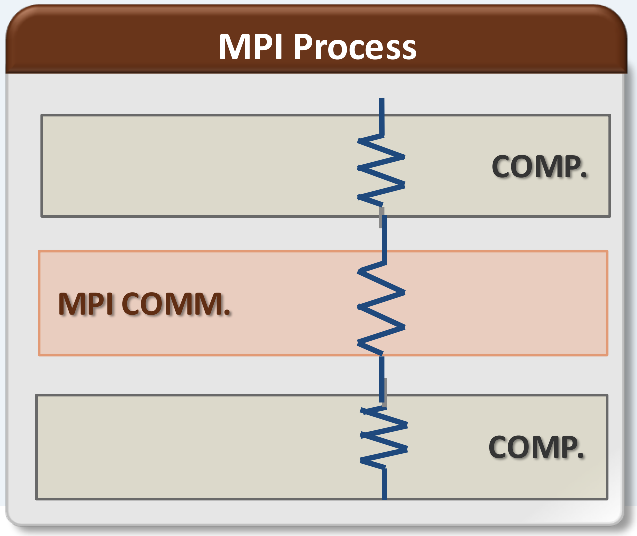
MPI's Four Levels of Thread Safety

- MPI defines four levels of thread safety -- these are commitments the application makes to the MPI
  - MPI_THREAD_SINGLE: only one thread exists in the application
  - MPI_THREAD_FUNNELED: multithreaded, but only the main thread makes MPI calls (the one that called MPI_Init_thread)
  - MPI_THREAD_SERIALIZED: multithreaded, but only one thread *at a time* makes MPI calls
  - MPI_THREAD_MULTIPLE: multithreaded and any thread can make MPI calls at any time (with some restrictions to avoid races – see next slide)
- 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(requested, 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

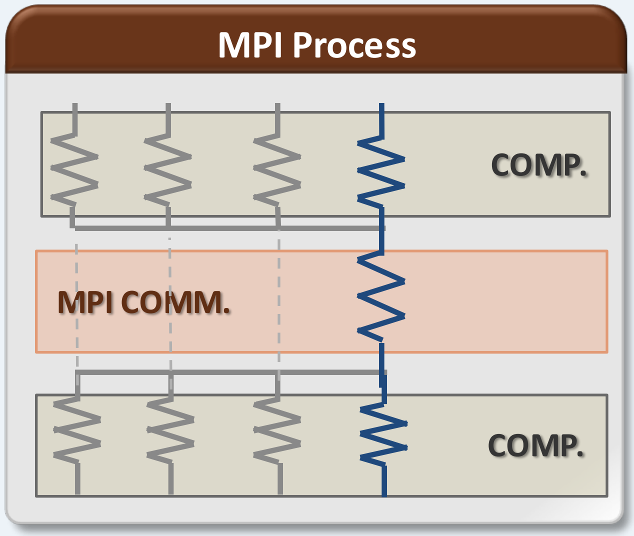
```
int main(int argc, char ** argv)
{
    int buf[100];

    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

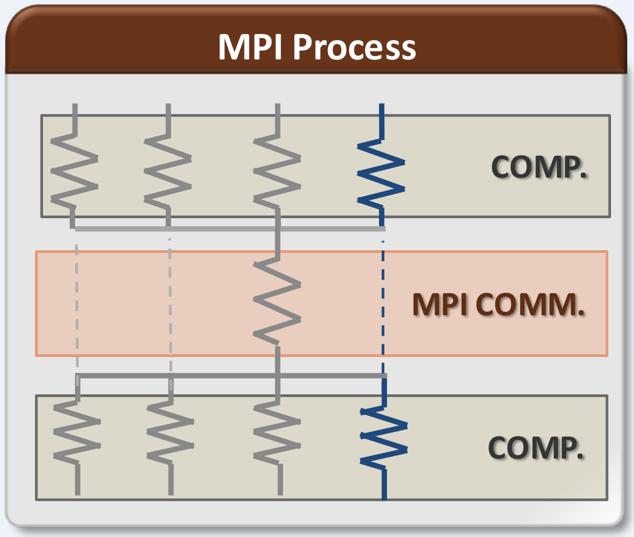
```
int main(int argc, char ** argv)
{
   int buf[100], provided;

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

#pragma omp parallel for
   for (i = 0; i < 100; i++)
       compute(buf[i]);

   /* Do MPI stuff */

   MPI_Finalize();
   return 0;
}
```



MPI_THREAD_SERIALIZED

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

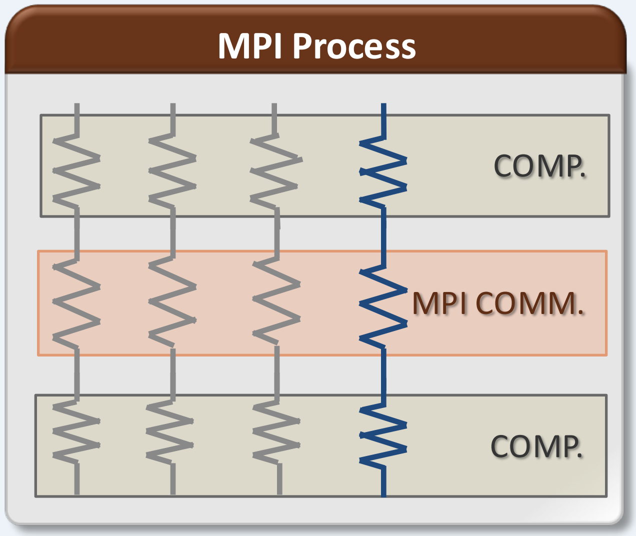
```
int main(int argc, char ** argv)
{
    int buf[100], provided;

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

#pragma omp parallel for
    for (i = 0; i < 100; i++) {
        compute(buf[i]);
#pragma omp critical
        /* Do MPI stuff */
    }

    MPI_Finalize();
    return 0;
}
```



MPI_THREAD_MULTIPLE

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

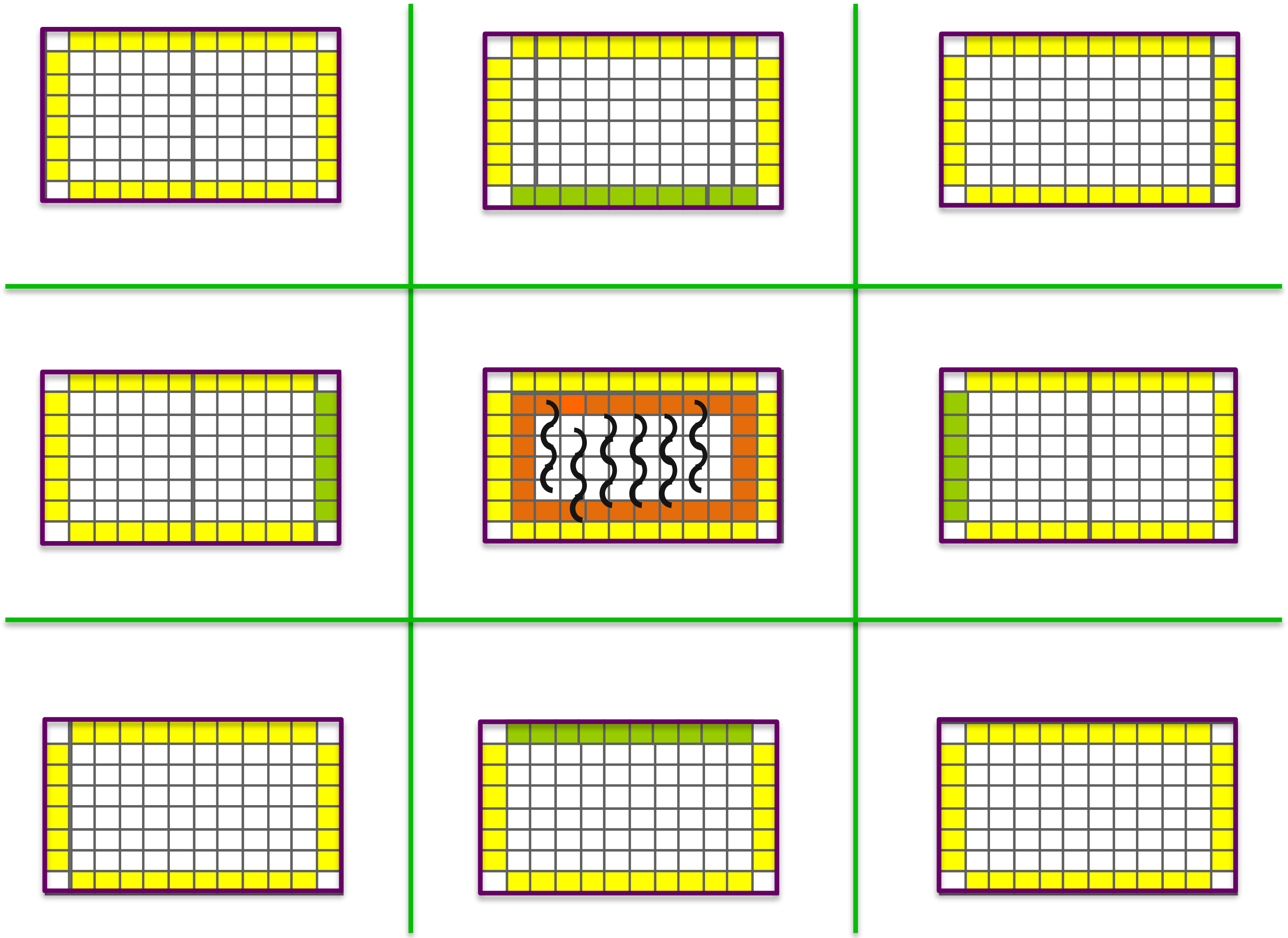
```
int main(int argc, char ** argv)
{
    int buf[100], provided;

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

#pragma omp parallel for
    for (i = 0; i < 100; i++) {
        compute(buf[i]);
        /* Do MPI stuff */
    }

    MPI_Finalize();
    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
  - MPI Standard *mandates* MPI_THREAD_SINGLE for MPI_Init
- *A threaded MPI program that does not call MPI_Init_thread is an incorrect program (common user error we see)*

Implementing Stencil Computation using MPI_THREAD_FUNNELED



Code Examples

- *stencil_mpi_ddt_funneled.c*
- Parallelize computation (OpenMP parallel for)
- Main thread does all communication

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 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

Ordering in MPI_THREAD_MULTIPLE: Incorrect Example with Object Management

Process 0

Thread 1 | Thread 2

MPI_Comm_free(comm)

MPI_Bcast(comm)

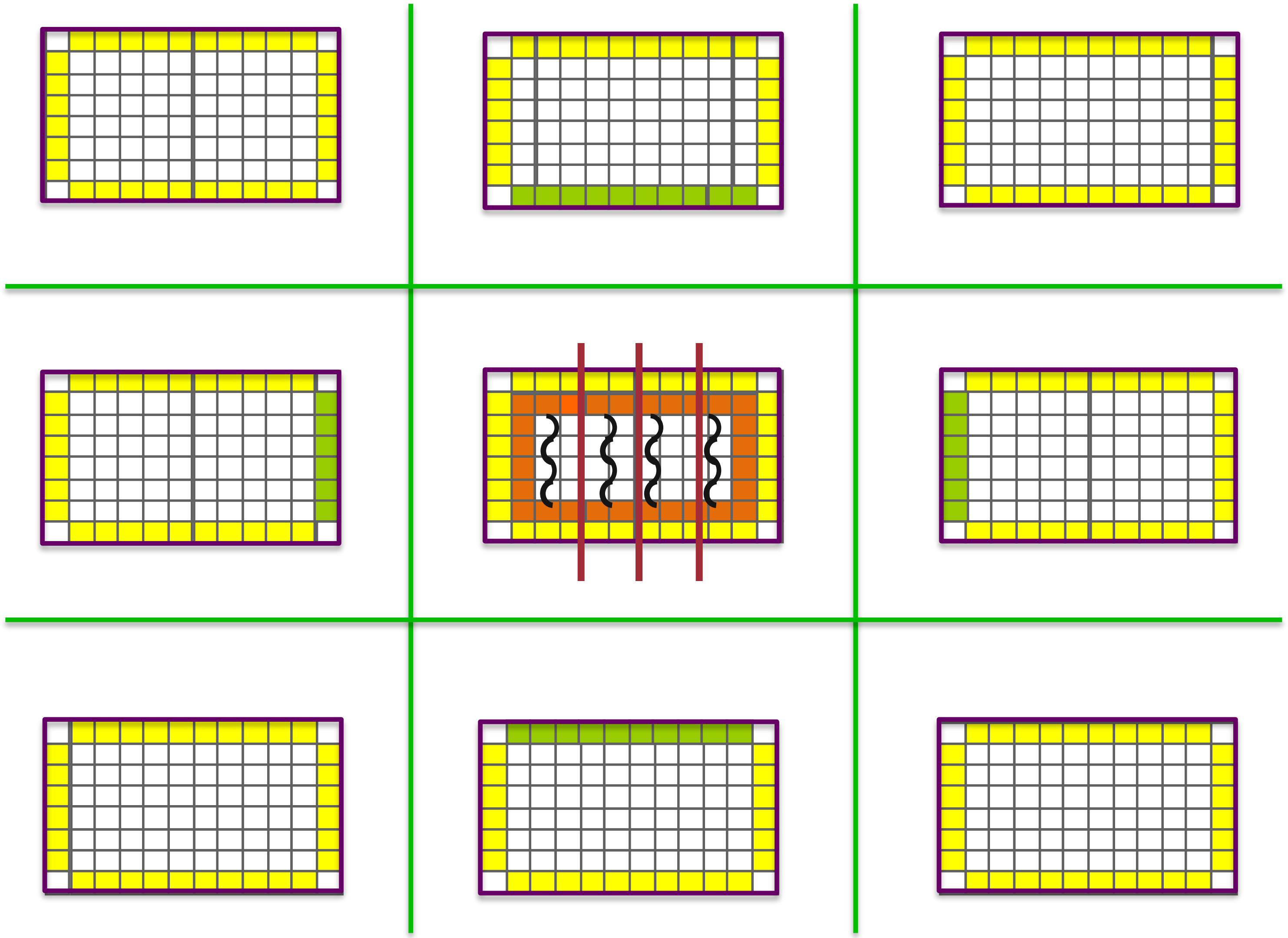
- The user has to make sure that one thread is not using an object while another thread is freeing it
  - This is essentially an ordering issue; the object might get freed before it is used

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.

Implementing Stencil Computation using MPI_THREAD_MULTIPLE



Code Examples

- *stencil_mpi_ddt_multiple.c*
- Divide the process memory among OpenMP threads
- Each thread responsible for communication and computation

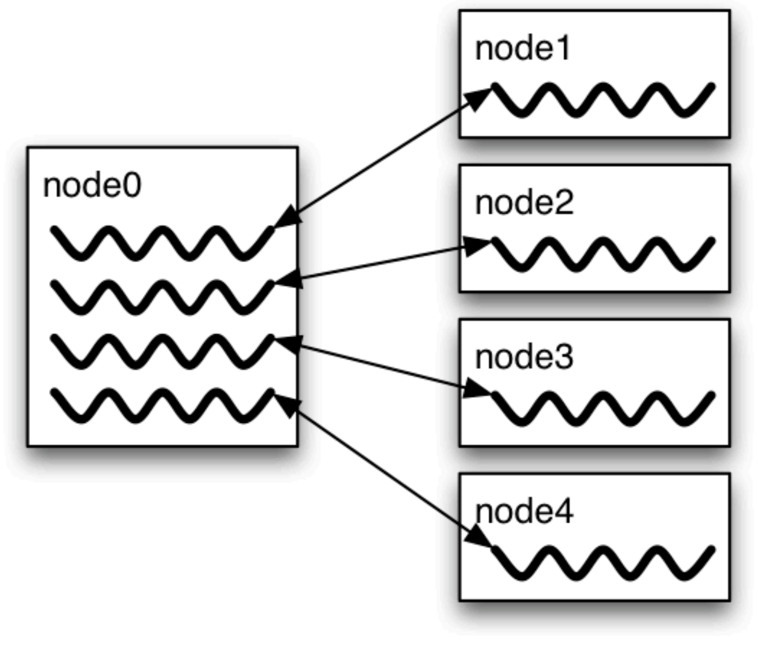
The Current Situation

- 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 "thread-safe" MPI for many hybrid programs
  - But watch out for Amdahl's Law!

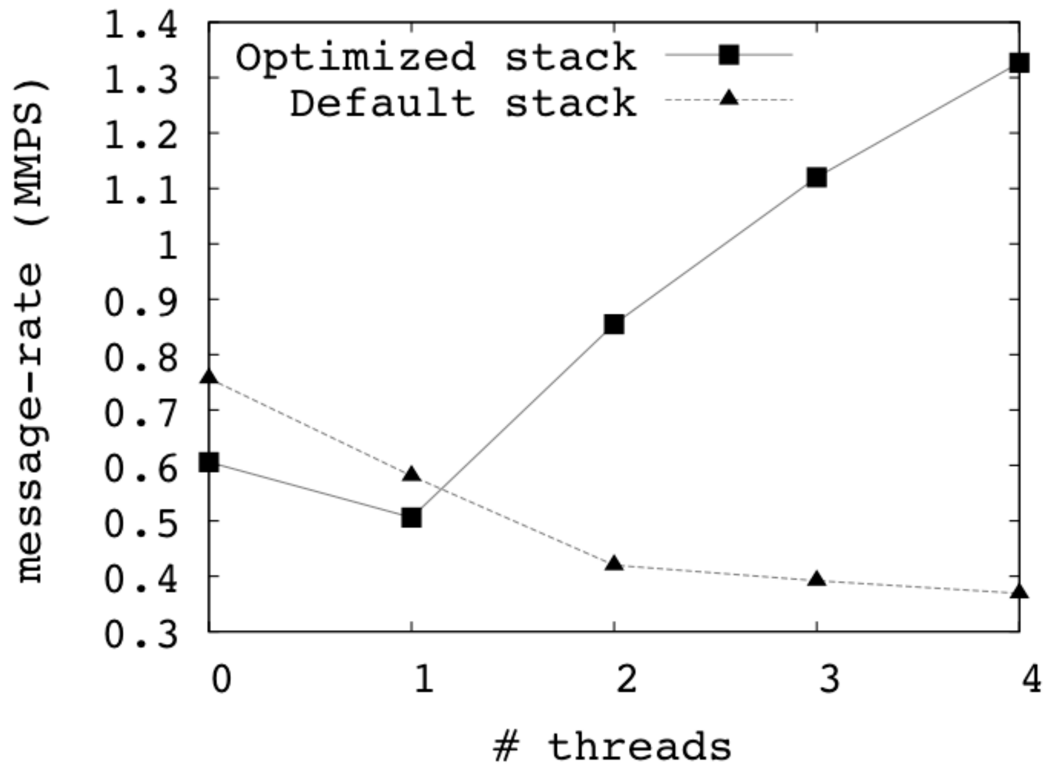
Performance with MPI_THREAD_MULTIPLE

- Thread safety does not come for free
- The implementation must access/modify several shared objects (e.g. message queues) in a consistent manner
- To measure the performance impact, we ran tests to measure communication performance when using multiple threads versus multiple processes
  - For results, see Thakur/Gropp paper: "Test Suite for Evaluating Performance of Multithreaded MPI Communication," *Parallel Computing*, 2009

Message Rate Results on BG/P



Message Rate Benchmark



"Enabling Concurrent Multithreaded MPI Communication on Multicore Petascale Systems" EuroMPI 2010

Why is it hard to optimize MPI_THREAD_MULTIPLE

- MPI internally maintains several resources
- Because of MPI semantics, it is required that all threads have access to some of the data structures
  - E.g., thread 1 can post an `Irecv`, and thread 2 can wait for its completion – thus the request queue has to be shared between both threads
  - Since multiple threads are accessing this shared queue, thread-safety is required to ensure a consistent state of the queue – adds a lot of overhead

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)

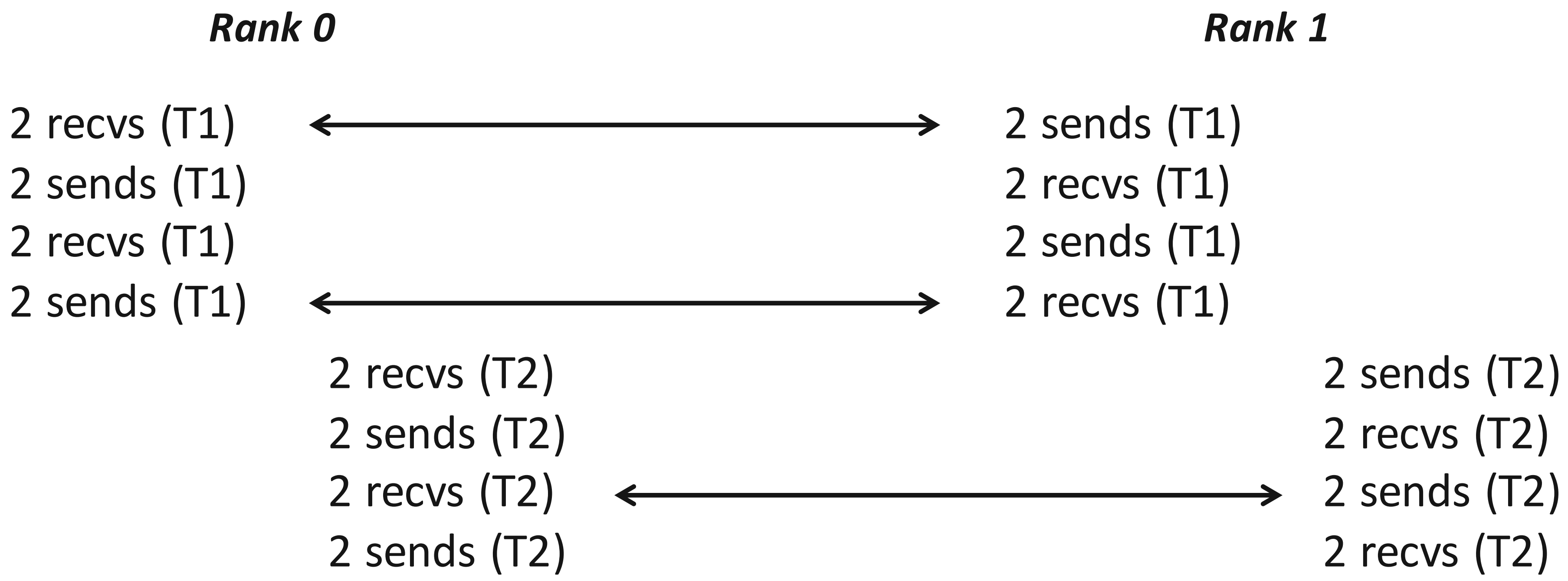
An Example we encountered

- 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

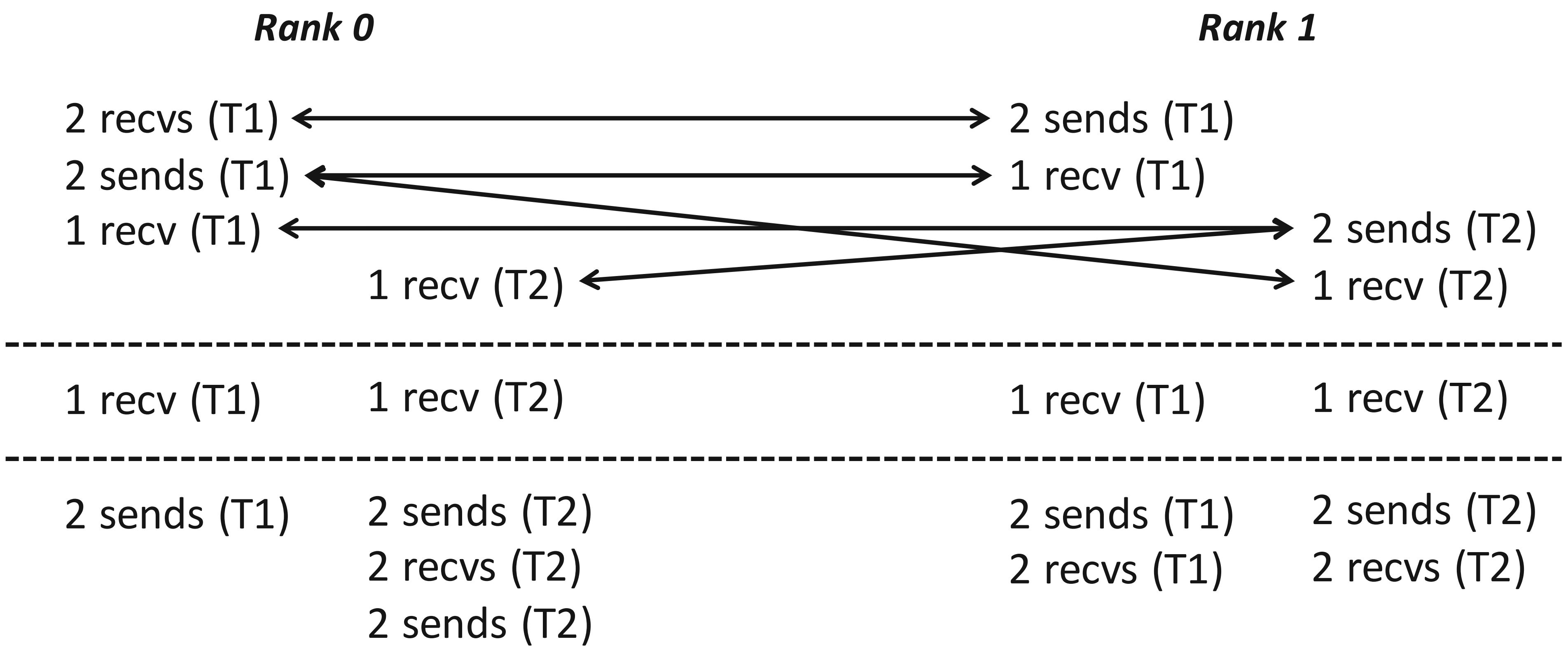
```
for (j = 0; j < 2; j++) {
    if (rank == 1) {
        for (i = 0; i < 2; i++)
            MPI_Send(NULL, 0, MPI_CHAR, 0, 0, MPI_COMM_WORLD);
        for (i = 0; i < 2; i++)
            MPI_Recv(NULL, 0, MPI_CHAR, 0, 0, MPI_COMM_WORLD, &stat);
    }
    else { /* rank == 0 */
        for (i = 0; i < 2; i++)
            MPI_Recv(NULL, 0, MPI_CHAR, 1, 0, MPI_COMM_WORLD, &stat);
        for (i = 0; i < 2; i++)
            MPI_Send(NULL, 0, MPI_CHAR, 1, 0, MPI_COMM_WORLD);
    }
}
```

Intended Ordering of Operations



- Every send matches a receive on the other rank

Possible Ordering of Operations in Practice



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

Some Things to Watch for in OpenMP

- Limited thread and no explicit memory affinity control (but see OpenMP 4.0 and the 4.1 Draft)
  - "First touch" (have intended "owning" thread perform first access) provides initial static mapping of memory
    - Next touch (move ownership to most recent thread) could help
  - No portable way to reassign memory affinity – reduces the effectiveness of OpenMP when used to improve load balancing.
- Memory model can require explicit "memory flush" operations
  - Defaults allow race conditions
  - Humans notoriously poor at recognizing all races
    - It only takes one mistake to create a hard-to-find bug

Some Things to Watch for in MPI + OpenMP

- No interface for apportioning resources between MPI and OpenMP
  - On an SMP node, how many MPI processes and how many OpenMP Threads?
    - Note the static nature assumed by this question
  - Note that having more threads than cores can be important for hiding latency
    - Requires very lightweight threads
- Competition for resources
  - Particularly memory bandwidth and network access
  - Apportionment of network access between threads and processes is also a problem, as we've already seen.

Where Does the MPI + OpenMP Hybrid Model Work Well?

- Compute-bound loops
  - Many operations per memory load
- Fine-grain parallelism
  - Algorithms that are latency-sensitive
- Load balancing
  - Similar to fine-grain parallelism; ease of
- Memory bound loops

Compute-Bound Loops

- Loops that involve many operations per load from memory
  - This can happen in some kinds of matrix assembly, for example.
  - Jacobi update not compute bound

Fine-Grain Parallelism

- Algorithms that require frequent exchanges of small amounts of data
- E.g., in blocked preconditioners, where fewer, larger blocks, each managed with OpenMP, as opposed to more, smaller, single-threaded blocks in the all-MPI version, gives you an algorithmic advantage (e.g., fewer iterations in a preconditioned linear solution algorithm).
- Even if memory bound

Load Balancing

- Where the computational load isn't exactly the same in all threads/processes; this can be viewed as a variation on fine-grained access.
- OpenMP schedules can handle some of this
  - For very fine grain cases, a mix of static and dynamic scheduling may be more efficient
  - Current research looking at more elaborate and efficient schedules for this case

Memory-Bound Loops

- Where read data is shared, so that cache memory can be used more efficiently.
- Example: Table lookup for evaluating equations of state
  - Table can be shared
  - If table evaluated as necessary, evaluations can be shared

Where is Pure MPI Better?

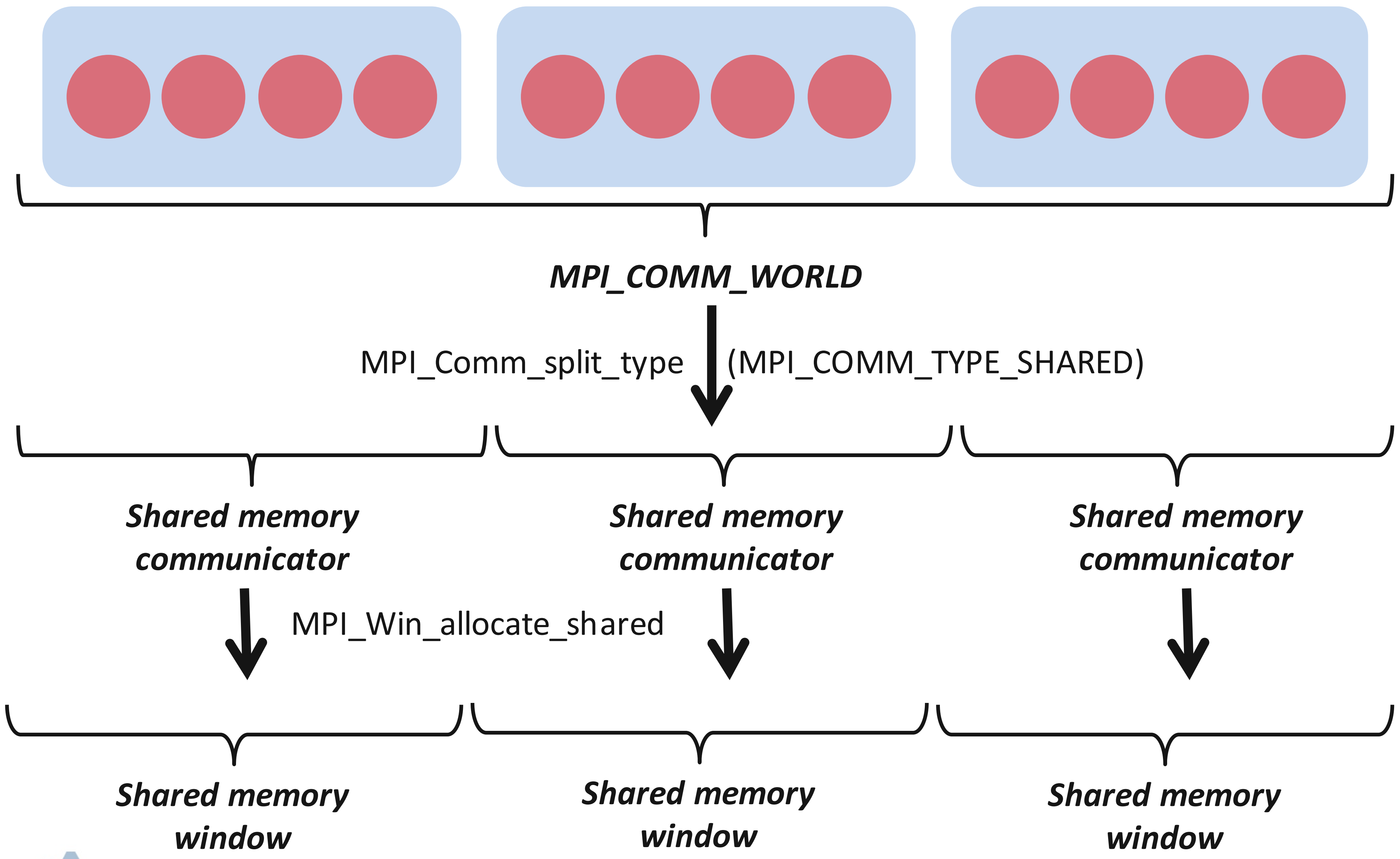
- Trying to use OpenMP + MPI on very regular, memory-bandwidth-bound computations is likely to lose because of the better, programmer-enforced memory locality management in the pure MPI version.
- Another reason to use more than one MPI process - if a single process (or thread) can't saturate the interconnect - then use multiple communicating processes or threads.
  - Note that threads and processes are not equal

MPI + Shared-Memory

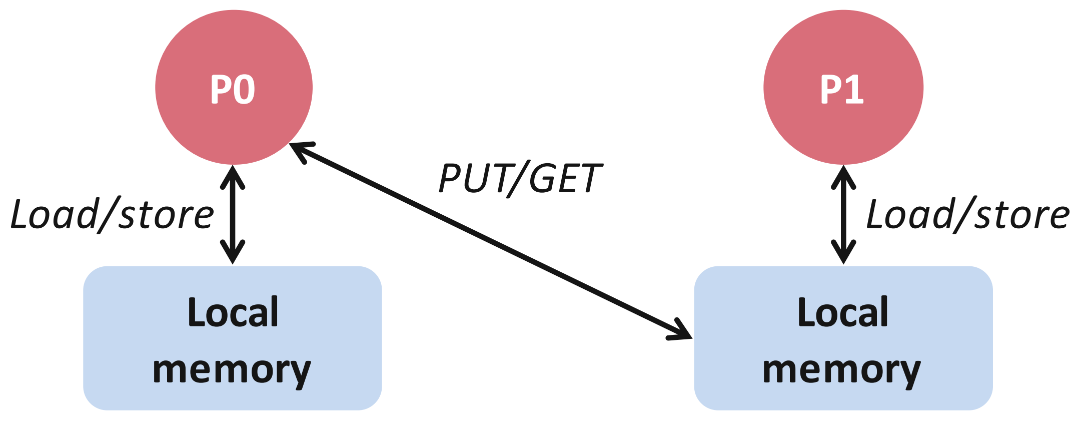
Hybrid Programming with Shared Memory

- 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

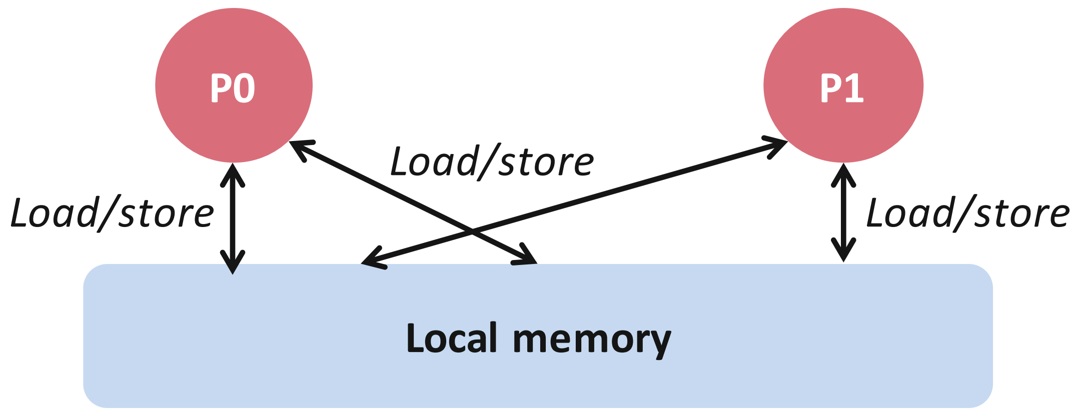
Creating Shared Memory Regions in MPI


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"
- 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)

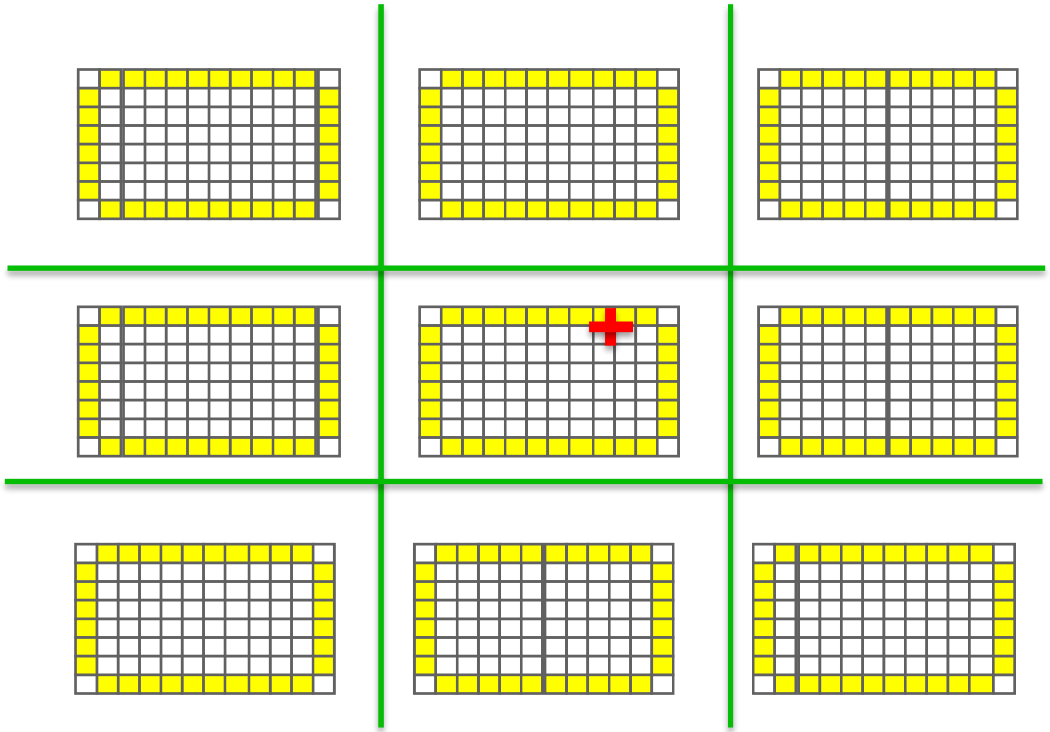
Shared Arrays with Shared memory windows

```
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;
}
```

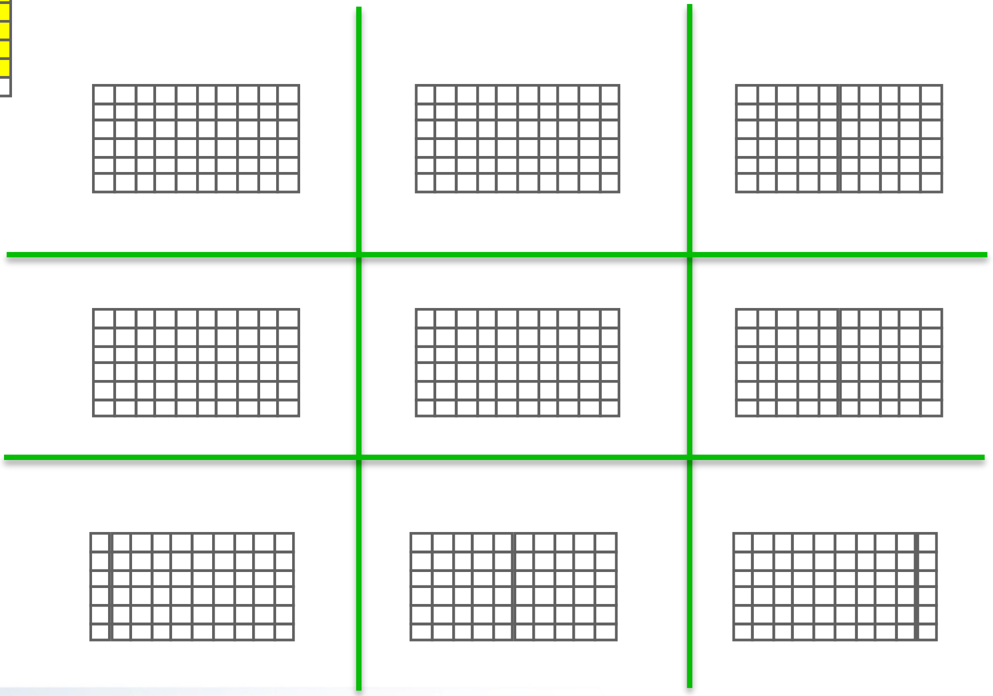
Memory allocation and placement

- 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

Example Computation: Stencil



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.

Walkthrough of 2D Stencil Code with Shared Memory Windows

- *stencil_mpi_shmem.c*

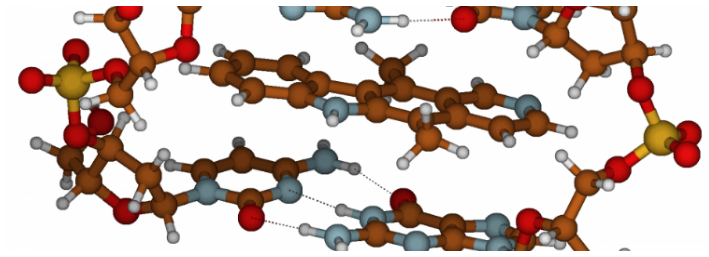
Which Hybrid Programming Method to Adopt?

- 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

Example: Quantum Monte Carlo

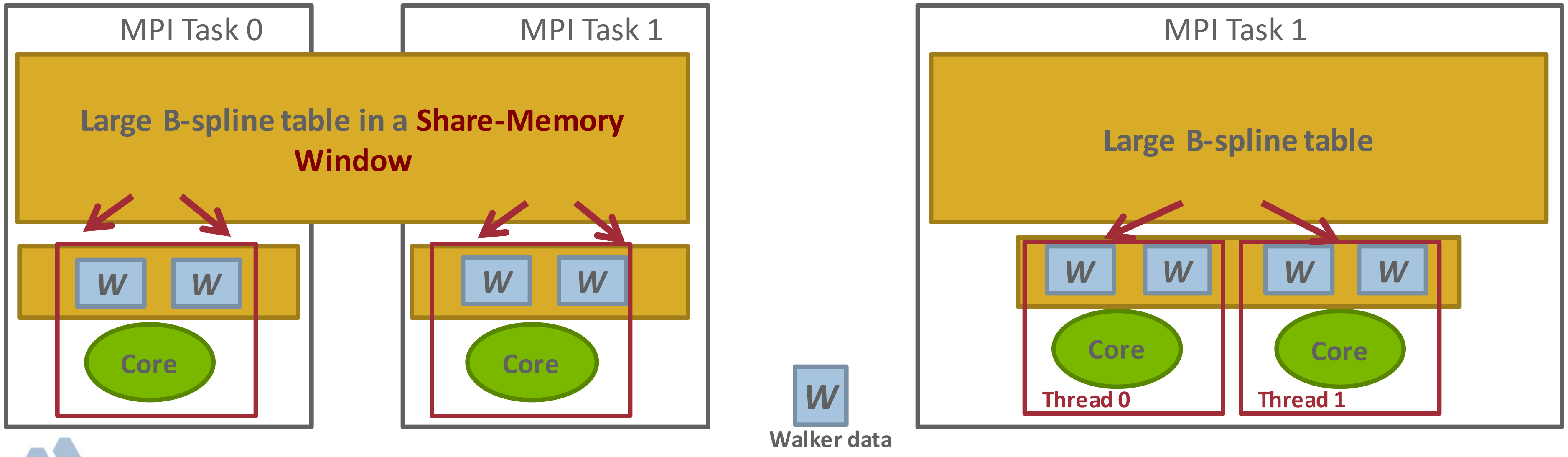
- Memory capacity bound with MPI-only
- Hybrid approaches
  - MPI + threads (e.g. X = OpenMP, Pthreads)
  - MPI + shared-memory (X = MPI)
- Can use direct load/store operations instead of message passing

QMCPACK



MPI + Shared-Memory (MPI 3.0)
- **Everything private by default**
- **Expose shared data explicitly**

MPI + Threads
- **Share everything by default**
- **Privatize data when necessary**



MPI + Accelerators

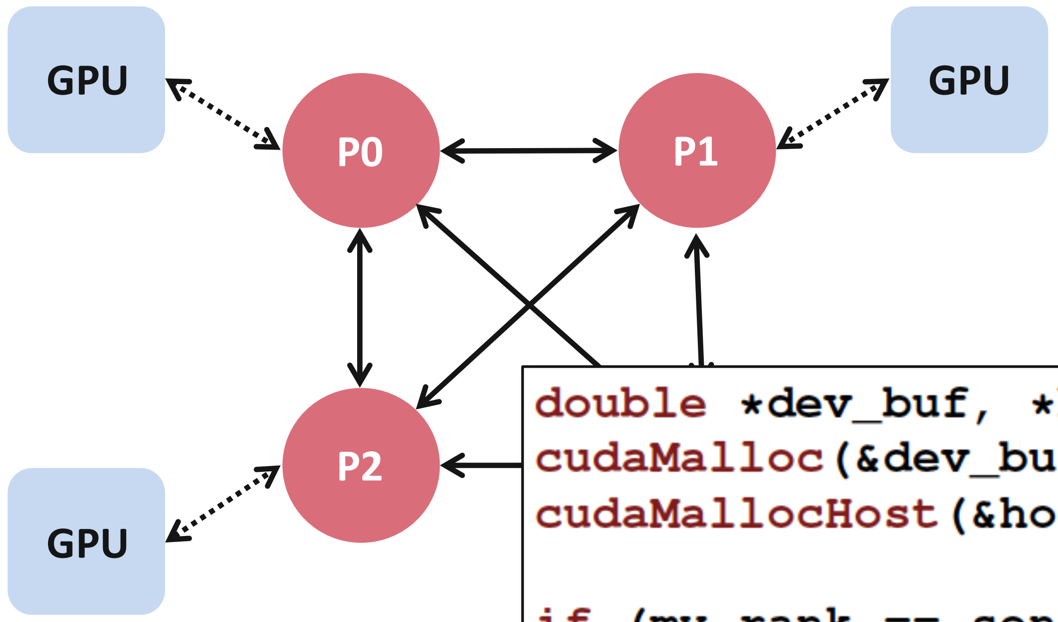
Accelerators in Parallel Computing

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

Hybrid Programming with Accelerators

- Many users are looking to use accelerators within their MPI applications
- The MPI standard does not provide any special semantics to interact with accelerators
  - Current MPI threading semantics are considered sufficient by most users
  - There are some research efforts for making accelerator memory directly accessibly by MPI, but those are not a part of the MPI standard

Current Model for MPI+Accelerator Applications



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

if (my_rank == sender) { /* sender */
  computation_on_GPU(dev_buf);
  cudaMemcpy(host_buf, dev_buf, size, ...);
  MPI_Send(host_buf, size, ...);
} else {                 /* receiver */
  MPI_Recv(host_buf, size, ...);
  cudaMemcpy(dev_buf, host_buf, size, ...);
  computation_on_GPU(dev_buf);
}
```

Alternate MPI+Accelerator models being studied

- Some MPI implementations (MPICH, Open MPI, MVAPICH) are investigating how the MPI implementation can directly send/receive data from accelerators
  - Unified virtual address (UVA) space techniques where all memory (including accelerator memory) is represented with a “void *”
  - Communicator and datatype attribute models where users can inform the MPI implementation of where the data resides
- Clear performance advantages demonstrated in research papers, but these features are not yet a part of the MPI standard (as of MPI-3.1)
  - Could be incorporated in a future version of the standard

Advanced Topics: Nonblocking Collectives, Topologies, and Neighborhood Collectives

Nonblocking Collective Communication

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

Nonblocking Collective Communication

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

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

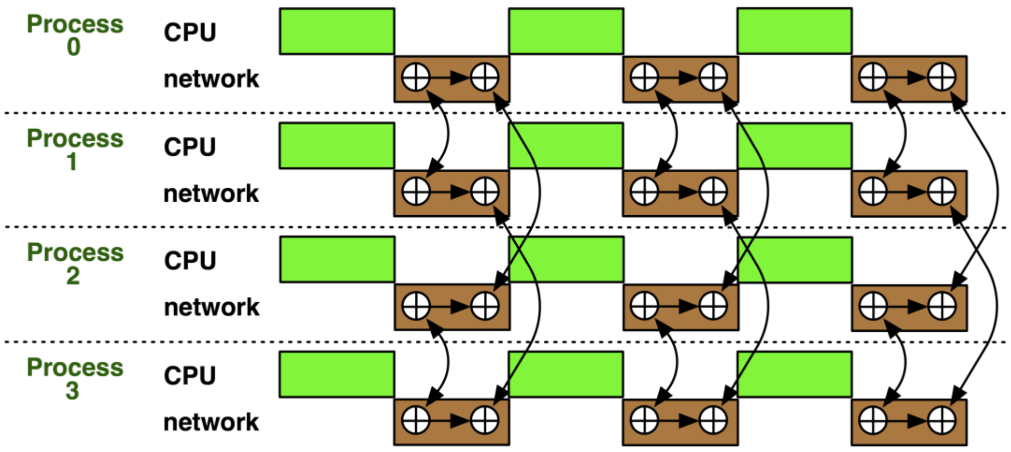
Nonblocking Collective Communication

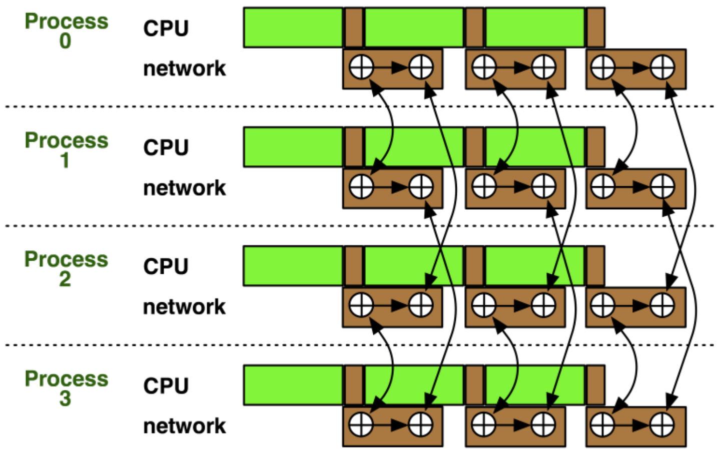
- Semantic advantages
  - Enable asynchronous progression (and manual)
    - Software pipelining
  - Decouple data transfer and synchronization
    - Noise resiliency!
  - Allow overlapping communicators
    - See also neighborhood collectives
  - Multiple outstanding operations at any time
    - Enables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

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

Nonblocking Collectives Overlap

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





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

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!

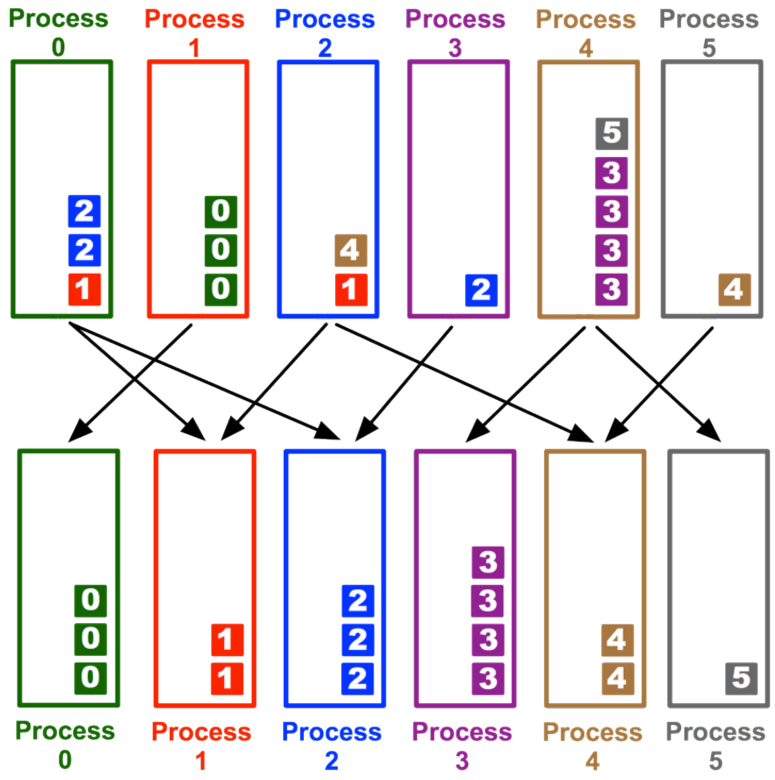
A Semantics Example: DSDE

- Dynamic Sparse Data Exchange
  - Dynamic: comm. pattern varies across iterations
  - Sparse: number of neighbors is limited (O(log P))
  - Data exchange: only senders know neighbors
- Main Problem: metadata
  - Determine who wants to send how much data to me

(I must post receive and reserve memory)

OR:

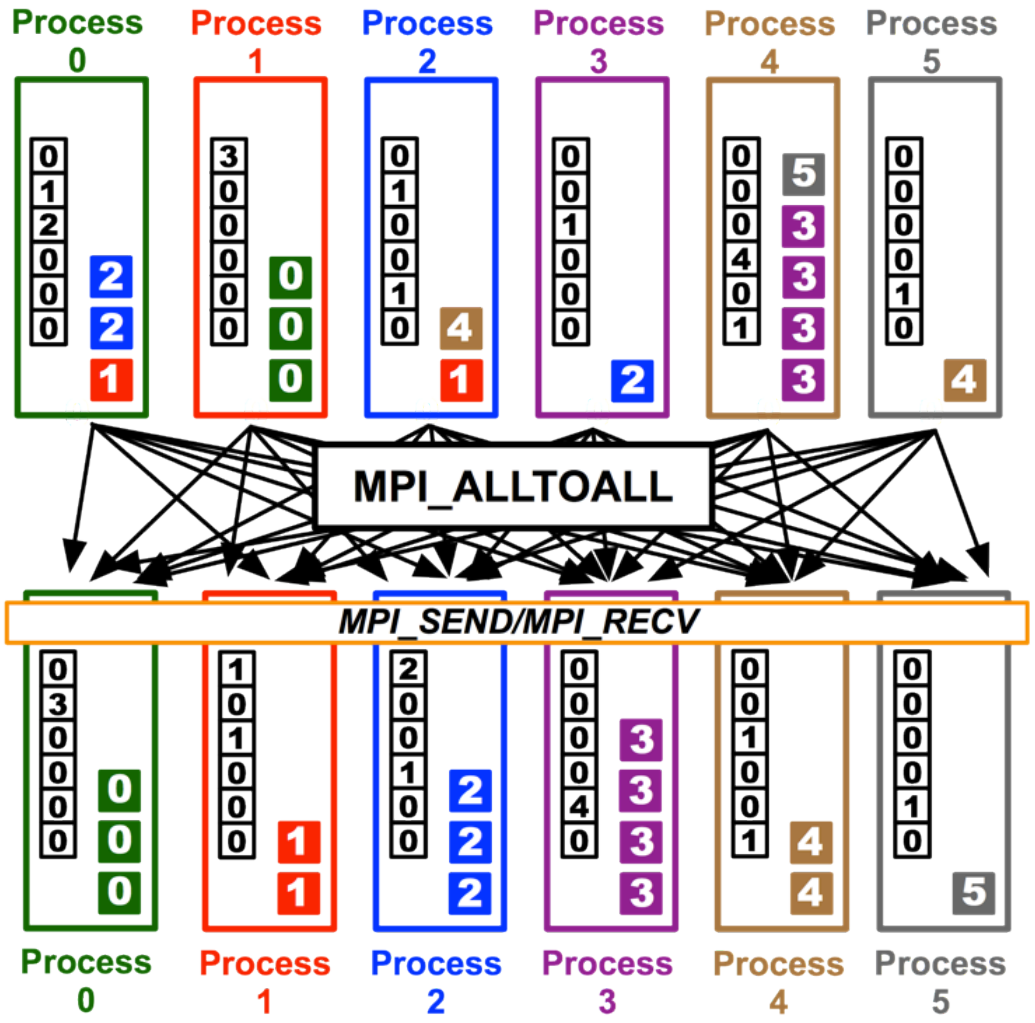
  - Use MPI semantics:
    - Unknown sender (MPI_ANY_SOURCE)
    - Unknown message size (MPI_PROBE)
    - Reduces problem to counting the number of neighbors
    - Allow faster implementation!



Hoefler et al.: Scalable Communication Protocols for Dynamic Sparse Data Exchange

Using Alltoall (PEX)

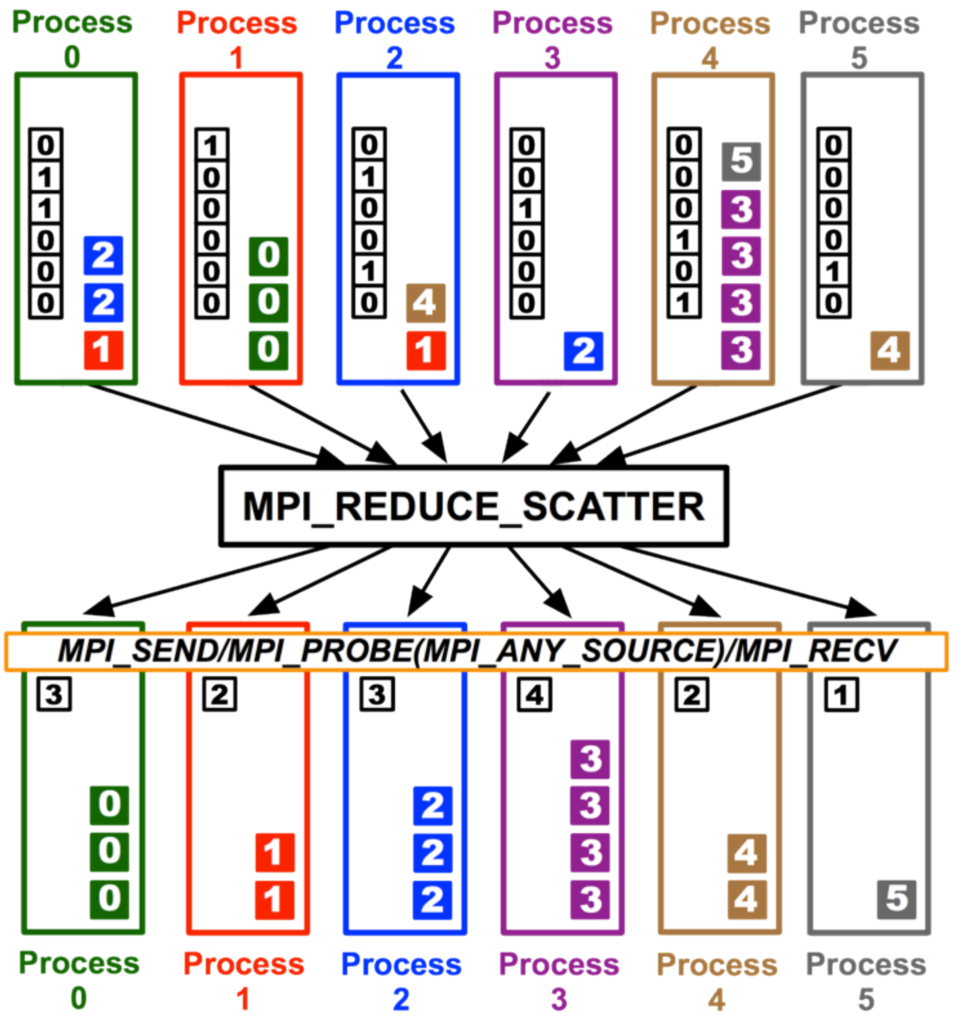
- Based on Personalized Exchange ($\Theta(P)$)
  - Processes exchange metadata (sizes) about neighborhoods with all-to-all
  - Processes post receives afterwards
  - Most intuitive but least performance and scalability!



T. Hoefler et al.: Scalable Communication Protocols for Dynamic Sparse Data Exchange

Reduce_scatter (PCX)

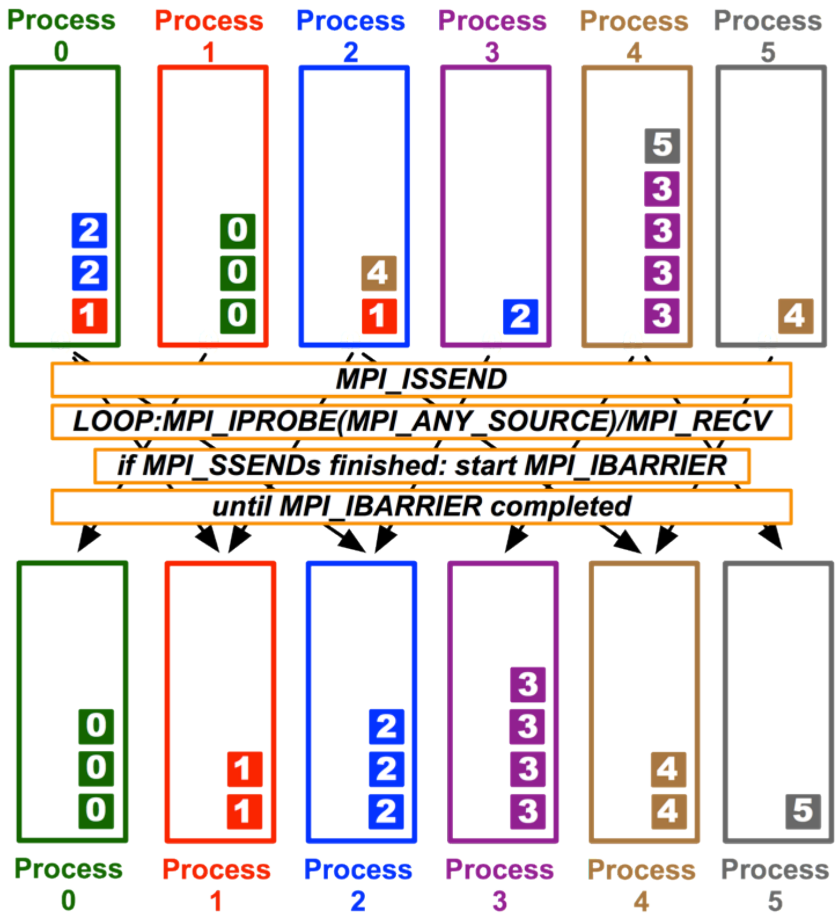
- Bases on Personalized Census ($\Theta(P)$)
  - Processes exchange metadata (counts) about neighborhoods with reduce_scatter
  - Receivers checks with wildcard MPI_IPROBE and receives messages
  - Better than PEX but non-deterministic!



T. Hoefler et al.:Scalable Communication Protocols for Dynamic Sparse Data Exchange

MPI_Ibarrier (NBX)

- Complexity - census (barrier): ($\Theta(\log(P))$)
  - Combines metadata with actual transmission
  - Point-to-point synchronization
  - Continue receiving until barrier completes
  - Processes start coll. synch. (barrier) when p2p phase ended
    - barrier = distributed marker!
  - Better than Alltoall, reduce-scatter!

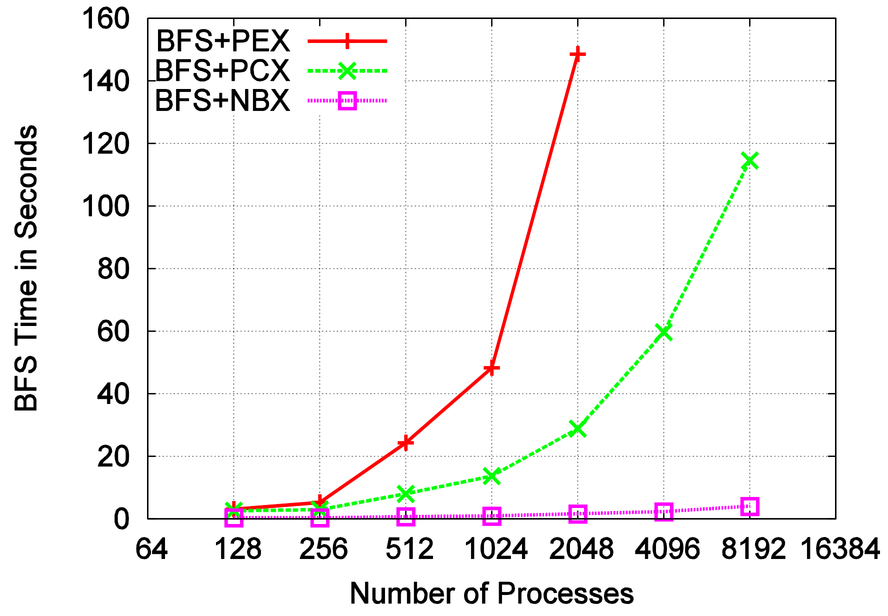


T. Hoefler et al.: Scalable Communication Protocols for Dynamic Sparse Data Exchange

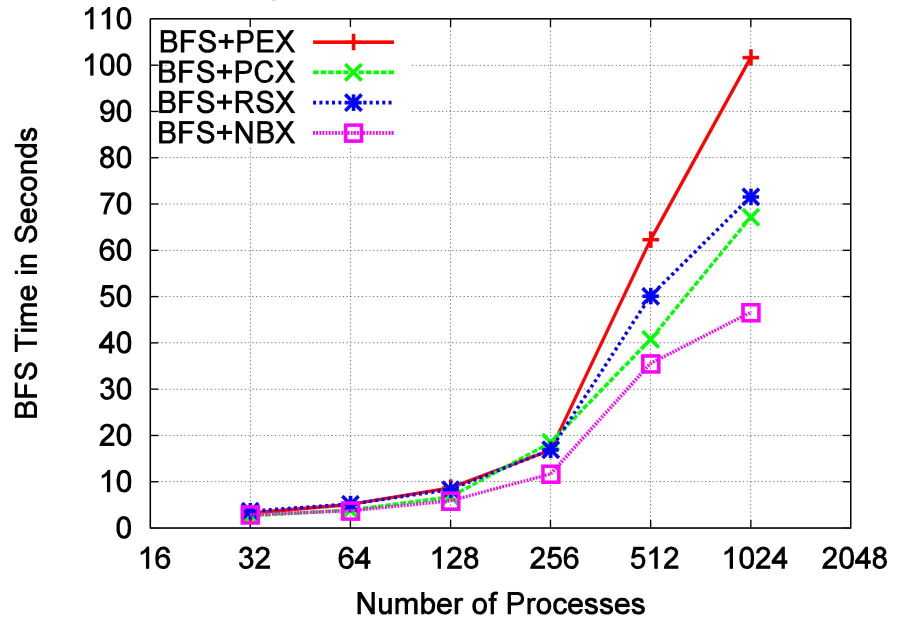
Parallel Breadth First Search

- On a clustered Erdős-Rényi graph, weak scaling
  - 6.75 million edges per node (filled 1 GiB)

BlueGene/P – with HW barrier!



Myrinet 2000 with LibNBC

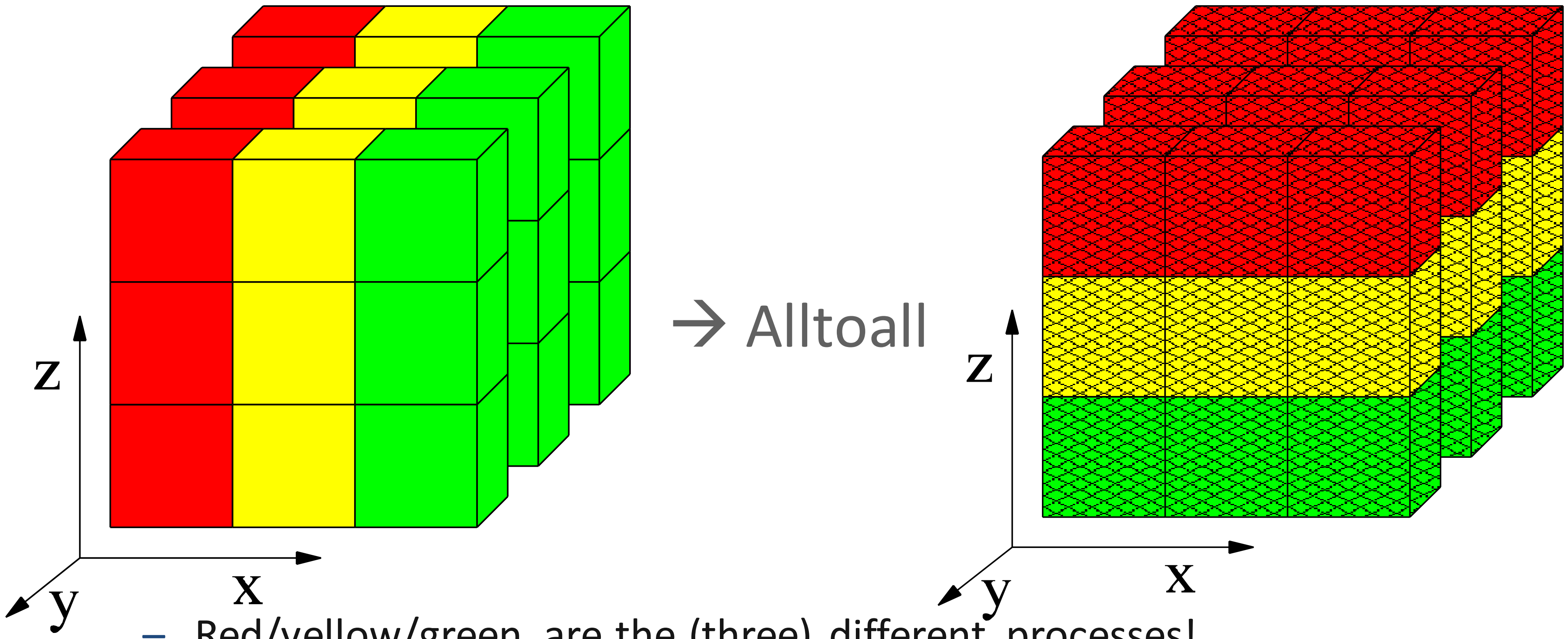


- HW barrier support is significant at large scale!

T. Hoefler et al.: Scalable Communication Protocols for Dynamic Sparse Data Exchange

Parallel Fast Fourier Transform

- 1D FFTs in all three dimensions
  - Assume 1D decomposition (each process holds a set of planes)
  - Best way: call optimized 1D FFTs in parallel → alltoall



  - Red/yellow/green are the (three) different processes!

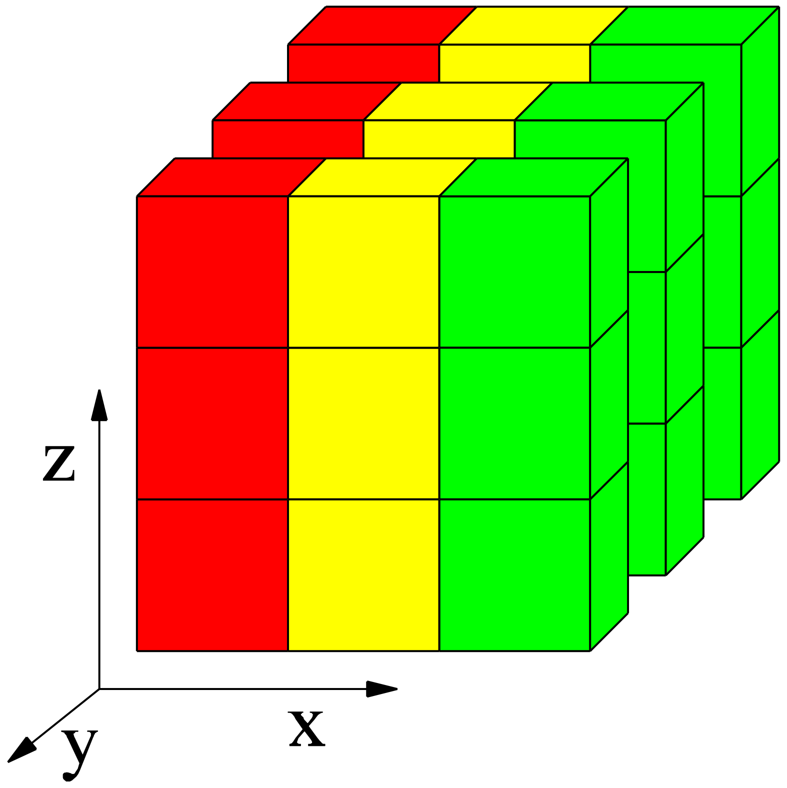
A Complex Example: FFT

```
for(int x=0; x<n/p; ++x) 1d_fft(/* x-th stencil */);

// pack data for alltoall
MPI_Alltoall(&in, n/p*n/p, cplx_t, &out, n/p*n/p, cplx_t, comm);
// unpack data from alltoall and transpose

for(int y=0; y<n/p; ++y) 1d_fft(/* y-th stencil */);

// pack data for alltoall
MPI_Alltoall(&in, n/p*n/p, cplx_t, &out, n/p*n/p, cplx_t, comm);
// unpack data from alltoall and transpose
```

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

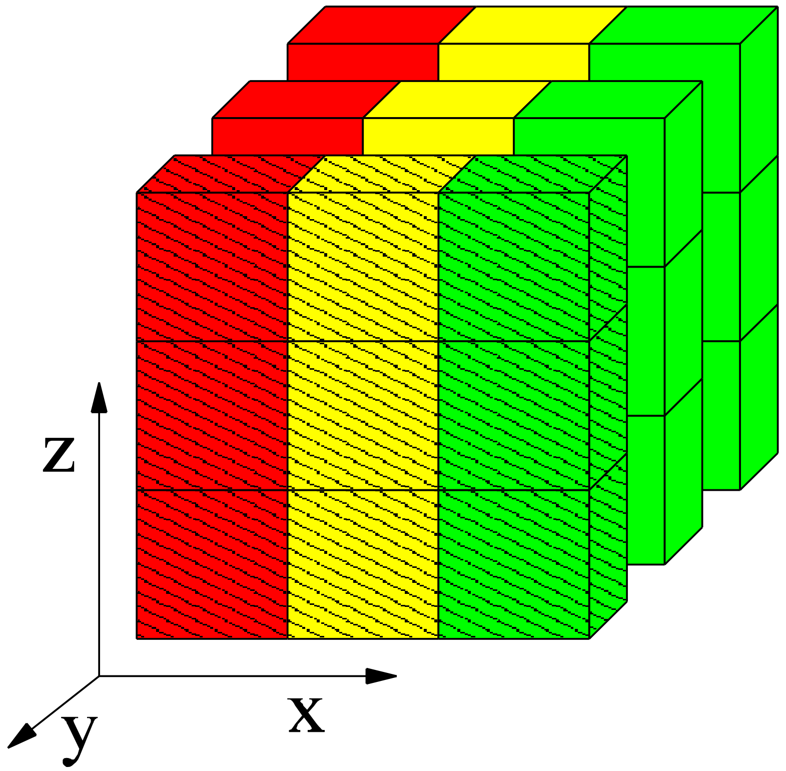
Parallel Fast Fourier Transform

- Data already transformed in y-direction



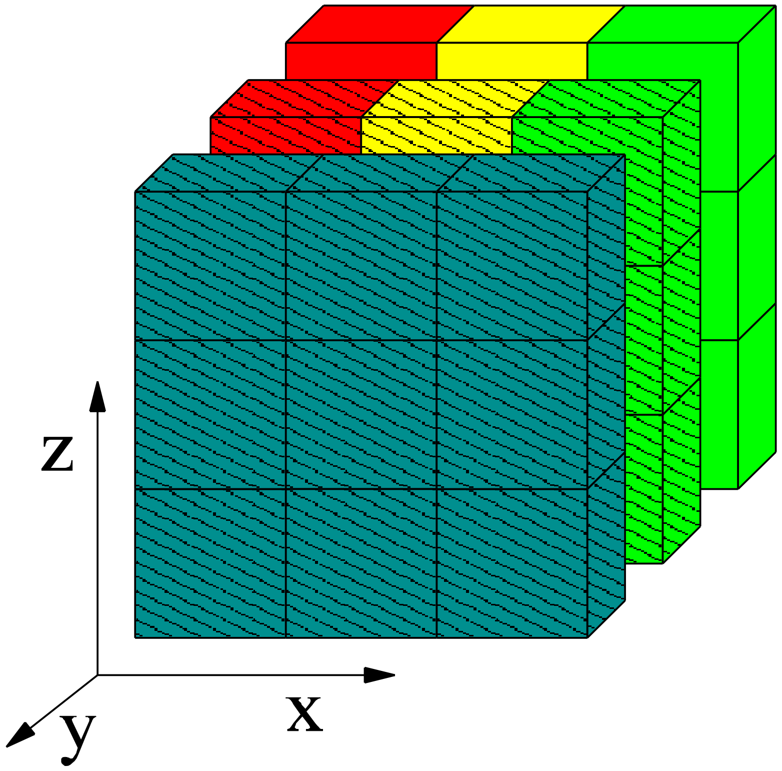
Parallel Fast Fourier Transform

- Transform first y plane in z



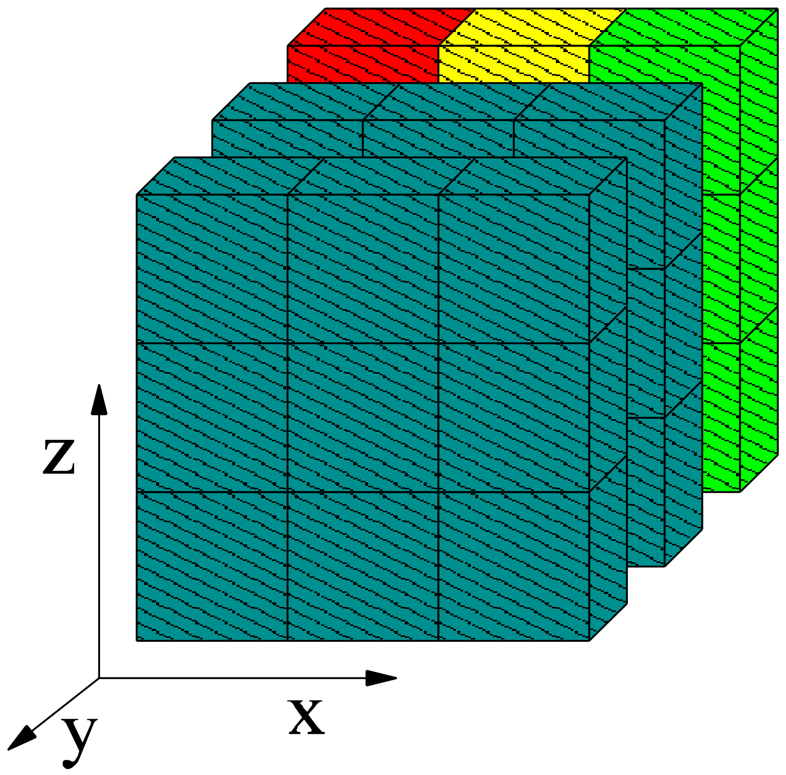
Parallel Fast Fourier Transform

- Start ialltoall and transform second plane



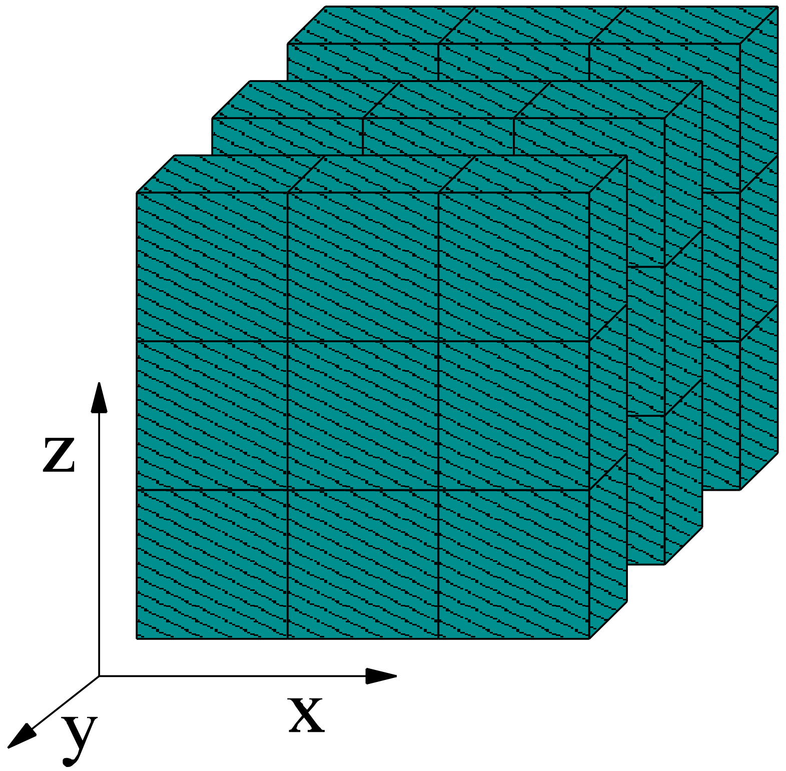
Parallel Fast Fourier Transform

- Start ialltoall (second plane) and transform third



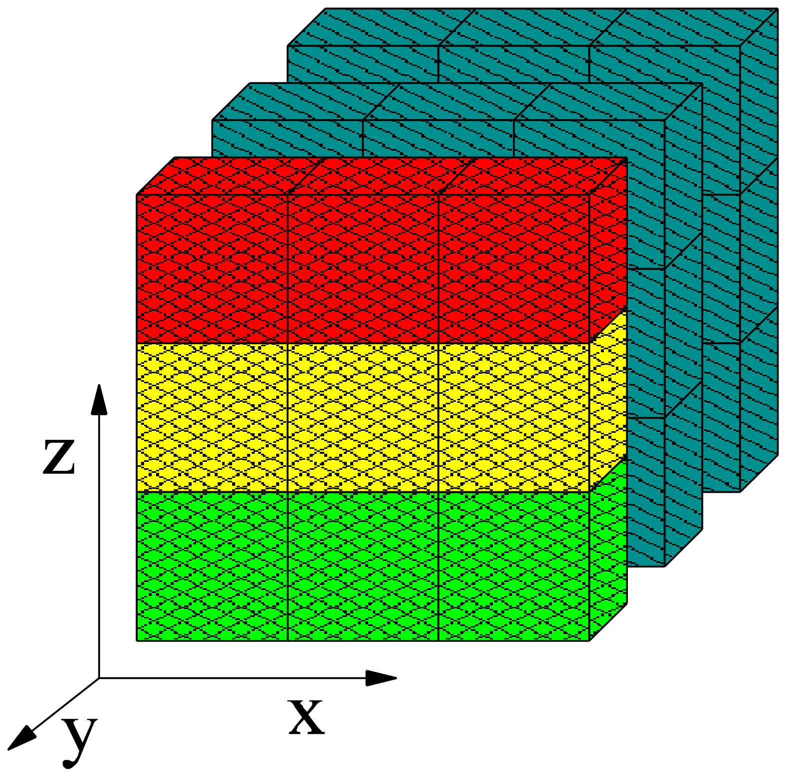
Parallel Fast Fourier Transform

- Start ialltoall of third plane and …



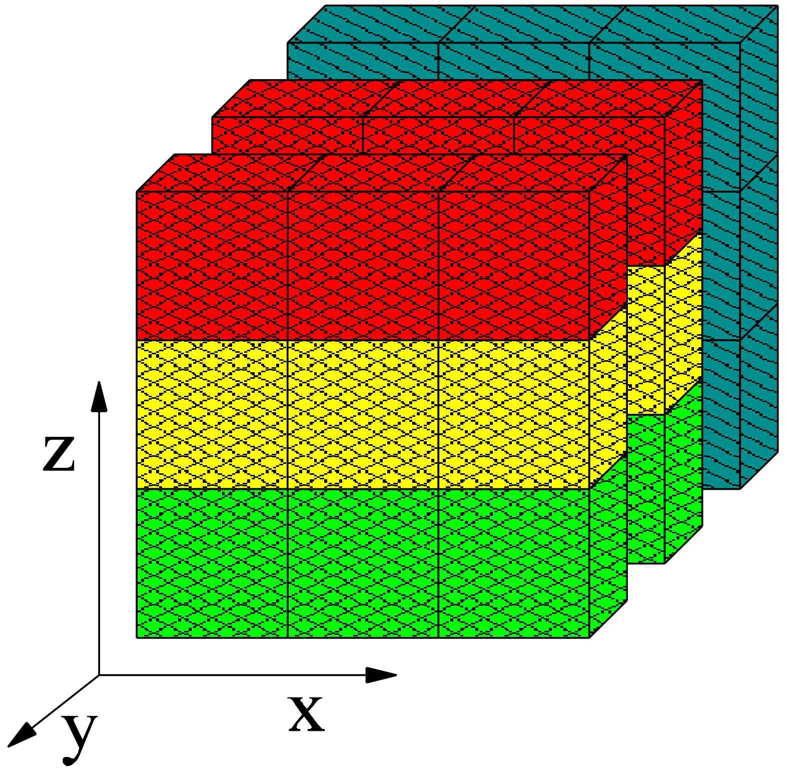
Parallel Fast Fourier Transform

- Finish ialltoall of first plane, start x transform



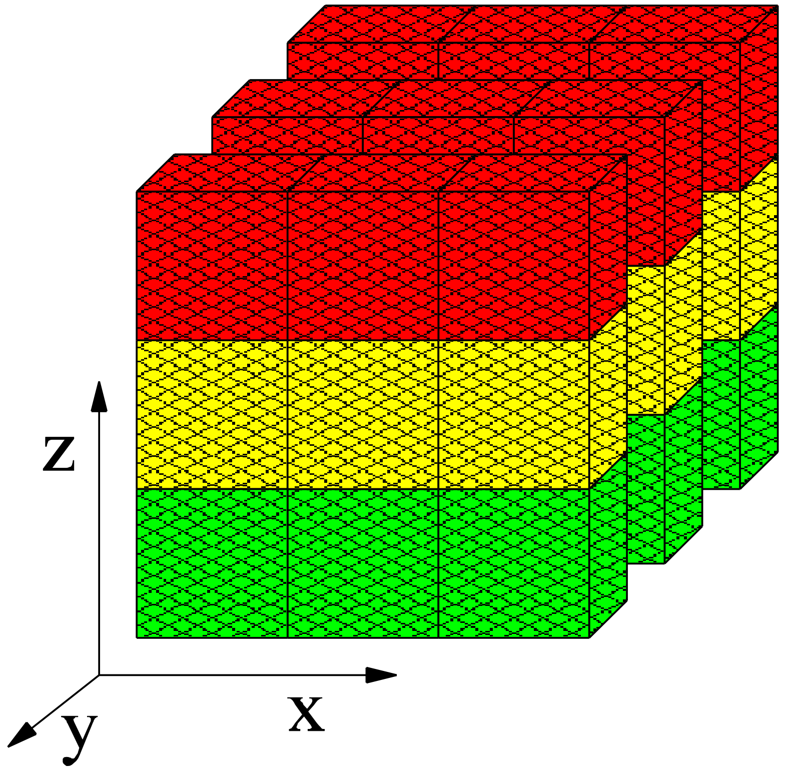
Parallel Fast Fourier Transform

- Finish second ialltoall, transform second plane



Parallel Fast Fourier Transform

- Transform last plane → done



FFT Software Pipelining

```
MPI_Request req[nb];
for(int b=0; b<nb; ++b) { // loop over blocks
  for(int x=b*n/p/nb; x<(b+1)n/p/nb; ++x) 1d_fft(/* x-th stencil*/);

  // pack b-th block of data for alltoall
  MPI_Ialltoall(&in, n/p*n/p/bs, cplx_t, &out, n/p*n/p, cplx_t, comm, &req[b]);
}
MPI_Waitall(nb, req, MPI_STATUSES_IGNORE);

// modified unpack data from alltoall and transpose
for(int y=0; y<n/p; ++y) 1d_fft(/* y-th stencil */);
// pack data for alltoall
MPI_Alltoall(&in, n/p*n/p, cplx_t, &out, n/p*n/p, cplx_t, comm);
// unpack data from alltoall and transpose
```

Nonblocking Collectives Summary

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

Topologies and Topology Mapping

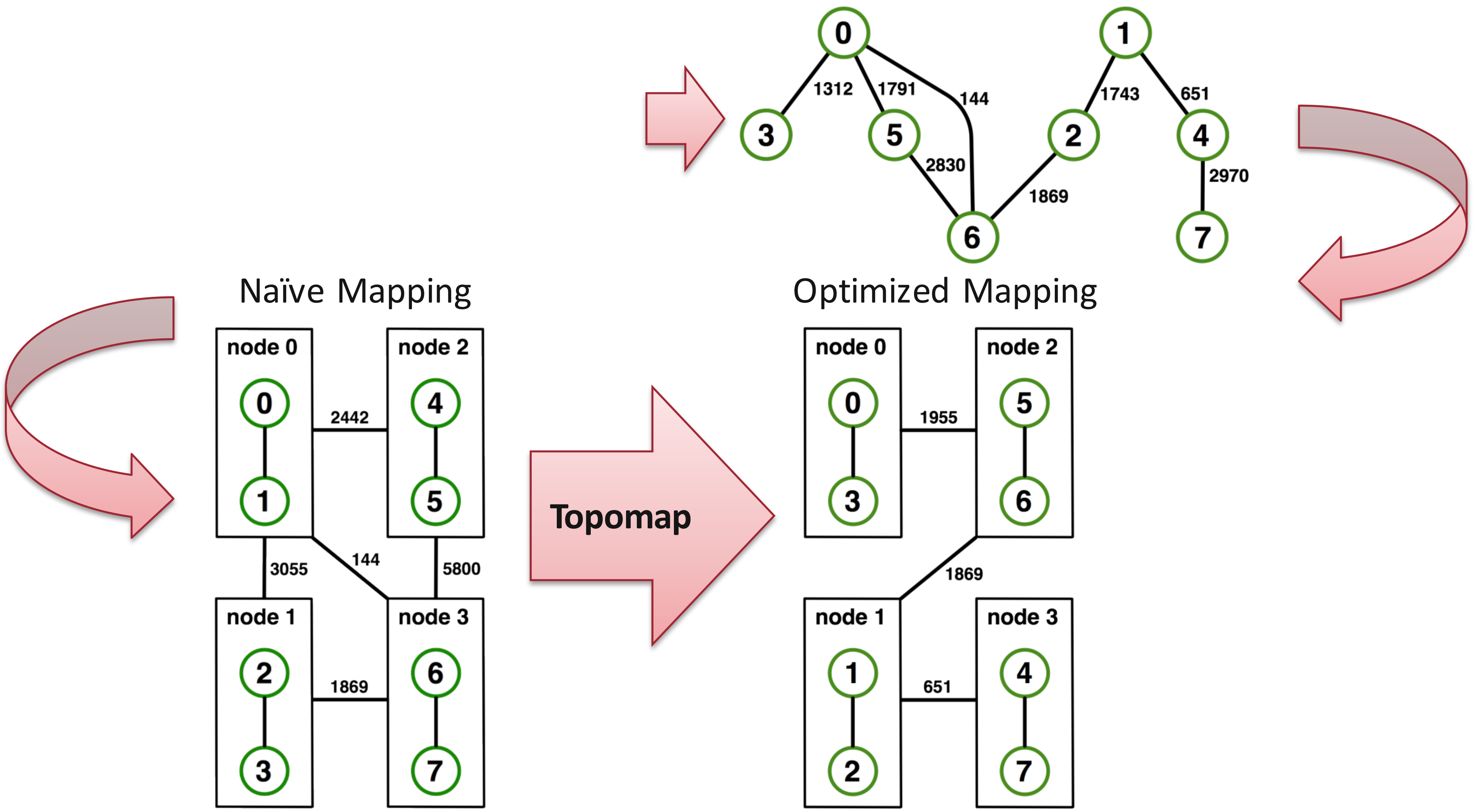
Topology Mapping and Neighborhood Collectives

- Topology mapping basics
  - Allocation mapping vs. rank reordering
  - Ad-hoc solutions vs. portability
- MPI topologies
  - Cartesian
  - Distributed graph
- Collectives on topologies – neighborhood collectives
  - Use cases

Topology Mapping Basics

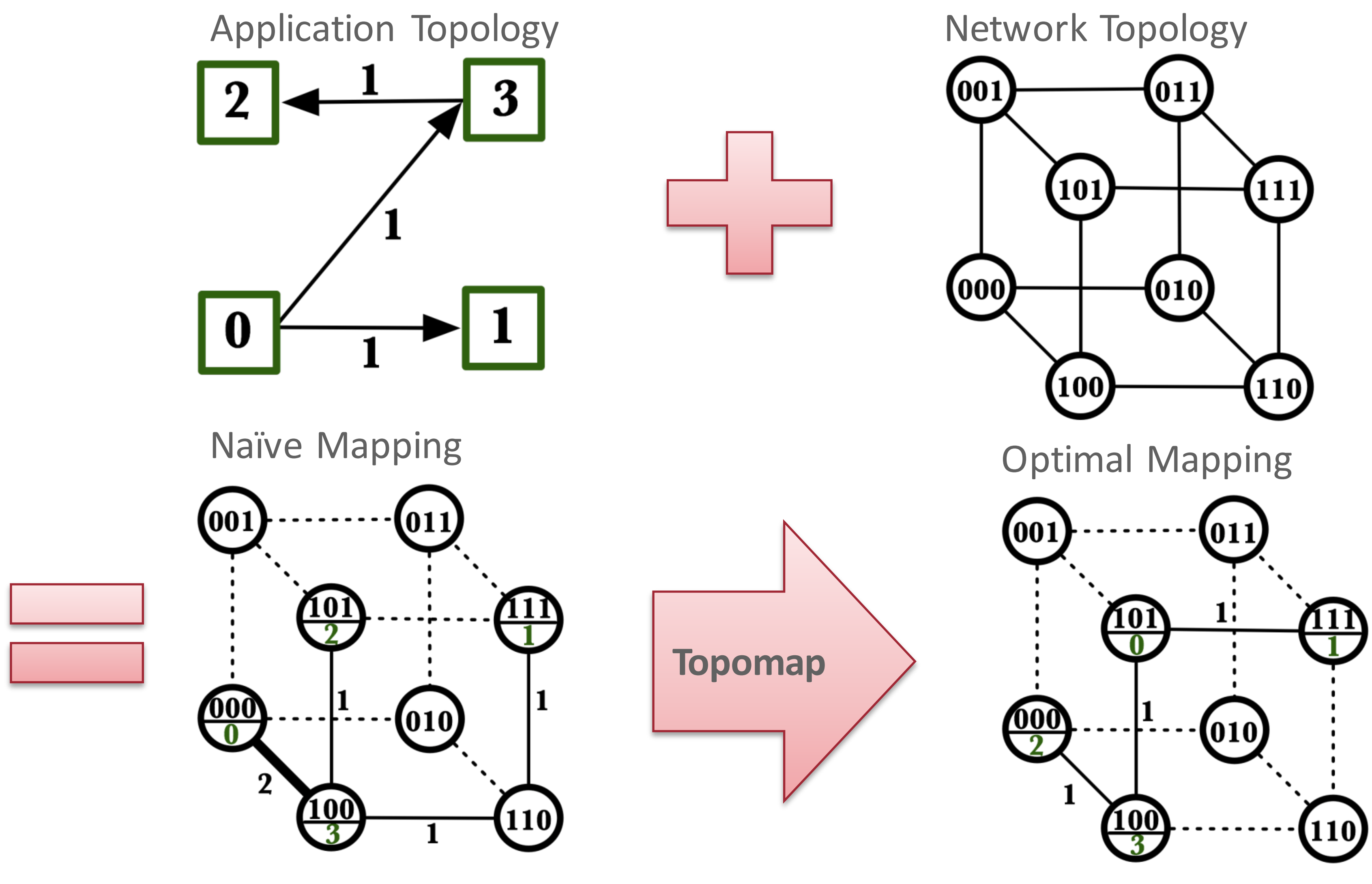
- MPI supports rank reordering
  - Change numbering in a given allocation to reduce congestion or dilation
  - Sometimes automatic (early IBM SP machines)
- Properties
  - Always possible, but effect may be limited (e.g., in a bad allocation)
  - Portable way: MPI process topologies
    - Network topology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

Example: On-Node Reordering



Gottschling et al.: Productive Parallel Linear Algebra Programming with Unstructured Topology Adaption

Off-Node (Network) Reordering



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_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 sum 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);
```

- Creates logical 3D Torus of size 5 x 5 x 5
- 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!

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

MPI_Dims_create Example

```
int p;
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

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

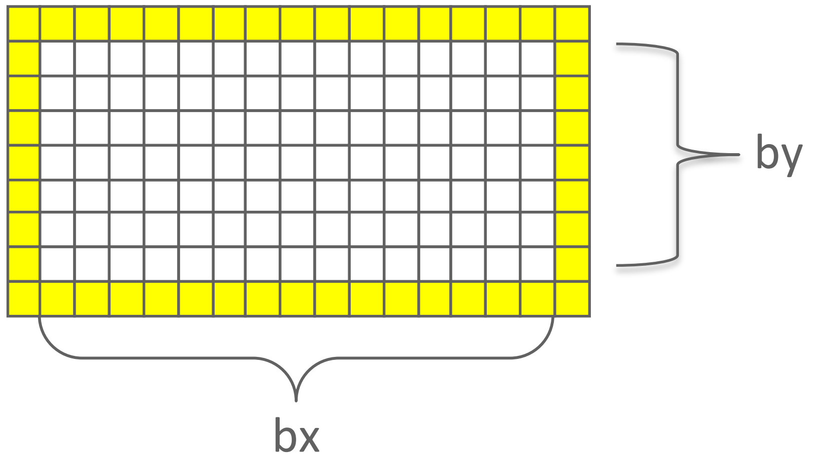
Cartesian Communication Helpers

```
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
  - No “over the edge” though

Code Example

- *stencil-mpi-carttopo.c*
- Adds calculation of neighbors with topology



MPI_Graph_create

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

- Don't use!!!!!
- nnodes is the total number of nodes
- index i stores the total number of neighbors for the first i nodes (sum)
  - Acts as offset into edges array
- edges stores the edge list for all processes
  - Edge list for process j starts at index[j] in edges
  - Process j has index[j+1]-index[j] edges

Distributed graph constructor

- MPI_Graph_create is discouraged
  - Not scalable
  - Not deprecated yet but hopefully soon
- New distributed interface:
  - Scalable, allows distributed graph specification
    - Either local neighbors **or** any edge in the graph
  - Specify edge weights
    - Meaning undefined but optimization opportunity for vendors!
  - Info arguments
    - Communicate assertions of semantics to the MPI library
    - E.g., semantics of edge weights

Hoefler et al.: The Scalable Process Topology Interface of MPI 2.2

MPI_Dist_graph_create_adjacent

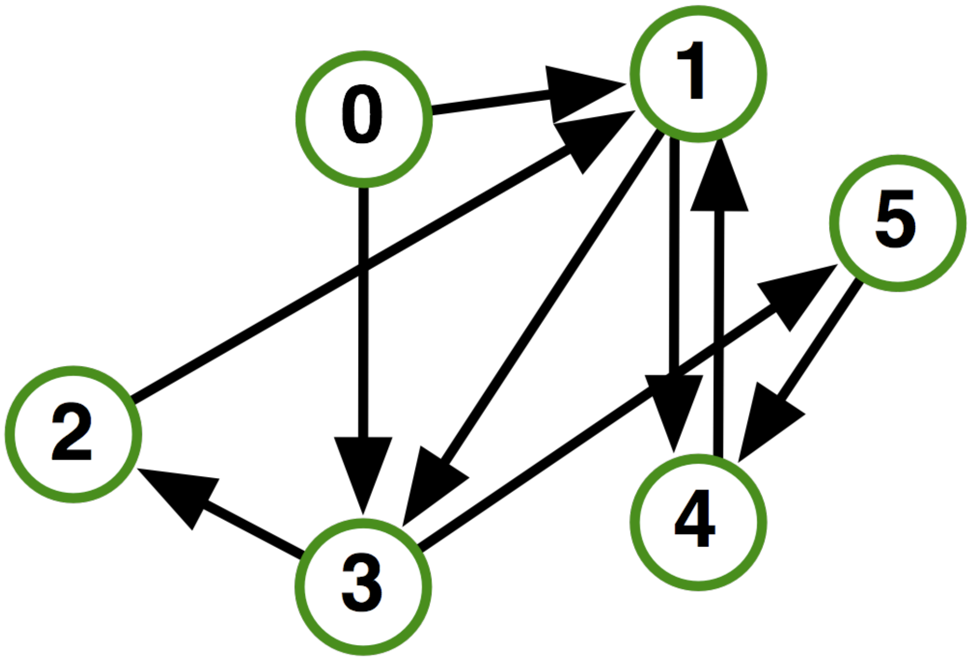
```
MPI_Dist_graph_create_adjacent(MPI_Comm  comm_old,
        int indegree, const int sources[], const int sourceweights[],
        int outdegree, const int destinations[],
        const int destweights[], MPI_Info info, int reorder,
        MPI_Comm *comm_dist_graph)
```

- indegree, sources, ~weights – source proc. Spec.
- outdegree, destinations, ~weights – dest. proc. spec.
- info, reorder, comm_dist_graph – as usual
- directed graph
- Each edge is specified twice, once as out-edge (at the source) and once as in-edge (at the dest)

Hoefler et al.: The Scalable Process Topology Interface of MPI 2.2

MPI_Dist_graph_create_adjacent

- Process 0:
  - Indegree: 0
  - Outdegree: 2
  - Dests: {3,1}
- Process 1:
  - Indegree: 3
  - Outdegree: 2
  - Sources: {4,0,2}
  - Dests: {3,4}
- …



Hoefler et al.: The Scalable Process Topology Interface of MPI 2.2

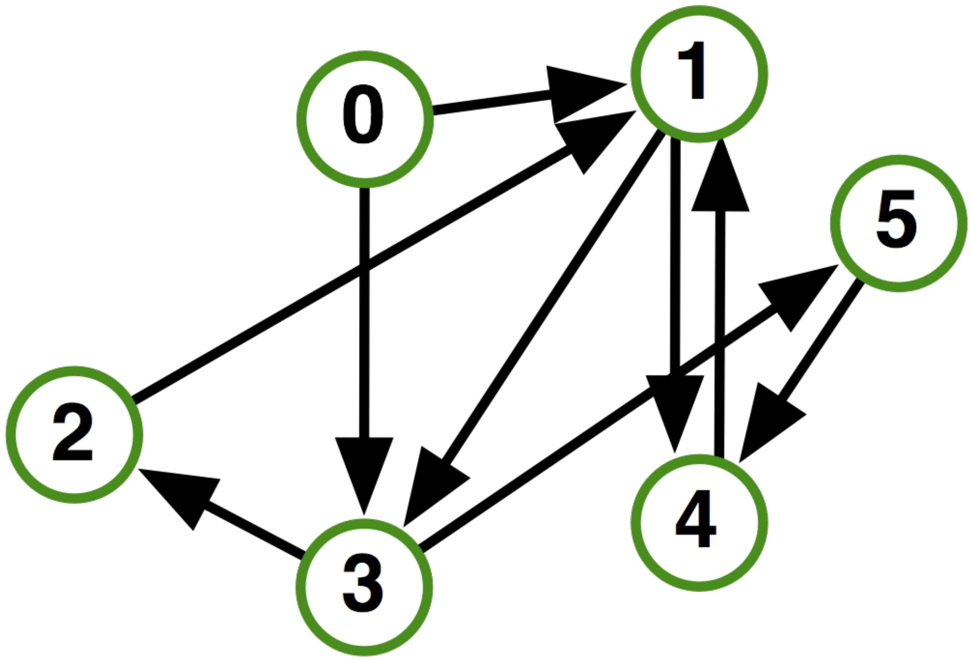
MPI_Dist_graph_create

```
MPI_Dist_graph_create(MPI_Comm comm_old, int n,
        const int sources[], const int degrees[],
        const int destinations[], const int weights[], MPI_Info info,
        int reorder, MPI_Comm *comm_dist_graph)
```

- n – number of source nodes
- sources – n source nodes
- degrees – number of edges for each source
- destinations, weights – dest. processor specification
- info, reorder – as usual
- More flexible and convenient
  - Requires global communication
  - Slightly more expensive than adjacent specification

MPI_Dist_graph_create

- Process 0:
  - N: 2
  - Sources: {0,1}
  - Degrees: {2,1}*
  - Dests: {3,1,4}
- Process 1:
  - N: 2
  - Sources: {2,3}
  - Degrees: {1,1}
  - Dests: {1,2}
- …



* Note that in this example, process 0 specifies only one of the two outgoing edges of process 1; the second outgoing edge needs to be specified by another process

Hoefler et al.: The Scalable Process Topology Interface of MPI 2.2

Distributed Graph Neighbor Queries

```
MPI_Dist_graph_neighbors_count(MPI_Comm  comm,
           int *indegree,int *outdegree, int *weighted)
```

- Query the number of neighbors of **calling process**
- Returns indegree and outdegree!
- Also info if weighted

```
MPI_Dist_graph_neighbors(MPI_Comm  comm, int maxindegree,
          int sources[], int sourceweights[], int maxoutdegree,
          int destinations[],int  destweights[])
```

- Query the neighbor list of **calling process**
- Optionally return weights

Hoefler et al.: The Scalable Process Topology Interface of MPI 2.2

Further Graph Queries

```
MPI_Topo_test(MPI_Comm  comm, int *status)
```

- Status is either:
  - MPI_GRAPH (ugs)
  - MPI_CART
  - MPI_DIST_GRAPH
  - MPI_UNDEFINED (no topology)
- Enables us to write libraries on top of MPI topologies!

Neighborhood Collectives

- Topologies implement no communication!
  - Just helper functions
- Collective communications only cover some patterns
  - E.g., no stencil pattern
- Several requests for “build your own collective” functionality in MPI
  - Neighborhood collectives are a simplified version
  - Cf. Datatypes for communication patterns!

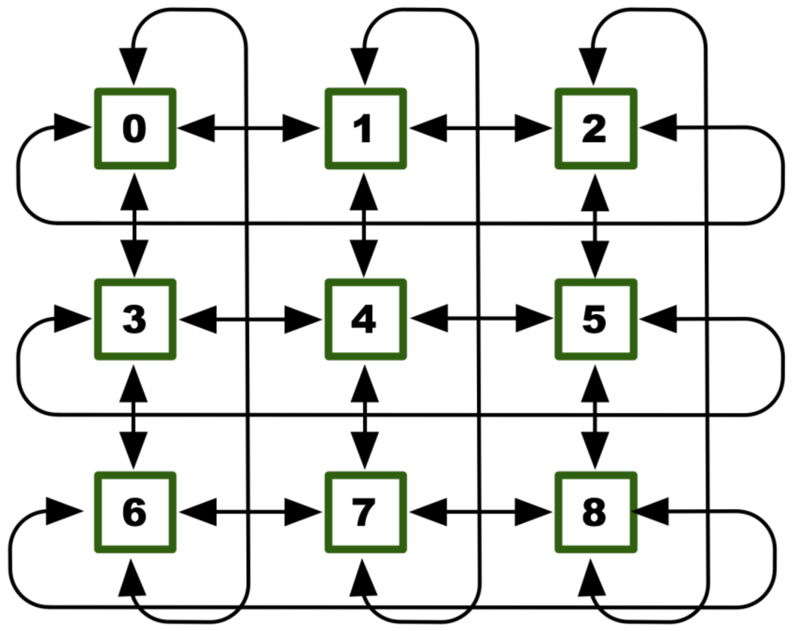
Cartesian Neighborhood Collectives

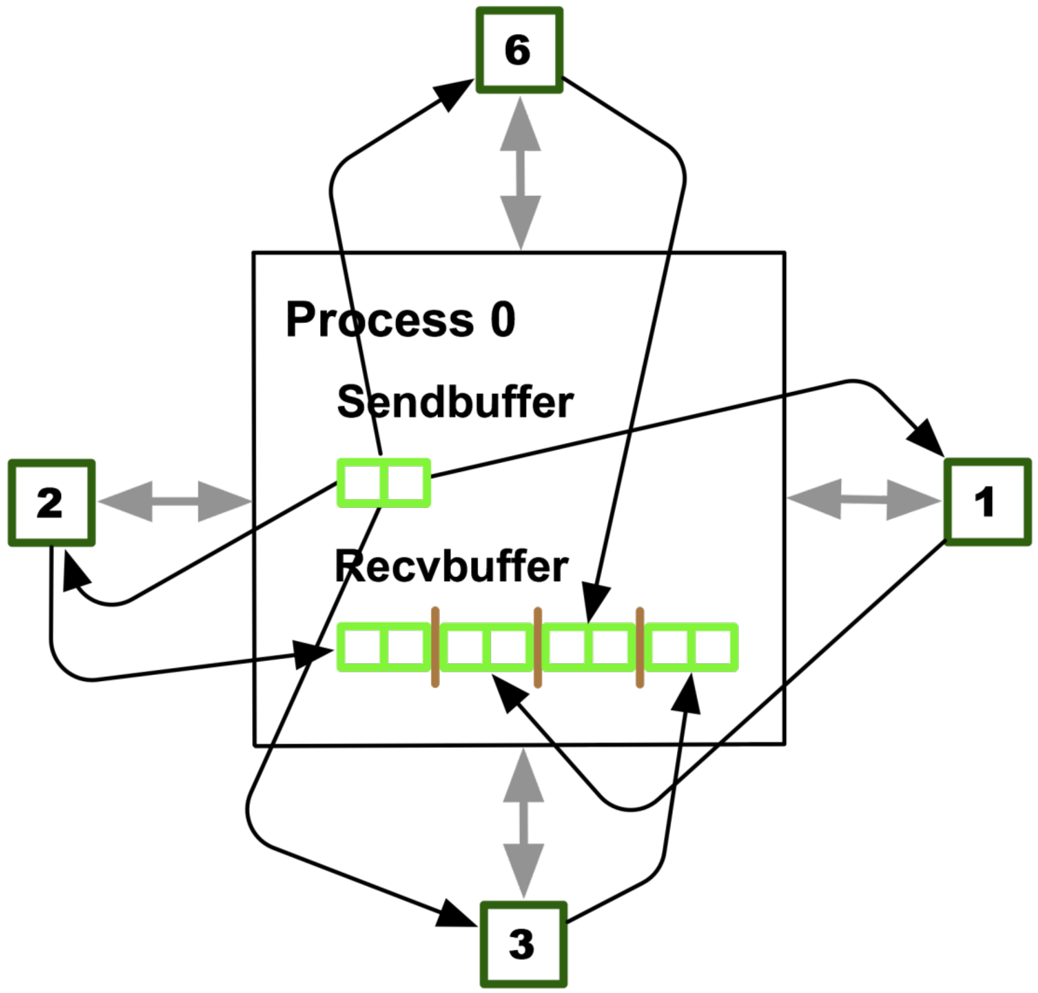
- Communicate with direct neighbors in Cartesian topology
  - Corresponds to cart_shift with disp=1
  - Collective (all processes in comm must call it, including processes without neighbors)
  - Buffers are laid out as neighbor sequence:
    - Defined by order of dimensions, first negative, then positive
    - 2*ndims sources and destinations
    - Processes at borders (MPI_PROC_NULL) leave holes in buffers (will not be updated or communicated)!

T. Hoefler and J. L. Traeff: Sparse Collective Operations for MPI

Cartesian Neighborhood Collectives

- Buffer ordering example:





Graph Neighborhood Collectives

- Collective Communication along arbitrary neighborhoods
  - Order is determined by order of neighbors as returned by (dist_)graph_neighbors.
  - Distributed graph is directed, may have different numbers of send/recv neighbors
  - Can express dense collective operations ☺
  - Any persistent communication pattern!

T. Hoefler and J. L. Traeff: Sparse Collective Operations for MPI

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
- Vector 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!

Code Example

- *stencil_mpi_carttopo_neighcolls.c*
- Adds neighborhood collectives to the topology

Why is Neighborhood Reduce Missing?

```
MPI_Ineighbor_allreducev(…);
```

- Was originally proposed (see original paper)
- High optimization opportunities
  - Interesting tradeoffs!
  - Research topic
- Not standardized due to missing use cases
  - My team is working on an implementation
  - Offering the obvious interface

T. Hoefler and J. L. Traeff: Sparse Collective Operations for MPI

Topology Summary

- Topology functions allow users to specify application communication patterns/topology
  - Convenience functions (e.g., Cartesian)
  - Storing neighborhood relations (Graph)
- Enables topology mapping (reorder=1)
  - Not widely implemented yet
  - May requires manual data re-distribution (according to new rank order)
- MPI does not expose information about the network topology (would be very complex)

Neighborhood Collectives Summary

- Neighborhood collectives add communication functions to process topologies
  - Collective optimization potential!
- Allgather
  - One item to all neighbors
- Alltoall
  - Personalized item to each neighbor
- High optimization potential (similar to collective operations)
  - Interface encourages use of topology mapping!

Section Summary

- Process topologies enable:
  - High-abstraction to specify communication pattern
  - Has to be relatively static (temporal locality)
    - Creation is expensive (collective)
  - Offers basic communication functions
- Library can optimize:
  - Communication schedule for neighborhood colls
  - Topology mapping

Recent Efforts of the MPI Forum for MPI-4 and Future MPI Standards

Introduction

- The MPI Forum continues to meet every 3 months to define future versions of the MPI Standard
- We describe some of the proposals the Forum is currently considering
- None of these topics are guaranteed to be in MPI-4
  - These are simply proposals that are being considered

MPI Working Groups

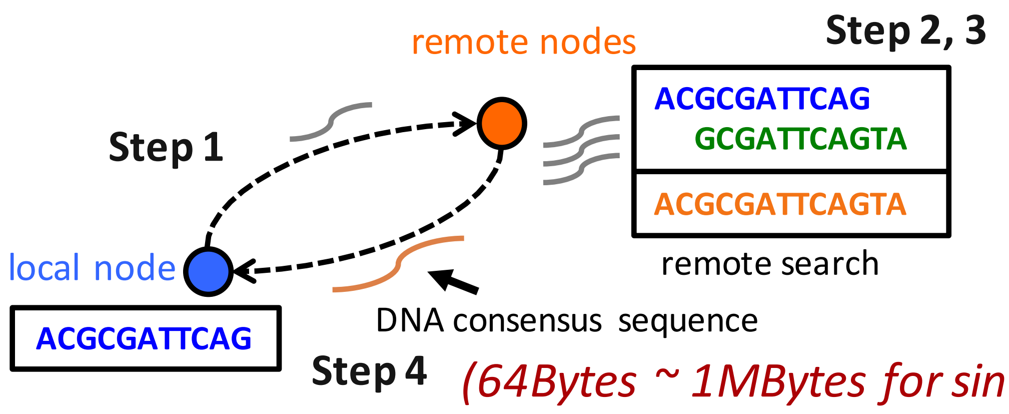
- Point-to-point communication
- Fault tolerance
- Hybrid programming
- Persistence
- Tools interfaces
- Large counts
- Others: RMA, Collectives, I/O

- http://meetings.mpi-forum.org/MPI_4.0_main_page.php

Point-to-Point Working Group

Example Application: Genome Assembly

Basic edge merging algorithm



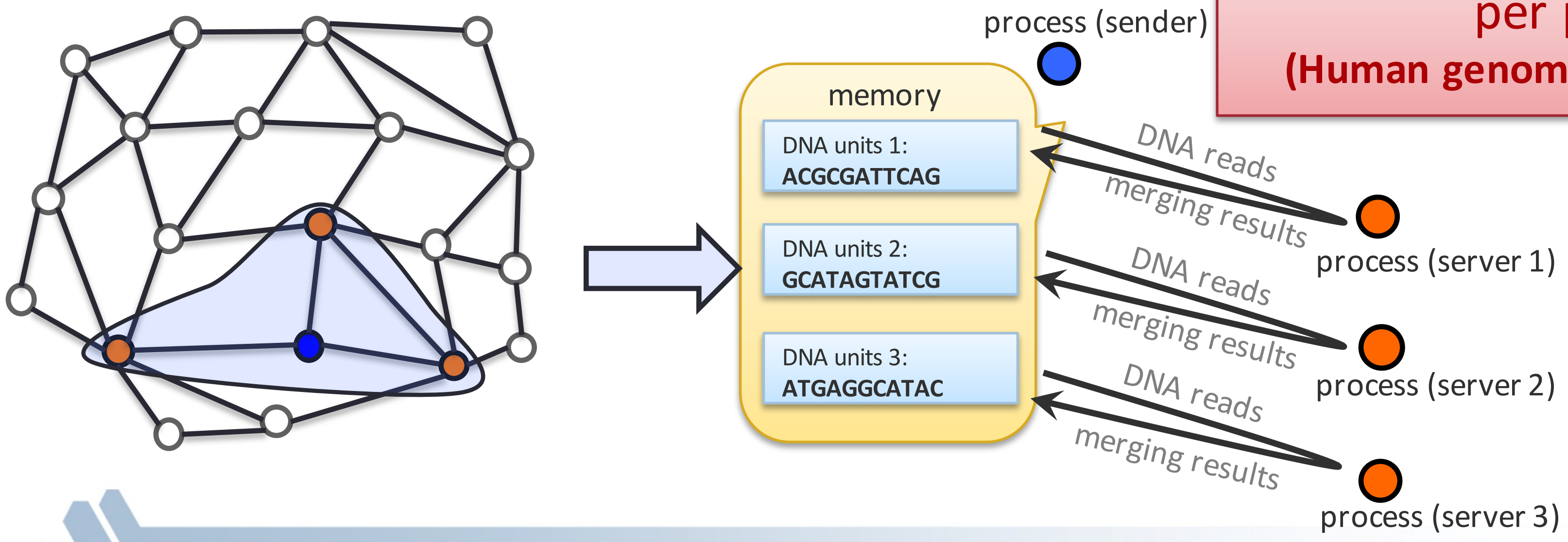
1. **Send local DNA unit to that node;**
2. **Search matching unit on that node;**
3. **Merge two units on that node;**
4. **Return merged unit.**

(64Bytes ~ 1MBytes for single message)

Large amount of outstanding data movement

10^6+ outstanding messages per process

(Human genome on Cray Edison *)



*** 64GB memory per node, 1KB memory per DNA reads, exclude runtime memory consumption.**

Proposal 1: Batched Communication Operations

- MPI-3.1 semantics
  - Each point-to-point operation creates a new request object
  - MPI library might run out of request objects after a few thousand operations
  - Application cannot issue a lot of messages to fully utilize the network
- Batched operations
  - RMA-like semantics for MPI send/recv communication
    - Application frees request as soon as the operation is issued
    - Batch completion of all operations on a communicator
      - MPI_COMM_WAITALL
  - Proportionally reduced number of requests
  - Can allow applications to consolidate multiple completions into a single request

Proposal 2: Communication Relaxation Hints

- mpi_assert_no_any_tag
  - The process will not use MPI_ANY_TAG
- mpi_assert_no_any_source
  - The process will not use MPI_ANY_SOURCE
- mpi_assert_exact_length
  - Receive buffers must be correct size for messages
- mpi_assert_overtaking_allowed
  - All messages are logically concurrent

Fault Tolerance Working Group

Improved Support for Fault Tolerance

- MPI always had support for error handlers and allows implementations to return an error code and remain alive
- MPI Forum working on additional support for MPI-4
- Current proposal handles fail-stop process failures (not silent data corruption or Byzantine failures)
  - If a communication operation fails because the other process has failed, the function returns error code MPI_ERR_PROC_FAILED
  - User can call MPI_Comm_shrink to create a new communicator that excludes failed processes
  - Collective communication can be performed on the new communicator

Proposal 1: Noncatastrophic Errors

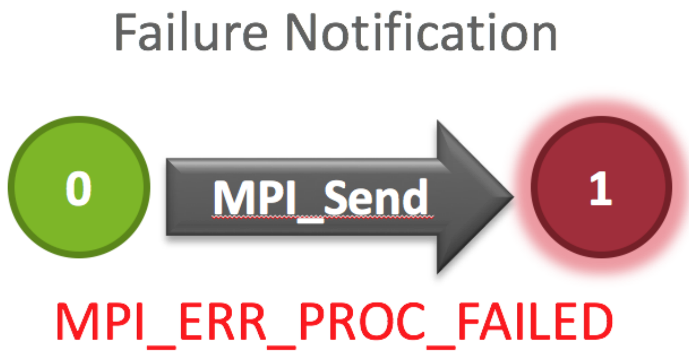
- Currently the state of MPI is undefined if any error occurs
- Even simple errors, such as incorrect arguments, can cause the state of MPI to be undefined
- Noncatastrophic errors are an opportunity for the MPI implementation to define some errors as “ignorable”
- For an error, the user can query if it is catastrophic or not
- If the error is not catastrophic, the user can simply pretend like (s)he never issued the operation and continue

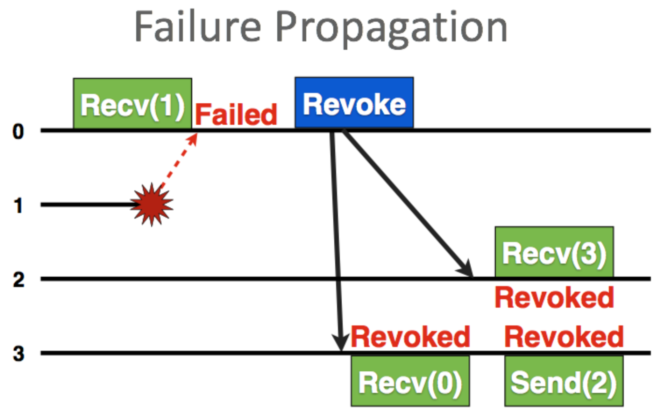
Proposal 2: Error Handlers

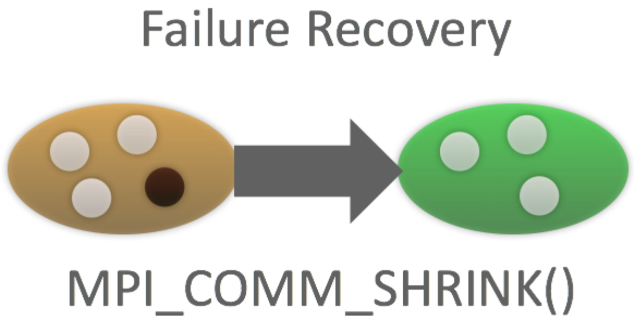
- Cleaner semantics for error handling
- Even with MPI-3.1, errors are not always fatal
  - But semantics of error handling are cumbersome to use
  - Their specification can use more precision
- How are error handlers inherited?
- Move default error handlers from MPI_COMM_WORLD to MPI_COMM_SELF

Proposal 3: User Level Failure Mitigation

- Enable application-level recovery by providing minimal FT API to prevent deadlock and enable recovery
- Don't do recovery for the application, but let the application (or a library) do what is best.
- Currently focused on process failure (not data errors or protection)







Hybrid Programming Working Group

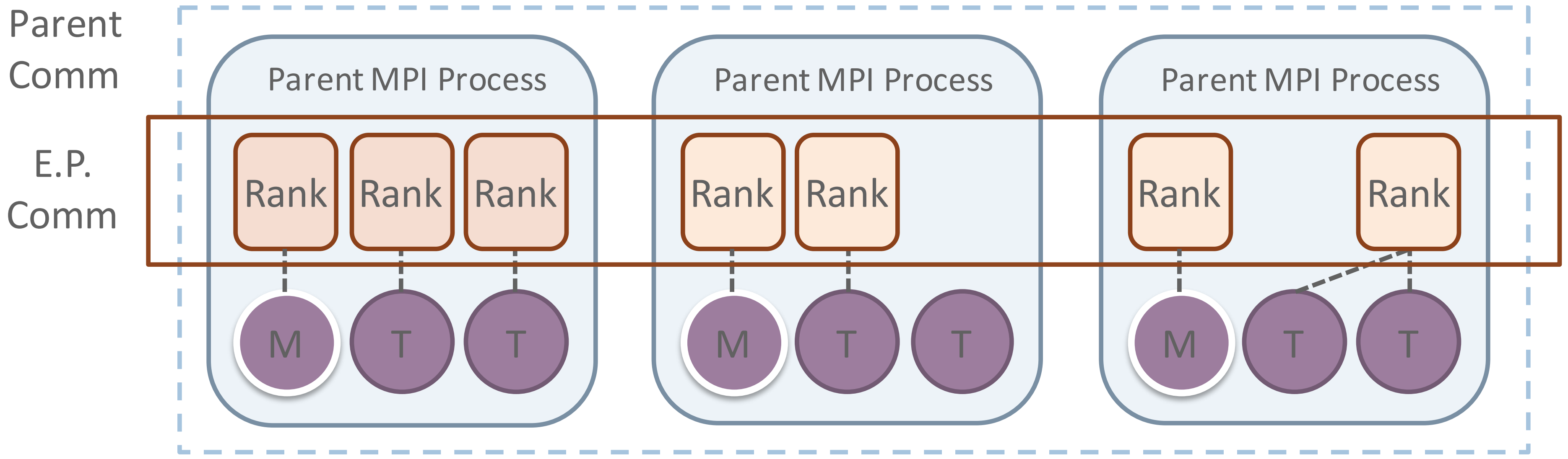
MPI-3.1 Performance/Interoperability Concerns

- Resource sharing between MPI processes
  - System resources do not scale at the same rate as processing cores
    - Memory, network endpoints, TLB entries, …
    - Sharing is necessary
  - MPI+threads gives a method for such sharing of resources
- Performance Concerns
  - MPI-3.1 provides a single view of the MPI stack to all threads
    - Requires all MPI objects (requests, communicators) to be shared between all threads
    - Not scalable to large number of threads
    - Inefficient when sharing of objects is not required by the user
  - MPI-3.1 does not allow a high-level language to interchangeably use OS processes or threads
    - No notion of addressing a single or a collection of threads
    - Needs to be emulated with tags or communicators

MPI Endpoints: Proposal for MPI-4

- Have multiple addressable communication entities within a single process
  - Instantiated in the form of multiple ranks per MPI process
- Each rank can be associated with one or more threads
- Lesser contention for communication on each “rank”
- In the extreme case, we could have one rank per thread (or some ranks might be used by a single thread)

MPI Endpoints Semantics



```
MPI_Comm_create_endpoints(MPI_Comm parent_comm, int my_num_ep,
         MPI_Info info, MPI_Comm out_comm_handles[])
```

- Creates new MPI ranks from existing ranks in parent communicator
  - Each process in parent comm. requests a number of endpoints
  - Array of output handles, one per local rank (i.e. endpoint) in endpoints communicator
  - Endpoints have MPI process semantics (e.g. progress, matching, collectives, …)
- Threads using endpoints behave like MPI processes
  - Provide per-thread communication state/resources
  - Allows implementation to provide process-like performance for threads

Persistence Working Group

Persistent Collective Operations

- An all-to-all transfer is done many times in an application
- The specific sends and receives represented never change (size, type, lengths, transfers)
- A nonblocking persistent collective operation can take the time to apply a heuristic and choose a faster way to move that data
- Fixed cost of making those decisions could be high (are amortized over all the times the function is used
- Static resource allocation can be done
- Choose fast(er) algorithm, take advantage of special cases
- Reduce queueing costs
- Special limited hardware can be allocated if available
- Choice of multiple transfer paths could also be performed

Basics

- Mirror regular nonblocking collective operations
- For each nonblocking MPI collective, add a persistent variant
- For every MPI_I<coll>, add MPI_<coll>_init
- Parameters are identical to the corresponding nonblocking variant
- All arguments "fixed" for subsequent uses
- Persistent collective operations cannot be matched with blocking or nonblocking collective calls

Init/Start

- The init function calls only perform initialization; do not start the operation
- E.g., MPI_Allreduce_init
  - Produces a persistent request (not destroyed by completion)
- Works with MPI_Start/MPI_Startall (cannot have multiple operations on the same communicator in Startall)
- Only inactive requests can be started
- MPI_Request_free can free inactive requests

Ordering of Inits and Starts

- Inits are nonblocking collective calls and must be ordered
- Persistent collective operations must be started in the same order at all processes
- Startall cannot contain multiple operations on the same communicator due to ordering ambiguity

Example

Nonblocking Collective APIs	Persistent Collective APIs
	MPI_Bcast_init(..., &req[0]);
	MPI_Reduce_init(..., &req[1]);
for (i=0; i<MAXITER; i++) {	for (i=0; i<MAXITER; i++) {
compute(bufA);	compute(bufA);
MPI_Ibcast(bufA,...,rowcomm, &req[0]);	MPI_Start(req[0]);
compute(bufB);	compute(bufB);
MPI_Ireduce(bufB,...,colcomm, &req[1]);	MPI_Start(req[1]);
MPI_Waitall(2, req, ...);	MPI_Waitall(2, req, ...);
}	}

Tools Working Group

Active Proposals (1/2)

- New interface to replace PMPI
  - Known, longstanding problems with the current profiling interface PMPI
    - One tool at a time can use it
    - Forces tools to be monolithic (a single shared library)
    - The interception model is OS dependent
  - New interface
    - Callback design
    - Multiple tools can potentially attach
    - Maintain all old functionality
- New feature for event notification in MPI_T
  - PERUSE
  - Tool registers for interesting event and gets callback when it happens

Active Proposals (2/2)

- Debugger support - MPIR interface
  - Fixing some bugs in the original “blessed” document
    - Missing line numbers!
  - Support non-traditional MPI implementations
    - Ranks are implemented as threads
  - Support for dynamic applications
    - Commercial applications/ Ensemble applications
    - Fault tolerance
  - Handle Introspection Interface
    - See inside MPI to get details about MPI Objects
      - Communicators, File Handles, etc.

Sessions Working Group

Before MPI-3.1, this could be erroneous

```
int main(int argc, char **argv) {
    MPI_Init_thread(…, MPI_THREAD_FUNNELED, …);
    pthread_create(…, my_thread1_main, NULL);
    pthread_create(…, my_thread2_main, NULL);
    // …
}
```

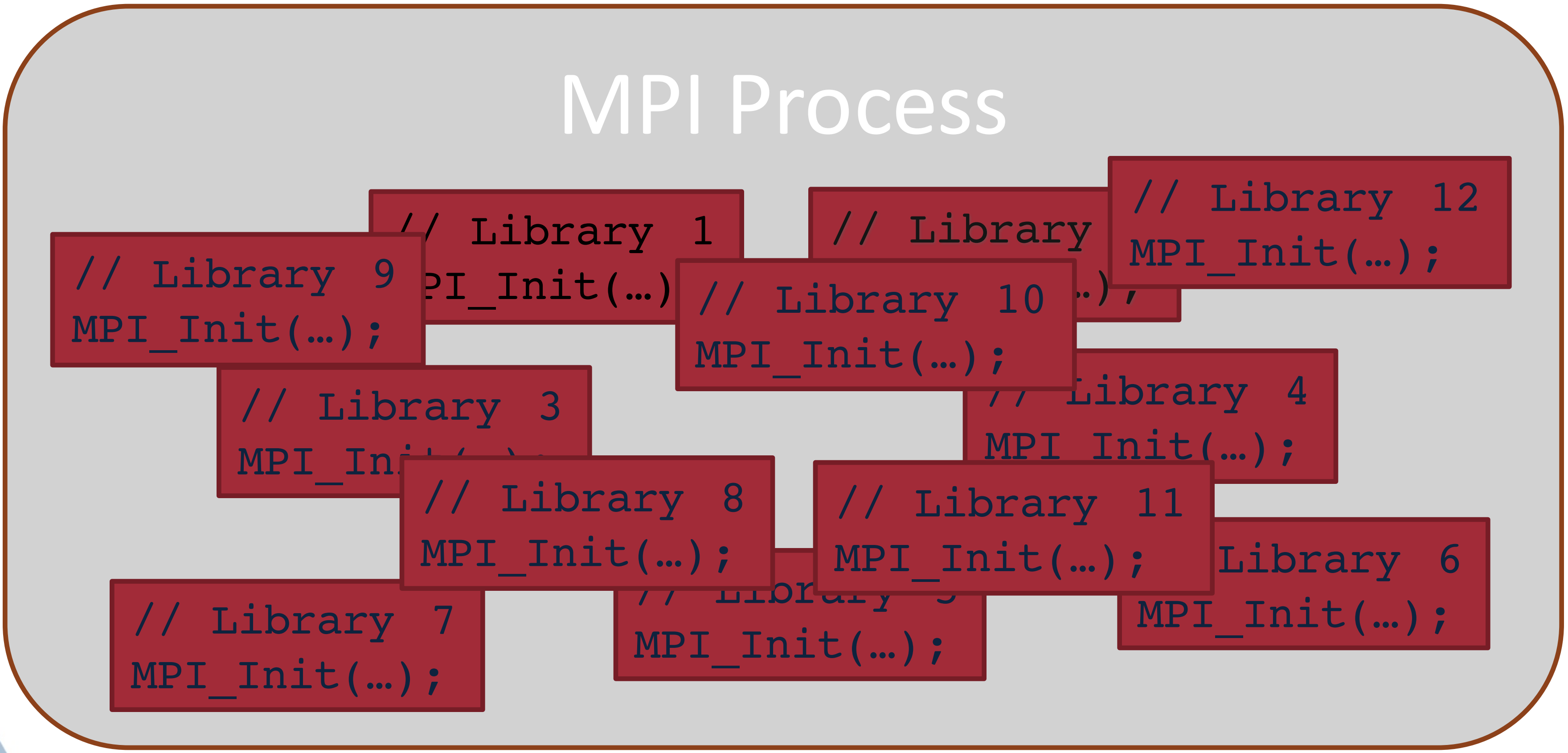
```
int my_thread1_main(void *context) {
    MPI_Initialized(&flag);
    // …
}
```

These might
run at the same time (!)

```
int my_thread2_main(void *context) {
    MPI_Initialized(&flag);
    // …
}
```

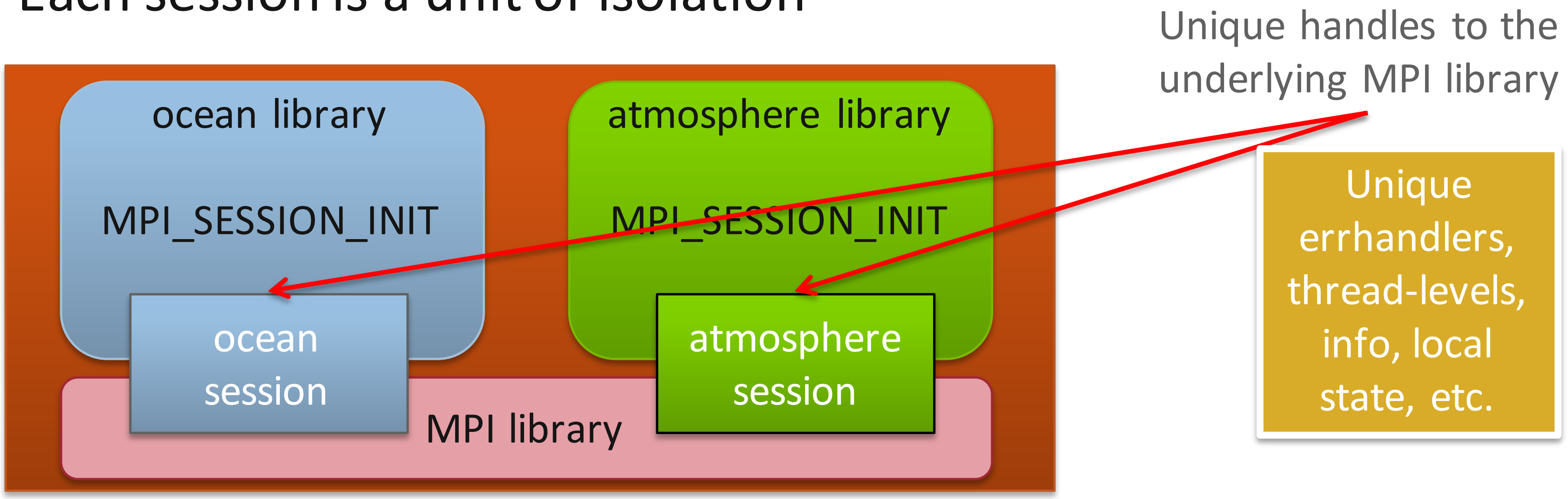
What we want

- Any thread (e.g., library) can use MPI any time it wants
- But still be able to totally clean up MPI if/when desired
- New parameters to initialize the MPI API



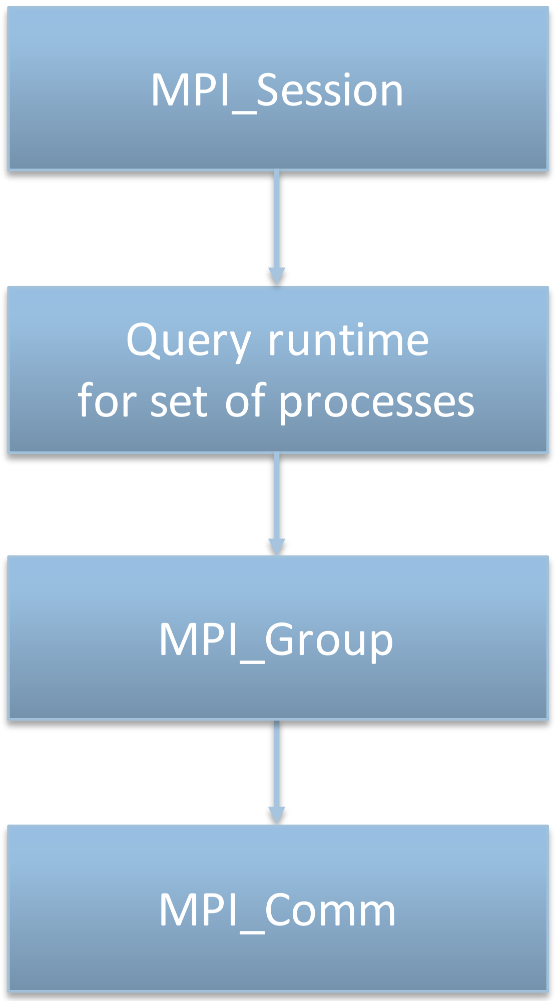
New Concept: “Session”

- A local handle to the MPI library
  - Implementation intent: lightweight / uses very few resources
  - Can also cache some local state
- Can have multiple sessions in an MPI process
  - MPI_Session_init(…, &session);
  - MPI_Session_finalize(…, &session);
- Each session is a unit of isolation



Overview

- General scheme:
  - Query the underlying run-time system
    - Get a “set” of processes
  - Determine the processes you want
    - Create an MPI_Group
  - Create a communicator with just those processes
    - Create an MPI_Comm



Static sets of processes

- Two sets are mandated to exist
  1. A set of processes effectively equivalent to the processes in MPI-3.1’s MPI_COMM_WORLD
  2. A set containing only a single process
- Sets are identified by string name
  - “mpi://WORLD”: refers to set #1, above
  - “mpi://SELF”: refers to set #2, above
- By definition, processes will be in more than one set

Large Counts Working Group

Problem with Large Counts

- MPI_Send/Recv and other functions take “int” as the count for data
  - What happens for data larger than 2GB x datatype size?
  - You create a new large “contiguous” derived datatype and send that
  - Possible, but clumsy
- What about duplicating all MPI functions to change “int” to “MPI_Count” (which is a large, typically 64-bit, integer)
  - Doubles the number of MPI functions
  - Possible, but clumsy

New C11 Bindings

- Use C11 _Generic type to provide multiple function prototypes
  - Like C++ function overloading, but done with compile time macro replacement
- MPI_Send will have two function signatures
  - One for traditional "int" arguments
  - One for new "MPI_Count" arguments
- Fully backward compatible for existing applications
- New applications can promote their data lengths to 64-bit without changing functions everywhere

Concluding Remarks

Conclusions

- Parallelism is critical today, given that it is the only way to achieve performance improvement with 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
- Your application can be next!

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

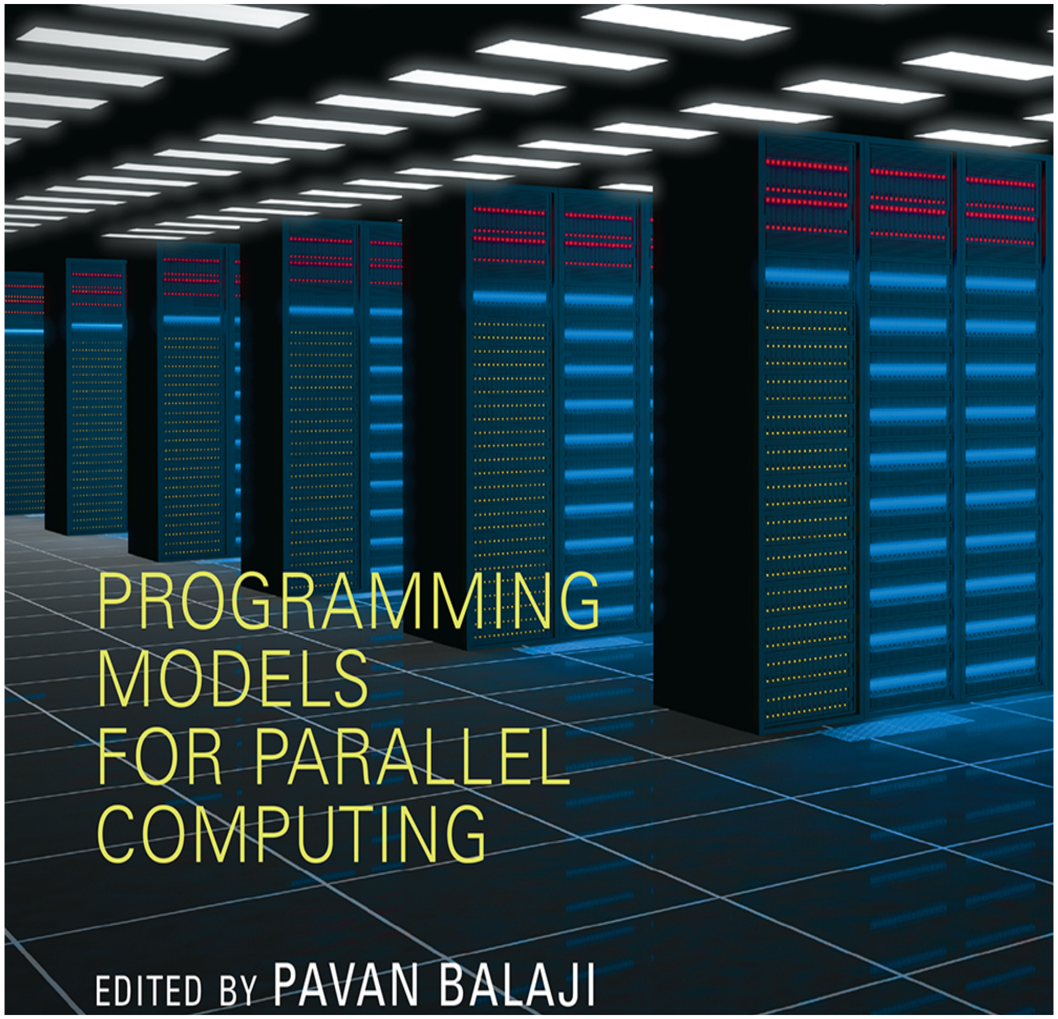
New Tutorial Books on MPI

- For basic MPI
  - ***Using MPI, 3rd edition, 2014***, by William Gropp, Ewing Lusk and Anthony Skjellum
  - https://mitpress.mit.edu/using-MPI-3ed
- For advanced MPI, including MPI-3
  - ***Using Advanced MPI, 2014,*** by William Gropp, Torsten Hoefler, Rajeev Thakur and Ewing Lusk
  - https://mitpress.mit.edu/using-advanced-MPI

New Book on Parallel Programming Models

Edited by Pavan Balaji

- ***MPI:*** W. Gropp and R. Thakur
- ***GASNet:*** P. Hargrove
- ***OpenSHMEM:*** J. Kuehn and S. Poole
- ***UPC:*** K. Yelick and Y. Zheng
- ***Global Arrays:*** S. Krishnamoorthy, J. Daily, A. Vishnu, and B. Palmer
- ***Chapel:*** B. Chamberlain
- ***Charm++:*** L. Kale, N. Jain, and J. Lifflander
- ***ADLB:*** E. Lusk, R. Butler, and S. Pieper
- ***Scioto:*** J. Dinan
- ***SWIFT:*** T. Armstrong, J. M. Wozniak, M. Wilde, and I. Foster
- ***CnC:*** K. Knobe, M. Burke, and F. Schlimbach
- ***OpenMP:*** B. Chapman, D. Eachempati, and S. Chandrasekaran
- ***Cilk Plus:*** A. Robison and C. Leiserson
- ***Intel TBB:*** A. Kukanov
- ***CUDA:*** W. Hwu and D. Kirk
- ***OpenCL:*** T. Mattson



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