Lecture 24: Parallel Programming on Distributed Systems with MPI

Concurrent and Multicore Programming, CSE536

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Slides borrowed from John Mellor-Crummey's Parallel Programming Courses from Rice University

Topics for Today

- Principles of message passing
  —building blocks (send, receive)
- MPI: Message Passing Interface
- Overlapping communication with computation
- Topologies
- Collective communication and computation
- Groups and communicators
- MPI derived data types
- Threading
- Remote Memory Access (RMA)
- Using MPI
- MPI Resources

Message Passing Overview

- The logical view of a message-passing platform
  - —p processes
  - —each with its own exclusive address space
- All data must be explicitly partitioned and placed
- All interactions (read-only or read/write) are two-sided
  - —process that has the data
  - —process that wants the data
- Typically use single program multiple data (SPMD) model
- The bottom line …
  - —strengths
    - – simple performance model: underlying costs are explicit
    - – portable high performance
  - —weakness: two-sided model can be awkward to program

Send and Receive

- **Prototype operations**

```
send(void *sendbuf, int nelems, int dest_rank)
receive(void *recvbuf, int nelems, int source_rank)
```

- **Consider the following code fragments:**

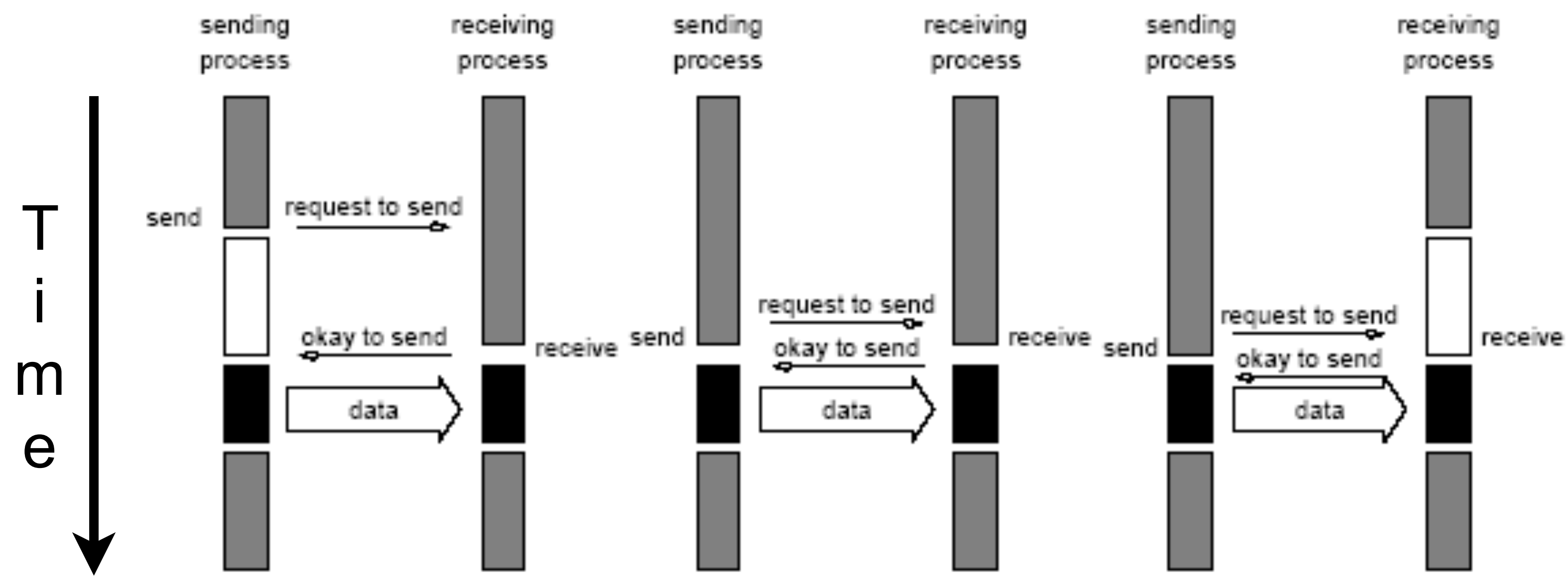
Processor 0	Processor 1
`a = 100;`	`receive(&a, 1, 0)`
`send(&a, 1, 1);`	`printf("%d\n", a);`
`a = 0;`	

- **The semantics of send**
  - value received by process P1 must be 100, not 0
  - motivates the design of send and receive protocols

Blocking Message Passing

- **Non-buffered, blocking sends**
  - —send does not return until the matching receive executes
- **Concerns**
  - —idling
  - —deadlock

Non-Buffered, Blocking Message Passing



(a) Sender comes first; idling at sender

(b) Sender and receiver come at about the same time; idling minimized

(c) Receiver comes first; idling at receiver

Handshaking for blocking non-buffered send/receive

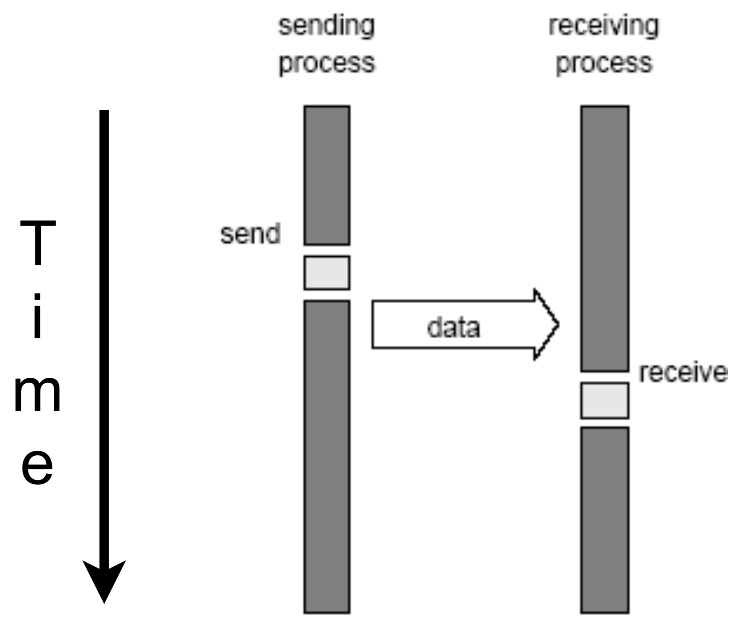
Idling occurs when operations are not simultaneous

(Case shown: no NIC support for communication)

Buffered, Blocking Message Passing

- **Buffered, blocking sends**
  - —sender copies the data into a buffer
  - —send returns after the copy completes
  - —data may be delivered into a buffer at the receiver as well
- **Tradeoff**
  - —buffering trades idling overhead for data copying overhead

Buffered, Blocking Message Passing



NIC moves the data behind the scenes

(illustrations show case when sender comes first)

Buffered Blocking Message Passing

Bounded buffer sizes can have significant impact on performance

```
Processor 0

for (i = 0; i < 1000; i++){
    produce_data(&a);
    send(&a, 1, 1);
  }
```

```
Processor 1

for (i = 0; i < 1000; i++){
   receive(&a, 1, 0);
   consume_data(&a);
}
```

Larger buffers enable the computation to tolerate asynchrony better

Buffered, Blocking Message Passing

Deadlocks are possible with buffering

since receive operations block

Processor 0

```
receive(&a, 1, 1);
send(&b, 1, 1);
```

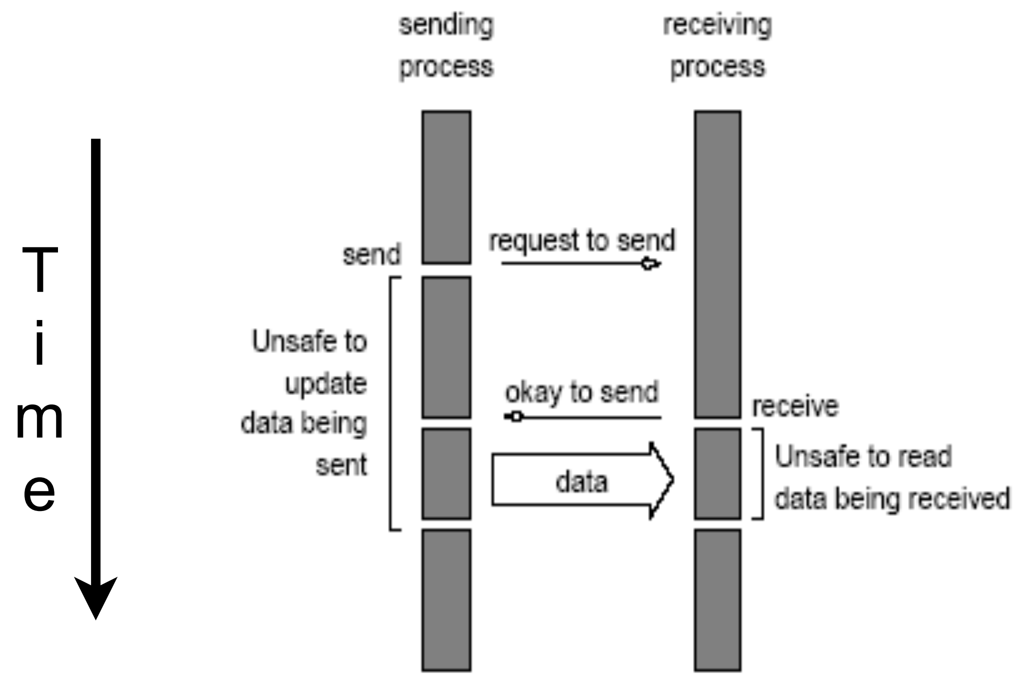
Processor 1

```
receive(&a, 1, 0);
send(&b, 1, 0);
```

Non-Blocking Message Passing

- **Non-blocking protocols**
  - send and receive return before it is safe
    - sender: data can be overwritten before it is sent
    - receiver: can read data out of buffer before it is received
  - ensuring proper usage is the programmer's responsibility
  - status check operation to ascertain completion
- **Benefit**
  - capable of overlapping communication with useful computation

Non-Blocking Message Passing



NIC moves the data behind the scenes

MPI: the Message Passing Interface

- **Standard library for message-passing**
  - —portable
  - —almost ubiquitously available
  - —high performance
  - —C and Fortran APIs
- **MPI standard defines**
  - —syntax of library routines
  - —semantics of library routines
- **Details**
  - —MPI routines, data-types, and constants are prefixed by “MPI_”
- **Simple to get started**
  - —fully-functional programs using only six library routines

Scope of the MPI Standards

- Communication contexts
- Datatypes
- Point-to-point communication
- Collective communication (synchronous, non-blocking)
- Process groups
- Process topologies
- Environmental management and inquiry
- The Info object
- Process creation and management
- One-sided communication (refined for MPI-3)
- External interfaces
- Parallel I/O
- Language bindings for Fortran, C and C++
- Profiling interface (PMPI)

MPI
MPI-2
MPI-3

MPI Primitives at a Glance

- Constants
- MPIO_Request_c2f
- MPIO_Request_f2c
- MPIO_Test
- MPIO_Wait
- MPI_Abort
- MPI_Address
- MPI_Allgather
- MPI_Allgatherv
- MPI_Allreduce
- MPI_Alltoall
- MPI_Alltoallv
- MPI_Attr_delete
- MPI_Attr_get
- MPI_Attr_put
- MPI_Barrier
- MPI_Bcast
- MPI_Bsend
- MPI_Bsend_init
- MPI_Buffer_attach
- MPI_Buffer_detach
- MPI_CHAR
- MPI_Cancel
- MPI_Cart_coords
- MPI_Cart_create
- MPI_Cart_get
- MPI_Cart_map
- MPI_Cart_rank
- MPI_Cart_shift
- MPI_Cart_sub
- MPI_Cartdim_get
- MPI_Comm_compare
- MPI_Comm_create
- MPI_Comm_dup
- MPI_Comm_free
- MPI_Comm_get_name
- MPI_Comm_group
- MPI_Comm_rank
- MPI_File_iwrite_shared
- MPI_File_open
- MPI_File_preallocate
- MPI_File_read
- MPI_File_read_all
- MPI_File_read_all_begin
- MPI_File_read_all_end
- MPI_File_read_at
- MPI_File_read_at_all
- MPI_File_read_at_all_begin
- MPI_File_read_at_all_end
- MPI_File_read_ordered
- MPI_File_read_ordered_begin
- MPI_File_read_ordered_end
- MPI_File_read_shared
- MPI_File_seek
- MPI_File_seek_shared
- MPI_File_set_atomicity
- MPI_File_set_errhandler
- MPI_File_set_info
- MPI_File_set_size
- MPI_File_set_view
- MPI_File_sync
- MPI_File_write
- MPI_File_write_all
- MPI_File_write_all_begin
- MPI_File_write_all_end
- MPI_File_write_at
- MPI_File_write_at_all
- MPI_File_write_at_all_begin
- MPI_File_write_at_all_end
- MPI_File_write_ordered
- MPI_File_write_ordered_begin
- MPI_File_write_ordered_end
- MPI_File_write_shared
- MPI_Finalize
- MPI_Finalized
- MPI_Gather
- MPI_Info_set
- MPI_Init
- MPI_Init_thread
- MPI_Initialized
- MPI_Int2handle
- MPI_Intercomm_create
- MPI_Intercomm_merge
- MPI_Iprobe
- MPI_Irecv
- MPI_Irsend
- MPI_Isend
- MPI_Issend
- MPI_Keyval_create
- MPI_Keyval_free
- MPI_NULL_COPY_FN
- MPI_NULL_DELETE_FN
- MPI_Op_create
- MPI_Op_free
- MPI_Pack
- MPI_Pack_size
- MPI_Pcontrol
- MPI_Probe
- MPI_Recv
- MPI_Recv_init
- MPI_Reduce
- MPI_Reduce_scatter
- MPI_Request_c2f
- MPI_Request_free
- MPI_Rsend
- MPI_Rsend_init
- MPI_Scan
- MPI_Scatter
- MPI_Scatterv
- MPI_Send
- MPI_Send_init
- MPI_Sendrecv
- MPI_Sendrecv_replace
- MPI_Ssend
- MPI_Comm_remote_group
- MPI_Comm_remote_size
- MPI_Comm_set_name
- MPI_Comm_size
- MPI_Comm_split
- MPI_Comm_test_inter
- MPI_DUP_FN
- MPI_Dims_create
- MPI_Errhandler_create
- MPI_Errhandler_free
- MPI_Errhandler_get
- MPI_Errhandler_set
- MPI_Error_class
- MPI_Error_string
- MPI_File_c2f
- MPI_File_close
- MPI_File_delete
- MPI_File_f2c
- MPI_File_get_amode
- MPI_File_get_atomicity
- MPI_File_get_byte_offset
- MPI_File_get_errhandler
- MPI_File_get_group
- MPI_File_get_info
- MPI_File_get_position
- MPI_File_get_position_shared
- MPI_File_get_size
- MPI_File_get_type_extent
- MPI_File_get_view
- MPI_File_iread
- MPI_File_iread_at
- MPI_File_iread_shared
- MPI_File_iwrite
- MPI_File_iwrite_at
- MPI_File_iwrite_shared
- MPI_Gatherv
- MPI_Get_count
- MPI_Get_elements
- MPI_Get_processor_name
- MPI_Get_version
- MPI_Graph_create
- MPI_Graph_get
- MPI_Graph_map
- MPI_Graph_neighbors
- MPI_Graph_neighbors_count
- MPI_Graphdims_get
- MPI_Group_compare
- MPI_Group_difference
- MPI_Group_excl
- MPI_Group_free
- MPI_Group_incl
- MPI_Group_intersection
- MPI_Group_range_excl
- MPI_Group_range_incl
- MPI_Group_rank
- MPI_Group_size
- MPI_Group_translate_ranks
- MPI_Group_union
- MPI_Ibsend
- MPI_Info_c2f
- MPI_Info_create
- MPI_Info_delete
- MPI_Info_dup
- MPI_Info_f2c
- MPI_Info_free
- MPI_Info_get
- MPI_Info_get_nkeys
- MPI_Info_get_nthkey
- MPI_Info_get_valuelen
- MPI_Info_set
- MPI_Ssend_init
- MPI_Start
- MPI_Startall
- MPI_Status_c2f
- MPI_Status_set_cancelled
- MPI_Status_set_elements
- MPI_Test
- MPI_Test_cancelled
- MPI_Testall
- MPI_Testany
- MPI_Testsome
- MPI_Topo_test
- MPI_Type_commit
- MPI_Type_contiguous
- MPI_Type_create_darray
- MPI_Type_create_subarray
- MPI_Type_extent
- MPI_Type_free
- MPI_Type_get_contents
- MPI_Type_get_envelope
- MPI_Type_hvector
- MPI_Type_lb
- MPI_Type_size
- MPI_Type_struct
- MPI_Type_ub
- MPI_Type_vector
- MPI_Unpack
- MPI_Wait
- MPI_Waitall
- MPI_Waitany
- MPI_Waitsome
- MPI_Wtick
- MPI_Wtime

http://www.mcs.anl.gov/research/projects/mpi/www/www3

MPI: the Message Passing Interface

Minimal set of MPI routines

`MPI_Init`	initialize MPI
`MPI_Finalize`	terminate MPI
`MPI_Comm_size`	determine number of processes in group
`MPI_Comm_rank`	determine id of calling process in group
`MPI_Send`	send message
`MPI_Recv`	receive message

Starting and Terminating the MPI Programs

- `int MPI_Init(int *argc, char ***argv)`
  - —initialization: must call this prior to other MPI routines
  - —effects
    - – strips off and processes any MPI command-line arguments
    - – initializes MPI environment
- `int MPI_Finalize()`
  - —must call at the end of the computation
  - —effect
    - – performs various clean-up tasks to terminate MPI environment
- **Return codes**
  - —MPI_SUCCESS
  - —MPI_ERROR

Communicators

- `MPI_Comm`: communicator = communication domain
  —group of processes that can communicate with one another
- Supplied as an argument to all MPI message transfer routines
- Process can belong to multiple communication domains
  —domains may overlap
- `MPI_COMM_WORLD`: root communicator
  — includes all the processes

Communicator Inquiry Functions

- `int MPI_Comm_size(MPI_Comm comm, int *size)`
  - determine the number of processes
- `int MPI_Comm_rank(MPI_Comm comm, int *rank)`
  - index of the calling process
  - $0 \le \text{rank} < \text{communicator size}$

“Hello World” Using MPI

```
#include <mpi.h>
#include <stdio.h>

int main(int argc, char *argv[])
{
        int npes, myrank;
        MPI_Init(&argc, &argv);
        MPI_Comm_size(MPI_COMM_WORLD, &npes);
        MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
        printf("From process %d out of %d, Hello World!\n",
                myrank, npes);
        MPI_Finalize();
       return 0;
}
```

Sending and Receiving Messages

- ```
  int MPI_Send(void *buf, int count, MPI_Datatype datatype,
               int dest_pe, int tag, MPI_Comm comm)
  ```

- ```
  int MPI_Recv(void *buf, int count, MPI_Datatype datatype,
              int source_pe, int tag, MPI_Comm comm,
              MPI_Status *status)
  ```

- **Message source or destination PE**
  - —index of process in the communicator `comm`
  - —receiver wildcard: `MPI_ANY_SOURCE`
    - any process in the communicator can be source
- **Message-tag: integer values, 0 ≤ tag < MPI_TAG_UB**
  - —receiver tag wildcard: `MPI_ANY_TAG`
    - messages with any tag are accepted
- **Receiver constraint**
  - — message size ≤ buffer length specified

MPI Primitive Data Types

MPI data type	C data type
`MPI_CHAR`	`signed char`
`MPI_SHORT`	`signed short int`
`MPI_INT`	`signed int`
`MPI_LONG`	`signed long int`
`MPI_UNSIGNED_CHAR`	`unsigned char`
`MPI_UNSIGNED_SHORT`	`unsigned short int`
`MPI_UNSIGNED`	`unsigned int`
`MPI_UNSIGNED_LONG`	`unsigned long int`
`MPI_FLOAT`	`float`
`MPI_DOUBLE`	`double`
`MPI_LONG_DOUBLE`	`long double`
`MPI_BYTE`	8 bits
`MPI_PACKED`	packed sequence of bytes

Receiver Status Inquiry

- `Mpi_Status`
  - —stores information about an `MPI_Recv` operation
  - —data structure

```
typedef struct MPI_Status {
  int MPI_SOURCE;
  int MPI_TAG;
  int MPI_ERROR; };
```

- `int MPI_Get_count(MPI_Status *status, MPI_Datatype datatype, int *count)`
  - —returns the count of data items received
    - – not directly accessible from status variable

Deadlock with MPI_Send/Recv?

destination

tag

```
int a[10], b[10], myrank;
MPI_Status s1, s2;
...
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
if (myrank == 0) {
    MPI_Send(a, 10, MPI_INT, 1, 1, MPI_COMM_WORLD);
    MPI_Send(b, 10, MPI_INT, 1, 2, MPI_COMM_WORLD);
}
else if (myrank == 1) {
    MPI_Recv(b, 10, MPI_INT, 0, 2, MPI_COMM_WORLD, &s1);
    MPI_Recv(a, 10, MPI_INT, 0, 1, MPI_COMM_WORLD, &s2);
}
...
```

Definition of MPI_Send says: “This routine may block until the message is received by the destination process”

Deadlock if MPI_Send is blocking

Another Deadlock Pitfall?

Send data to neighbor to your right on a ring ...

```
int a[10], b[10], npes, myrank;
MPI_Status status;
...
MPI_Comm_size(MPI_COMM_WORLD, &npes);

MPI_Comm_rank(MPI_COMM_WORLD, &myrank);

MPI_Send(a, 10, MPI_INT, (myrank+1)%npes, 1,
         MPI_COMM_WORLD);

MPI_Recv(b, 10, MPI_INT, (myrank-1+npes)%npes, 1,
          MPI_COMM_WORLD, &status);
...
```

Deadlock if MPI_Send is blocking

Avoiding Deadlock with Blocking Sends

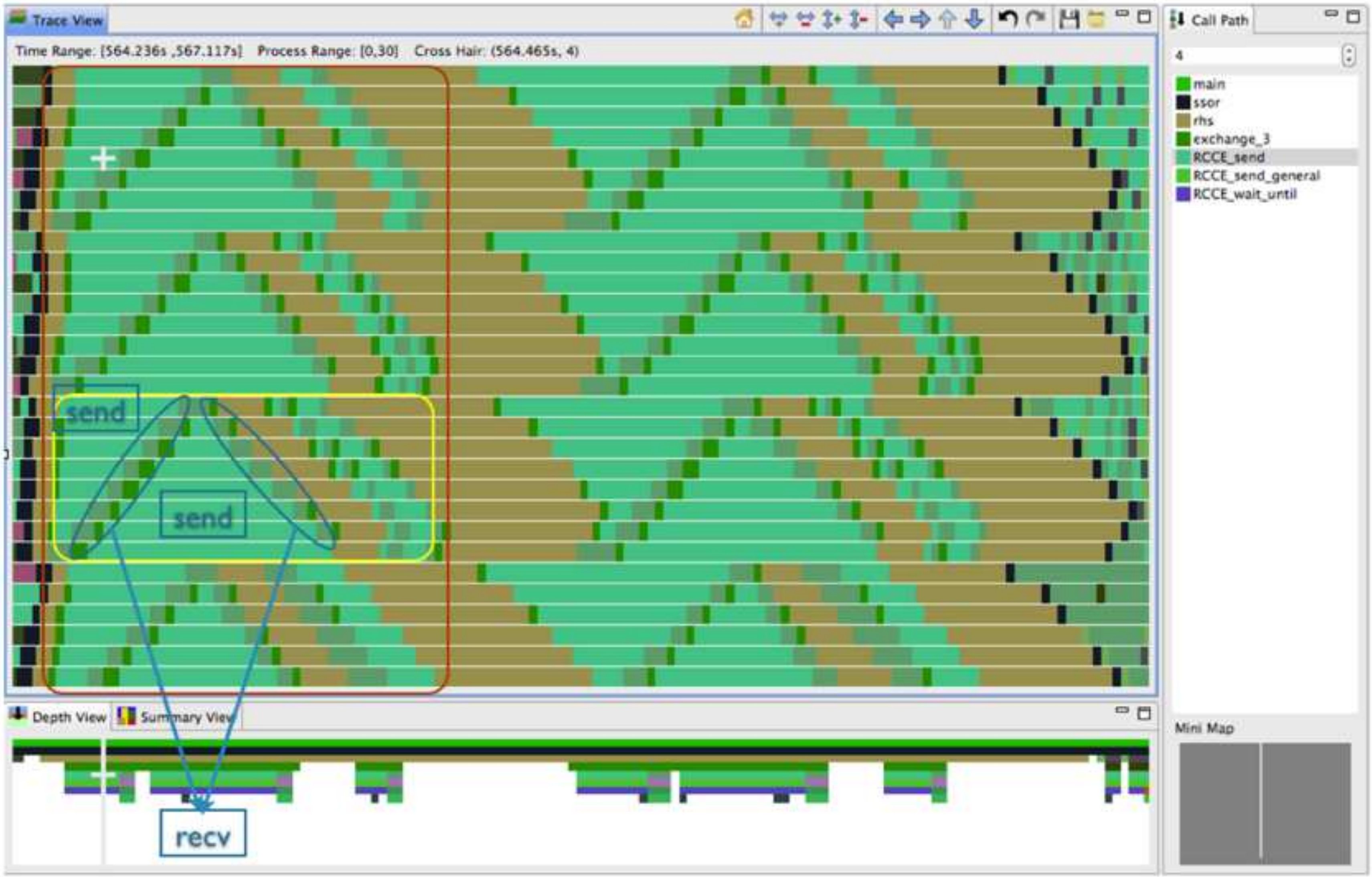
Send data to neighbor to your right on a ring ...

Break the circular wait

```
int a[10], b[10], npes, myrank;
MPI_Status status;
...
MPI_Comm_size(MPI_COMM_WORLD, &npes);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);

if (myrank%2 == 1) {    // odd processes send first, receive second
       MPI_Send(a, 10, MPI_INT, (myrank+1)%npes, 1,
              MPI_COMM_WORLD);
       MPI_Recv(b, 10, MPI_INT, (myrank-1+npes)%npes, 1,
              MPI_COMM_WORLD, &status);
}
else {                  // even processes receive first, send second
       MPI_Recv(b, 10, MPI_INT, (myrank-1+npes)%npes, 1,
              MPI_COMM_WORLD, &status);
       MPI_Send(a, 10, MPI_INT, (myrank+1)%npes, 1,
              MPI_COMM_WORLD);
}
...
```

Serialization in NAS LU on Intel SCC



Primitives for Non-blocking Communication

- Non-blocking send and receive return before they complete

```
int MPI_Isend(void *buf, int count, MPI_Datatype datatype,
              int dest, int tag, MPI_Comm comm,
              MPI_Request *request)
int MPI_Irecv(void *buf, int count, MPI_Datatype datatype,
              int source, int tag, MPI_Comm comm,
              MPI_Request *request)
```

- `MPI_Test:` has a particular non-blocking request finished?

```
int MPI_Test(MPI_Request *request, int *flag,
        MPI_Status *status)
```

- `MPI_Waitany:` block until some request in a set completes

```
int MPI_Wait_any(int req_cnt, MPI_Request *req_array,
                 int *req_index, MPI_Status *status)
```

- `MPI_Wait:` block until a particular request completes

```
int MPI_Wait(MPI_Request *request, MPI_Status *status)
```

Avoiding Deadlocks with NB Primitives

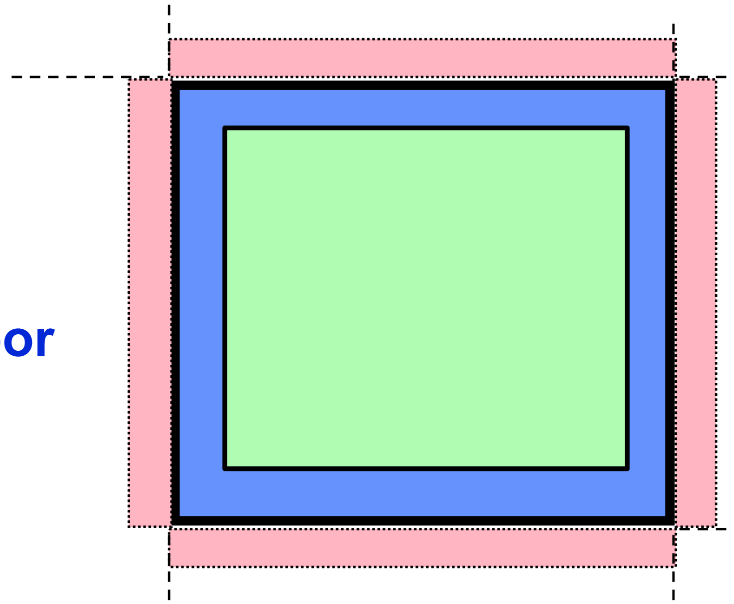
Using non-blocking operations avoids most deadlocks

tag

```
int a[10], b[10], myrank;
MPI_Request r1, r2;
...
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
if (myrank == 0) {
   MPI_ISend(a, 10, MPI_INT, 1, 1, MPI_COMM_WORLD, &r1);
   MPI_ISend(b, 10, MPI_INT, 1, 2, MPI_COMM_WORLD, &r2);
}
else if (myrank == 1) {
   MPI_IRecv(b, 10, MPI_INT, 0, 2, &status, MPI_COMM_WORLD, &r1);
   MPI_IRecv(a, 10, MPI_INT, 0, 1, &status, MPI_COMM_WORLD, &r2);
}
...
```

Overlapping Communication Example

- Original
  - —send boundary layer (blue) to neighbors with blocking send
  - —receive boundary layer (pink) from neighbors
  - —compute data volume (green + blue)
- Overlapped
  - —send boundary layer (blue) to neighbor with non-blocking send
  - —compute interior region (green) from
  - —receive boundary layer (pink)
  - —wait for non-blocking sends to complete (blue)
  - —compute boundary layer (blue)



Message Exchange

To exchange messages in a single call (both send and receive)

```
int MPI_Sendrecv(void *sendbuf, int sendcount,
  MPI_Datatype senddatatype, int dest, int sendtag,
  void *recvbuf, int recvcount, MPI_Datatype recvdatatype,
  int source, int recvtag, MPI_Comm comm,
  MPI_Status *status)
```

Requires both send and receive arguments

Why Sendrecv?

Sendrecv is useful for executing a shift operation along a chain of processes. If blocking send and recv are used for such a shift, then one needs to avoid deadlock with an odd/even scheme. When Sendrecv is used, MPI handles these issues.

To use same buffer for both send and receive

```
int MPI_Sendrecv_replace(void *buf, int count,
  MPI_Datatype datatype, int dest, int sendtag,
  int source, int recvtag, MPI_Comm comm,
  MPI_Status *status)
```

Collective Communication in MPI

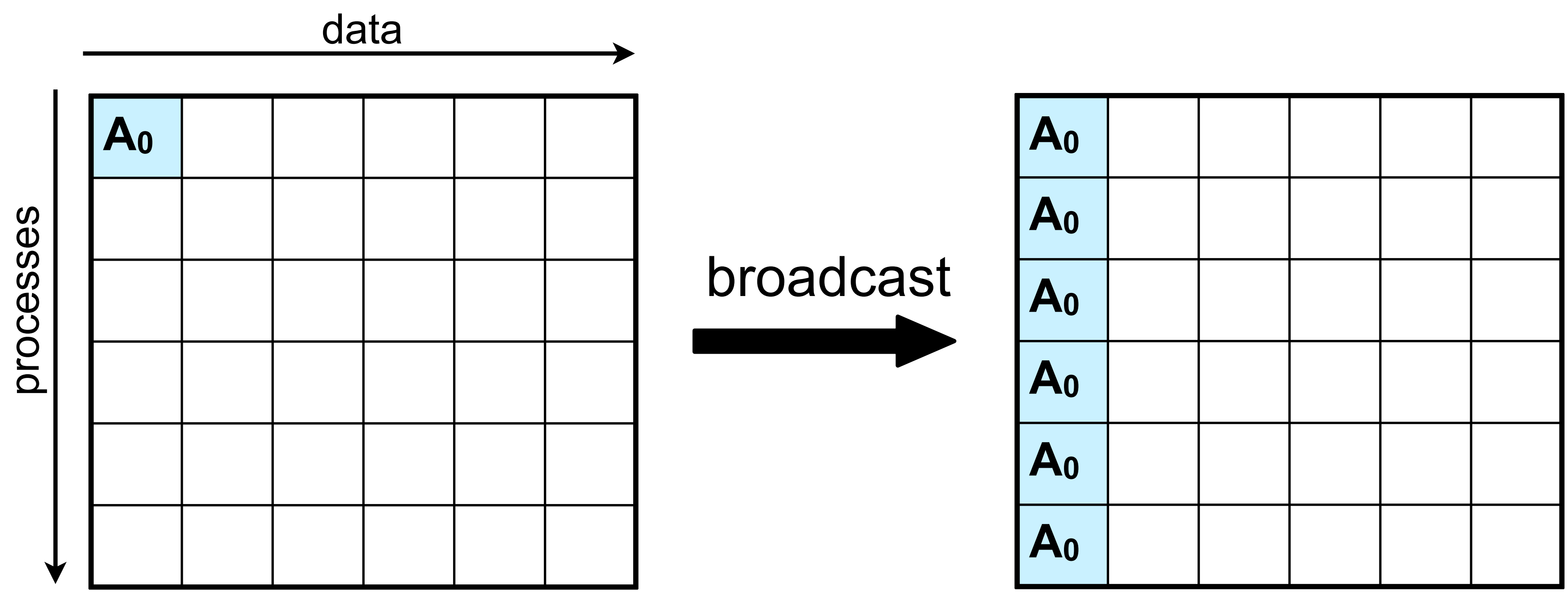
- MPI provides an extensive set of collective operations
- Operations defined over a communicator's processes
- All processes in a communicator must call the same collective operation
  - —e.g. all participants in a one-to-all broadcast call the broadcast primitive, even though all but the root are conceptually just "receivers"
- Simplest collective: barrier synchronization

```
int MPI_Barrier(MPI_Comm comm)
```

  - wait until all processes arrive

One-to-all Broadcast

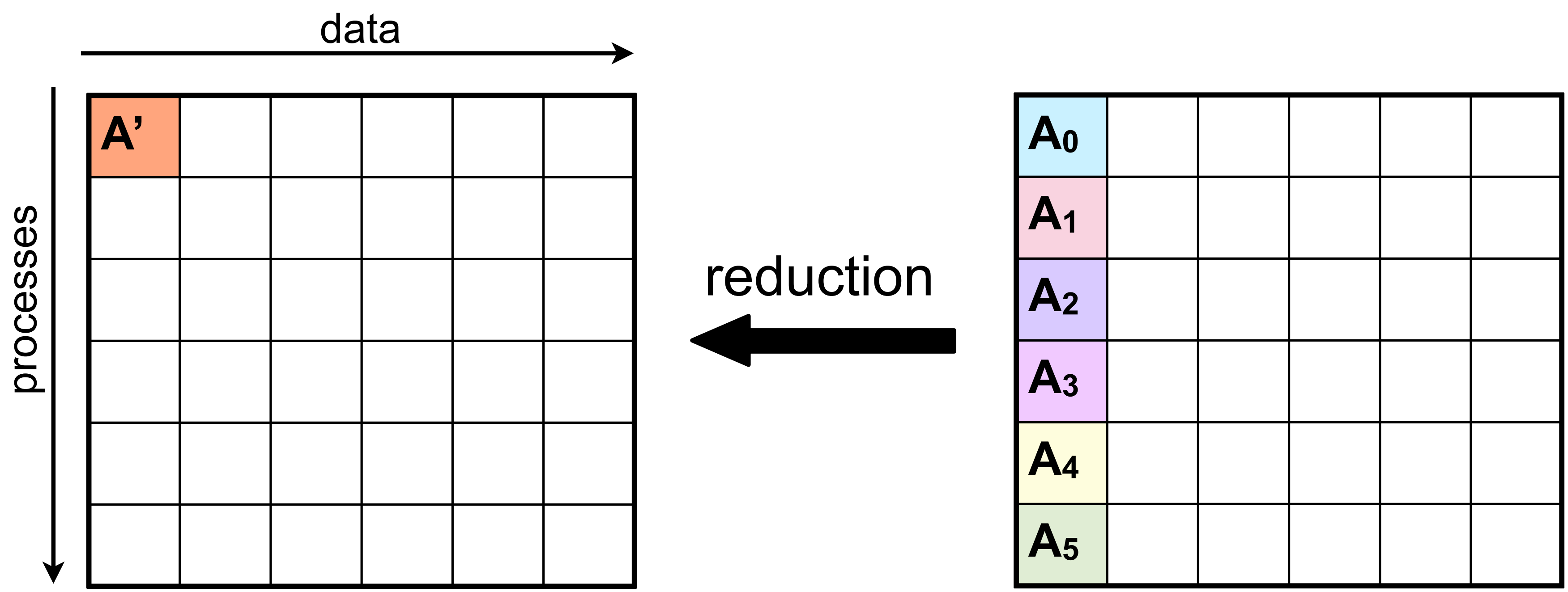
```
int MPI_Bcast(void *buf, int count,
              MPI_Datatype datatype, int source,
              MPI_Comm comm)
```



All-to-one Reduction

```
int MPI_Reduce(void *sendbuf, void *recvbuf,
               int count, MPI_Datatype datatype,
               MPI_Op op, int target, MPI_Comm comm)
```

MPI_Op examples: sum, product, min, max, ... (see next page)



$A' = op(A_0, \ldots A_{p-1})$

MPI_Op Predefined Reduction Operations

Operation	Meaning	Datatypes
`MPI_MAX`	Maximum	integers and floating point
`MPI_MIN`	Minimum	integers and floating point
`MPI_SUM`	Sum	integers and floating point
`MPI_PROD`	Product	integers and floating point
`MPI_LAND`	Logical AND	integers
`MPI_BAND`	Bit-wise AND	integers and byte
`MPI_LOR`	Logical OR	integers
`MPI_BOR`	Bit-wise OR	integers and byte
`MPI_LXOR`	Logical XOR	integers
`MPI_BXOR`	Bit-wise XOR	integers and byte
`MPI_MAXLOC`	Max value-location	Data-pairs
`MPI_MINLOC`	Min value-location	Data-pairs

MPI_MAXLOC and MPI_MINLOC

- `MPI_MAXLOC`
  - —combines pairs of values (v_i, l_i)
  - —returns the pair (v, l) such that
    - – v is the maximum among all v_i's
    - – l is the corresponding l_i

      if non-unique, it is the smallest among l_i's
- `MPI_MINLOC` analogous

Value	15	17	11	12	17	11
Process	0	1	2	3	4	5

```
MinLoc(Value, Process) = (11, 2)
MaxLoc(Value, Process) = (17, 1)
```

Data Types for MINLOC and MAXLOC Reductions

`MPI_MAXLOC` and `MPI_MINLOC` reductions operate on data pairs

MPI Datatype	C Datatype
`MPI_2INT`	**pair of** ints
`MPI_SHORT_INT`	short **and** int
`MPI_LONG_INT`	long **and** int
`MPI_LONG_DOUBLE_INT`	long double **and** int
`MPI_FLOAT_INT`	float **and** int
`MPI_DOUBLE_INT`	double **and** int

All-to-All Reduction and Prefix Sum

- **All-to-all reduction - every process gets a copy of the result**

```
int MPI_Allreduce(void *sendbuf, void *recvbuf,
                  int count, MPI_Datatype datatype,
                  MPI_Op op, MPI_Comm comm)
```

—semantically equivalent to MPI_Reduce + MPI_Bcast

- **Parallel prefix operations**

—inclusive scan: processor i result = op(v_0, ... v_i)

```
int MPI_Scan(void *sendbuf, void *recvbuf, int count,
     MPI_Datatype datatype, MPI_Op op,
             MPI_Comm comm)
```

—exclusive scan: processor i result = op(v_0, ... v_{i-1})

```
int MPI_Exscan(void *sendbuf, void *recvbuf, int count,
              MPI_Datatype datatype, MPI_Op op,
              MPI_Comm comm)
```

Exscan example MPI_SUM

input	[2	4	1	1	0	1	-3	2	0	6	1	5]
output	[0	2	6	7	8	8	9	6	8	8	14	15]

Scatter/Gather

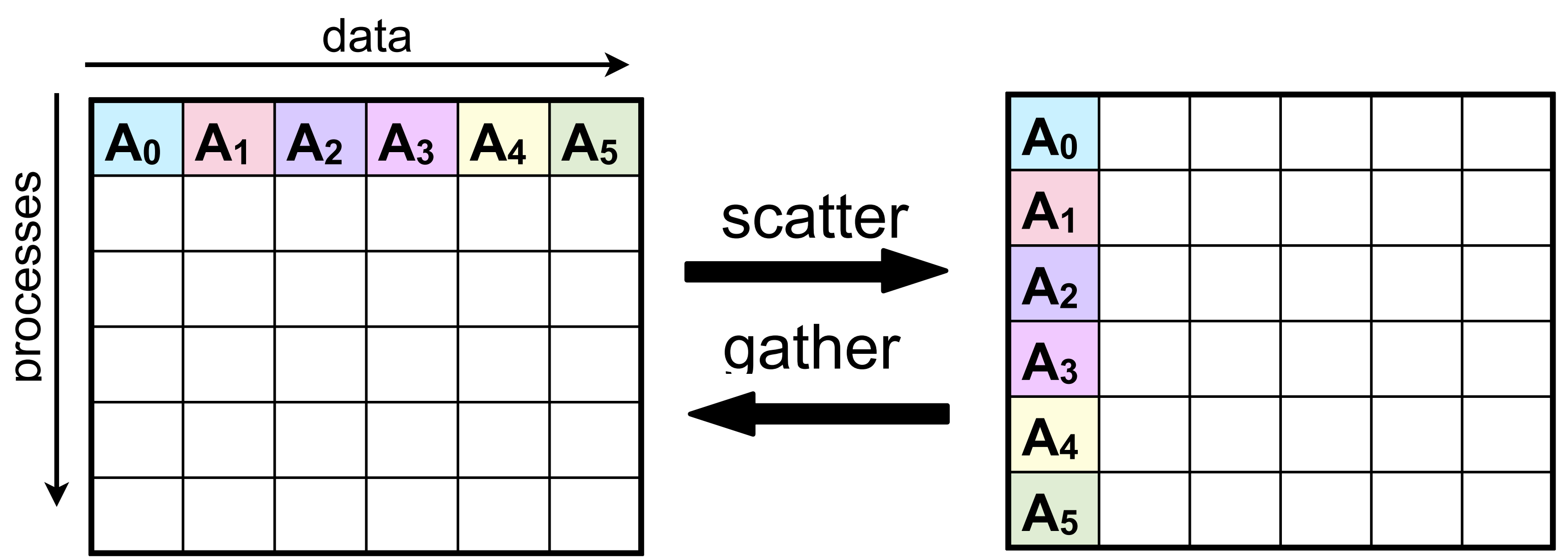
- **Scatter data p-1 blocks from root process delivering one to each other**

```
int MPI_Scatter(void *sendbuf, int sendcount,
         MPI_Datatype senddatatype, void *recvbuf,
         int recvcount, MPI_Datatype recvdatatype,
         int source, MPI_Comm comm)
```

sendcount = number sent to each

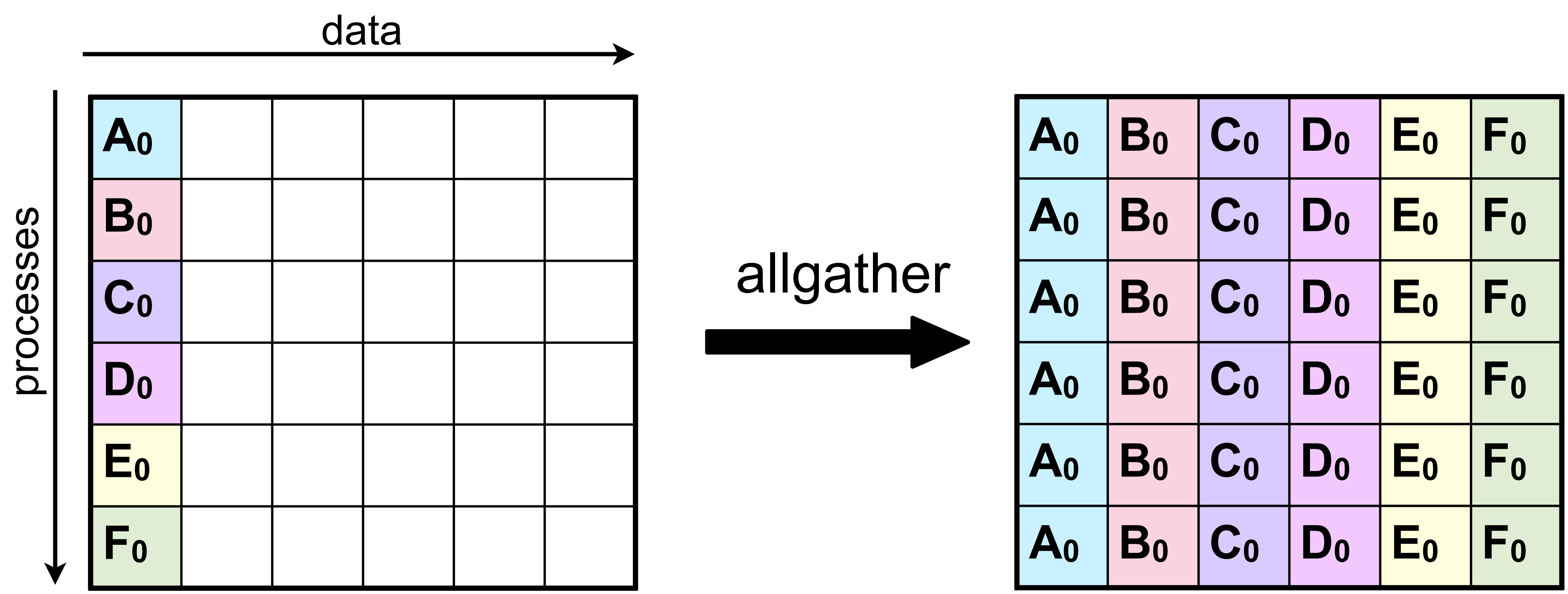
- **Gather data at one process**

```
int MPI_Gather(void *sendbuf, int sendcount,
         MPI_Datatype senddatatype, void *recvbuf,
         int recvcount, MPI_Datatype recvdatatype,
         int target, MPI_Comm comm)
```



Allgather

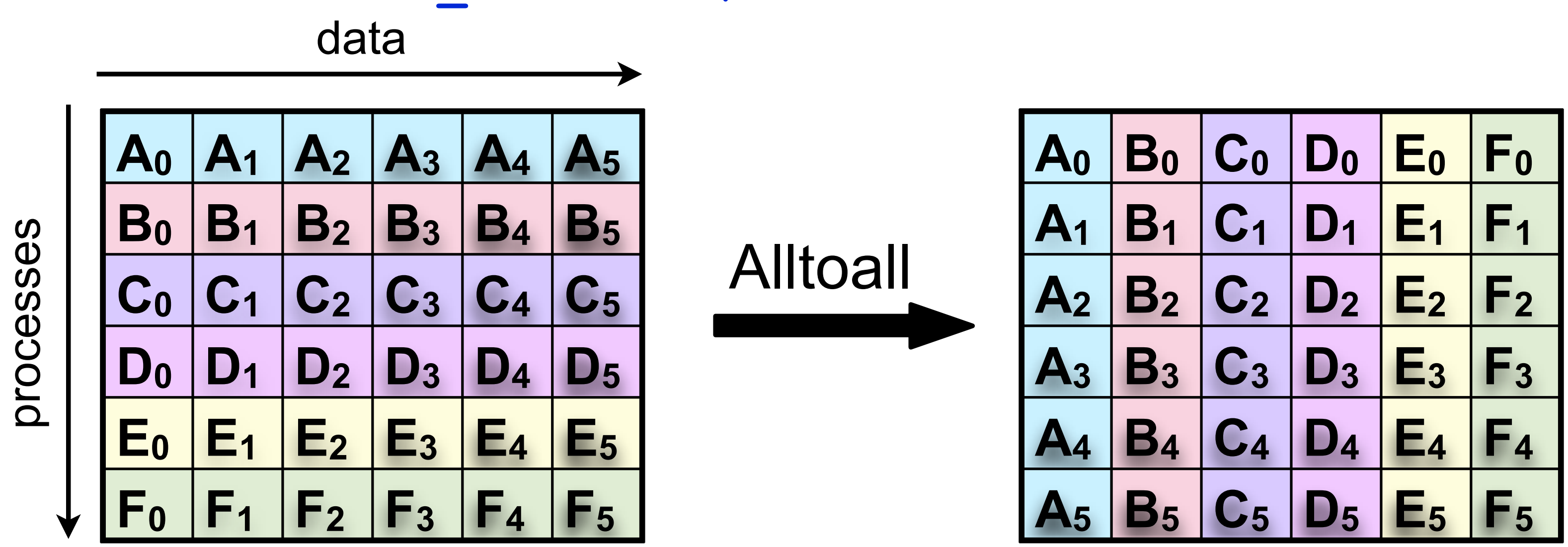
```
int MPI_AllGather(void *sendbuf, int sendcount,
                  MPI_Datatype senddatatype, void *recvbuf,
                  int recvcount, MPI_Datatype recvdatatype,
                  MPI_Comm comm)
```



All-to-All Personalized Communication

- Each process starts with its own set of blocks, one destined for each process
- Each process finishes with all blocks destined for itself
- Analogous to a matrix transpose

```
int MPI_Alltoall(void *sendbuf, int sendcount,
        MPI_Datatype senddatatype, void *recvbuf,
        int recvcount, MPI_Datatype recvdatatype,
        MPI_Comm comm)
```



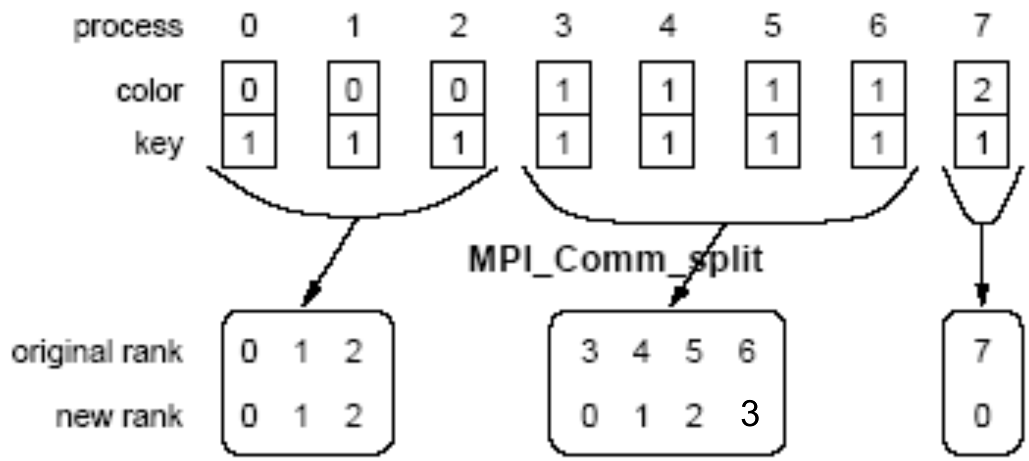
Splitting Communicators

- **Useful to partition communication among process subsets**
- **MPI provides mechanism for partitioning a process group**
  - **—splitting communicators**
- **Simplest such mechanism**

```
int MPI_Comm_split(MPI_Comm comm, int color, int key,
                   MPI_Comm *newcomm)
```

  - **—effect**
    - **group processes by color**
    - **sort resulting groups by key**

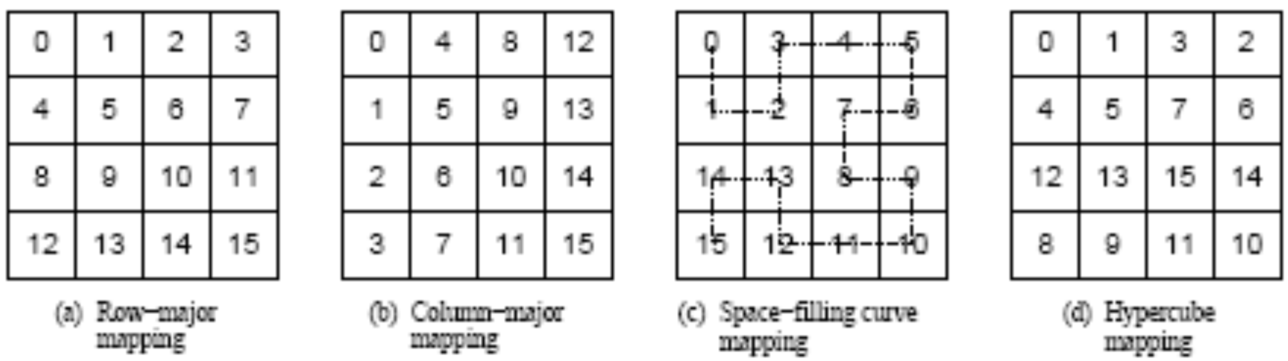
Splitting Communicators



Using `MPI_Comm_split` to split a group of processes in a communicator into subgroups

Topologies and Embeddings

- Processor ids in `MPI_COMM_WORLD` can be remapped
  - —higher dimensional meshes
  - —space-filling curves



- Goodness of any mapping
  - — determined by the interaction pattern
    - program
    - topology of the machine
  - —MPI does not provide any explicit control over these mappings

Cartesian Topologies

- **For regular problems a multidimensional mesh organization of processes can be convenient**
- **Creating a new communicator augmented with a mesh view**

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

- **Map processes into a mesh**
  - ndims = number of dimensions
  - dims = vector with length of each dimension
  - periods = vector indicates which dims are periodic
  - reorder = flag - ranking may be reordered
- **Processor coordinate in cartesian topology**
  - a vector of length ndims

Using Cartesian Topologies

- Sending and receiving still requires 1-D ranks
- Map Cartesian coordinates ⇔ rank

```
int MPI_Cart_coord(MPI_Comm comm_cart, int rank, int maxdims,
                   int *coords)
```

```
int MPI_Cart_rank(MPI_Comm comm_cart, int *coords, int *rank)
```

- Most common operation on cartesian topologies is a shift
- Determine the rank of source and destination of a shift

```
int MPI_Cart_shift(MPI_Comm comm_cart, int dir, int s_step,
                   int *rank_source, int *rank_dest)
```

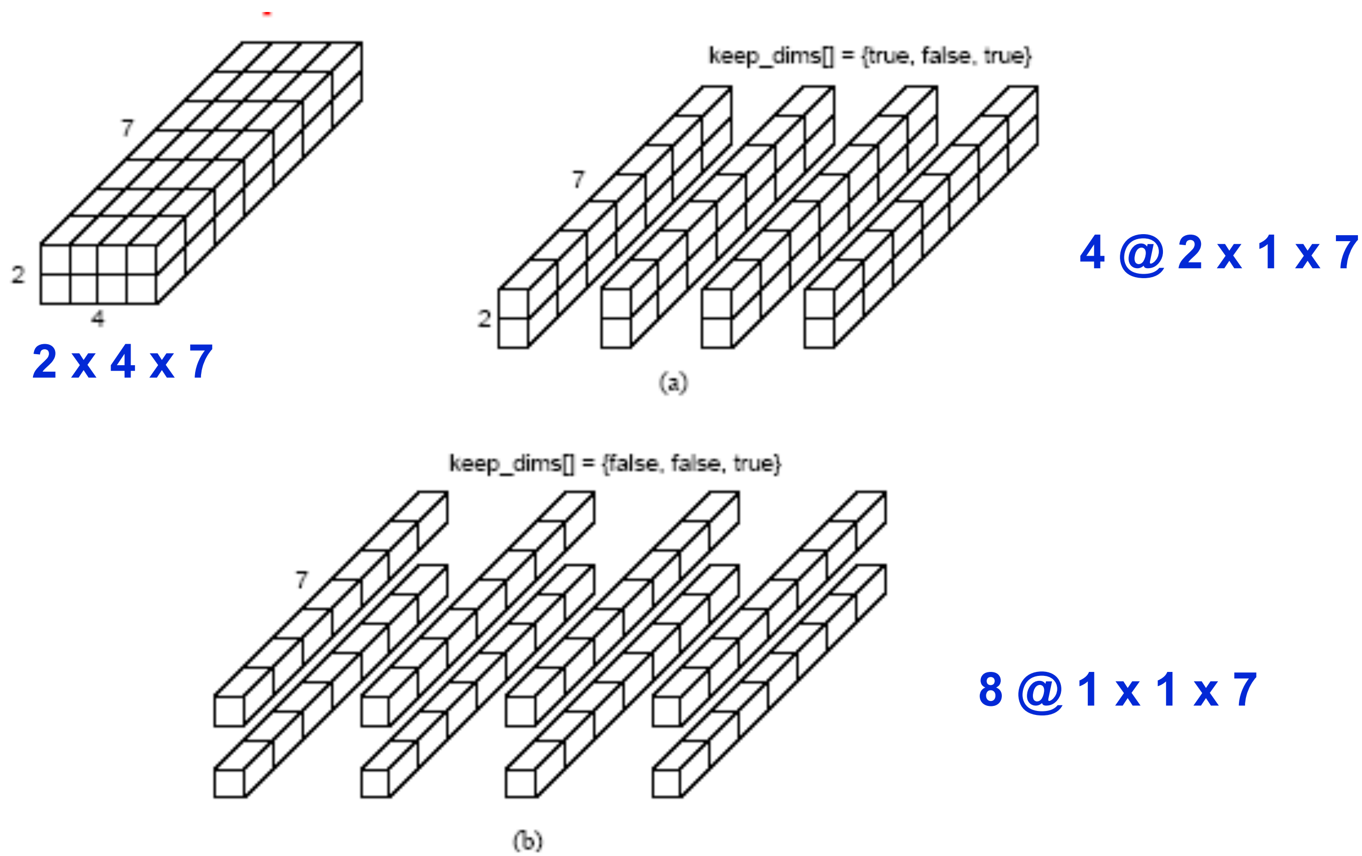
Splitting Cartesian Topologies

- Processes arranged in a virtual grid using Cartesian topology
- May need to restrict communication to a subset of the grid
- Partition a Cartesian topology to form lower-dimensional grids

```
int MPI_Cart_sub(MPI_Comm comm_cart, int *keep_dims,
                 MPI_Comm *comm_subcart)
```

- If `keep_dims[i]` is true (i.e. non-zero in C)
  - `i`th dimension is retained in the new sub-topology
- Process coordinates in a sub-topology
  - derived from coordinate in the original topology
  - disregard coordinates for dimensions that were dropped

Splitting Cartesian Topologies



Graph Toplogies

- For irregular problems a graph organization of processes can be convenient

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

- Map processes into a graph
  - nnodes = number of nodes
  - index = vector of integers describing node degrees
  - edges = vector of integers describing edges
  - reorder = flag indicating ranking may be reordered

process	neighbors
0	1, 3
1	0
2	3
3	0, 2

nnodes =	4
index =	2, 3, 4, 6
edges =	1, 3, 0, 3, 0, 2

Operations on Graph Topologies

- **Interrogating a graph topology with MPI_Graphdims_get**

```
int MPI_Graphdims_get(MPI_Comm comm, int *nnodes,
                      int *nedges)
```

  - **inquire about length of node and edge vectors**

- **Extracting a graph topology with MPI_Graph_get**

```
int MPI_Graph_get(MPI_Comm comm, int maxindex,
                  int maxedges, int *index,
                  int *edges)
```

  - **read out the adjacency list structure in index and edges**

MPI Derived Data Types

- A general datatype is an opaque object that specifies 2 things
  - —a sequence of basic data types
  - —a sequence of integer (byte) displacements
    - not required to be positive, distinct, or in increasing order
- Some properties of general data types
  - —order of items need not coincide with their order in memory
  - —an item may appear more than once
- Type map = pair of type & displacement sequences (equivalently, a sequence of pairs)
- Type signature = sequence of basic data types

Building an MPI Data Type

```
int MPI_Type_struct(int count, int blocklens[],
MPI_Aint indices[], MPI_Datatype old_types[],
MPI_Datatype *newtype )
```

if you define a structure datatype and wish to send or receive multiple items, you should explicitly include an MPI_UB entry as the last member of the structure.

Example

struct { int a; char b; } foo;

```
blen[0]=1; indices[0] = 0;                // offset of a
oldtypes[0]=MPI_INT;
blen[1]=1; indices[1] = &foo.b - &foo.a; // offset of b
oldtypes[1]=MPI_CHAR;
blen[2]=1; indices[2] = sizeof(foo);     // offset of UB
oldtypes[2]= MPI_UB;
MPI_Type_struct( 3, blen, indices, oldtypes, &newtype );
```

MPI Data Type Constructor Example 1

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

—newtype is the datatype obtained by concatenating count copies of oldtype

- Example
  —consider constructing newtype from the following
    - oldtype with type map *{ (double, 0), (char, 8) }* , with extent 16
    - let count = 3

  —type map of newtype is
    - *{ (double, 0), (char, 8),*
      (double, 16), (char, 24),
      (double, 32), (char, 40) }
    - namely, alternating double and char elements, with displacements *0, 8, 16, 24, 32, 40*

MPI Data Type Constructor Example 2

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

- **Let oldtype have type map**

  { (double, 0), (char, 8) } with extent 16

- **A call to `MPI_Type_vector`(2, 3, 4, oldtype, newtype) will create the datatype with type map**
  - two blocks with three copies each of the old type, with a stride of 4 elements (*4* x *16* bytes) between the blocks

{ (double, 0), (char, 8), (double, 16), (char, 24), (double, 32), (char, 40),
(double, 64), (char, 72), (double, 80), (char, 88), (double, 96), (char, 104) }

Threads and MPI

- **MPI does not define if an MPI process is a thread or an OS process**
  - —threads are not addressable
  - —MPI_Send(... thread_id ...) is not possible
- **MPI-2 Specification**
  - —does not mandate thread support
  - —specifies what a thread-compliant MPI should do
  - —specifies four levels of thread support

Initializing MPI for Threading

```
int MPI_Init_thread(int *argc, char ***argv,
                    int required, int *provided)
```

Used instead of MPI_Init; MPI_Init_thread has a provision to request a certain level of thread support in required

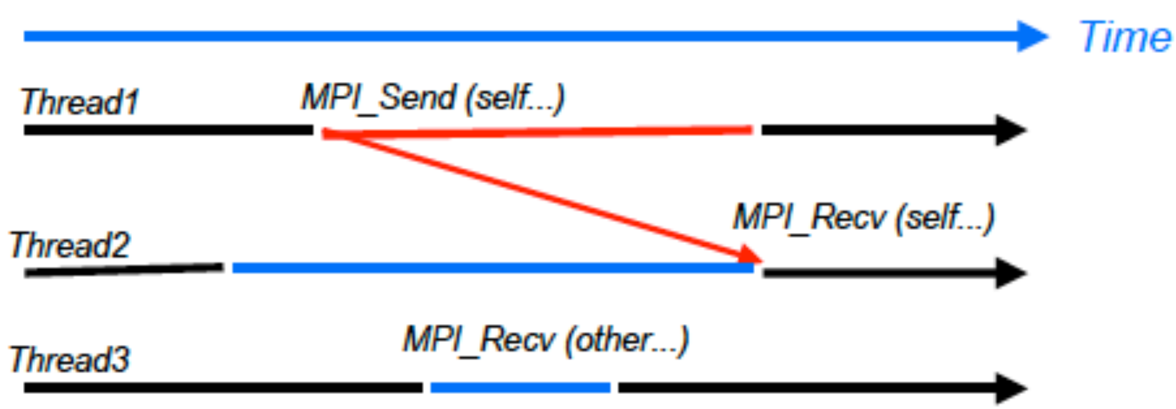
- MPI_THREAD_SINGLE: only one thread will execute
- MPI_THREAD_FUNNELED: if the process is multithreaded, only the thread that called MPI_Init_thread will make MPI calls
- MPI_THREAD_SERIALIZED: if the process is multithreaded, only one thread will make MPI library calls at one time
- MPI_THREAD_MULTIPLE: if the process is multithreaded, multiple threads may call MPI at once with no restrictions

Require the lowest level that you need

MPI_Init is equivalent to supplying MPI_THREAD_SINGLE to MPI_Init_thread

Thread-compliant MPI

- **All MPI library calls are thread safe**
- **Blocking calls block the calling thread only**
  - —other threads can continue executing



MPI Threading Inquiry Primitives

- Inquire about what kind of thread support MPI has provided to your application

```
int MPI_Query_thread(int *provided)
```

- Inquire whether this thread called MPI_Init or MPI_Init_thread

```
int MPI_Is_thread_main(int *flag)
```

MPI + Threading Example

```
#include "mpi.h"
#include <stdio.h>

int main( int argc, char *argv[] )
{
    int errs = 0;
    int provided, flag, claimed;
    pthread_t thread;

    MPI_Init_thread( 0, 0, MPI_THREAD_MULTIPLE, &provided );

    MPI_Is_thread_main( &flag );
    if (!flag) {
        errs++;
        printf( "This thread called init_thread but Is_thread_main gave false\n" );
        fflush(stdout);
    }
    MPI_Query_thread( &claimed );
    if (claimed != provided) {
        errs++;
        printf( "Query thread gave thread level %d but Init_thread gave %d\n", claimed, provided );
        fflush(stdout);
    }
    pthread_create(&thread, NULL, mythread_function, NULL);
    ...

    MPI_Finalize();
    return errs;
}
```

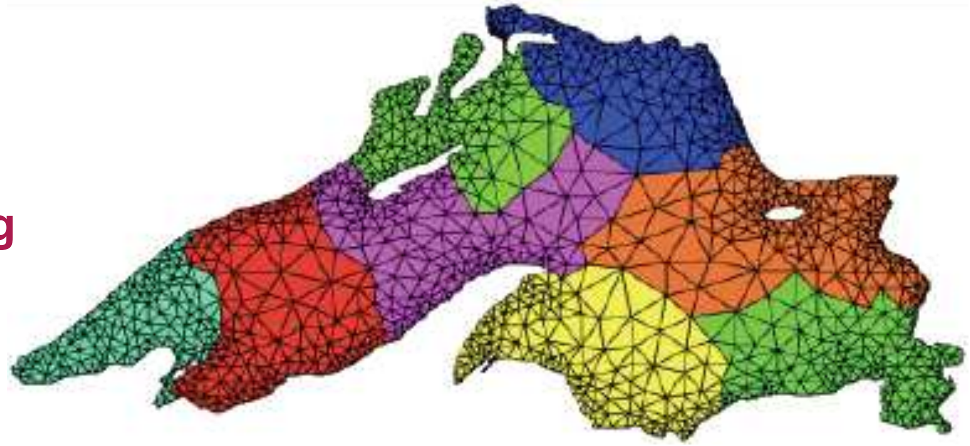
One-Sided vs. Two-Sided Communication

- **Two-sided: data transfer and synchronization are conjoined**
  - —message passing communication is two-sided
    - – sender and receiver issue explicit send or receive operations to engage in a communication
- **One-sided: data transfer and synchronization are separate**
  - —a process or thread of control can read or modify remote data without explicit pairing with another process
  - —terms
    - – origin process: process performing remote memory access
    - – target process: process whose data is being accessed

Why One-Sided Communication?

- **If communication pattern is not known a priori, using a two-sided (send/recv) model requires an extra step to determine how many sends-recvs to issue on each processor**

Consider the communication associated with acquiring information about neighboring vertices in a partitioned graph



- **Easier to code using one-sided communication because only the origin or target process needs to issue the put or get call**
- **Expose hardware shared memory**
  - **—more direct mapping of communication onto HW using load/store**
    - **avoid SW overhead of message passing; let the HW do its thing!**

Figure credit: "Introduction to Parallel Computing" A. Grama, A. Gupta, G. Karypis, and V. Kumar. Addison Wesley, 2003

One-Sided Communication in MPI-2

- **MPI-2 Remote Memory Access (RMA)**
  - processes in a communicator can read, write, and accumulate values in a region of "shared" memory
- **Two aspects of RMA-based communication**
  - data transfer, synchronization
- **RMA advantages**
  - multiple data transfers with a single synchronization operation
  - can be significantly faster than send/recv on some platforms
    - e.g. systems with hardware support for shared memory

MPI-2 RMA Operation Overview

- **MPI_Win_create**
  - —collective operation to create new window object
  - —exposes memory to RMA by other processes in a communicator
- **MPI_Win_free**
  - —deallocates window object
- **Non-blocking data movement operations**
  - —MPI_Put
    - moves data from local memory to remote memory
  - —MPI_Get
    - retrieves data from remote memory into local memory
  - —MPI_Accumulate
    - updates remote memory using local values
- **Synchronization operations**

Active Target vs. Passive Target RMA

- **Passive target RMA**
  - target process makes no synchronization call
- **Active target RMA**
  - requires participation from the target process in the form of synchronization calls (fence or post/wait, start/complete)
- **Illegal to have overlapping active and passive RMA epochs**

Synchronization for Passive Target RMA

- MPI_Win_lock(locktype, target_rank, assert, win) “beginning RMA”
  - locktype values
    - MPI_LOCK_EXCLUSIVE
      - one process at a time may access
      - use when modifying the window
    - MPI_LOCK_SHARED
      - multiple processes
        - (as long as none hold MPI_LOCK_EXCLUSIVE)
      - useful when accessing window only with MPI_Get
  - assert values
    - 0
    - MPI_MODE_NOCHECK
- MPI_Win_unlock(target_rank, win) “ending RMA”

Active Target Synchronization

- **MPI_Win_start**
  - —begins an RMA epoch on origin process
- **MPI_Win_post**
  - —starts RMA exposure for a local window on a target process
- **MPI_Win_wait/test**
  - —end RMA exposure on local window on a target process
- **MPI_Win_complete**
  - —forces local completion an RMA epoch on origin
- **MPI_Win_fence**
  - —collective forces remote completion of put/get/acc before fence

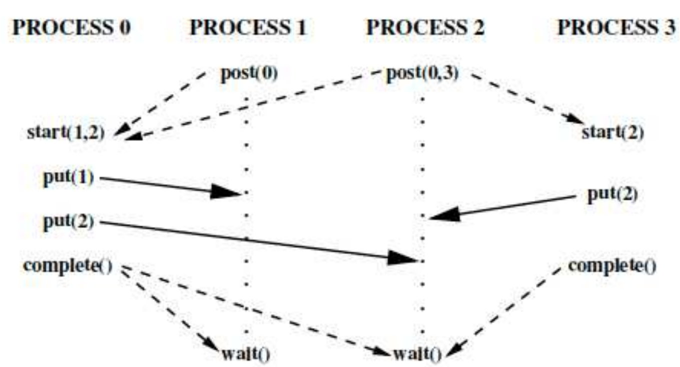


Figure credit: MPI-3 draft specification, Nov. 2010.

MPI RMA Active Target Example 1

Generic loosely synchronous, iterative code, using fence synchronization

The window at each process consists of array A, which contains the origin and target buffers of the Get calls

```
   ...
   while(!converged(A)){
      update_boundary(A);
      MPI_Win_fence(MPI_MODE_NOPRECEDE, win);
      for(i=0; i < toneighbors; i++)
         MPI_Get(&tobuf[i], 1, totype[i], fromneighbor[i],
                 fromdisp[i], 1, fromtype[i], win);
 update_core(A);
      MPI_Win_fence(MPI_MODE_NOSUCCEED,win);
    }
```

Similar code could be written with Put rather than Get

MPI RMA Active Target Example 2

Generic loosely synchronous, iterative code, using fence synchronization

The window at each process consists of array A, which contains the origin and target buffers of the Get calls

```
   ...
   while(!converged(A)){
      update_boundary(A);
      MPI_Win_post(togroup, win);
MPI_Win_start(fromgroup, win);
      for(i=0; i < toneighbors; i++)
         MPI_Get(&tobuf[i], 1, totype[i], fromneighbor[i],
                     fromdisp[i], 1, fromtype[i], win);
update_core(A);
      MPI_Win_complete(win);
    }
```

Similar code could be written with Put rather than Get

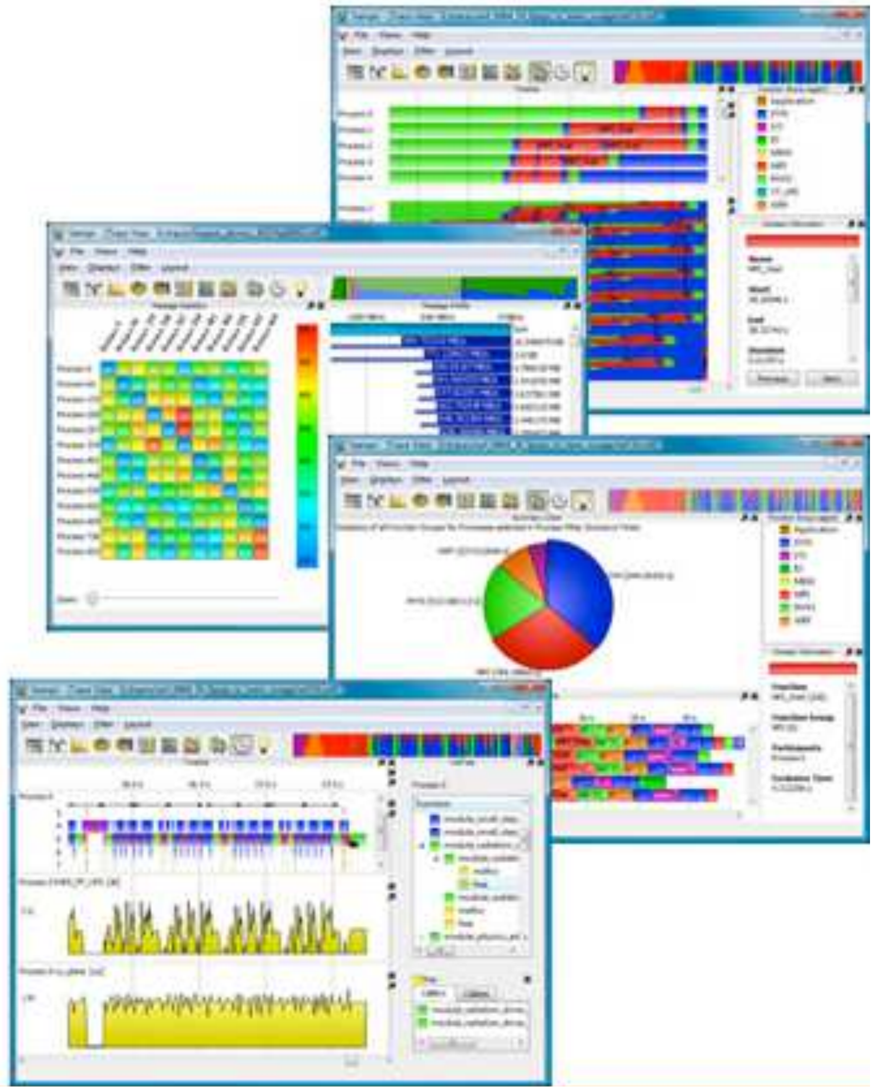
MPI-1 Profiling Interface - PMPI

- To support tools, MPI implementations define two interfaces to every MPI function
  - MPI_xxx
  - PMPI_xxx
- One can "wrap" MPI functions with a tool library to observe execution of an MPI program

```
int MPI_Send(void* buffer, int count, MPI_Datatype dtype,
             int dest, int tag, MPI_Comm comm)
  {
    double tstart = MPI_Wtime(); /* Pass on all arguments */
    int extent;
    int result = PMPI_Send(buffer,count,dtype,dest,tag,comm);
    MPI_Type_size(datatype, &extent); /* Compute size */
    totalBytes += count*extent;
    totalTime += MPI_Wtime() - tstart; /* and time */
    return result;
  }
```

Some MPI Tools

- MPICH MPI implementation
  - —MPI tracing library
  - —Jumpshot trace visualization tool
- Vampir: MPI trace analysis tools
  - —http://www.vampir.eu/
- MPIp library for profiling MPI operations
  - —http://mpip.sourceforge.net
- memcheck
  - —OpenMPI + valgrind checks correct use of comm buffers
  - —http://www.open-mpi.org
- marmot
  - —checks usage of MPI routines
  - —http://www.hlrs.de/organization/av/amt/projects/marmot



Vampir displays

MPI Libraries

- **SCALAPACK - dense linear algebra using block-cyclic tilings**
  - —http://www.netlib.org/scalapack/scalapack_home.html
- **PetSC - Portable Extensible, Toolkit for Scientific Computation**
  - —data structures and routines for solution of scientific applications modeled by partial differential equations
  - —http://www.mcs.anl.gov/petsc/petsc-as
- **Trilinos - software framework for solving large-scale, complex multi-physics engineering and scientific problems**
  - —http://trilinos.sandia.gov

MPI-3 Additions

Nonblocking collective operations

- —barrier synchronization
- —broadcast
- —gather
- —scatter
- —gather-to-all
- —all-to-all scatter/gather
- —reduce
- —reduce-scatter
- —inclusive scan
- —exclusive scan

Building MPI Programs

- **Each MPI installation defines compilation scripts**
  - —mpicc: C
  - —mpif90: Fortran 90
  - —mpif77: Fortran 77
  - —mpicxx, mpiCC: C++
- **Benefits of using these scripts**
  - —they supply the appropriate paths
    - for MPI include files
    - for MPI library files
  - —they link appropriate libraries into your executable

Common Errors and Misunderstandings

- Expecting argc and argv to be passed to all processes
  - some MPI implementations pass them to all processes, but the MPI standard does not require it
- Doing things before MPI_Init or after MPI_Finalize
  - the MPI standard says nothing about the state of an execution outside this interval
- Matching MPI_Bcast with MPI_Recv; all should use MPI_Bcast
- Assuming your MPI implementation is thread safe

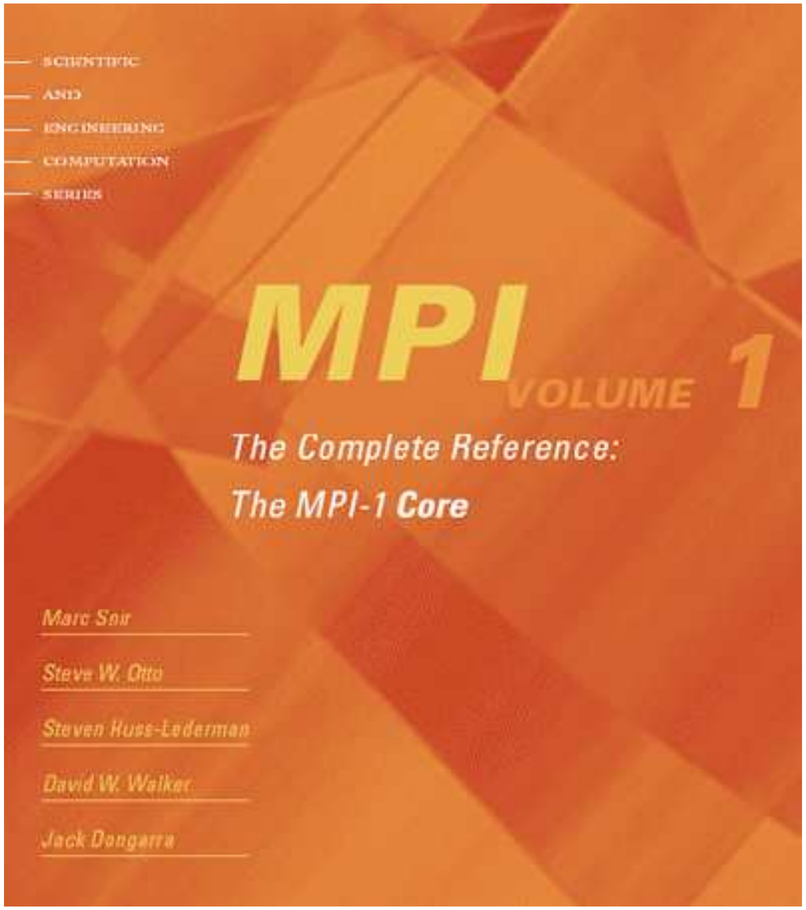
Running MPI Programs

- Each MPI installation provides one or more launch scripts
  - mpirun
  - mpiexec
- On networks of workstations, launch MPI as follows
  - mpirun [-np PE] [--hostfile <filename>] <pgm>
    - mpirun will use rsh or ssh to launch jobs on machines in hostfile
    - without a hostfile, it will run all jobs on the local node
- If running under a resource manager (e.g. PBS)
  - `mpirun [-np ncores] yourprogram`
  - `mpiexec [-np ncores] yourprogram`

MPI Online Resources

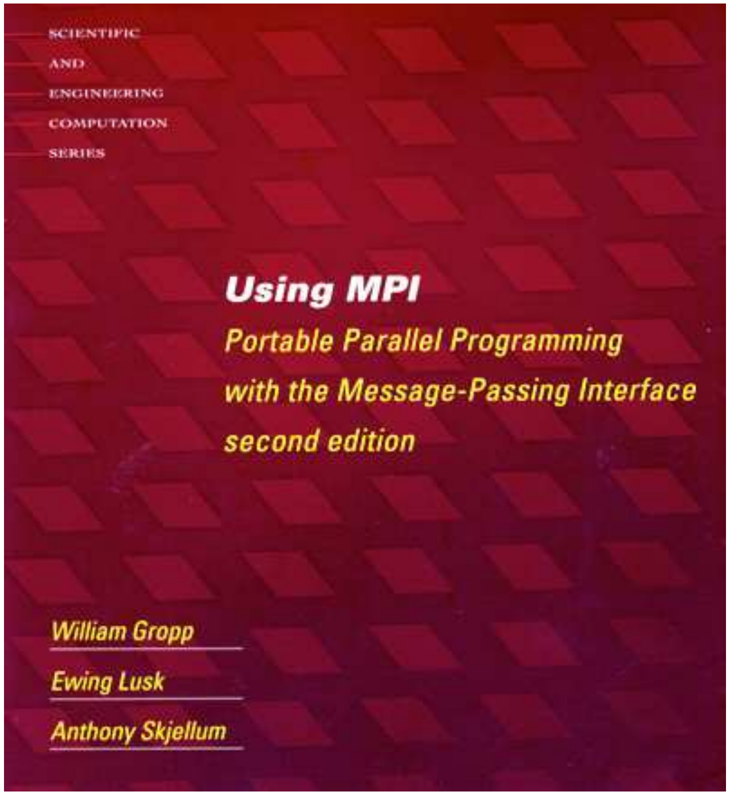
- **http://www.mpi-forum.org**
  - **—http://www.mpi-forum.org/docs/docs.html**
    - **MPI standards documents (all official releases)**
- **http://www.mcs.anl.gov/research/projects/mpi/**
  - **—tutorials http://www.mcs.anl.gov/research/projects/mpi/learning.html**
  - **—MPICH and MPICH2 implementations by ANL**

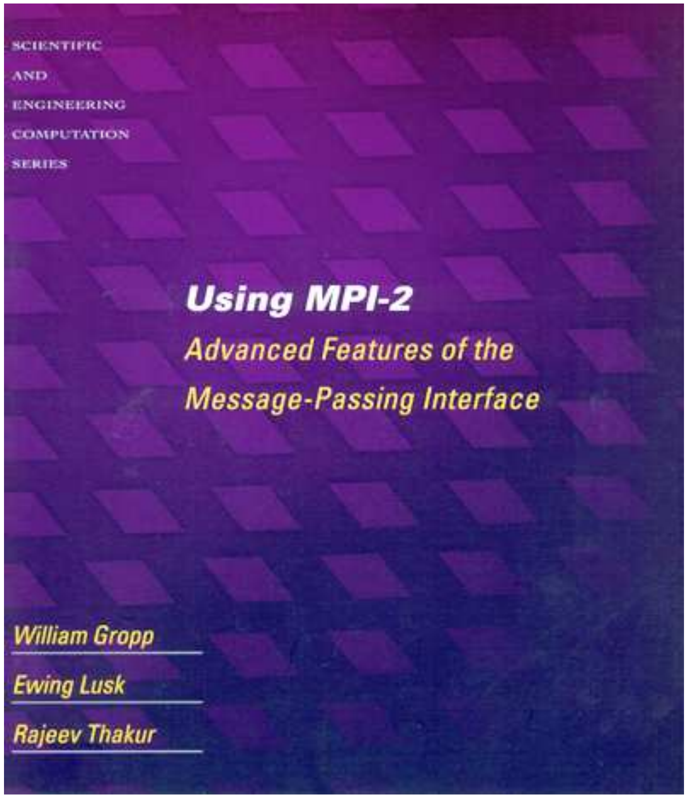
The MPI and MPI-2 Standards



- **MPI: The Complete Reference, Volume 1 (2nd Edition) - The MPI Core, MIT Press, 1998.**
- **MPI: The Complete Reference, Volume 2 - The MPI-2 Extensions, MIT Press, 1998.**

Guides to MPI and MPI-2 Programming





- **Using MPI: http://www.mcs.anl.gov/mpi/usingmpi**
- **Using MPI-2: http://www.mcs.anl.gov/mpi/usingmpi2**

References

- William Gropp, Ewing Lusk and Anthony Skjellum. Using MPI, 2nd Edition Portable Parallel Programming with the Message Passing Interface. MIT Press, 1999; ISBN 0-262-57132-3
- Ananth Grama, Anshul Gupta, George Karypis, and Vipin Kumar. "Introduction to Parallel Computing," Chapter 6. Addison Wesley, 2003.
- Athas, W. C. and Seitz, C. L. 1988. Multicomputers: Message-Passing Concurrent Computers. Computer 21, 8 (Aug. 1988), 9-24. DOI= http://dx.doi.org/10.1109/2.73