Advanced MPI

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What we know already

- Everything to write typical MPI programs
  - Program structure
  - Point-to-point communication
  - Communication modes
  - Blocking/non-blocking communication
  - Collective Communication
  - Data types
  - Groups and communicators
  - Performance considerations

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MPI provides additional, advanced features

- Virtual topologies
- MPI-IO
- One-sided communication
- Profiling Interface

- Very useful in special cases – go beyond an introductory lecture

- We will touch these issues only on the surface

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MPI Profiling Interface

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Profiling Interface Overview

- To understand program performance it is important to understand what the program is actually doing
- Simple printf's are not sufficient to understand the complex behavior of message passing programs
  - Where does synchronization occur?
  - Which process is waiting for input when?
  - Etc.

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A side note: Timing in MPI

- To simply understand how long a program/a certain part of a program took MPI provides an interface to system timer:

```
double MPI_Wtime();
DOUBLE PRECISION MPI_WTIME()
```

- Timing resolution can be explored by

```
Double MPI_Wtick();
```

  - Resolution on the Cray is 1 microsecond
- Not enough to understand complex behavior

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Profiling Interface

- MPI allows to log certain events to a log file that can be analyzed post-mortem
- Part of the MPI MultiProcessing Environment
  - Prefix MPE
  - **Tracing Library** This traces all MPI calls. Each MPI call is preceded by a line that contains the rank in MPI_COMM_WORLD of the calling process, and followed by another line indicating that the call has completed..
  - **Animation Library** This is a simple form of real-time program animation and requires X window routines.
  - **Logging Library** This is the most useful and widely used profiling libraries in MPE. They form the basis to generate log files from user MPI programs. There are currently 3 different log file formats allowed in MPE.

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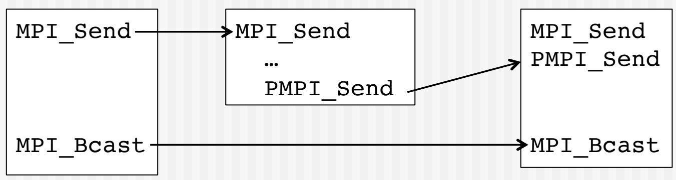
MPI Profiling Interface

- You normally don't instrument and log events in your MPI program directly
- MPI provides a mechanism for tool developer to dynamically replace (at link time) standard MPI routines with instrumented ones through a nameshift
  - Each MPI call is also defined as PMPI



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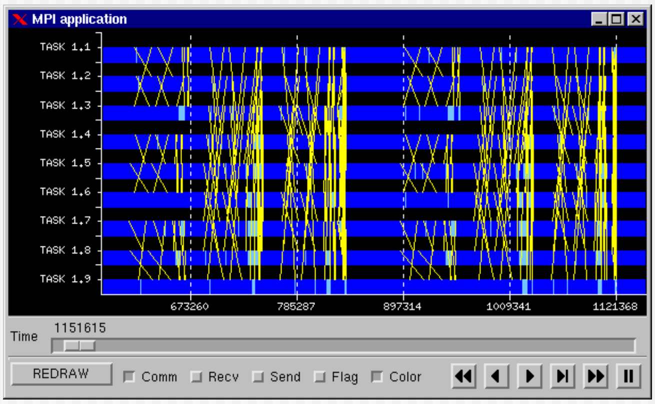
Using MPI Profiling

- Link against profiled MPI implementation
- This will produce a trace file
- Use performance tools (see performance lecture) to analyze the data



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Virtual Topologies

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Ordering of Processes

- So far we have worked with a flat process space
  - Rank 0 … n-1
- Many application have however an inherent structure of their data
  - E.g. 2D or 3D matrices
- Likewise, the underlying network has a specific structure
  - E.g. fat tree, 3d torus, dragonfly
- Can we take advantage of this and map processes in a similar fashion?

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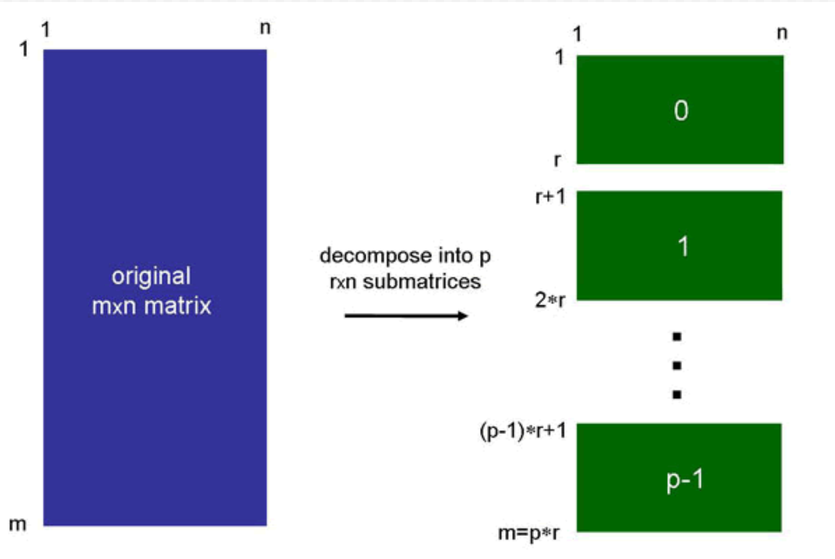
Example – Simple (flat) topology



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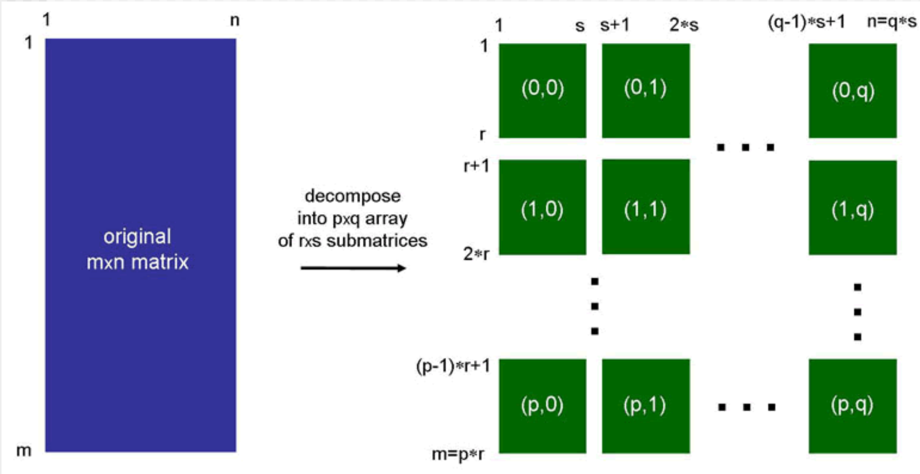
Example – 2D Topology



- Can still use flat process space but requires tedious and error prone mapping

MPI Virtual Topologies

- MPI provides 2 types of virtual topologies
  - Cartesian
  - Graphs
- Cartesian topology (generalization of a grid function)
  - Each process is connected to its neighbors in a virtual grid
  - Boundaries can be cyclic (or not)
  - Processes are identified by (discrete) Cartesian coordinates
    - Eg. x,y,z
- Graph topology
  - Describe communication patterns by means of graphs
  - The most general description of communication patterns
  - Not covered here

Benefits of Virtual Topologies

- Convenient process naming
- Naming scheme to fit communication pattern
- Simplifies writing code
- Can allow MPI to optimize communications
  - Vendors can optimize mappings on their network topology
- Used in Neighborhood Collectives
  - New MPI3 feature

How do Virt. Topologies work?

- Creating a virtual topology produces a new communicator
- MPI provides mapping functions between the serial process enumeration and the virtual topology
- Mapping functions compute processor ranks based on the topology naming scheme

Virtual Grid

0,0 (0)	0,1 (1)
1,0 (2)	1,1 (3)
2,0 (4)	2,1 (5)

Main Cartesian Commands

- **MPI_CART_CREATE**: creates a new communicator using a Cartesian topology
- **MPI_CART_COORDS**: returns the corresponding Cartesian coordinates of a (linear) rank in a Cartesian communicator.
- **MPI_CART_RANK**: returns the corresponding process rank of the Cartesian coordinates of a Cartesian communicator.
- **MPI_CART_SUB**: creates new communicators for subgrids of up to (N-1) dimensions from an N-dimensional Cartesian grid.
- **MPI_CART_SHIFT**: finds the resulting source and destination ranks, given a shift direction and amount.

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MPI_CART_CREATE

```
int MPI_Cart_create(MPI_Comm old_comm, int ndims,
    int *dim_size, int *periods, int reorder,
    MPI_Comm *new_comm)
```

```
MPI_CART_CREATE(OLD_COMM, NDIMS, DIM_SIZE, PERIODS,
                REORDER, NEW_COMM, IERR)
```

`periods:` Array of size ndims specifying periodicity status of each dimension

`reorder:` whether process rank reordering by MPI is permitted

`New_comm:` Communicator handle

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Example

```
#include "mpi.h"
MPI_Comm old_comm, new_comm;
int ndims, reorder, periods[2], dim_size[2];

old_comm = MPI_COMM_WORLD;
ndims = 2;            /*  2-D matrix/grid */
dim_size[0] = 3;      /* rows */
dim_size[1] = 2;      /* columns */
periods[0] = 1;       /* row periodic (each column forms a
                         ring) */
periods[1] = 0;       /* columns nonperiodic */
reorder = 1;          /* allows processes reordered for
                         efficiency */

MPI_Cart_create(old_comm, ndims, dim_size,
                periods, reorder, &new_comm);
```

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Example Cont'd

	-1,0 (4)	-1,1 (5)	
0,-1(-1)	0,0 (0)	0,1 (1)	0,2(-1)
1,-1(-1)	1,0 (2)	1,1 (3)	1,2 (-1)
2,-1(-1)	2,0 (4)	2,1 (5)	2,2 (-1)
	3,0 (0)	3,1 (1)	

periods(0)=.true.;periods(1)=.false.

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Note

- MPI_CART_CREATE is a collective communication function so it must be called by all processes in the group. Like other collective communication routines, MPI_CART_CREATE uses blocking communication. However, it is not required to be synchronized among processes in the group and hence is implementation dependent.
- If the total size of the Cartesian grid is smaller than available processes, those processes not included in the new communicator will return MPI_COMM_NULL.
- If the total size of the Cartesian grid is larger than available processes, the call results in error.

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MPI-IO

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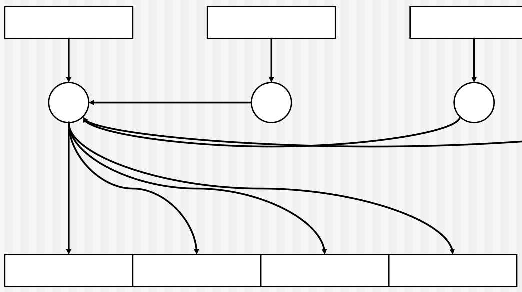
Common Ways of Doing I/O in Parallel Programs

- Sequential I/O:
  - All processes send data to process 0, and 0 writes it to the file

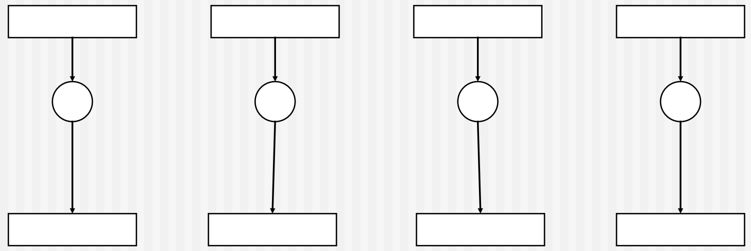


Pros and Cons of Sequential I/O

- Pros:
  - parallel machine may support I/O from only one process
    - (e.g., no common file system)
  - Some I/O libraries (e.g. HDF-4, NetCDF) not parallel
  - resulting single file is handy for **`ftp`**, **`mv`**
  - big blocks improve performance
  - short distance from original, serial code
- Cons:
  - lack of parallelism limits scalability, performance (single node bottleneck)

Another Way

- Each process writes to a separate file



- Pros:
  - parallelism, high performance
- Cons:
  - lots of small files to manage
  - difficult to read back data from different number of processes
  - Lots of requests can make trouble to the file system

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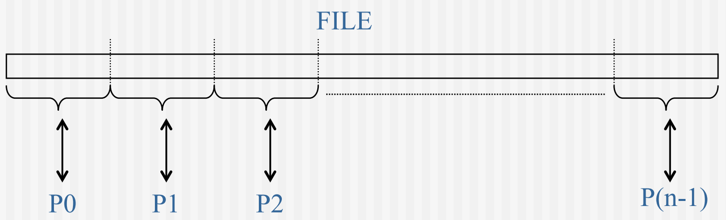
What is Parallel I/O?

- Multiple processes of a parallel program accessing data (reading or writing) from a *common* file



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Why Parallel I/O?

- Non-parallel I/O is simple but
  - Poor performance (single process writes to one file) or
  - Awkward and not interoperable with other tools (each process writes a separate file)
- Parallel I/O
  - Provides high performance
  - Can provide a single file that can be used with other tools (such as visualization programs)

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What is MPI-IO

- I/O interface specification for use in MPI applications
- Data model is a stream of bytes in a file
  - Same as POSIX and stdio
- Features
  - Noncontiguous I/O with **MPI datatypes** and file views
  - Collective I/O
  - Nonblocking I/O
  - Language bindings

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MPI File Structure

- MPI defines how multiple processes access and modify data in a shared file.
- Necessary to thin[k] … this file
  - Similar to how derived d… …thin memory
- MPI-IO works with … ple datatypes and derived datatypes
  - Derived datatypes are preferred because of performance benefits
- A view defines the current set of data, visible and accessible, from an open file.
  - Each process has its own view of the shared file that defines what data it can access.
  - A view can be changed by the user during program execution.

> One big file access instead of many small ones
> (see e.g. http://www.mcs.anl.gov/~thakur/dtype/)

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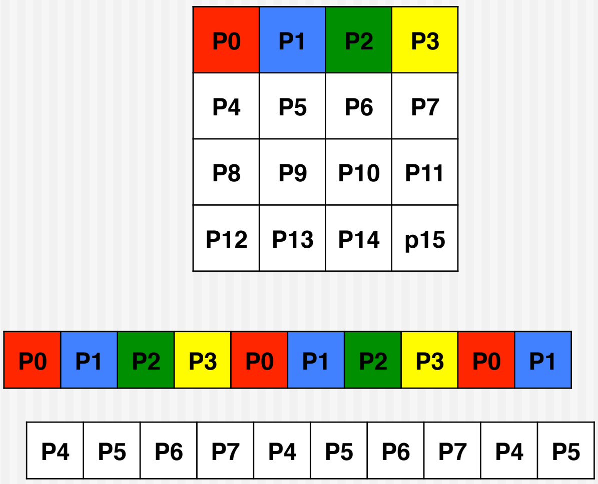
Why Derived Data Types?



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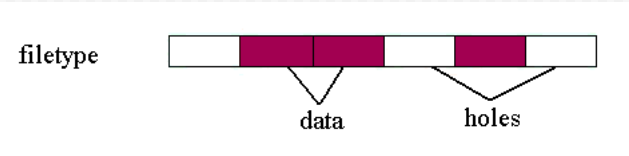
Essential Concepts

- Displacement
  - describes where to start in the file
- Elementary datatype (etype)
  - the type of data that is to be written or read
  - Basic or derived datatype
- Filetype
  - the pattern of how the data is partitioned in the file
  - A filetype is a defined sequence of etypes, which can have data or be considered blank



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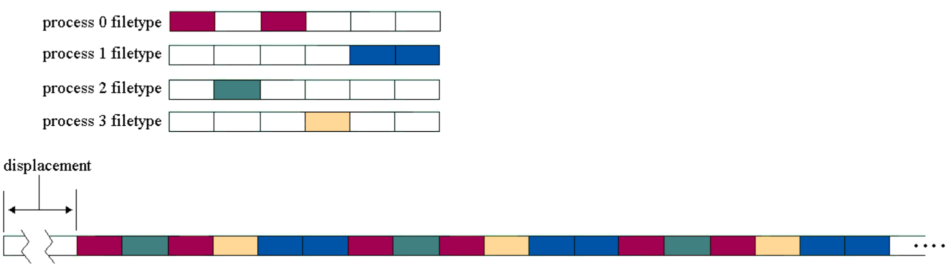
Example: File views



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Simple Example

```
MPI_File fh;
MPI_Status status;
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
bufsize = FILESIZE/nprocs;
nints = bufsize/sizeof(int);

MPI_File_open(MPI_COMM_WORLD, "/pfs/datafile",
              MPI_MODE_RDONLY, MPI_INFO_NULL, &fh);
MPI_File_seek(fh, rank * bufsize, MPI_SEEK_SET);
MPI_File_read(fh, buf, nints, MPI_INT, &status);
MPI_File_close(&fh);
```

offset

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More about MPI-IO

- See for instance

*www.npaci.edu/ahm2002/ahm_ppt/**Parallel_IO_MPI_2**.ppt*
Rajeev Thakur. Mathematics and Computer Science Division. Argonne National Laboratory

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One-sided Communication

Recap: Point-to-point Communication

- Both sender and receiver must issue matching MPI calls
  - Depending on buffering semantics may require handshake
- Sometimes it is difficult to know in advance when messages have to be sent/received and what characteristics these messages have
  - Could solve such situations with extra control messages
    - Requires polling, introduces overhead, and is cumbersome
- MPI provides Remote Memory Access (RMA), or one-sided communication
  - Allows one process to specify all communication parameters for both the sender and receiver

One-sided Communication

- Communication and Synchronization are separated
- Allows remote processes to
  - Write into local memory (**put**)
  - Read local memory (**get**)
- Accessible memory areas are called “windows”
- Communication can happen without synchronization
- Access to windows is synchronized

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Looks a bit like shared-memory programming?

- In fact, tries to bring the advantages of shared-memory programming to MPI programs
- Effective implementation needs shared memory or hardware support for RDMA
  - Available e.g. in infiniband or Cray networks
- Need synchronization to ensure correct behavior
  - Same issues as in shared-memory programming
  - MPI provides **window objects** for synchronization
- How to implement synchronization is a great optimization field

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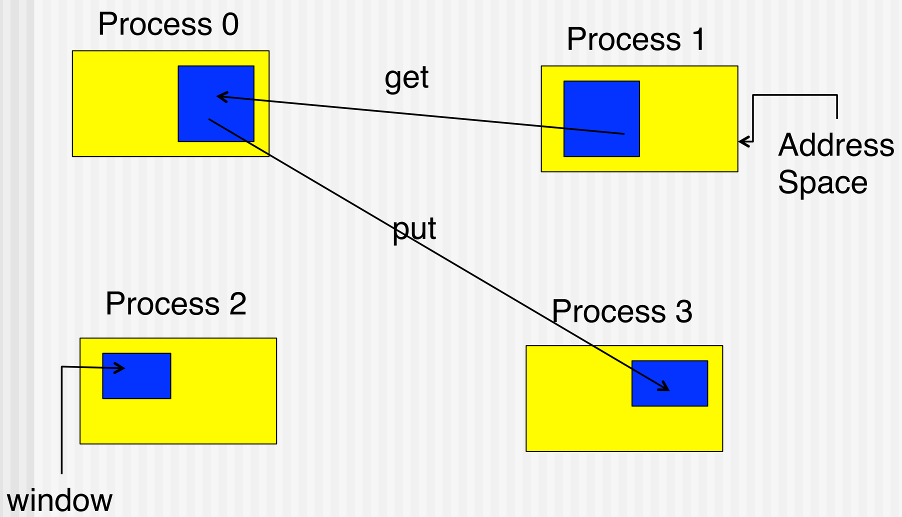
Window Objects



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Main Commands

- **`MPI_Win_create`** exposes local memory to RMA operation by other processes in a communicator
  - Collective operation
  - Creates window object
- **`MPI_Win_free`** deallocates window object
- **`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
- Data movement operations are non-blocking
- **Subsequent synchronization on window object needed to ensure operation is complete**

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Advantages of one-sided communication

- Can do multiple data transfers with a single synchronization operation
- Bypass tag matching
  - effectively precomputed as part of remote offset
- Some irregular communication patterns can be more economically expressed
- Can be significantly faster than send/receive on systems with hardware support for remote memory access, such as shared memory systems
  - **BUT**: can also be significantly slower depending on synchronization need and access patterns!

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Synchronization

- `Put/Get/Accumulate` are non-blocking
  - Subsequent synchronization on window object is needed to ensure operations are complete
- MPI_Win_fence is used to synchronize access to windows
  - Should be called before and after RMA
  - Similar to a barrier in shared memory

Process 0	Process 1
`MPI_Win_fence(win)`	`MPI_Win_fence(win)`
`MPI_Put`	
`MPI_Put`	
`MPI_Win_fence(win)`	`MPI_Win_fence(win)`

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New Modes in MPI-3

- PSCW Synchronization

- `MPI_Win_post(MPI_Group group, int assert, MPI_Win win)`
  - Start exposure
- `MPI_Win_start(MPI_Group group, int assert, MPI_Win win)`
  - Start access (may wait for post)
- `MPI_Win_complete(MPI_Win win)`
  - Finish access (origin only)
- `MPI_Win_wait(MPI_Win win)`
  - Wait for completion (at target)

- As asynchronous as possible

Other MPI-3 Features

- Lock-based synchronization
  - Locks window for access by one or all ranks

- Flush
  - Complete all outstanding operations at target and/or origin

- Request-based put and get (Rput, Rget)
  - Returns a request handle that can be tested for completion

Summary

- One-sided communication provides convenient means for irregular applications
- Communication can be more efficient with proper hardware support
- Great care needs to be put on (efficient) synchronization

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Summary

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Recap: Basic MPI Concepts

- Message **buffers** described by address, data type, and count
- Processes identified by their **ranks**
- **Communicators** identifying communication contexts/ groups

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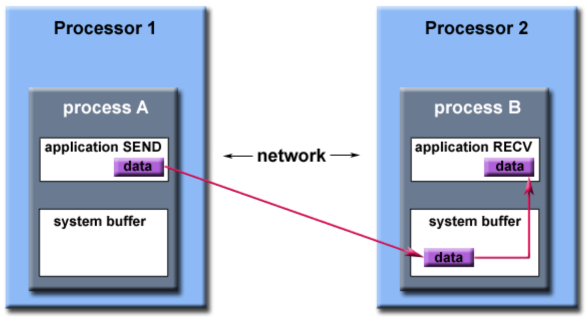
What is not specified

- Certain aspects are not specified in the MPI standard but left as implementation detail:
  - Process startup (how to start an MPI program)
    - All what happens before `MPI_Init` is executed
  - Richer error codes are allowed
  - Message buffering



Path of a message buffered at the receiving process

Basic Send/Receive Commands

```
int MPI_Send(void *buf, int count, MPI_Datatype
dtype, int dest, int tag, MPI_Comm comm);

MPI_SEND(BUF, COUNT, DTYPE, DEST, TAG, COMM, IERR)
```

Buffer, Count, Datatype } Body

Destination, Tag, Communicator } Envelope

```
int MPI_Recv(void *buf, int count, MPI_Datatype
dtype, int source, int tag, MPI_Comm comm, MPI_Status
*status);

MPI_RECV(BUF, COUNT, DTYPE, SOURCE, TAG, COMM,
STATUS, IERR)
```

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Wildcards

- Instead of specifying everything in the envelope explicitly, wildcards can be used for sender and tag:

  `MPI_ANY_SOURCE` and `MPI_ANY_TAG`
- Actual source and tag are stored in `STATUS` variable

C:

```
MPI_Status status;
MPI_Recv(b, 100, MPI_DOUBLE,
         MPI_ANY_SOURCE, MPI_ANY_TAG,
         MPI_COMM_WORLD, &status );

source = status.MPI_SOURCE;
tag = status.MPI_TAG;
```

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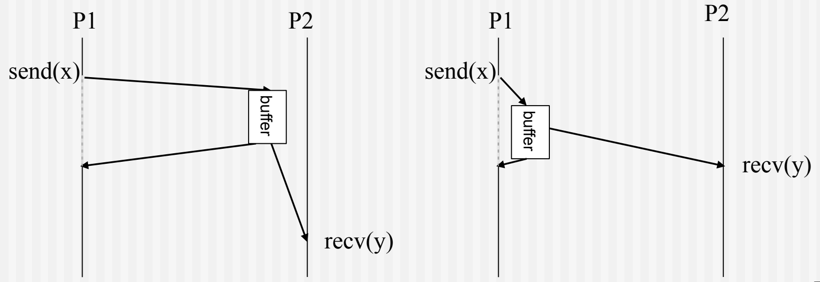
A Word on Buffering

- MPI implementations typically use (**internal**) message buffers
  - Sending process can safely modify the sent data once it is copied into the buffer, irrespectively of status of receiving process
  - Receiving process can buffer incoming messages even if no (user space) receiving buffer is provided, yet
  - Buffers can be on both sides



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Note

This system buffer is **DIFFERENT** to the message buffer you specify in the `MPI_Send` or `MPI_Recv` calls!

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Blocking and Completion

- Both `MPI_Send` and `MPI_Recv` are blocking
  - They program only continues after they are completed
- The command is completed once it is safe to (re)use the data
  - `MPI_Recv`: data has been fully received
  - `MPI_Send`: can be completed even if no non-local action has been taking place. WHY?
  - Once data is copied into a send buffer `MPI_Send` can complete

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Deadlocks

- Deadlocks are common (and hard to debug) errors in message passing programs
- A deadlock occurs when two (or more) processes wait on the progress of each other:

```
if( myrank == 0 ) {
   /* Receive, then send a message */
   MPI_Recv( b, 100, MPI_DOUBLE, 1, 19, MPI_COMM_WORLD,
             &status );
   MPI_Send( a, 100, MPI_DOUBLE, 1, 17, MPI_COMM_WORLD );
 }
 else if( myrank == 1 ) {
   /* Receive, then send a message */
   MPI_Recv( b, 100, MPI_DOUBLE, 0, 17, MPI_COMM_WORLD,
             &status );
   MPI_Send( a, 100, MPI_DOUBLE, 0, 19, MPI_COMM_WORLD );
```

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Help to avoid Deadlocks Cont'd

- Careful message ordering
  - Always a good idea!
- Buffered communication
  - But comes with (quite substantial) overhead
- Non-blocking calls

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Non-blocking Communication

- For all send/receive calls there is a non-blocking equivalent named `I(x)send/Irecv`
- Non-blocking calls will return immediately irrespectively of the send/receive status
  - They actually only **initiate** the action
  - Actual sending/receiving of messages will be handled internally in the MPI implementation
  - Calls return a handle that allows to check the progress of sending/ receiving
- Blocking and non-blocking calls can be intermixed
  - A blocking receive can match a non-blocking send and vice-versa.

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Completion of non-blocking send/receives

```
int MPI_Wait( MPI_Request *request, MPI_Status
*status );
MPI_WAIT(REQUEST, STATUS, IERR )
```

- `MPI_Wait` is blocking and will only return when the message has been sent/received
  - After `MPI_Wait` returns it is safe to access the data again

```
int MPI_Test( MPI_Request *request, int *flag,
              MPI_Status *status );
MPI_TEST(REQUEST, FLAG, STATUS, IERR)
```

- MPI_Test returns immediately
  - Status of request is returned in flag (true for done, false when still ongoing)

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Collective Communication Cont'd

- Communication involving all processes in a **group** (i.e. a **communicator**)
  - MPI-3 defines "neighborhood collectives"
- All processes in a group **MUST** participate to the collective operation
- No tag mechanism, only order of program execution
  - Remember that MPI messages cannot overtake another one
- Until MPI-2 all collective routines were only blocking
  - With the standard completion semantics of blocking communication – thus no guarantee there is a full synchronization
  - MPI-3 introduced non-blocking collectives
    - Important difference to non-blocking p2p: no matching with non-blocking collectives!

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List of Collective Routines

- Barrier synchronization across all processes.
- Broadcast from one process to all other processes
- Global reduction operations such as sum, min, max or user-defined reductions
- Gather data from all processes to one process
- Scatter data from one process to all processes
- All-to-all exchange of data
- Scan across all processes

Take a deeper look

- Usage of data types
  - So far we used the pre-defined data types; what if we need to deal with more complex structures?
- Usage of communicators
  - How to group processes in individual groups
- Improving Communication Performance
  - Aka how to speed up programs

Performance Considerations

- Simple and effective performance model:
  - More parameters == slower
- **contig < vector < index < struct**
- Some (most) MPIs are inconsistent
  - But this rule is portable
- Advice to users:
  - Try datatype “compression” bottom-up

Loss of performance

- Transfer time = latency + message length/bandwidth + synchronization time
- You cannot do much about bandwidth but
- Reduce latency
  - Combine many small into a single large message
  - Hide communication with computation
- Reduce message length
  - Only communicate what is absolutely needed
- Avoid synchronization

And finally …

- The top MPI Errors according to

Advanced MPI: I/O and One-Sided Communication, presented at SC2005, by William Gropp, Rusty Lusk, Rob Ross, and Rajeev Thakur
http://www.mcs.anl.gov/research/projects/mpi/tutorial/advmpi/sc2005-advmpi.pdf)

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Top MPI Errors

- Fortran: missing ierr argument
- Fortran: missing MPI_STATUS_SIZE on status
- Fortran: Using integers where MPI_OFFSET_KIND or MPI_ADDRESS_KIND integers are required (particularly in I/O)
- Fortran 90: Using array sections to nonblocking routines (e.g., MPI_Isend)
- All: MPI_Bcast not called collectively (e.g., sender bcasts, receivers use MPI_Recv)
- All: Failure to wait (or test for completion) on MPI_Request
- All: Reusing buffers on nonblocking operations
- All: Using a single process for all file I/O
- All: Using MPI_Pack/Unpack instead of Datatypes
- All: Unsafe use of blocking sends/receives
- All: Using MPI_COMM_WORLD instead of comm in libraries
- All: Not understanding implementation performance settings
- All: Failing to install and use the MPI implementation according to its documentation.

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Summary

- MPI allows to write portable parallel code across many different architectures
- Writing simple MPI programs is easy (6 commands)
- Writing efficient MPI programs is difficult
  - Need also to understand MPI implementation and underlying hardware
  - Experiment with different options
  - Also experiment with hybrid approaches: use Open-MP within a nodes and MPI across nodes

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