Message-Passing Programming: MPI

National Tsing Hua University

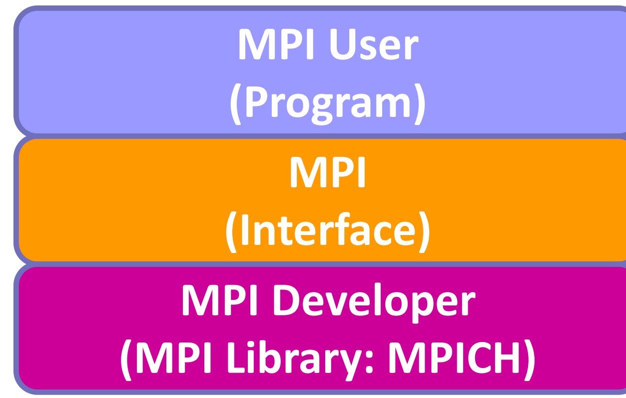
2025, Fall Semester

Outline

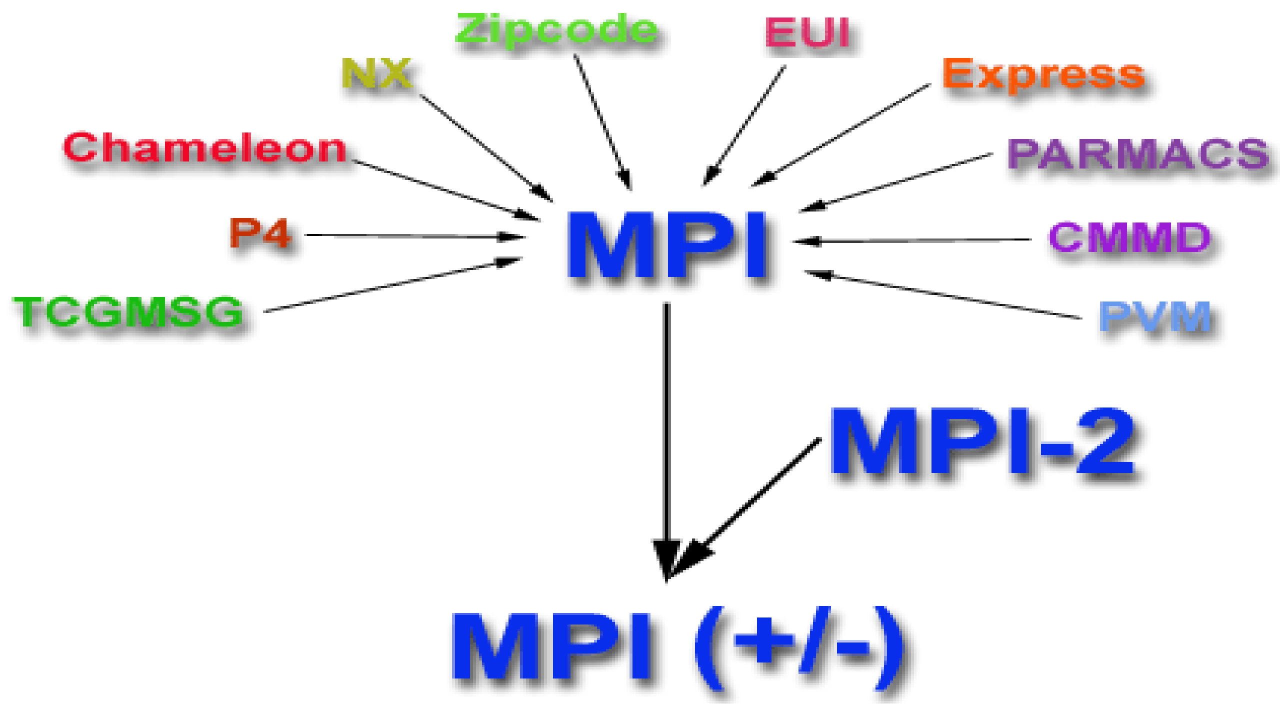
- MPI Introduction
  - History & Evolution
- Communication Methods
  - Synchronous / Asynchronous
  - Blocking / Non-Blocking
- MPI API
  - Point-to-Point Communication Routines
  - Collective Communication Routines
  - Group and Communicator Management Routines
- MPI-IO

What is MPI

- MPI = Message Passing **Interface**
- A **specification** for the developers and users of message passing libraries
  - By itself, it is an **interface NOT a library**
- Commonly used for **distributed memory system & high-performance computing**
- Goal:
  - **Portable**: Run on different machines or platforms
  - Scalable: Run on million of compute nodes
  - Flexible: Isolate MPI developers from MPI programmers (users)

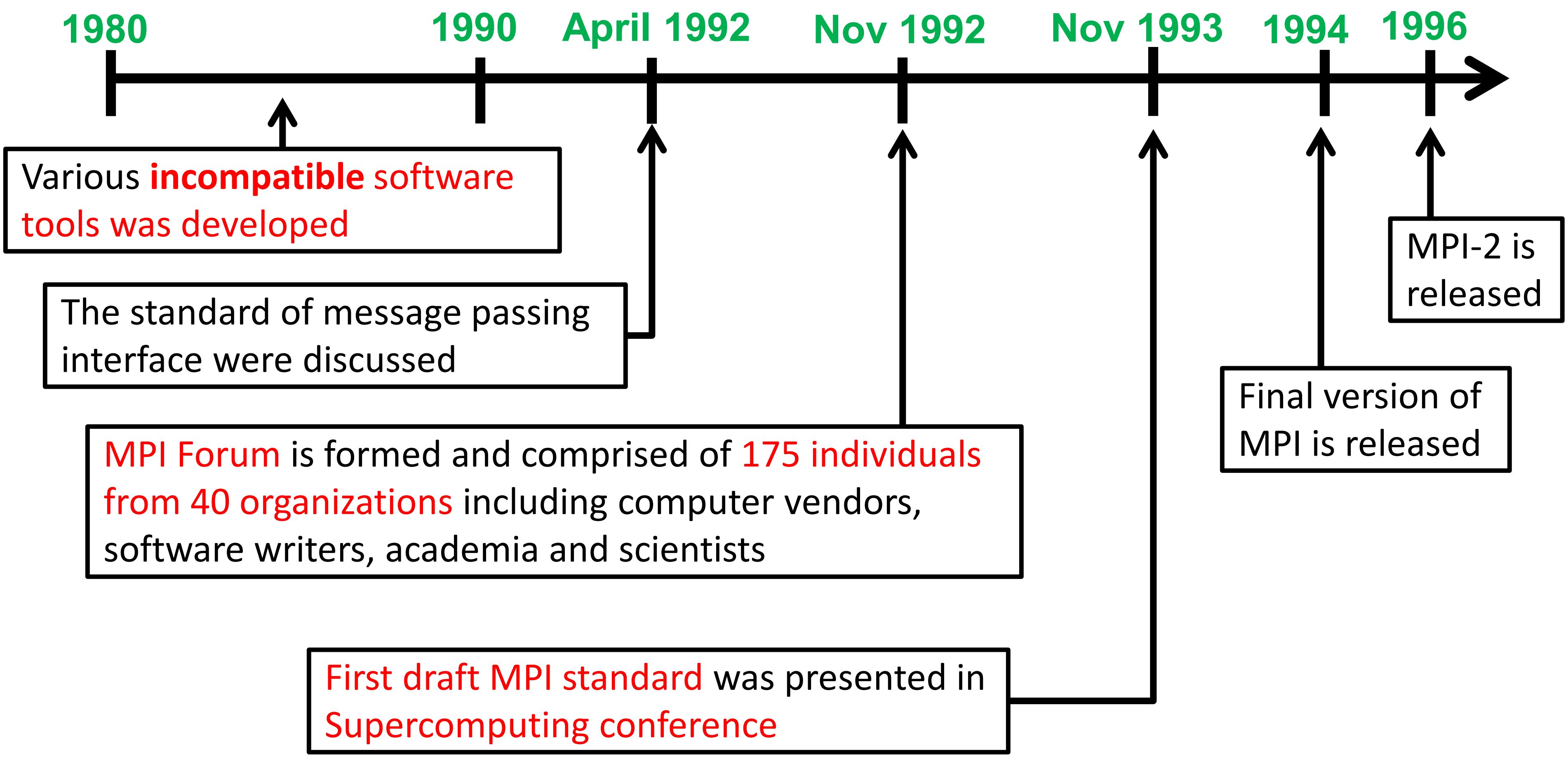


History and Evolution



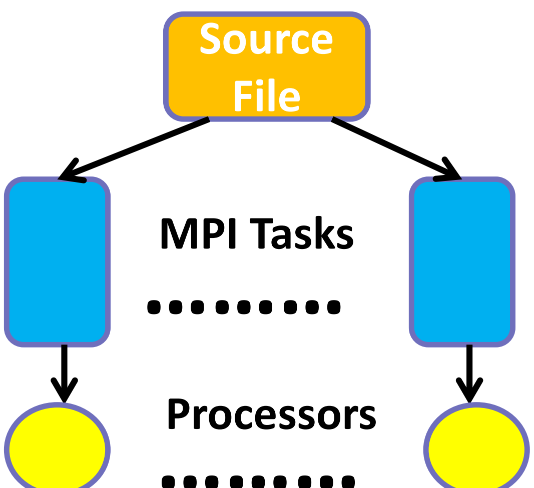
- MPI resulted from the efforts of numerous individuals and groups
- Today, MPI implementations are a combination of MPI-1 and MPI-2. A few implementations include the full functionality of both
- The MPI Forum is now drafting the MPI-3 standard

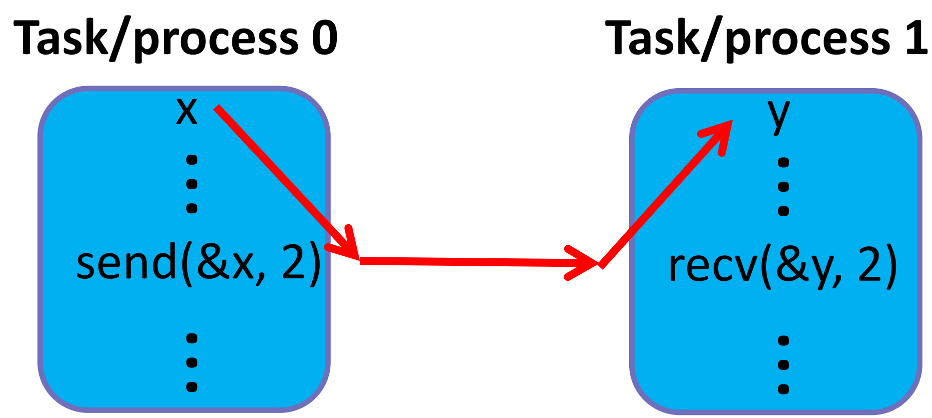
History and Evolution



Programming Model

- SPMD: Single Program Multiple Data
  - Allow **tasks** to branch or conditionally execute only parts of the program they are designed to execute
  - MPI tasks of a parallel program can not be dynamically spawned during run time. (MPI-2 addresses this issue).
- Distributed memory
  - MPI provide method of sending & receiving message





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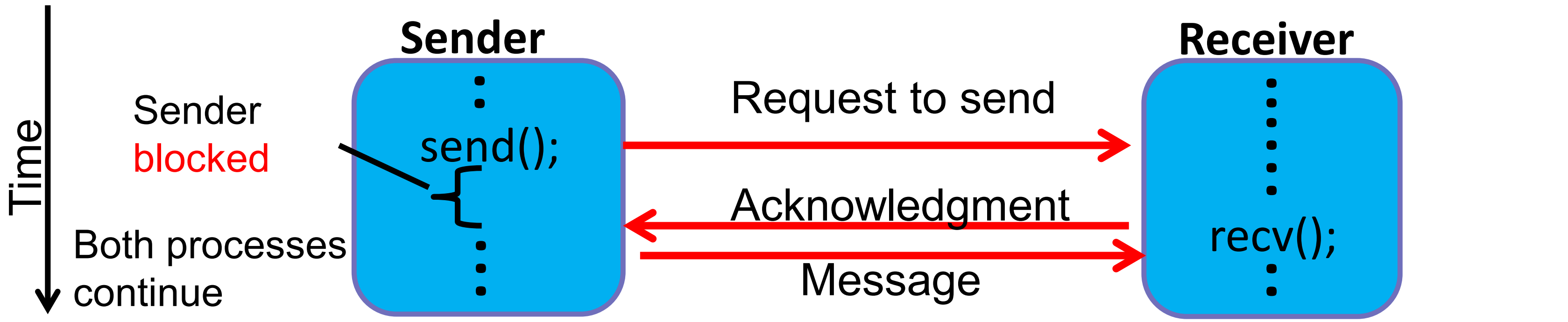
Communication Methods

- From the view of the pair of communicated processes
  - **Synchronous communication** --- sending and receiving data occurs simultaneously
  - **Asynchronous communication** --- sending and receiving data occurs non-simultaneously
- From the view of individual function call
  - **Blocking** --- has been used to describe routines that do not return until the transfer is completed
  - **Non-blocking** --- has been used to describe routines that return whether or not the message had been received
- Synchronous vs. blocking:
  - Synchronous comm. commonly implemented by blocking call
  - Synchronous comm. intrinsically performs two action: **Transfer Data** & **Synchronize Processes**

Synchronous/Blocking Message Passing

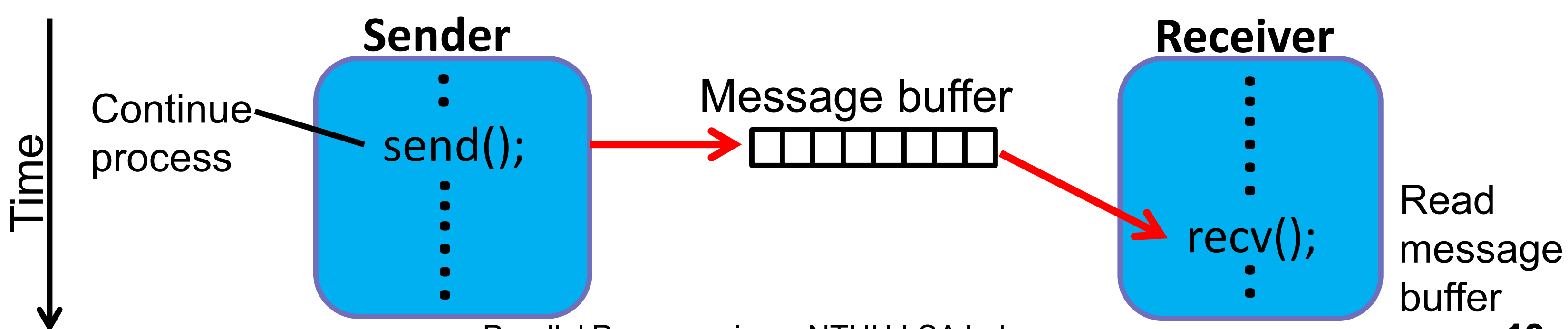
- **Sender**: wait until the complete message can be accepted by the receiver before sending the message



- **Receiver**: wait until the message it is expecting arrives

Asynchronous/Non-Blocking Message Passing

- How message-passing routines can return before the message transfer has been completed?
  - Generally, a ***message buffer*** needed between source and destination to hold message
  - Message buffer is a memory space at the sender and/or receiver side
  - For send routine, once the local actions have been completed and the message is safely on its way, the process can continue with subsequent work



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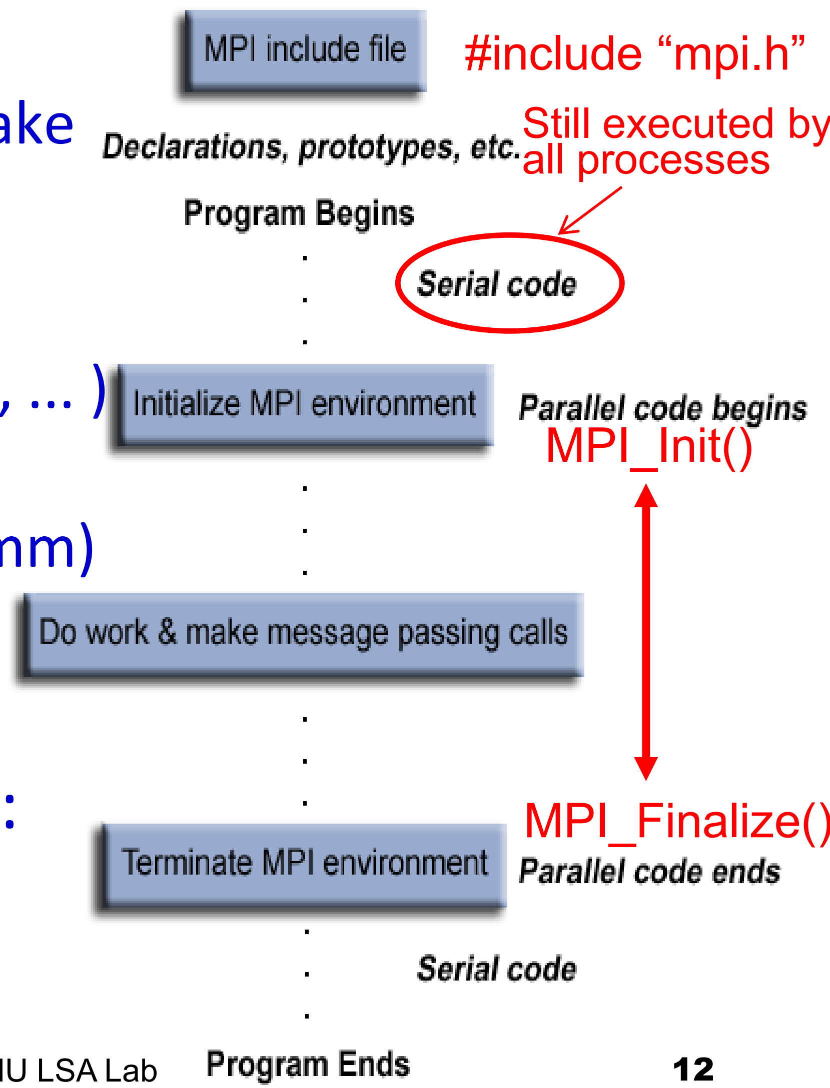
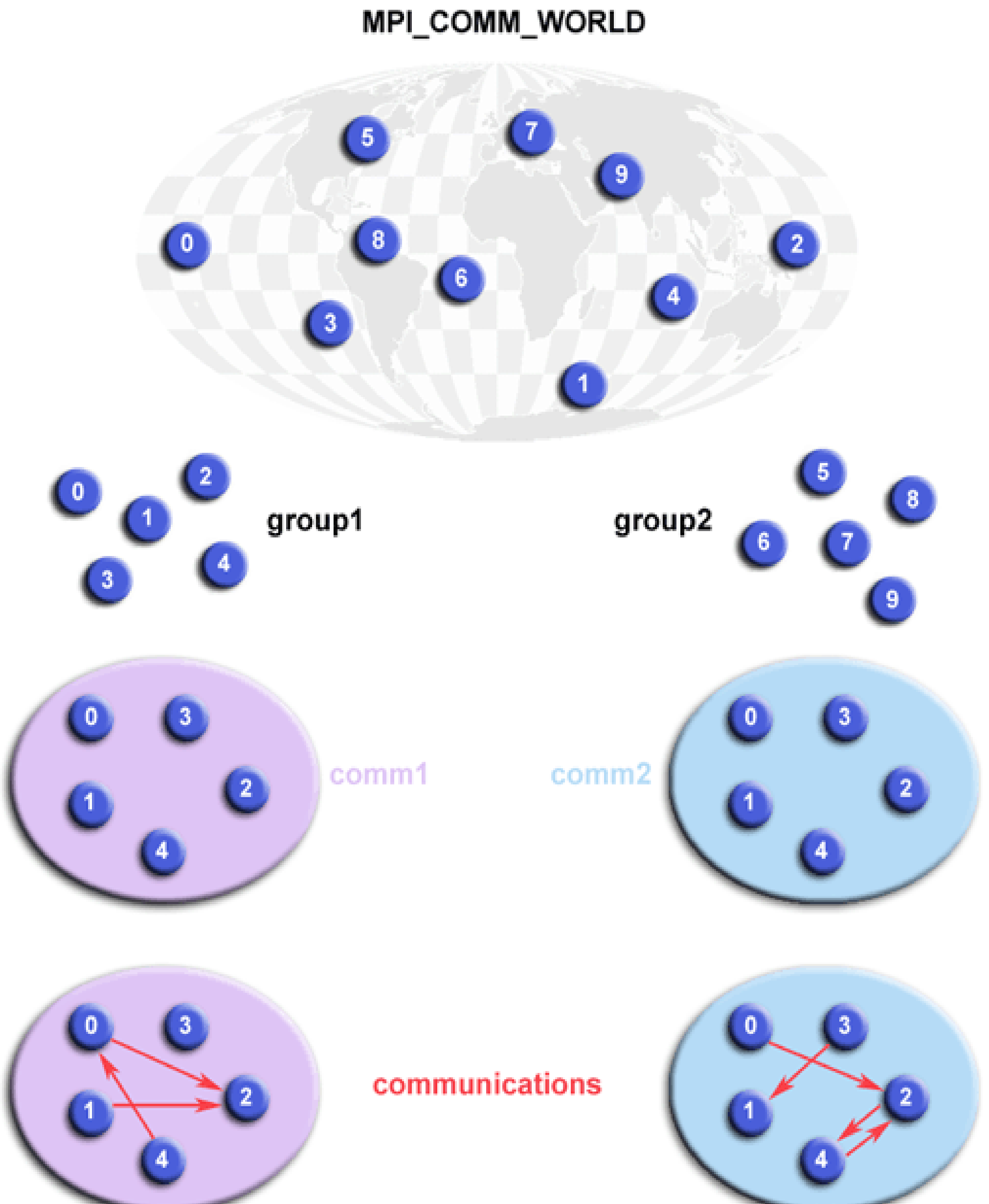
Getting Start

- Header file: **“mpi.h”**
  - Required for all programs that make MPI library call
- MPI calls:
  - Format: rc = MPI_Xxx(parameter, ...)
  - Example: rc = MPI_Bcast (&buffer,count,datatype,root,comm)
  - Error code: return as “rc”; rc=MPI_SUCCESS if successful
- General MPI program structure:



Getting Start

- Communicators and Groups:
  - **Groups** define which **collection of processes** may communicate with each other
  - Each group is associated with a **communicator** to perform its communication function calls
  - **MPI_COMM_WORLD** is the **pre-defined** communicator for all processors
- Rank
  - An **unique identifier** (task ID) for each process in a **communicator**
  - Assigned by the system when the process initializes
  - Contiguous and begin at zero



Environment Management Routines

- **MPI_Init ()**
  - Initializes the MPI execution environment
  - Must be called before any other MPI functions
  - Must be called only once in an MPI program
- **MPI_Finalize ()**
  - Terminates the MPI execution environment
  - No other MPI routines may be called after it
- **MPI_Comm_size (comm, &size)**
  - Determines the number of processes in the group associated with a communicator
- **MPI_Comm_rank (comm, &rank)**
  - Determines the rank of the calling process within the communicator
  - This rank is often referred to as a task ID

Example

```
#include "mpi.h"
int main (int argc, char *argv[]) {
    int numtasks, rank, rc;
    rc = MPI_Init (&argc,&argv);
    if (rc != MPI_SUCCESS) {
            printf ("Error starting MPI program. Terminating.\n");
            MPI_Abort (MPI_COMM_WORLD, rc);
    }
    MPI_Comm_size (MPI_COMM_WORLD, &numtasks);
    MPI_Comm_rank (MPI_COMM_WORLD, &rank);
    printf ("Number of tasks= %d My rank= %d\n", numtasks, rank);
    MPI_Finalize ();
}
```

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Point-to-Point Communication Routines

Blocking send	MPI_Send(buffer,count,type,dest,tag,comm)
Non-blocking send	MPI_Isend(buffer,count,type,dest,tag,comm,request)
Blocking receive	MPI_Recv(buffer,count,type,source,tag,comm,status)
Non-blocking receive	MPI_Irecv(buffer,count,type,source,tag,comm,request)

- buffer: **Address space** that references the data to be sent or received
- type: MPI_CHAR, MPI_SHORT, MPI_INT, MPI_LONG, MPI_DOUBLE, …
- count: Indicates the number of **data elements** of a particular type to be sent or received
- comm: indicates the communication context
- source/dest: the **rank** (task ID) of the sender/receiver
- tag: arbitrary non-negative integer assigned by the programmer to uniquely **identify** a message. Send and receive operations must match message tags. **MPI_ANY_TAG** is the wild card.
- status: status after operation
- request: used by **non-blocking** send and receive operations

Blocking Example

Blocking send	MPI_Send(buffer,count,type,dest,tag,comm)
Blocking receive	MPI_Recv(buffer,count,type,source,tag,comm,status)

```
MPI_Comm_rank(MPI_COMM_WORLD, &myRank); /* find process rank */
if (myRank == 0) {
    int x=10;
    MPI_Send(&x, 1, MPI_INT, 1, 0, MPI_COMM_WORLD);
} else if (myRank == 1) {
    int x;
    MPI_Recv(&x, 1, MPI_INT, 0, MPI_ANY_TAG, MPI_COMM_WORLD, status);
}
```

Non-Blocking Example

Non-Blocking send	MPI_ISend(buffer,count,type,dest,tag,comm,request)
Non-Blocking receive	MPI_IRecv(buffer,count,type,source,tag,comm,requst)

```
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);/* find process rank */
if (myrank == 0) {
   int x=10;
   MPI_Isend(&x, 1, MPI_INT, 1, 0, MPI_COMM_WORLD, req1);
   compute();
} else if (myrank == 1) {
   int x;
   MPI_Irecv(&x, 1, MPI_INT, 0, MPI_ANY_TAG, MPI_COMM_WORLD, req1);
}
MPI_Wait(req1, status);
```

- **MPI_Wait()** **blocks** until the operation has actually completed
- **MPI_Test()** returns with a flag set indicating whether operation completed at that time.

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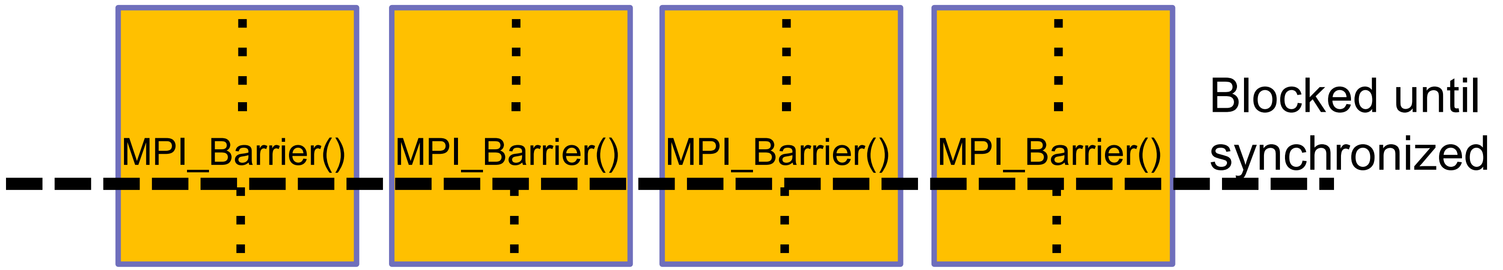
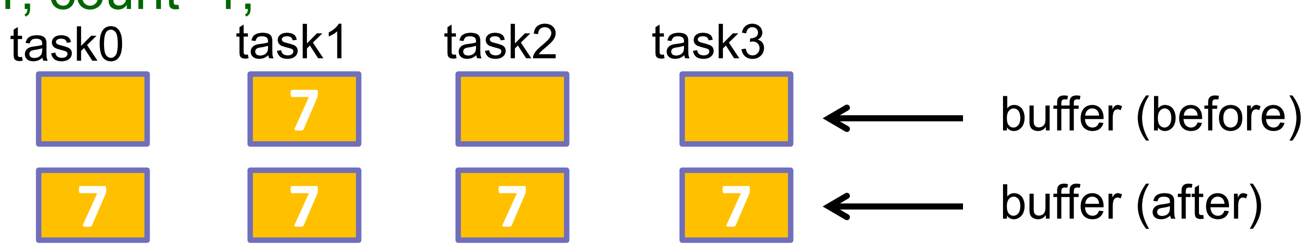
Collective Communication Routines

- MPI_Barrier (comm)
  - Creates a barrier **synchronization** in a group
  - Blocks until **all tasks** in the **group** reach the same MPI_Barrier call



- MPI_Bcast (&buffer, count, datatype, root, comm)
  - Broadcasts (sends) a message from the process with rank "root" to all other processes in the group

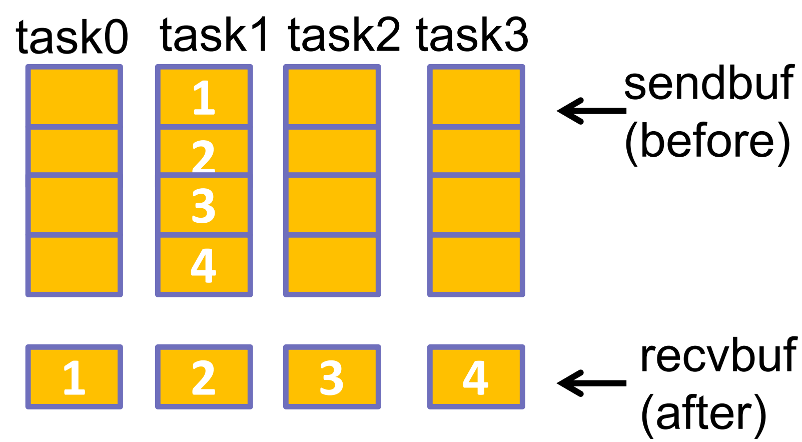
root=1; count=1;



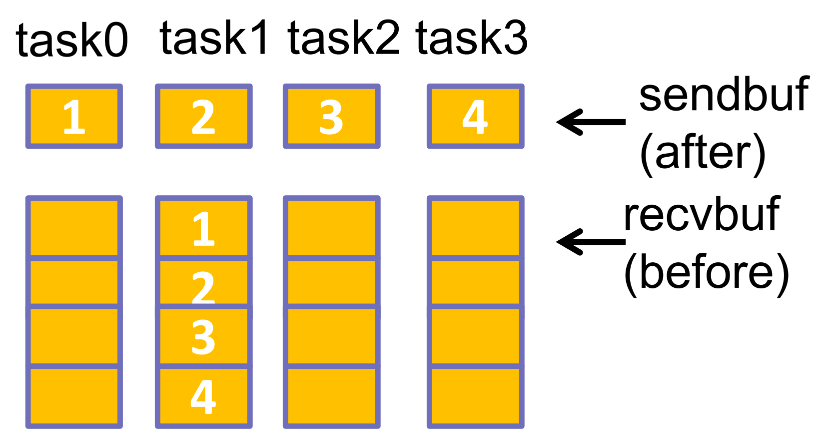
Collective Communication Routines

- MPI_Scatter (&sendbuf, sendcnt, sendtype, &recvbuf, recvcnt, recvtype, root, comm)
  - Distributes **distinct** messages from a source task to all tasks

root=1; sendcnt=recvcnt=1;



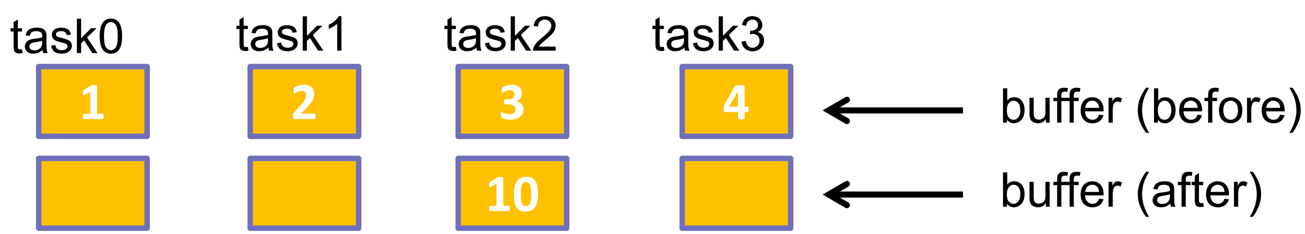
- MPI_Gather (&sendbuf, sendcnt, sendtype, &recvbuf, recvcnt, recvtype, root, comm)
  - Gathers **distinct** messages from each task in the group to a single destination task
  - This routine is the reverse operation of MPI_Scatter



Collective Communication Routines

- MPI_Reduce (&sendbuf, &recvbuf, count, datatype, op, dest, comm)
  - Applies a **reduction operation** on **all tasks** in the group and places the result in **one task**

    dest=2, count=1; op=MPI_SUM

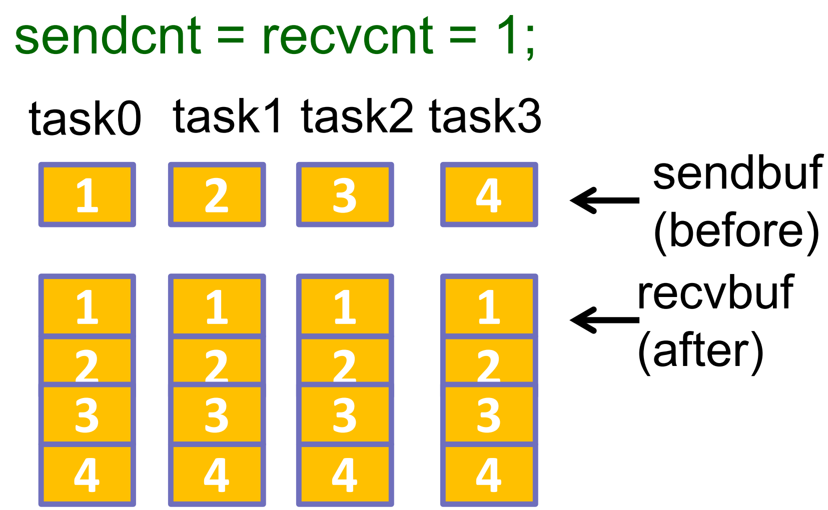


- **Pre-defined** Reduction Operations

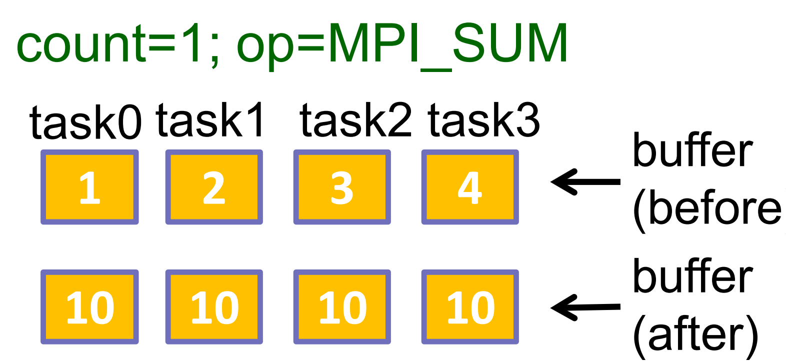
MPI_MAX	Maximum	MPI_MIN	Minimum
MPI_SUM	Sum	MPI_PROD	Product
MPI_LAND	Logical AND	MPI_BAND	Bit-wise AND
MPI_LOR	Logical OR	MPI_BOR	Bit-wise OR
MPI_LXOR	Logical XOR	MPI_BXOR	Bit-wise XOR

Collective Communication Routines

- MPI_Allgather (&sendbuf, sendcount, sendtype, &recvbuf, recvcount, recvtype, comm)
  - Concatenation of data to all tasks
  - This is equivalent to an MPI_Gather followed by an MPI_Bcast



- MPI_Allreduce(&sendbuf, &recvbuf, count, datatype, op, comm)
  - Applies a reduction operation and places the result in all tasks
  - This is equivalent to an MPI_Reduce followed by an MPI_Bcast



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Group and Communicator Routines

* All these calls are collective call that needs to be called by all the processes in the communicator

- Group & Communicator Data Type
  - MPI_Group
  - MPI_Comm
- MPI_Comm_group(Comm, &Group)
  - Access the group associated with a given communicator
- MPI_Group_incl(Group, size, ranks[], &NewGroup)
  - Produce a group by including a subset of members from an existing group
  - all members must be distinct
- MPI_Comm_create(Comm, NewGroup, &NewComm)
  - Create a new communicator
  - The new communicator must be a subset of the original group

Examples: Divide MPI tasks into two groups

```
int  rank, numtasks;
MPI_Group   orig_group, new_group;
MPI_Comm   new_comm

MPI_Init();
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_size(MPI_COMM_WORLD, &numtasks);

/* Extract the original group handle */
MPI_Comm_group(MPI_COMM_WORLD, &orig_group);

/* Divide tasks into two distinct groups based upon rank */
int rank1[4] = {0,1,2,3}; int rank2[4] = {5,6,7,8};
if (rank < numtasks/2)   MPI_Group_incl(orig_group, 4, ranks1, &new_group);
else                     MPI_Group_incl(orig_group, 4, ranks2, &new_group);

/* Create new communicator  & Broadcast within the new group */
MPI_Comm_create(MPI_COMM_WORLD, new_group, &new_comm);
MPI_Barrier(new_comm);
MPI_Finalize();
```

All MPI tasks must call MPI_Group_incl, but they don't necessary to be included in the new group

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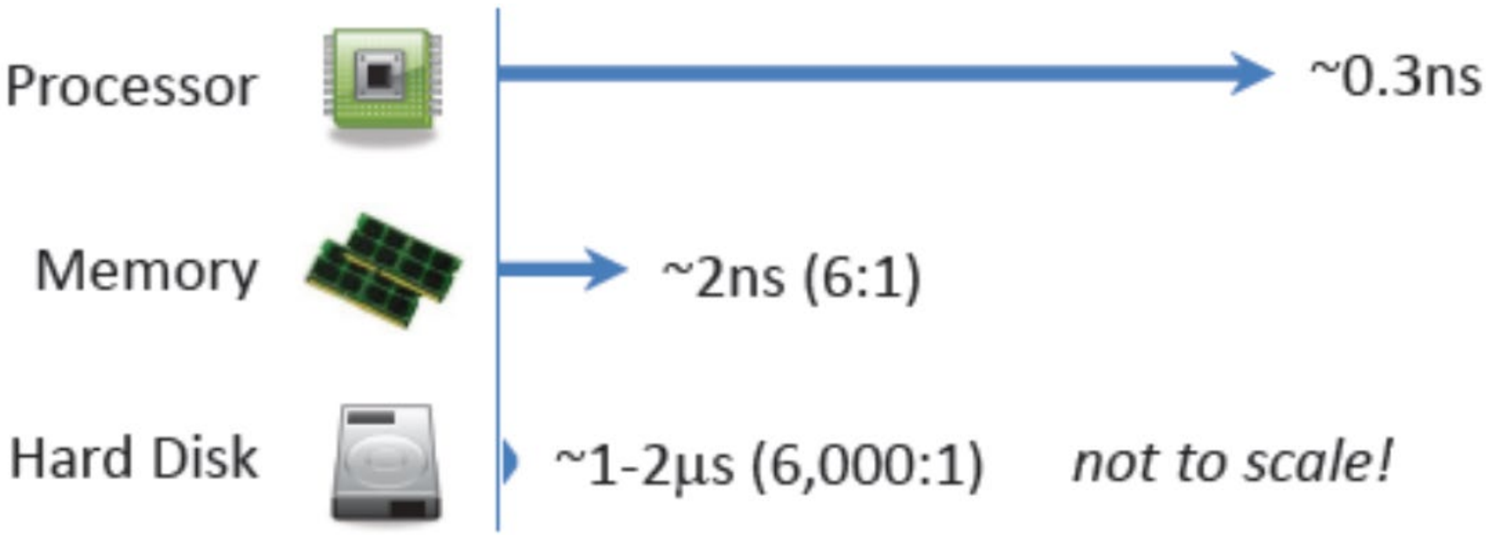
Relative Speed of Components in HPC Platform

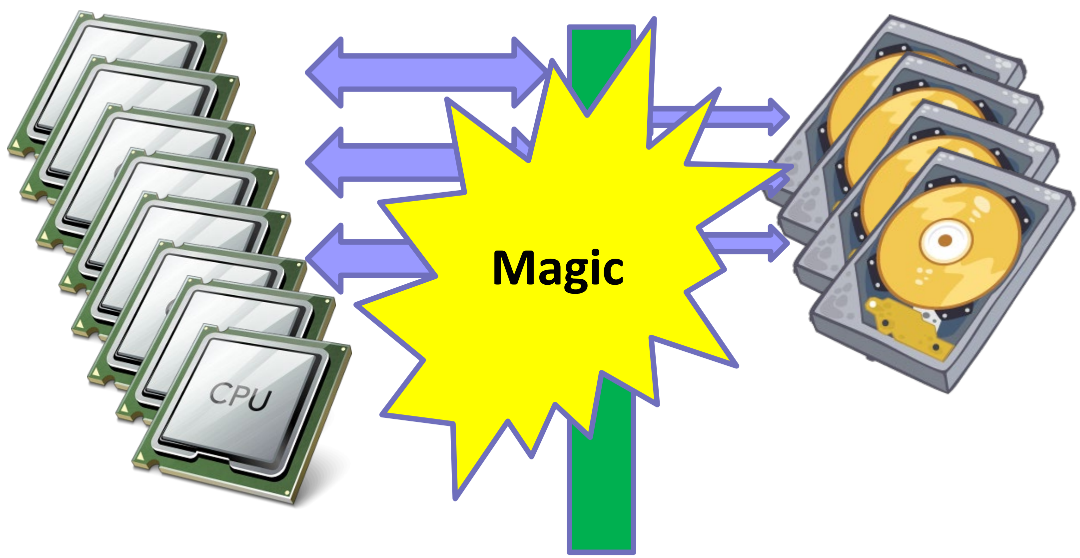
- An HPC platform's I/O subsystems are typically slow as compared to its other parts
- The I/O gap between memory speed and average disk access stands at roughly 10^{-3}



Concurrent Data Access in a Cluster

We need some magic to make the collection of spinning disks act like a single disk …

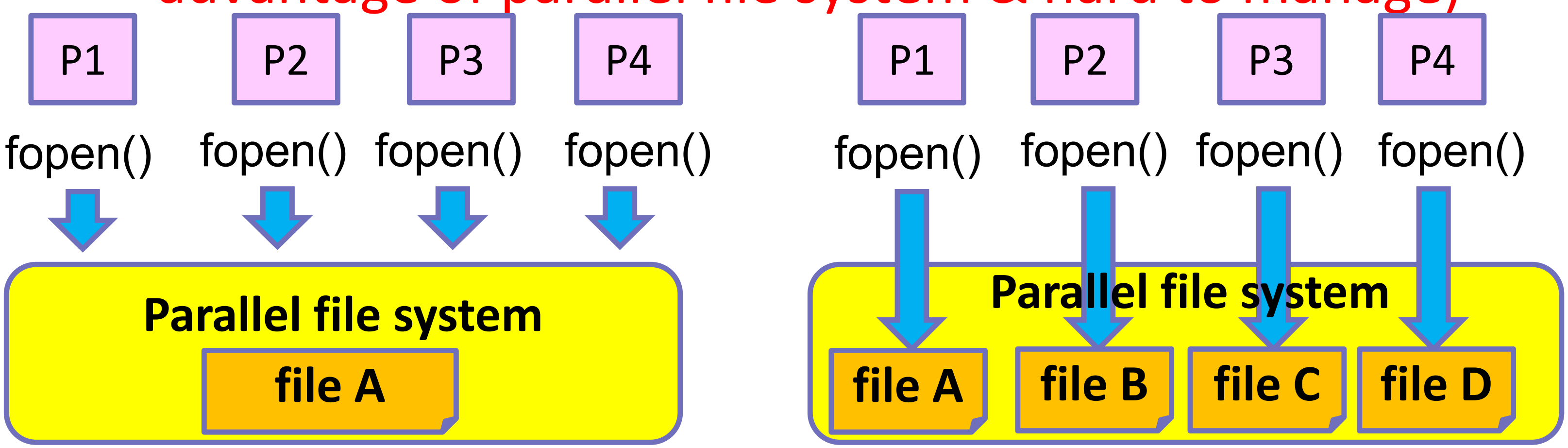
a few hundreds spinning disks



hundreds of thousands of processors

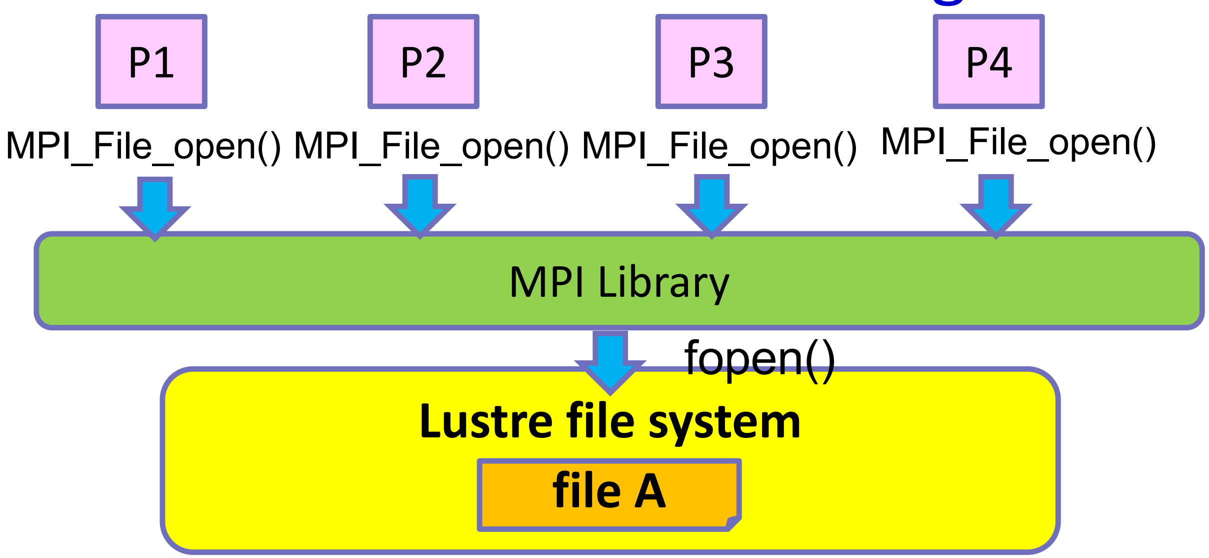
POSIX File Access Operations

- POSIX file system call "fopen()":
  - The same is opened by each processes → multiple file handlers across your MPI processes
  - Open the same file with read permission is OK
  - But can't open with write permission together due file system locking mechanism → data inconsistency
  - To write simultaneously must create multiple files (can't take advantage of parallel file system & hard to manage)



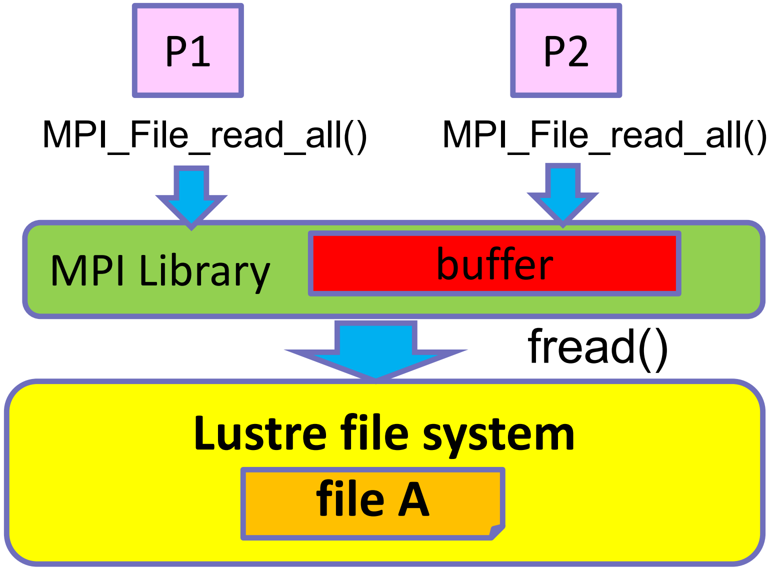
MPI-IO File Access Operations

- MPI-IO call "MPI_File_open()"
  - File is opened only once in a collective manner
  - MPI library will share and synchronize with each other to use the same file handler
  - Can handle both read and write together

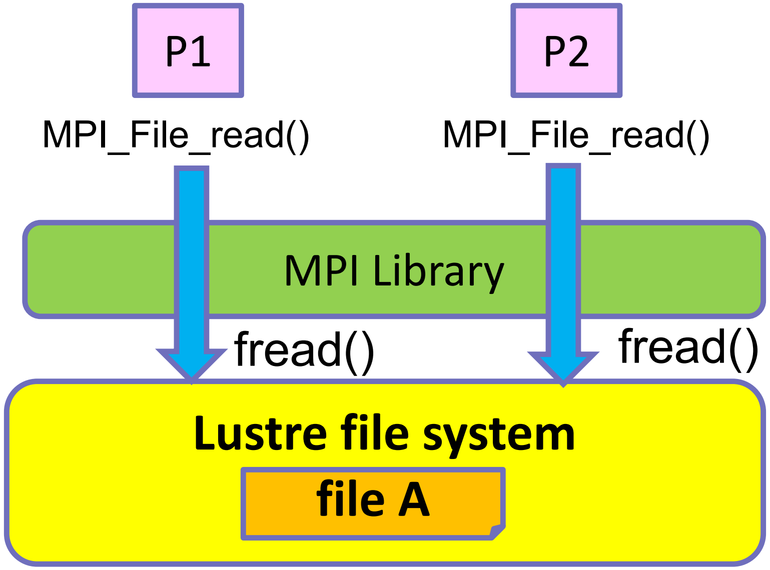


MPI-IO Independent/Collective I/O

- Collective I/O
  - Read/write to a shared memory buffer, then issue ONE file request
  - Reduce #I/O request
    ➔ Good for small I/O
  - Require synchronization



- Independent I/O
  - Read/write individually
  - Prevent synchronization
  - One request per process
  - Request is serialized if access the **same OST**
  - Good for large I/O



MPI-IO API

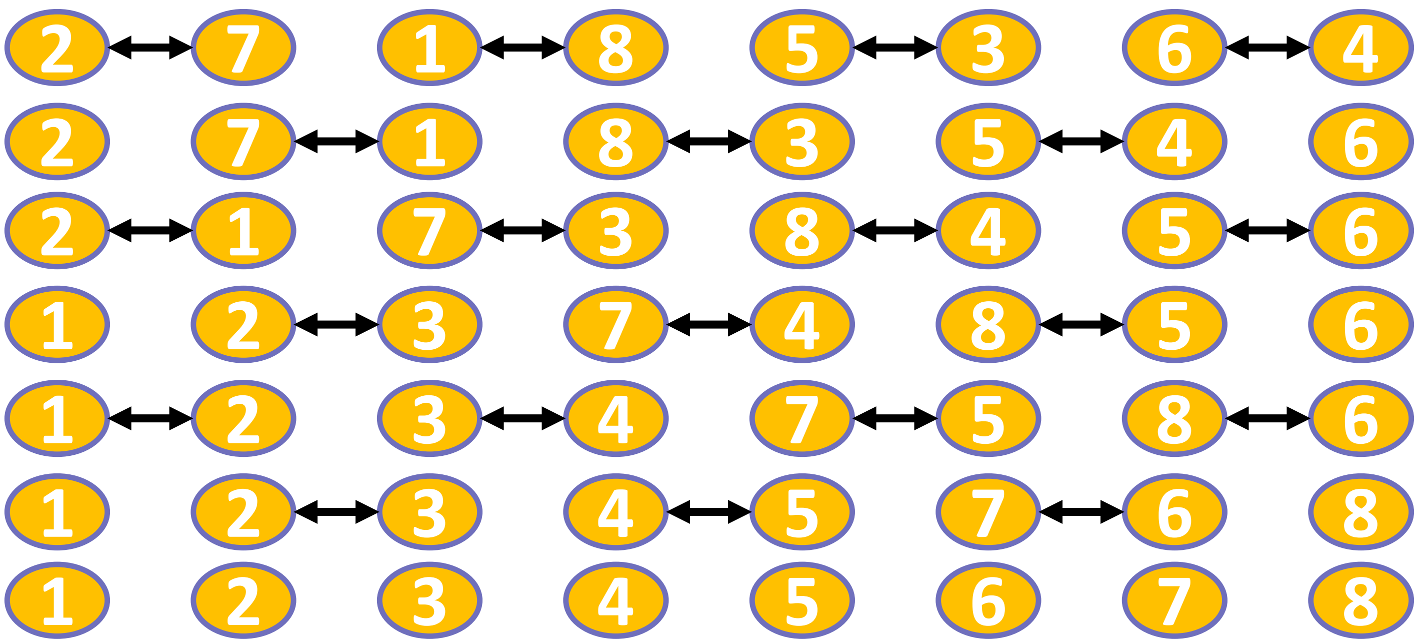
- **MPI_File_open(MPI_Comm comm, char *filename, int amode, MPI_Info info, MPI_File *fh)**
  - Open a file
- **MPI_File_close(**MPI_File *fh**)**
  - Close a file
- **MPI_File_read/write(MPI_File fh, void *buf, int count, MPI_Datatype datatype, MPI_Status *status)**
  - Independent read/write using individual file pointer
- **MPI_File_read/write_all(MPI_File fh, void *buf, int count, MPI_Datatype datatype, MPI_Status *status)**
  - Collectively read/write using individual file pointer
- **MPI_File_sync(MPI_File fh)**
  - Flush all previous writes to the storage device

Reference

- Textbook:
  - Parallel Computing Chap2
- MPI Tutorial:
  - https://computing.llnl.gov/tutorials/mpi/
- MPI API:
  - http://www.mcs.anl.gov/research/projects/mpi/www/www3/

HW1: Odd-Even Sort

- Algo:
  - comparing & switch in order between all (odd, even)-indexed pairs of adjacent elements in the list
  - comparing & switch in order between all (even,odd)-indexed pairs of adjacent elements in the list
  - Repeat until the list is sorted



HW1: Odd-Even Sort

- Sequential code:

```
/* Assumes a is an array of values to be sorted. */
var sorted = false;
while(!sorted) {
    sorted=true;
    for(var i = 1; i < list.length-1; i += 2) {
        if(a[i] > a[i+1]) { swap(a, i, i+1); sorted = false; }
    }
    for(var i = 0; i < list.length-1; i += 2) {
        if(a[i] > a[i+1]) { swap(a, i, i+1); sorted = false; }
    }
}
```

HW1: Odd-Even Sort

- Parallel Code:
  1. For each process with odd rank *P*, send its number to the process with rank *P*-1.
  2. For each process with rank *P*-1, compare its number with the number sent by the process with rank *P* and send the larger one back to the process with rank *P*.
  3. For each process with even rank *Q*, send its number to the process with rank *Q*-1.
  4. For each process with rank *Q*-1, compare its number with the number sent by the process with rank *Q* and send the larger one back to the process with rank *Q*.
  5. Repeat 1-4 until the numbers are sorted.