Programming with MPI: Advanced Topics

Steve Lantz

Senior Research Associate

Cornell CAC

Workshop: Introduction to Parallel Computing on Ranger, July 14, 2010

Based on materials developed by by Bill Barth at TACC

Goals

- To gain an awareness of specialized features in MPI that you may want to use right away in writing parallel applications
- To create a little mental catalog of MPI’s more advanced capabilities for future reference

At the end of each section, let’s ask:

- Why was this set of routines included? What might they be good for?
- Can we think of an example where they would be useful?

Introduction and Outline

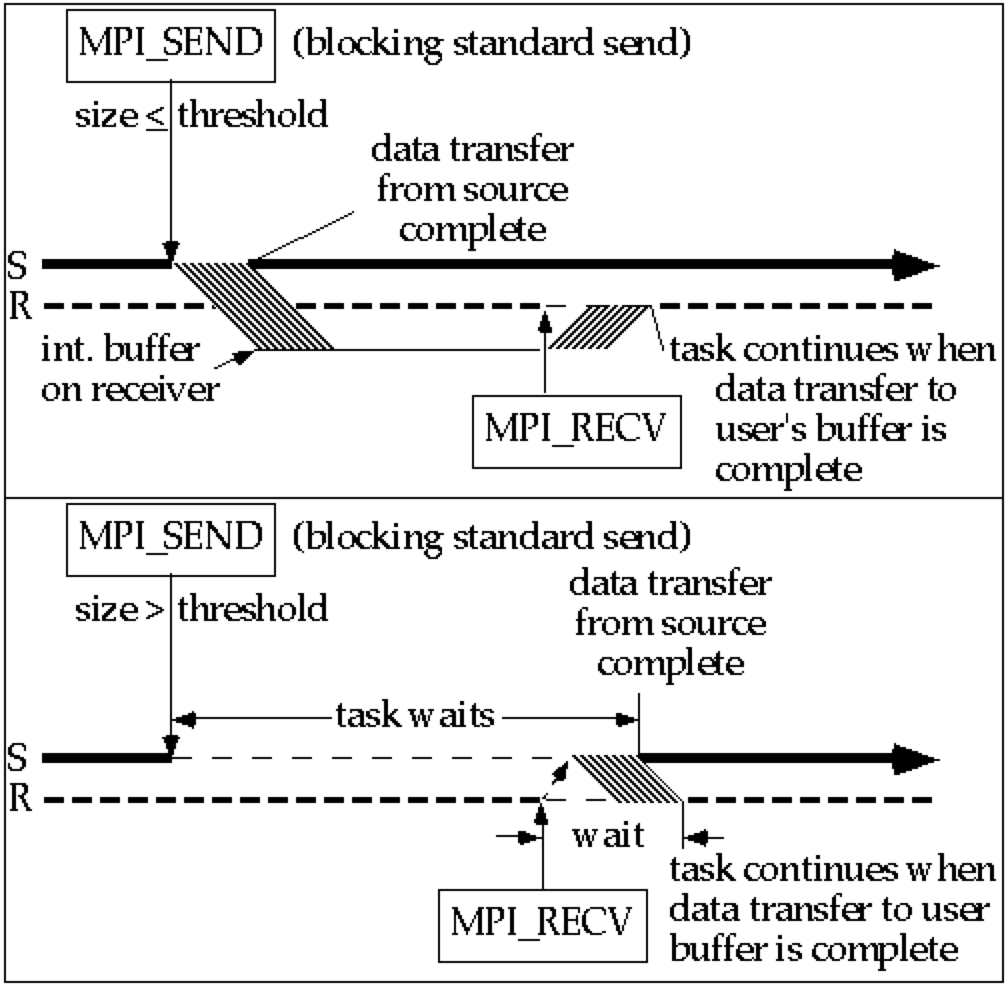
1. Advanced point-to-point communication
2. Collective communication with non-contiguous data
3. Derived datatypes
4. Communicators and groups
5. Persistent communication
6. Parallel I/O (MPI-2)
7. Status of MPI-2

1. Advanced Point-to-Point Communication

Standard Send, Receive

Standard-Mode Blocking Calls:
MPI_Send, MPI_Recv

- MPI_Send returns only when the buffer is safe to reuse:
  - the small message has been copied elsewhere, or
  - the large message has actually been transferred;
  - the small/large threshold is implementation dependent
- Rule of thumb: a send only completes if a matching receive is posted/executed


MPI_SEND
(blocking standard send)
size ≤ threshold
data transfer from source complete
S
R
int. buffer on receiver
MPI_RECV
task continues when data transfer to user's buffer is complete
MPI_SEND
(blocking standard send)
size > threshold
data transfer from source complete
task waits
S
R
wait
MPI_RECV
task continues when data transfer to user buffer is complete

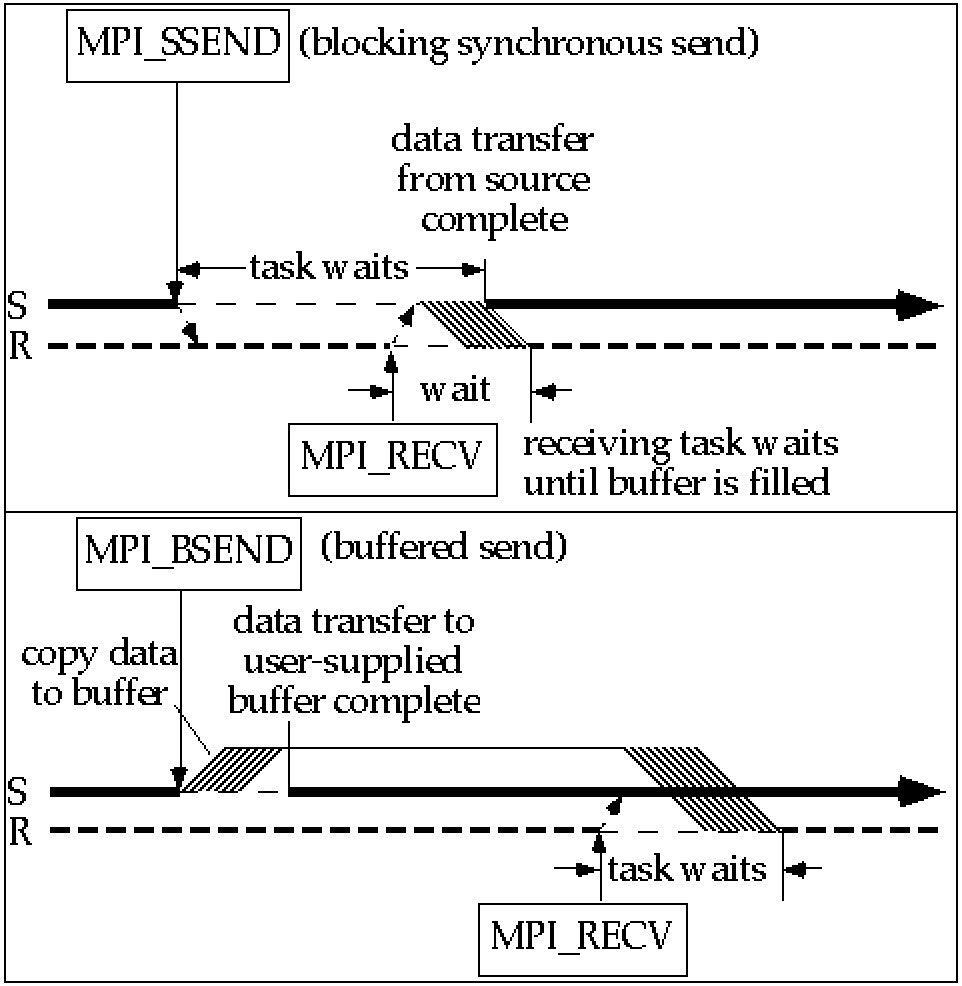
Synchronous and Buffered Modes

Synchronous Mode: MPI_Ssend

- Transfer is not initiated until matching receive is posted
- Non-local: handshake needed
- Returns after message is sent

Buffered Mode: MPI_Bsend

- Completes as soon as the message is copied into the user-provided buffer
- Buffer must be provided using MPI_Buffer_attach
- One buffer per process



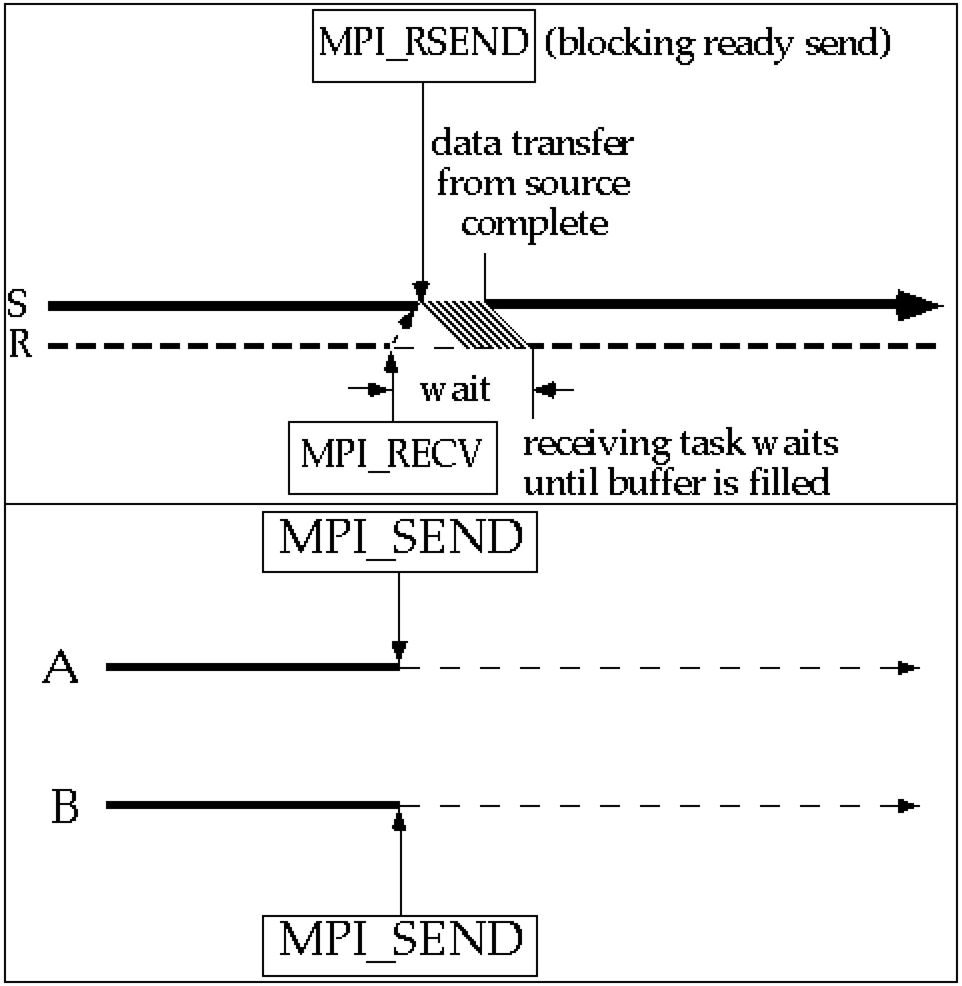
Ready Mode and Deadlock

Ready Mode: MPI_Rsend

- Initiates transfer immediately
- Assumes that a matching receive has already been posted
- Error if receiver isn't ready

Deadlock

- All tasks are waiting for events that yet haven't been initiated
- Can be avoided by reordering calls, by using non-blocking calls, or with MPI_Sendrecv


MPI_RSEND
(blocking ready send)
data transfer from source complete
S
R
wait
MPI_RECV
receiving task waits until buffer is filled
MPI_SEND
A
B
MPI_SEND

Discussion of Send Modes

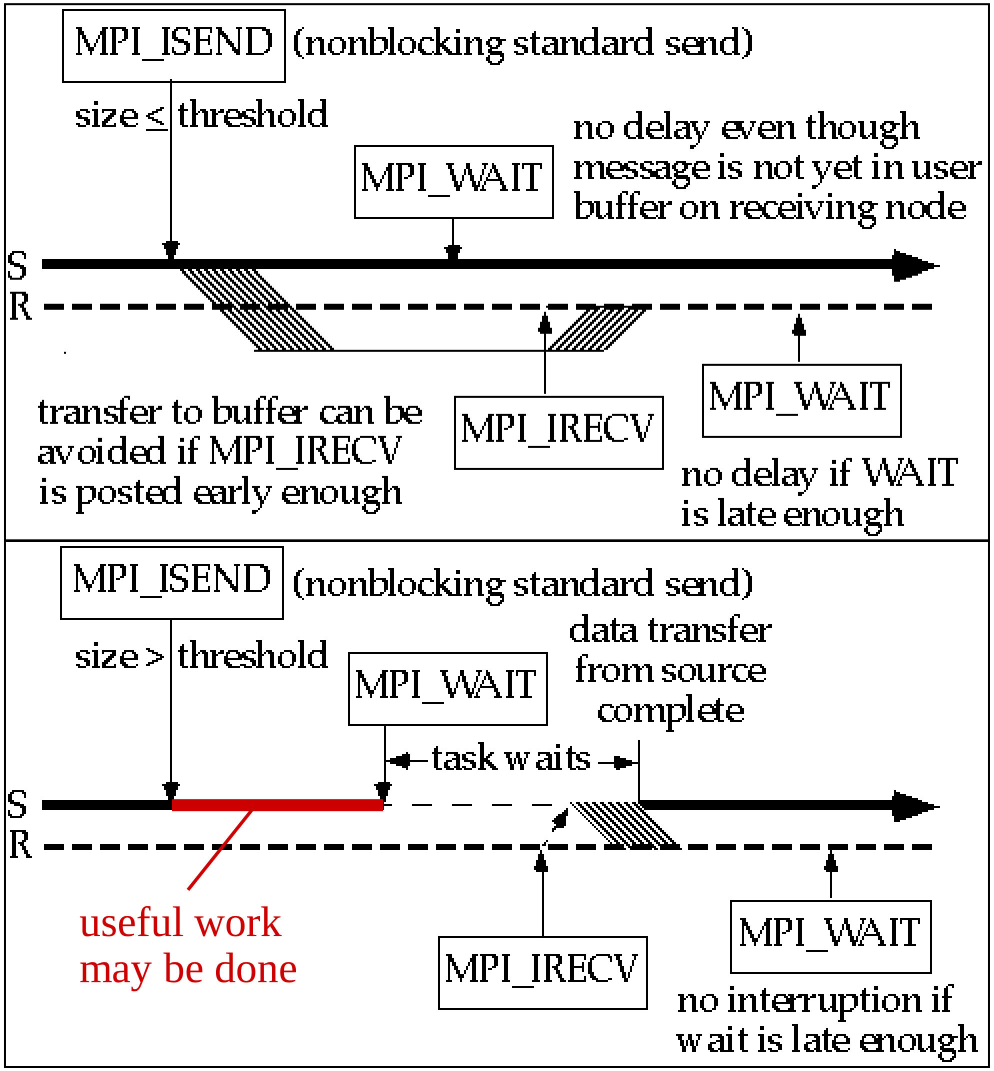
- Synchronous mode is portable and “safe”
  - does not depend on order (ready mode) or buffer space (buffered mode)
  - incurs substantial overhead
- Ready mode has least total overhead, but how can error be avoided?
  - sometimes the logic of the code implies the receiver must be ready
- Buffered mode decouples sender and receiver
  - sender doesn’t have to sync; receiver doesn’t have to be ready
  - time and memory overheads are incurred by copying to the buffer
  - sender can control size of message buffers and total amount of space
- Standard mode tries to strike a balance
  - small messages are buffered on receiver’s side (avoiding sync overhead)
  - large messages are sent synchronously (avoiding big buffer space)

MPI_Sendrecv and MPI_Sendrecv_replace

- MPI_Sendrecv (blocking)
  - send message A from one buffer; receive message B in another buffer
  - destination of A, source of B can be same or different
- MPI_Sendrecv_replace (blocking)
  - send message A from one buffer; receive message B in *SAME* buffer
  - again, destination of A, source of B can be same or different
  - system takes care of the extra internal buffering
- Illustration 1: data swap between processors
  - destination and source are identical
- Illustration 2: chain of processors
  - send result to **`myrank+1`**, receive next input from **`myrank-1`**

Non-Blocking Calls

- Calls return immediately
- System handles buffering
- Not “safe” to access message contents until action is known to be completed
- With MPI_Isend, message buffer is reusable right away if tag or receiver is different; otherwise, check status
- With MPI_Irecv, user must always check for data; only small messages are buffered


MPI_ISEND
(nonblocking standard send)
size ≤ threshold
MPI_WAIT
no delay even though message is not yet in user buffer on receiving node
S
R
transfer to buffer can be avoided if MPI_IRECV is posted early enough
MPI_IRECV
MPI_WAIT
no delay if WAIT is late enough
MPI_ISEND
(nonblocking standard send)
size > threshold
MPI_WAIT
data transfer from source complete
task waits
S
R
useful work may be done
MPI_IRECV
MPI_WAIT
no interruption if wait is late enough

Use of Non-Blocking Communication

- Non-blocking calls permit overlap of computation and communication
- All send modes are available: MPI_Irsend, MPI_Ibsend, MPI_Issend
- Non-blocking calls must normally be resolved through a second call
  - main options: MPI_Wait, MPI_Test, MPI_Request_free
  - variants like MPI_Waitany help to resolve calls in arbitrary order
  - reason for doing this: avoid running out of request handles
- Outline for typical code:

```
for (i=0;i<M;i++) MPI_Irecv( <declare receive buffers> );
for (i=0;i<N;i++) MPI_Isend( <mark data for sending> );
    /* Do local operations */
MPI_Waitall( <make sure all receives finish> )
    /* Operate on received data */
MPI_Waitall( <clear request handles for all sends> )
```

MPI_Wait and MPI_Test

- **`MPI_Wait`** halts progress until a *specific* non-blocking request (send or receive) is satisfied; the related message buffer is then safe to use
  - **`MPI_Waitall`** does the same thing for a *whole array* of requests
  - **`MPI_Waitany`** waits for *any one* request from an array
  - **`MPI_Waitsome`** waits for *one or more* requests from an array
- **`MPI_Test`** immediately returns the status (no waiting!) of a specific non-blocking operation, again identified by a request handle
  - returns **`flag = true`** only if the operation is complete
  - allows alternative instructions to be carried out if operation isn't complete
  - has the same variants: MPI_Testall, MPI_Testany, MPI_Testsome

```
MPI_Testany(int count, MPI_Request *array_of_reqs,
            int *index, int *flag, MPI_Status *status);
```

Other Ways to Gain Flexibility in Communication

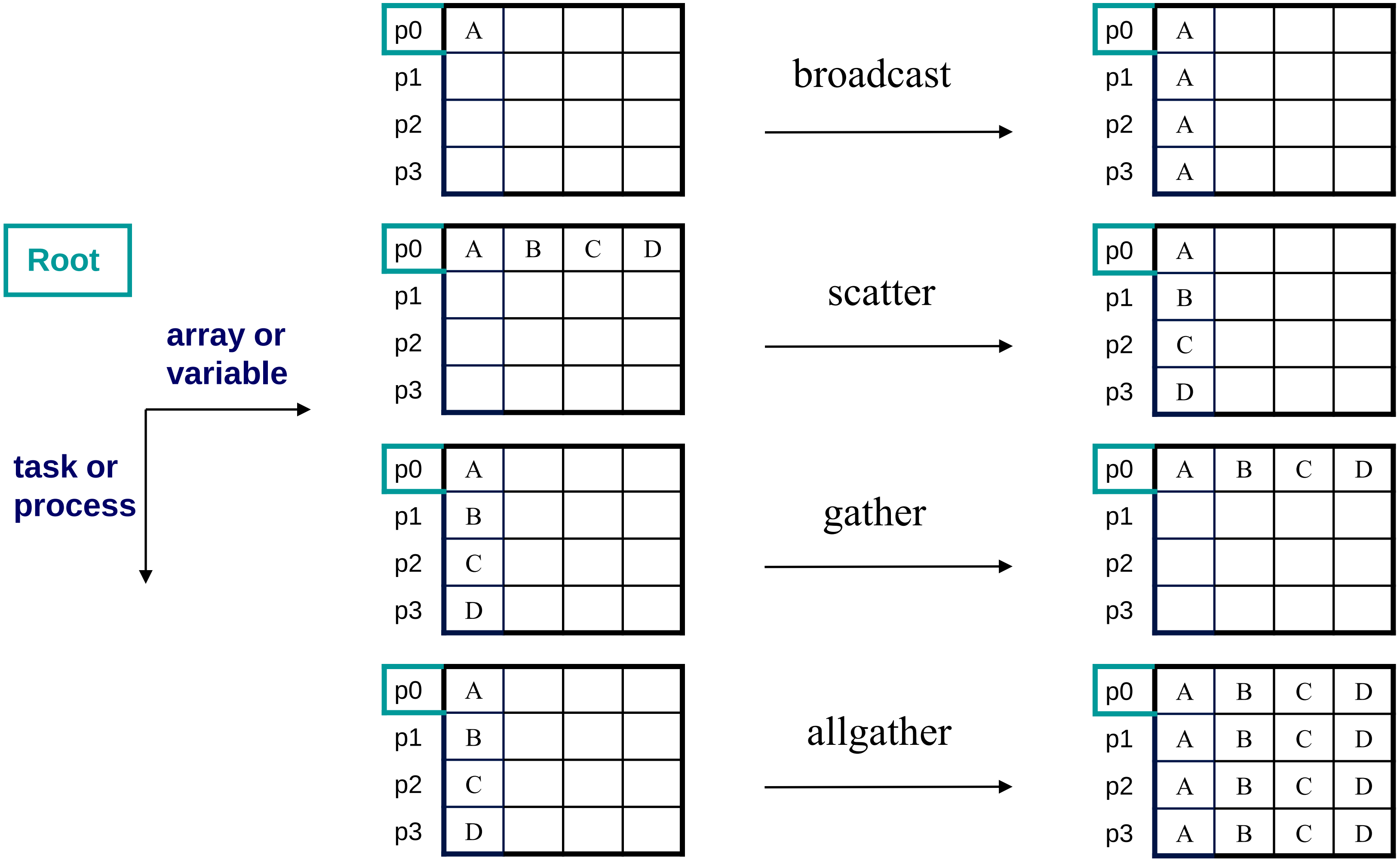
- **MPI_ANY_SOURCE, MPI_ANY_TAG** are “wildcards” that may be used by receives (blocking and non-blocking) in situations where the source or tag of a message does not need to be known in advance
  - the **status** argument returns source, tag, and error status
  - a separate call to **MPI_Get_count** determines the size of the message
  - but… what if you need to know a message’s size *before* receiving it?
- **MPI_Iprobe** returns the properties of any message that has arrived without receiving it into a buffer (maybe you need to do a big malloc!)

```
MPI_Iprobe(int source, int tag, MPI_Comm comm,
           int *flag, MPI_Status *status);
```

- **MPI_Probe** blocks until such a message arrives (no flag)

2. Collective Communication with Non-Contiguous Data

Review: Scatter and Gather



broadcast

p0	A			
p1				
p2				
p3				

p0	A			
p1	A			
p2	A			
p3	A			

scatter

p0	A	B	C	D
p1				
p2				
p3				

p0	A			
p1	B			
p2	C			
p3	D			

gather

p0	A			
p1	B			
p2	C			
p3	D			

p0	A	B	C	D
p1				
p2				
p3				

allgather

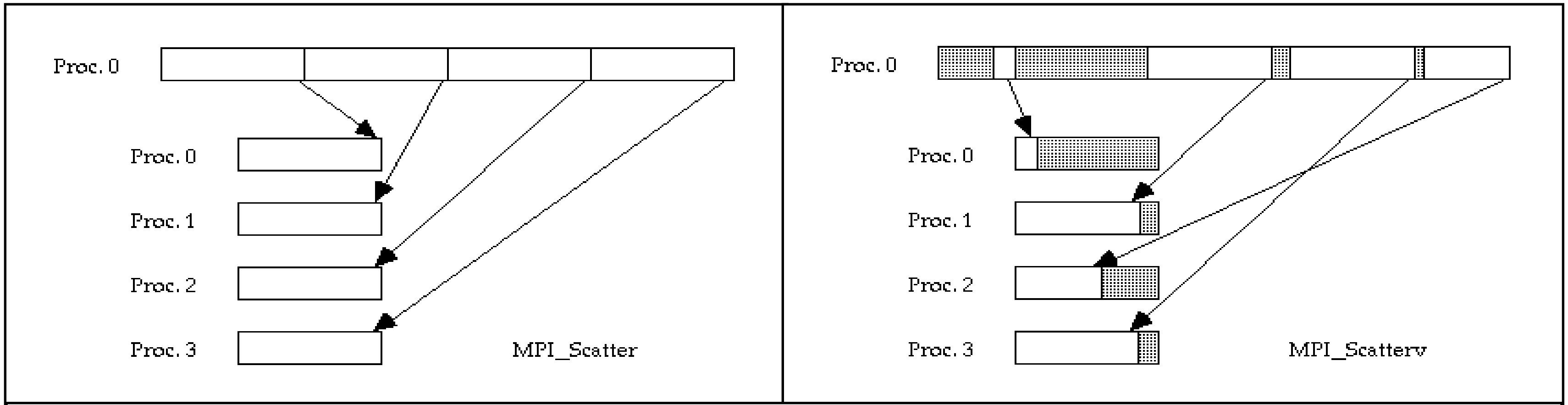
p0	A			
p1	B			
p2	C			
p3	D			

p0	A	B	C	D
p1	A	B	C	D
p2	A	B	C	D
p3	A	B	C	D

Introducing Scatterv, Gatherv

- MPI_{Scatter,Gather,Allgather}***v***
- What does ***v*** stand for?
  - varying size and relative location of messages
- Advantages
  - more flexibility
  - less need to copy data into temporary buffers
  - more compact
- Disadvantage
  - harder to program

Scatter vs. Scatterv



```
CALL mpi_scatterv ( SENDBUF, SENDCOUNTS, DISPLS, SENDTYPE,
                    RECVBUF, RECVCOUNT,          RECVTYPE,
                    ROOT, COMM, IERR )
```

- **SENDCOUNTS(J)** is the number of items of type **SENDTYPE** to send from process **ROOT** to process **J**. Defined on **ROOT**.

- **DISPLS(J)** is the displacement from **SENDBUF** to the beginning of the **J**-th message, in units of **SENDTYPE**. Defined on **ROOT**.

Allgatherv Example

```
MPI_Comm_size(comm,&ntids);
sizes = (int*)malloc(ntids*sizeof(int));
MPI_Allgather(&n,1,MPI_INT,sizes,1,MPI_INT,comm);
offsets = (int*)malloc(ntids*sizeof(int));
s=0;
for (i=0; i<ntids; i++)
  {offsets[i]=s; s+=sizes[i];}
N = s;
result_array = (int*)malloc(N*sizeof(int));
MPI_Allgatherv
   ((void*)local_array,n,MPI_INT,(void*)result_array,
    sizes,offsets,MPI_INT,comm);
free(sizes); free(offsets);
```

3. Derived Datatypes

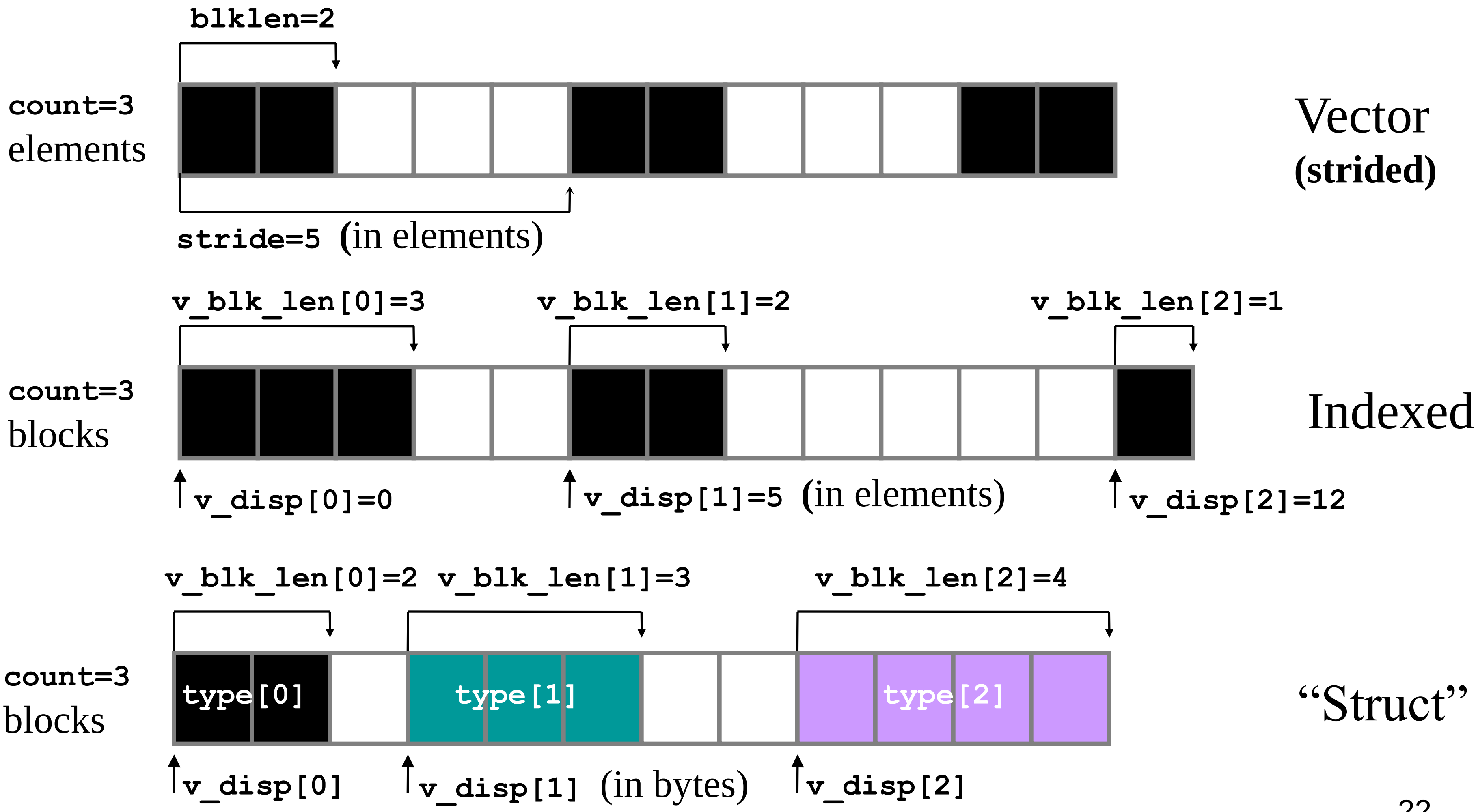
Derived Datatypes: Motivation

- MPI basic datatypes are predefined for contiguous data of single type
- What if an application needs to communicate data of mixed type or in non-contiguous locations?
  - solutions that involve making multiple MPI calls, copying data into a buffer and packing, etc., are slow, clumsy and wasteful of memory
  - better solution is to create/derive datatypes for these special needs from existing datatypes
- Derived datatypes can be created recursively at runtime
- Packing and unpacking is done automatically

MPI Datatypes

- **Elementary**: Language-defined types
- **Contiguous**: Vector with stride of one
- **Vector**: Elements separated by constant “stride”
- **Hvector**: Vector, with stride in bytes
- **Indexed**: Array of indices (for scatter/gather)
- **Hindexed**: Indexed, with indices in bytes
- **Struct**: General mixed types (for C structs etc.)

Picturing Some Derived Datatypes



Using MPI’s Vector Type

- Function **MPI_TYPE_VECTOR** allows creating non-contiguous vectors with constant stride. Where might one use it?

```
mpi_type_vector(count,blocklen,stride,oldtype,vtype,ierr)
```

ncols = 4
nrows = 5

Array A

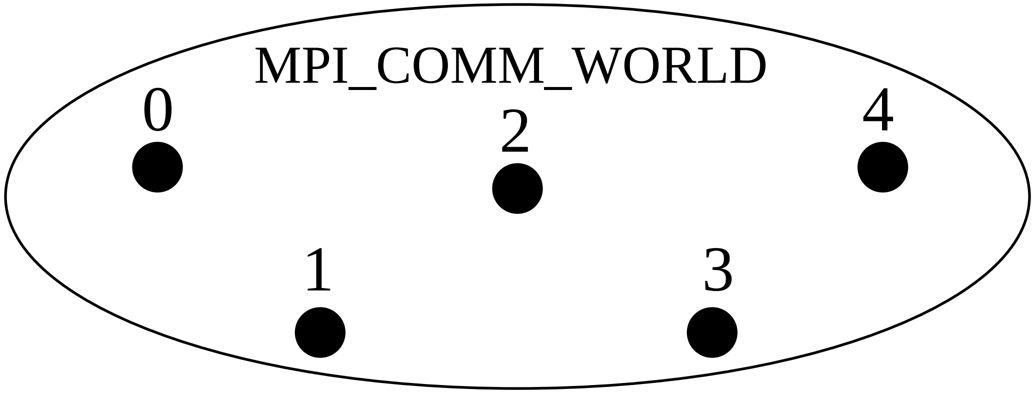
1	6	11	16
2	7	12	17
3	8	13	18
4	9	14	19
5	10	15	20

```
call MPI_Type_vector(ncols,1,nrows,MPI_DOUBLE_PRECISION,&
                     vtype,ierr)
call MPI_Type_commit(vtype,ierr)
call MPI_Send(A(nrows,1),1,vtype...)
```

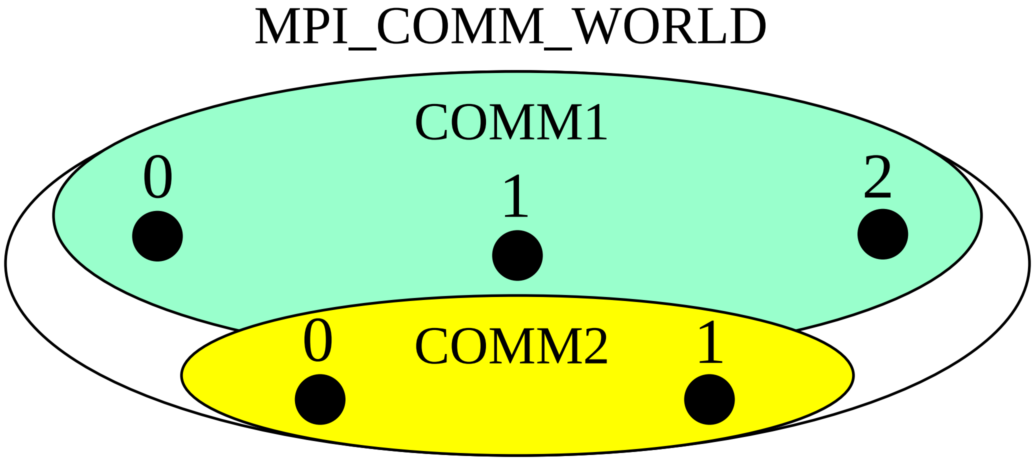
4. Communicators and Groups

Communicators and Groups: Definitions

- All MPI communication is relative to a *communicator* which contains a *context* and a *group*. The group is just a set of processes.



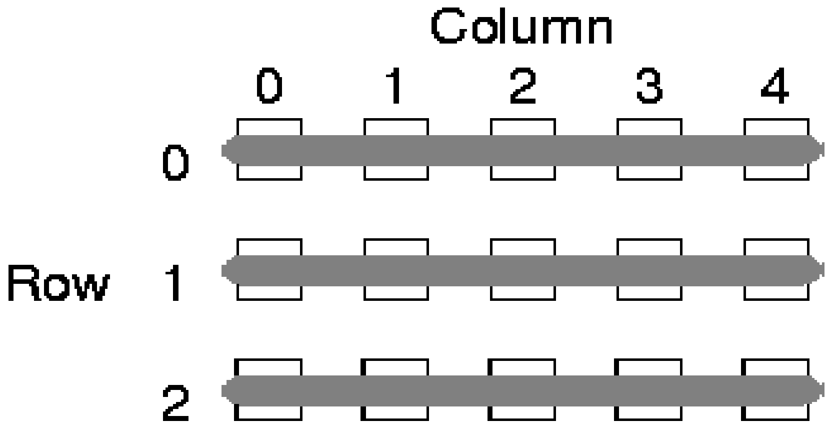
- Processes may have different ranks in different communicators.



Subdividing Communicators: Approach #1

- To subdivide a communicator into multiple non-overlapping communicators, one approach is to use **`MPI_Comm_split`**

```
MPI_Comm_rank(MPI_COMM_WORLD,&rank);
myrow = (int)(rank/ncol);
MPI_Comm_split(MPI_COMM_WORLD,myrow,rank,row_comm);
```



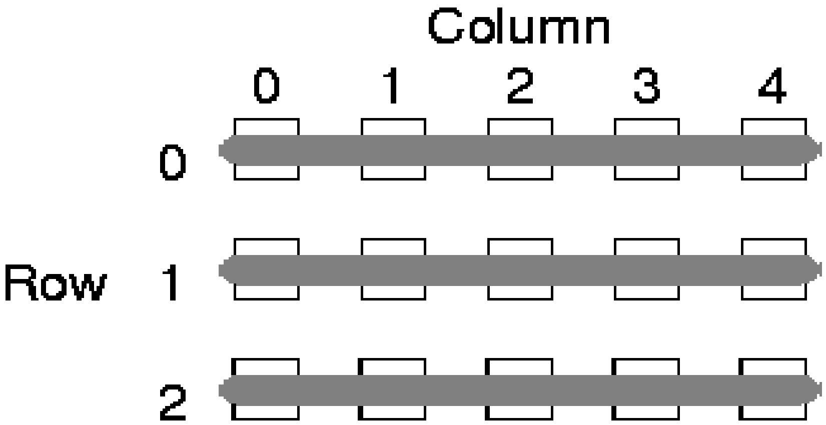
Arguments to MPI_Comm_split

```
MPI_Comm_rank(MPI_COMM_WORLD,&rank);
myrow = (int)(rank/ncol);
MPI_Comm_split(MPI_COMM_WORLD,myrow,rank,row_comm);
```

1. Communicator to split
2. Key – all processes with the same key go in the same communicator
3. Value to determine ordering in the result communicator (optional)
4. Result communicator

Subdividing Communicators: Approach #2

- The same goal can be accomplished using groups
- **`MPI_Comm_group`** – extract the group defined by a communicator
- **`MPI_Group_incl`** – make a new group from selected members of the existing group (e.g., members in the same row of a 2D layout)
- **`MPI_Comm_create`** – form a communicator based on this group



Code for Approach #2

```
MPI_Group base_grp,grp;  MPI_Comm row_comm,temp_comm;
int row_list[NCOL], irow, myrank_in_world;

MPI_Comm_group(MPI_COMM_WORLD,&base_grp); //get base
MPI_Comm_rank(MPI_COMM_WORLD,&myrank_in_world);

irow = (myrank_in_world/NCOL);
for (i=0; i <NCOL; i++)  row_list[i] = i;
for (i=0; i <NROW; i++){
   MPI_Group_incl(base_grp,NCOL,row_list,&grp);
   MPI_Comm_create(MPI_COMM_WORLD,grp,&temp_comm);
   if (irow == i) *row_comm=temp_comm;
   for (j=0;j<NCOL;j++) row_list[j] += NCOL;
}
```

Communicators and Groups: Summary

- In Approach #1, we used **`MPI_Comm_split`** to split one communicator into multiple non-overlapping communicators.
- This approach is relatively compact and is suitable for regular decompositions.

- In Approach #2, we broke the communicator into (sub)groups and made these into new communicators to suit our needs.
- We did this using **`MPI_Comm_group`**, **`MPI_Group_incl`**, and **`MPI_Comm_create`**.
- This approach is quite flexible and is more generally applicable.
- A number of other group functions are available: union, intersection, difference, include, exclude, range-include, range-exclude.

5. Persistent Communication

How Persistent Communication Works

- Motivation: we'd like to save the argument list of an MPI call to reduce overhead for subsequent calls with the same arguments
- INIT takes the original argument list of a send or receive call and creates a persistent *communication request* from it
  - **`MPI_Send_init`** (for *nonblocking* send)
  - **`MPI_Bsend_init`** (for buffered send – can do Rsend or Ssend as well)
  - **`MPI_Recv_init`** (for *nonblocking* receive)
- START starts an operation based on the *communication request*
  - **`MPI_Start`**
  - **`MPI_Startall`**
- REQUEST_FREE frees the persistent communication request
  - **`MPI_Request_free`**

Typical Situation Where Persistence Might Be Used

```
MPI_Recv_init(buf1, count,type,src,tag,comm,&req[0]);
MPI_Send_init(buf2, count,type,src,tag,comm,&req[1]);

for (i=1; i < BIGNUM; i++)
{
      MPI_Start(&req[0]);
      MPI_Start(&req[1]);
      MPI_Waitall(2,req,status);
      do_work(buf1, buf2);
}

MPI_Request_free(&req[0]);
MPI_Request_free(&req[1]);
```

Performance Benefits from Using Persistence

Improvement in Wallclock Time (IBM SP2)
Persistent vs. Conventional Communication

size, bytes	mode	improvement	mode	improvement
8	async	19 %	sync	15 %
4096	async	11 %	sync	4.7 %
8192	async	5.9 %	sync	2.9 %
800,000	-	-	sync	0 %
8,000,000	-	-	sync	0 %

- **Takeaway**: it’s most effective when applied to lots of small messages

6. Parallel I/O (MPI-2)

What is Parallel I/O?

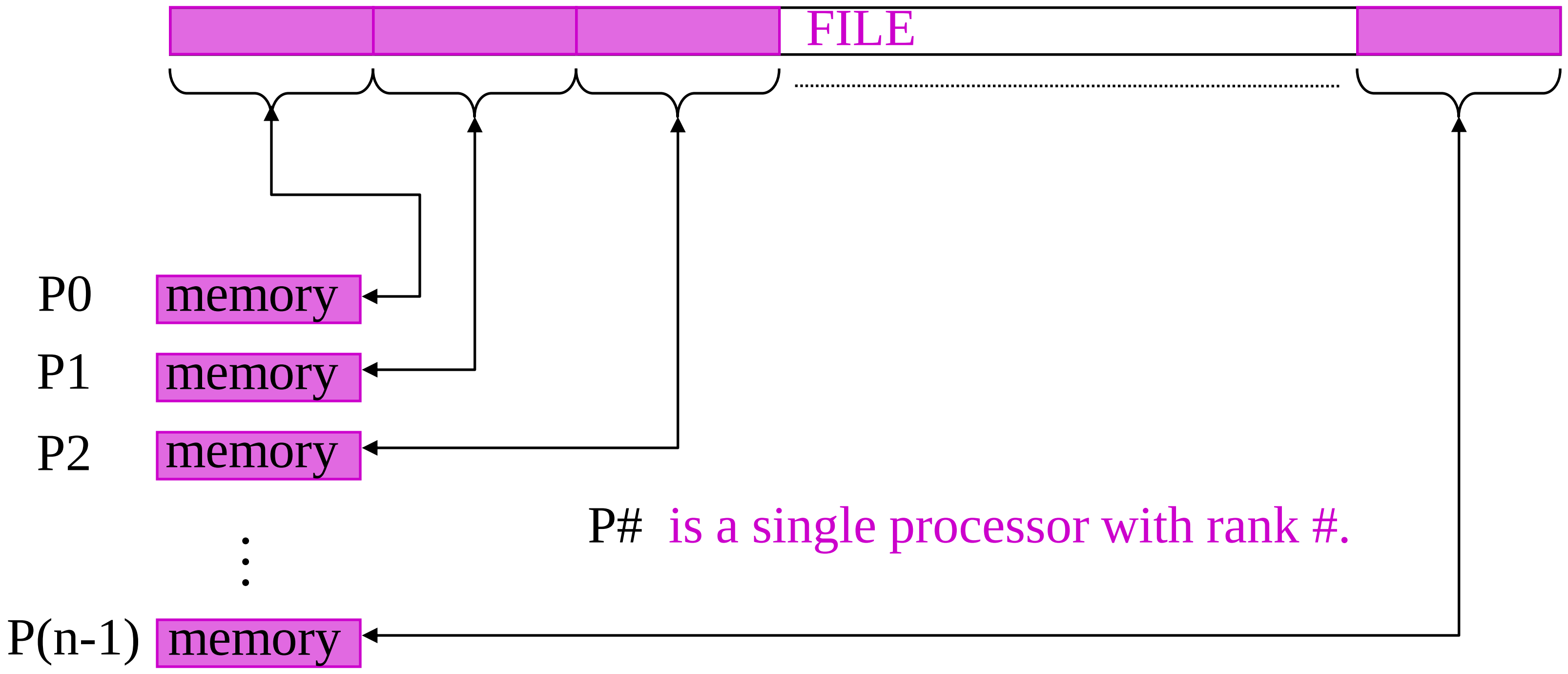
- HPC Parallel I/O occurs when:
  - multiple MPI tasks can read or write simultaneously,
  - from or to a single file,
  - in a parallel file system,
  - through the MPI-IO interface.
- A parallel file system works by:
  - appearing as a normal Unix file system, while
  - employing multiple I/O servers (usually) for high sustained throughput.
- Two common alternatives to parallel MPI-IO are:
  1. Rank 0 accesses a file; it gathers/scatters file data from/to other ranks.
  2. Each rank opens a separate file and does I/O to it independently.

Why Parallel I/O?

- I/O was lacking from the MPI-1 specification
- Due to need, it was defined independently, then subsumed into MPI-2
- HPC Parallel I/O requires some extra work, but it
  - potentially provides high throughput and
  - offers a single (unified) file for viz and pre/post processing.
- Alternative I/O schemes are simple enough to code, but have either
  - poor scalability (e.g., single task is a bottleneck) or
  - file management challenges (e.g., files must be collected from local disk).
- MPI-IO provides
  - mechanisms for performing synchronization,
  - syntax for data movement, and
  - means for defining noncontiguous data layout in a file (MPI datatypes).

Simple MPI-IO

Each MPI task reads/writes a single block:



P# is a single processor with rank #.

Reading by Using Individual File Pointers – C Code

```
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);
```

Reading by Using Explicit Offsets – F90 Code

```
include 'mpif.h'
integer status(MPI_STATUS_SIZE)
integer (kind=MPI_OFFSET_KIND) offset

nints  = FILESIZE/(nprocs*INTSIZE)
offset = rank * nints * INTSIZE

call MPI_FILE_OPEN( MPI_COMM_WORLD, '/pfs/datafile', &
                    MPI_MODE_RDONLY,                 &
                    MPI_INFO_NULL, fh, ierr)
call MPI_FILE_READ_AT( fh, offset, buf, nints,
                       MPI_INTEGER, status, ierr)
call MPI_FILE_CLOSE(fh, ierr)
```

Writing with Pointers and Offsets; Shared Pointers

- Use MPI_File_write or MPI_File_write_at
- MPI_File_open flags:
  - **`MPI_MODE_WRONLY`** (write only)
  - **`MPI_MODE_RDWR`** (read and write)
  - **`MPI_MODE_CREATE`** (create file if it doesn't exist)
  - Use bitwise-or '|' in C, or addition '+" in Fortran, to combine multiple flags

Shared Pointers

- Create one implicitly-maintained pointer per collective file open
  - **`MPI_File_read_shared`**
  - **`MPI_File_write_shared`**
  - **`MPI_File_seek_shared`**

Noncontiguous Accesses

- Common in parallel applications
  - example: distributed arrays stored in files

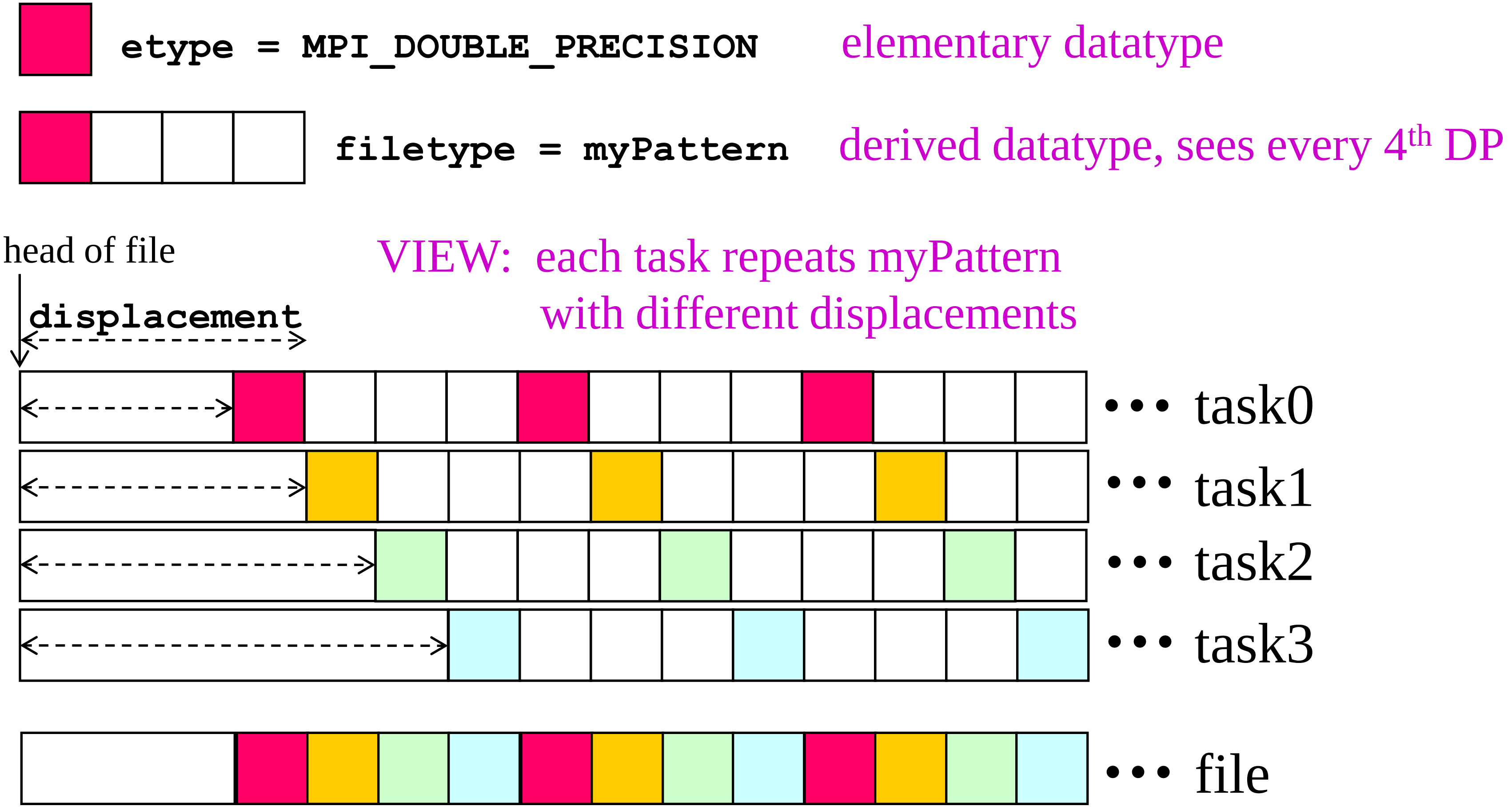
- A big advantage of MPI I/O over Unix I/O is the ability to specify noncontiguous accesses in a file **and** a memory buffer
  - do this by using derived datatypes within a single MPI function call
  - allows implementation to optimize the access

- Collective I/O combined with noncontiguous accesses yields the highest performance

File Views

- A *view* is a triplet of arguments (*displacement*, *etype*, *filetype*) that is passed to **MPI_File_set_view**
- *displacement* = number of bytes to be skipped from the start of the file
- *etype* = basic unit of data access (can be any basic or derived datatype)
- *filetype* = specifies layout of etypes within file

Example #1: File Views for a Four-Task Job



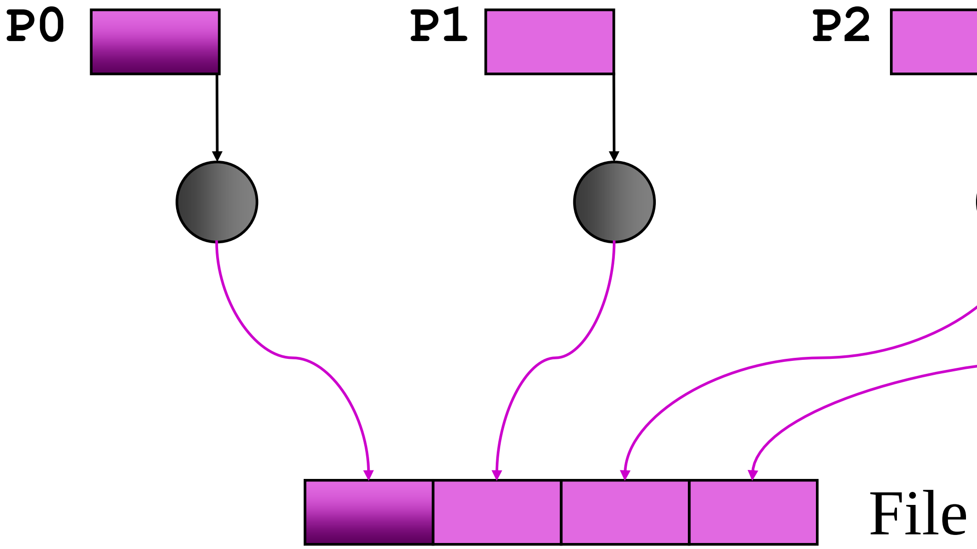
etype = MPI_DOUBLE_PRECISION elementary datatype

filetype = myPattern derived datatype, sees every 4th DP

VIEW: each task repeats myPattern
with different displacements

Example #2: File Views for a Four-Task Job

- 1 block from each task, written in task order



`MPI_File_set_view` assigns regions of the file to separate processes

Code for Example #2

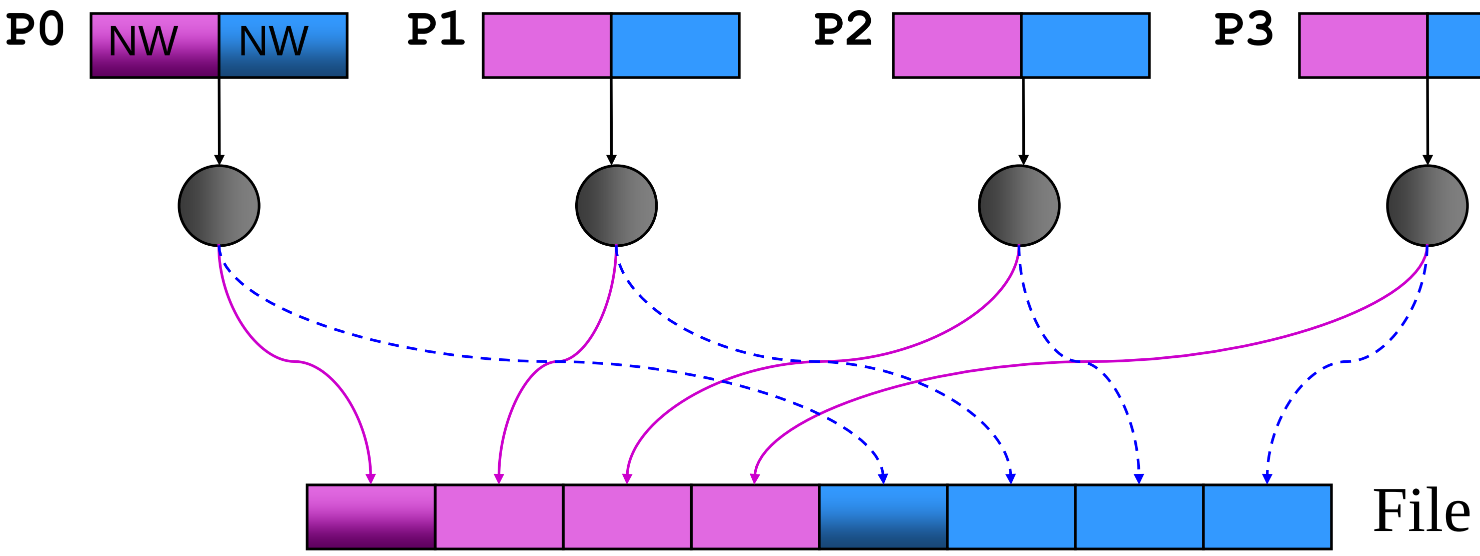
```
#define N 100
MPI_Datatype arraytype;
MPI_Offset disp;

disp = rank*sizeof(int)*N; etype = MPI_INT;
MPI_Type_contiguous(N, MPI_INT, &arraytype);
MPI_Type_commit(&arraytype);

MPI_File_open(    MPI_COMM_WORLD, "/pfs/datafile",
                  MPI_MODE_CREATE | MPI_MODE_RDWR,
                  MPI_INFO_NULL, &fh);
MPI_File_set_view(fh, disp, etype, arraytype,
                  "native", MPI_INFO_NULL);
MPI_File_write(fh, buf, N, etype, MPI_STATUS_IGNORE);
```

Example #3: File Views for a Four-Task Job

- 2 blocks from each task, written in round-robin fashion to a file



`MPI_File_set_view` assigns regions of the file to separate processes

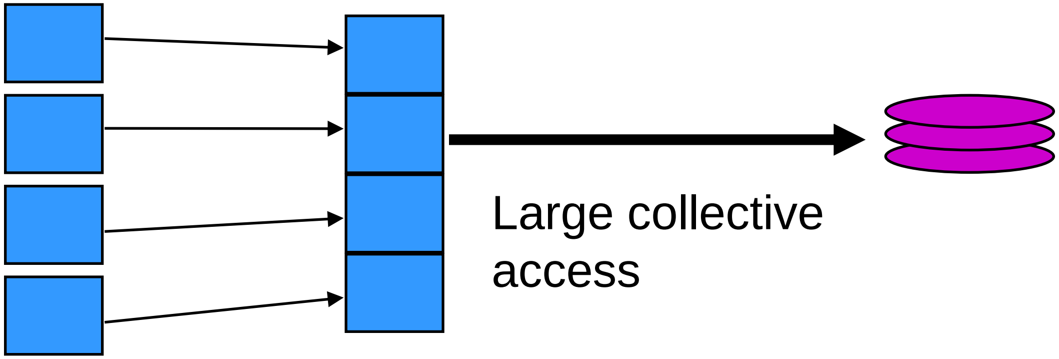
Code for Example #3

```
int buf[NW*2];
   MPI_File_open(MPI_COMM_WORLD, "/data2",
                 MPI_MODE_RDWR, MPI_INFO_NULL, &fh);
/* want to see 2 blocks of NW ints, NW*npes apart */
   MPI_Type_vector(2, NW, NW*npes, MPI_INT, &fileblk);
   MPI_Type_commit(                         &fileblk);
   disp = (MPI_Offset)rank*NW*sizeof(int);
   MPI_File_set_view(fh, disp, MPI_INT, fileblk,
                     "native", MPI_INFO_NULL);

/* processor writes 2 'ablk', each with NW ints */
   MPI_Type_contiguous(NW,   MPI_INT, &ablk);
   MPI_Type_commit(&ablk);
   MPI_File_write(fh, (void *)buf, 2, ablk, &status);
```

Collective I/O in MPI

- A critical optimization in parallel I/O
- Allows communication of “big picture” to file system
- Framework for 2-phase I/O, in which communication precedes I/O (uses MPI machinery)
- Basic idea: build large blocks, so that reads/writes in I/O system will be large



Small individual requests

Large collective access

MPI Routines for Collective I/O

- Typical routine names:
  - **`MPI_File_read_all`**
  - **`MPI_File_read_at_all`**, etc.
- The **`_all`** indicates that all processes in the group specified by the communicator passed to **`MPI_File_open`** will call this function
- Each process provides nothing beyond its own access information; therefore, the argument list is the same as for the non-collective functions

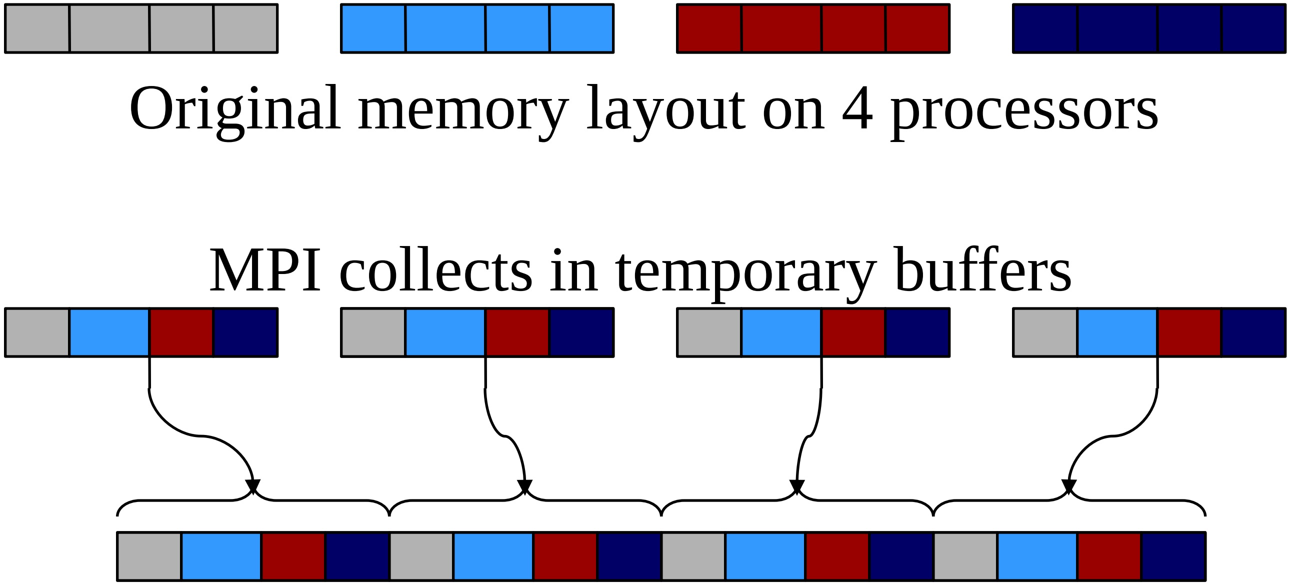
Advantages of Collective I/O

- By calling the collective I/O functions, the user allows an implementation to optimize the request based on the combined requests of all processes

- The implementation can merge the requests of different processes and service the merged request efficiently

- Particularly effective when the accesses of different processes are noncontiguous and interleaved

Collective I/O: Memory Layout, Communication



Original memory layout on 4 processors

MPI collects in temporary buffers

then writes to File layout

More Advanced I/O

- Asynchronous I/O:
  - **`iwrite/iread`**
  - terminate with **`MPI_Wait`**

- Split operations:
  - **`read_all_begin/end`**
  - **`write_all_begin/end`**
  - give the system more chance to optimize

Passing Hints to the Implementation

```
MPI_Info info;
MPI_Info_create(&info);

/* no. of I/O devices to be used for file striping */
MPI_Info_set(info, "striping_factor", "4");

/* the striping unit in bytes */
MPI_Info_set(info, "striping_unit", "65536");

MPI_File_open(MPI_COMM_WORLD, "/pfs/datafile",
              MPI_MODE_CREATE | MPI_MODE_RDWR,
              info, &fh);

MPI_Info_free(&info);
```

Examples of Hints (Used in ROMIO)

- `striping_unit`
- `striping_factor`
- `cb_buffer_size`
- `cb_nodes`

MPI-2 predefined hints

- `ind_rd_buffer_size`
- `ind_wr_buffer_size`

New algorithm parameters

- `start_iodevice`
- `pfs_svr_buf`
- `direct_read`
- `direct_write`

Platform-specific hints

Summary of Parallel I/O Issues

- MPI-IO has many features that can help users achieve high performance
- The most important of these features are:
  - the ability to specify noncontiguous accesses
  - the collective I/O functions
  - the ability to pass hints to the implementation
- Use is encouraged, because I/O is expensive!
- In particular, when accesses are noncontiguous, users must:
  - create derived datatypes
  - define file views
  - use the collective I/O functions

7. Status of MPI-2

Features of MPI-2

- Parallel I/O (MPI-IO) – probably the most popular
- One-sided communication (put / get)
- Dynamic process management (spawn)
- Expanded collective communication operations (e.g., non-blocking)
- Support for multithreading
- Additional support for programming languages
  - C++ interface
  - limited F90 support
  - interfaces for debuggers, profilers

MPI-2 Status Assessment

- Virtually all vendors offer MPI-1
  - Well-established free implementations (MPICH, OpenMPI) support networks of heterogeneous workstations, e.g.
  - The functionality of MPI-1 (or even a subset) is sufficient for most applications
- Partial MPI-2 implementations are available from most vendors
- MPI-2 implementations tend to appear piecemeal, with I/O first
  - MPI-IO now available in most MPI implementations
  - One-sided communication available in some
  - OpenMPI (aka LAM) and MPICH2 now becoming complete
  - Dynamic process management may not mesh well with batch systems

References

- William Gropp, Ewing Lusk, and Anthony Skjellum, *Using MPI, Second Edition* (MIT Press, 1999)
- William Gropp, Ewing Lusk, and Rajeev Thakur, *Using MPI-2* (MIT Press, 1999)

  http://www.scribd.com/doc/28220855/Using-MPI-2-Advanced-Features
- Index to the MPI 1.1 standard

  http://www.mpi-forum.org/docs/mpi-11-html/node182.html
- Index to the MPI 2 standard

  http://www.mpi-forum.org/docs/mpi-20-html/node306.htm
- The I/O Stress Benchmark Codes

  https://asc.llnl.gov/computing_resources/purple/archive/benchmarks/ior/