ICHEC
Irish Centre for High-End Computing

PRACE Course: Intermediate MPI

9-11 November 2022

MPI Collective Communication

Collective Communication

- Communications involving a group of processes.
- Must be called by all processes in a communicator.
- Examples:
  - Barrier synchronization.
  - Broadcast, scatter, gather.
  - Global sum, global maximum, etc.
  - Neighbor communication in a virtual process grid

From MPI-3.0

Characteristics of Collective Communication

- Optimised Communication routines involving a group of processes
- Collective action over a communicator, i.e. all processes must call the collective routine.
- No tags.
- Receive buffers must be exactly the right size.
- In MPI-1.0 – MPI-2.2, all collective operations are blocking. Nonblocking versions since MPI-3.0.

Barrier Synchronisation

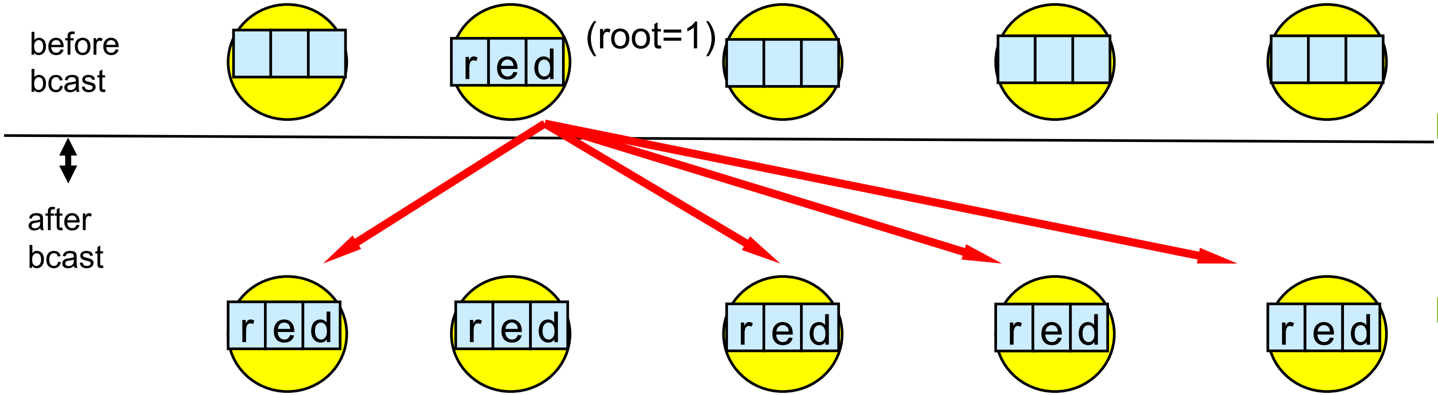
- C:
  int MPI_Barrier(MPI_Comm comm)
- Fortran:
  MPI_BARRIER(COMM, IERROR)
  TYPE(MPI_Comm) :: comm
  INTEGER, OPTIONAL :: ierror

- MPI_Barrier is normally never needed:
  - all synchronization is done automatically by the data communication;
  - if used for debugging, please guarantee, that it is removed in production.
  - can be used for time measurement

Broadcast

- C:
  int MPI_Bcast(void *buf, int count, MPI_Datatype datatype, int root, MPI_Comm comm)
- Fortran:
  MPI_Bcast(BUF, COUNT, DATATYPE, ROOT, COMM, IERROR)
      TYPE(*), DIMENSION(..) :: buf; TYPE(MPI_Datatype) :: datatype
      INTEGER COUNT, ROOT; TYPE(MPI_Comm) :: comm
      INTEGER, OPTIONAL :: ierror

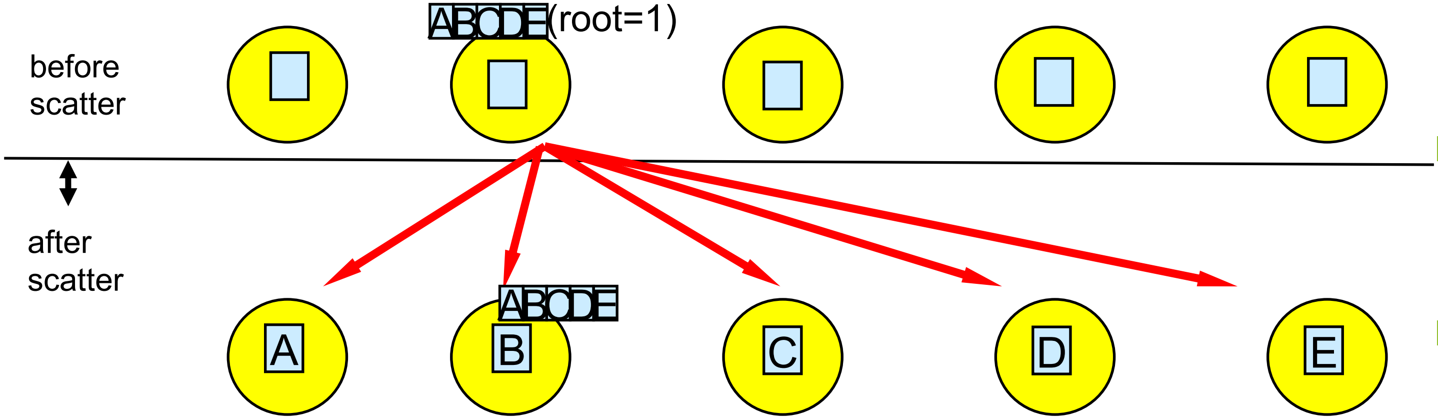
MPI_Bcast(buf, 3, MPI_CHAR, 1, MPI_COMM_WORLD);



Scatter

- C:
  int MPI_Scatter(void *sendbuf, int sendcount, MPI_Datatype sendtype, void *recvbuf, int recvcount, MPI_Datatype recvtype, int root, MPI_Comm comm)
- Fortran:
  MPI_SCATTER(SENDBUF, SENDCOUNT, SENDTYPE, RECVBUF, RECVCOUNT, RECVTYPE, ROOT, COMM, IERROR)
  TYPE(*), DIMENSION(..) :: sendbuf, recvbuf; INTEGER :: sendcount, recvcount, root
  TYPE(MPI_Datatype) :: sendtype, recvtype; TYPE(MPI_Comm) :: comm; INTEGER, OPTIONAL :: ierror

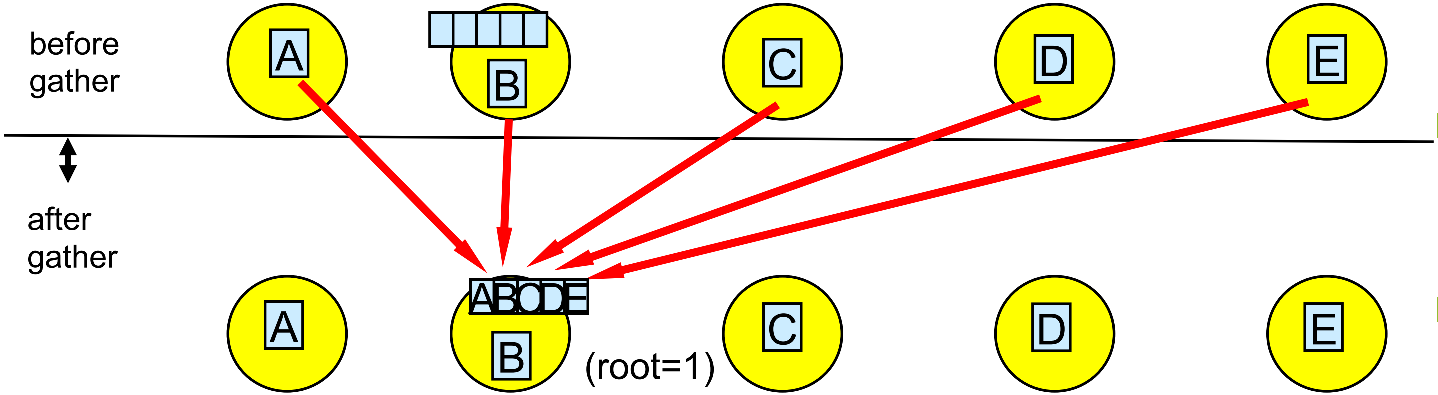
MPI_Scatter(sbuf, 1, MPI_CHAR, rbuf, 1, MPI_CHAR, 1, MPI_COMM_WORLD);



Gather

- C:
  int MPI_Gather(void *sendbuf, int sendcount, MPI_Datatype sendtype, void *recvbuf, int recvcount, MPI_Datatype recvtype, int root, MPI_Comm comm)
- Fortran:
  MPI_GATHER(SENDBUF, SENDCOUNT, SENDTYPE, RECVBUF, RECVCOUNT, RECVTYPE, ROOT, COMM, IERROR)
  TYPE(*), DIMENSION(..) :: sendbuf, recvbuf; INTEGER :: sendcount, recvcount, root;
  TYPE(MPI_Datatype) :: sendtype, recvtype; TYPE(MPI_Comm) :: comm; INTEGER, OPTIONAL :: ierror

MPI_Gather(sbuf, 1, MPI_CHAR, rbuf, 1, MPI_CHAR, 1, MPI_COMM_WORLD);



Example – MPI Scatter

```
#include <stdio.h>
#include <mpi.h>
#define SIZE 4

int main( int argc, char **argv ) {
  int myRank, uniSize, ierror;
  int sendbuf[SIZE][SIZE]={
  {1, 2, 3, 4},
  {5, 6, 7, 8},
  {9, 10, 11, 12},
  {13, 14, 15, 16},
  };
  int recvbuf[SIZE];

  ierror=MPI_Init(&argc, &argv);
  ierror=MPI_Comm_size(MPI_COMM_WORLD, &uniSize);
  ierror=MPI_Comm_rank(MPI_COMM_WORLD, &myRank);

  if(uniSize==SIZE){
    ierror = MPI_Scatter(sendbuf, SIZE, MPI_INT, recvbuf, SIZE, MPI_INT, 0, MPI_COMM_WORLD );
    printf("rank= %d  Results: %d %d %d %d\n", myRank,recvbuf[0],recvbuf[1],recvbuf[2],recvbuf[3]);
  }

  ierror = MPI_Finalize();
  return ierror;
}
```

Run with 4 processors

```
rank= 0  Results: 1.0 2.0 3.0 4.0
rank= 1  Results: 5.0 6.0 7.0 8.0
rank= 2  Results: 9.0 10.0 11.0 12.0
rank= 3  Results: 13.0 14.0 15.0 16.0
```

Global Reduction Operations

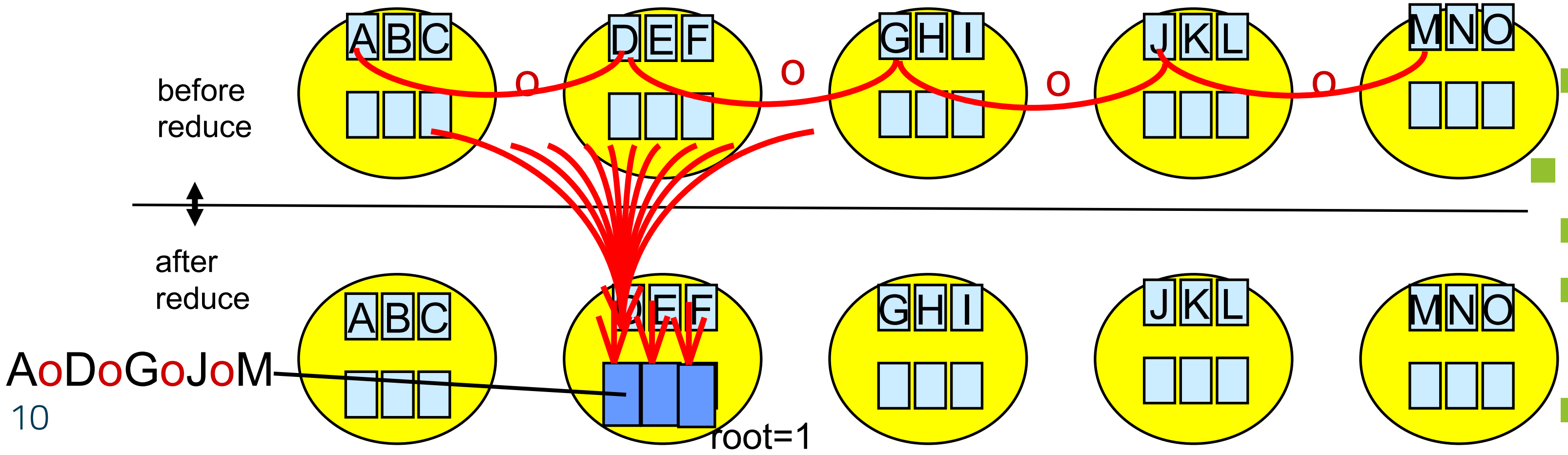
- To perform a global reduce operation across all members of a group.
- $d_0 \circ d_1 \circ d_2 \circ d_3 \circ \ldots \circ d_{s-2} \circ d_{s-1}$
  - di : data in process rank i (single variable, or vector)
  - $\circ$: commutative and associative operation
  - Example:
    global sum or product
    global maximum or minimum
    global user-defined operation
- floating point rounding may depend on usage of associative law:
  - $[(d_0 \circ d_1) \circ (d_2 \circ d_3)] \circ [\ldots \circ (d_{s-2} \circ d_{s-1})]$
  - $((((((d_0 \circ d_1) \circ d_2) \circ d_3) \circ \ldots) \circ d_{s-2}) \circ d_{s-1})$

Reduce

- C:
  int MPI_Reduce(void *sendbuf, void *recvbuf, int count, MPI_Datatype datatype, MPI_Op op, int root, MPI_Comm comm);
- Fortran:
  MPI_REDUCE(SENDBUF, RECVBUF, COUNT, DATATYPE, OP, ROOT, COMM, IERROR)
  TYPE(*), DIMENSION(..) :: sendbuf, recvbuf; INTEGER :: count, root
  TYPE(MPI_Datatype) :: datatype; TYPE(MPI_Comm) :: comm;
  TYPE(MPI_Op) :: op; INTEGER, OPTIONAL :: ierror

To reuse the same buffer: MPI_IN_PLACE

MPI_Reduce(&sendbuf, &recvbuf, 1, MPI_INT, MPI_SUM, root, MPI_COMM_WORLD);



Predefined Reduction Operation Handles

Predefined operation handle	Function
MPI_MAX	Maximum
MPI_MIN	Minimum
MPI_SUM	Sum
MPI_PROD	Product
MPI_LAND	Logical AND
MPI_BAND	Bitwise AND
MPI_LOR	Logical OR
MPI_BOR	Bitwise OR
MPI_LXOR	Logical exclusive OR
MPI_BXOR	Bitwise exclusive OR
MPI_MAXLOC	Maximum and location of the maximum
MPI_MINLOC	Minimum and location of the minimum

User-Defined Reduction Operations

- Operator handles
  - predefined – see table above
  - user-defined

- User-defined operation □:
  - Associative
  - Can be commutative
  - user-defined function must perform the operation vector_A □ vector_B

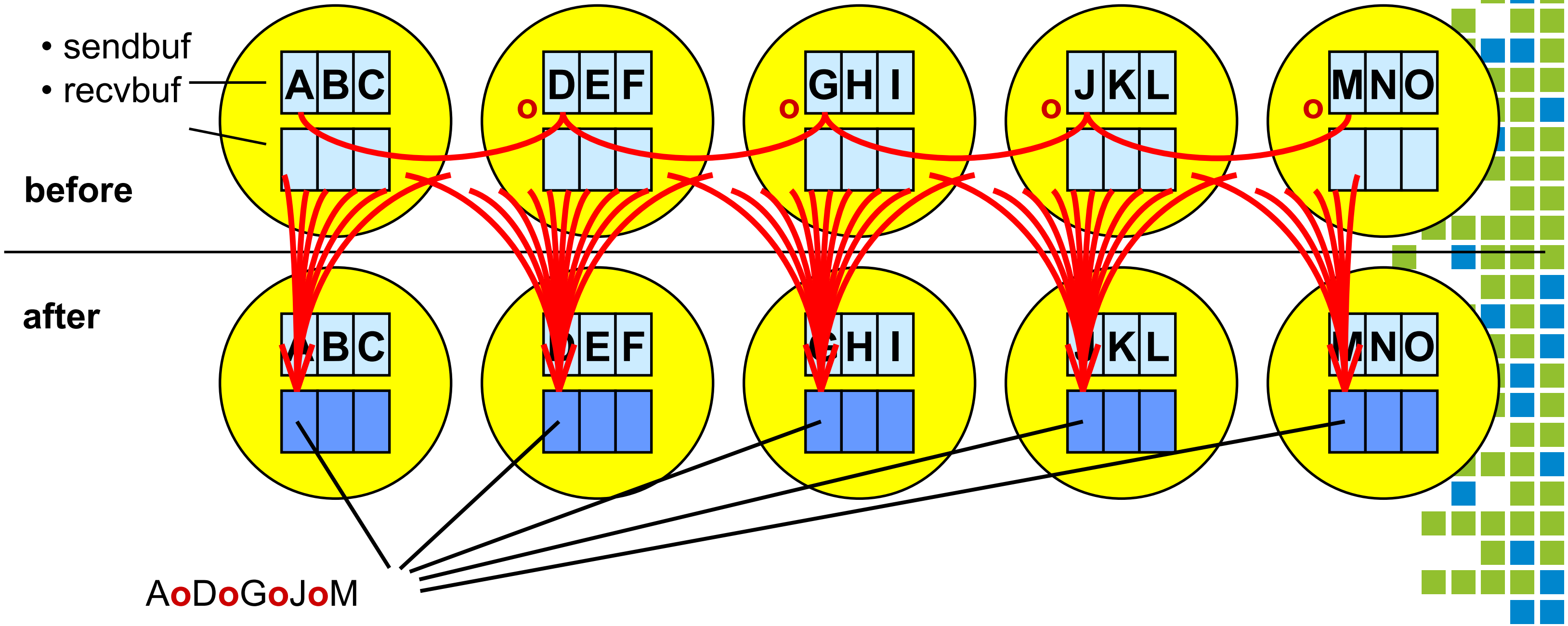
- User-defined function: MPI_User_function, FUNCTION USER_FUNCTION

- Registering a user-defined reduction function:
  - C: MPI_Op_create(MPI_User_function *func, int commute, MPI_Op *op)
  - Fortran: MPI_OP_CREATE(FUNC, COMMUTE, OP, IERROR)

Variants of Reduction Operations

- MPI_ALLREDUCE *(see next slide)*
  - no root,
  - returns the result in all processes
- MPI_REDUCE_SCATTER _BLOCK and MPI_REDUCE_SCATTER
  - result vector of the reduction operation is scattered to the processes
- MPI_SCAN *(see the next second slide)*
  - prefix reduction
  - result at process with rank i :=
    reduction of inbuf-values from rank 0 to rank i
- MPI_Exscan
  - result at process with rank i :=
    reduction of inbuf-values from rank 0 to rank i-1

MPI_Allreduce



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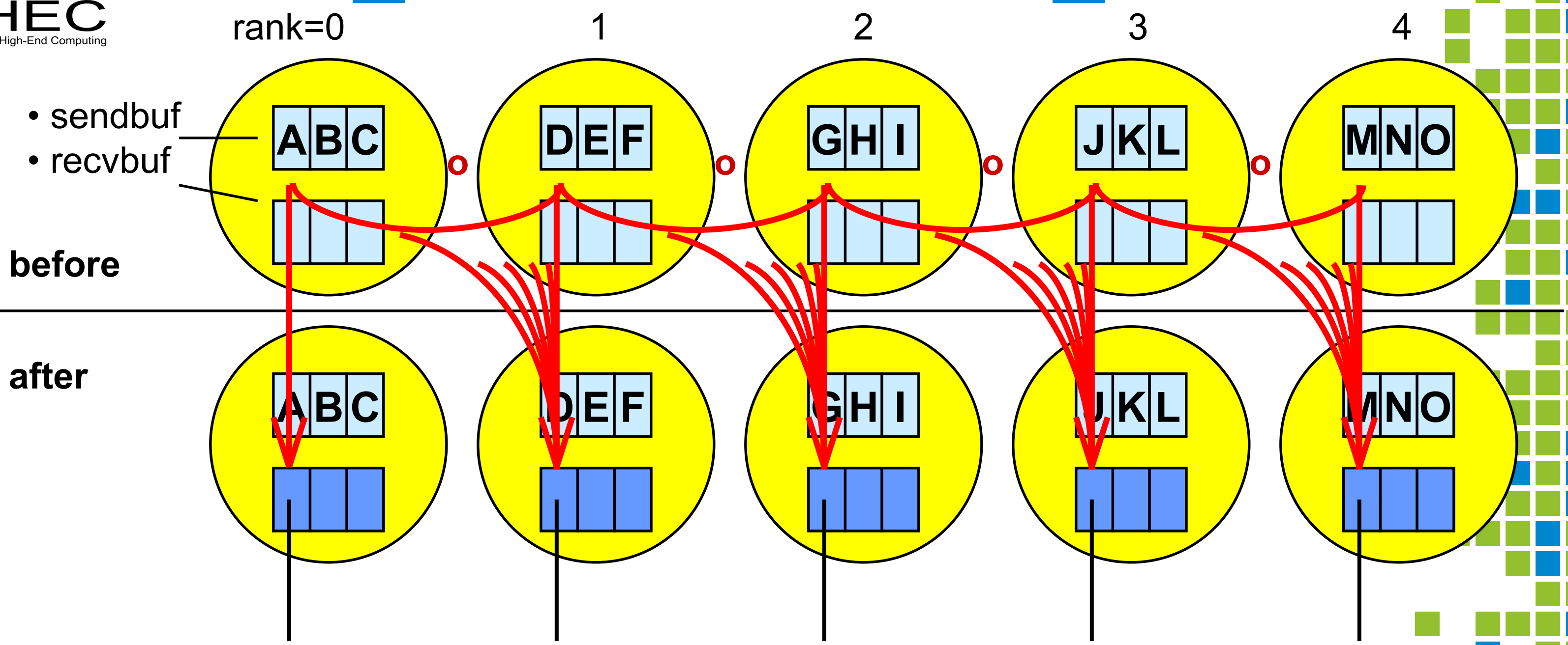
MPI_Scan and MPI_Exscan



MPI_Scan:	A	AoD	AoDoG	AoDoGoJ	AoDoGoJoM
MPI_Exscan:	-	A	AoD	AoDoG	AoDoGoJ

done in parallel

```
MPI_Scan(&myRank, &scansum, 1, MPI_INT, MPI_SUM, MPI_COMM_WORLD);
```

Other Collective Communication Routines

- MPI_Gatherv, MPI_Scatterv
    - Each message has a different count and displacement
    - array of counts and array of displs

- MPI_Allgather, MPI_Allgatherv
    - similar to MPI_Gather, but all processes receive the result vector

- MPI_Alltoall, MPI_Alltoallv, MPI_Alltoallw
    - each process sends messages to all processes

MPI_Gatherv

- C:

  ```
  int MPI_Gatherv(void *sendbuf, int sendcount, MPI_Datatype sendtype, void *recvbuf,
  int *recvcounts, int *displs, MPI_Datatype recvtype, int root, MPI_Comm comm
  ```

- Fortran:

  ```
  MPI_GATHERV(SENDBUF, SENDCOUNT, SENDTYPE, RECVBUF,
  RECVCOUNTS, DISPLS, RECVTYPE, ROOT, COMM, IERROR)
  TYPE(*), DIMENSION(..) :: sendbuf, recvbuf; TYPE(MPI_Comm) :: comm
   INTEGER :: sendcount, recvcounts(*), displs(:), root;
  TYPE(MPI_Datatype) :: sendtype, recvtype; INTEGER, OPTIONAL :: ierror
  ```

- recvcounts: the number of elements that is received from each process. Each element in the array corresponds to the rank of the sending process.
- displs: The location, relative to the recvbuf parameter, of the data from each communicator process. The data that is received from process j is placed into the receive buffer of the root process offset displs[j] elements from the sendbuf pointer.

Example - MPI_Gatherv

```
recvcounts[4]={0, 1, 2, 3};
int displs[4]={0, 0, 1, 3};

MPI_Gatherv(sendbuf, rank, MPI_INT, recvbuf, recvcounts, displs,
MPI_INT, 0, MPI_COMM_WORLD);
```

```
rank=1: sendbuf[0]=1
rank=2: sendbuf[0]=2
rank=2: sendbuf[1]=2
rank=3: sendbuf[0]=3
rank=3: sendbuf[1]=3
rank=3: sendbuf[2]=3
```

```
recvbuf[0]=1
recvbuf[1]=2
recvbuf[2]=2
recvbuf[3]=3
recvbuf[4]=3
recvbuf[5]=3
```

MPI_AllGather

- C:

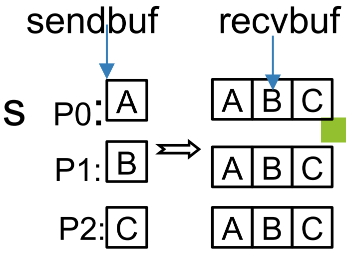
  int MPI_Allgather(void *sendbuf, int sendcount, MPI_Datatype sendtype, void *recvbuf, int recvcount, MPI_Datatype recvtype, MPI_Comm comm)
- Fortran:

  MPI_ALLGATHER(SENDBUF, SENDCOUNT, SENDTYPE, RECVBUF, RECVCOUNT, RECVTYPE, COMM, IERROR)

  TYPE(*), DIMENSION(..) :: sendbuf, recvbuf; TYPE(MPI_Comm) :: comm

  INTEGER :: sendcount, recvcount; INTEGER, OPTIONAL :: ierror

  TYPE(MPI_Datatype) :: sendtype, recvtype



- Gathers data from all members of a group and sends the data to all members of the group.
- similar to the MPI_Gather, except that it sends the data to all processes instead of only to the root.

Nonblocking Collective Communication Routines

- Combines nonblocking functionality with a collective communication
- Preventing deadlocks, overlapping communication with computation and deferring synchronization together with a group communication.

- Nonblocking variants of all collective communication:
  - MPI_Ibarrier, MPI_Ibcast, MPI_Iscatter, MPI_Igather, MPI_Ireduce, …   *(Chapter 5 mpi31-report.pdf)*

- MPI_I… calls are local (i.e., not synchronizing), whereas the corresponding MPI_Wait collectively synchronizes in same way as corresponding blocking collective procedure
- The output request is the same request object with p2p comm.
- All completion calls are supported:. MPI_Waitall, MPI_Waitany, MPI_Testall, …

Nonblocking Collective Communication Routines

- Nonblocking p2p operations can be canceled by MPI_CANCEL but nonblocking collectives not.
- Nonblocking collective operations do not match with blocking collective operations.
- Send and recv buffers must not be modified while the operation is in progress.

With point-to-point message passing, such matching is allowed

- May have multiple outstanding collective communications on same communicator
- Ordered initialization on each communicator

References: [1], [4] and [8]

Nonblocking Barrier

- C:
  int MPI_Ibarrier(MPI_Comm comm, MPI_Request *request)
- Fortran:
  MPI_IBARRIER(COMM, REQUEST, IERROR)
  TYPE(MPI_Comm) :: comm; TYPE(MPI_Request) :: request
  INTEGER, OPTIONAL :: ierror

- Performs a barrier synchronization across all members of a group in a non-blocking way
- MPI_Ibarrier is very useful routine:
  - each process starts the barrier after it finishes its local part and serves the requests of other processes until the barrier is reached by all others and completes

Example - Nonblocking Barrier

```
MPI_Request reqs[m], barrier_request; //We send m messages

int barrier_done=0, barrier_active=0;

for(i=0;i<m;i++) MPI_Issend(sbuf[i], size[i], type, dst[i], tag, comm, &reqs[i]);

while(!barrier_done)
  MPI_Iprobe(MPI_ANY_Source, tag, comm, &flag, &stat);

  if(flag){ //allocate buffer and receive message }

  if(!barrier_active){
    int flag;
    MPI_Testall(m, reqs, &flag, MPI_STATUSES_IGNORE);

    if(flag){
      MPI_Ibarrier(comm, &barrier_request);
      barrier_active=1;
    }
    else{
      MPI_Test(&barrier_request, &barrier_done, MPI_STATUS_IGNORE);
    }
  }
```

Each as a sender loops over its neighbors,sending the data

Loop until all signaled that all receives are called

Check if there is a message

Check whether all Issend calls are finished

Start MPI_Ibarrier to signal to all that all MPI_Issend of this process are already received

T. Hoefler, C. Siebert, A. Lumsdaine, “Scalable communication protocols for dynamic sparse data exchange”

Nonblocking Reduce

- C:

  ```
  int MPI_Ireduce(const void *sendbuf, void *recvbuf, int count,
  MPI_Datatype datatype, MPI_Op op, int root, MPI_Comm comm,
  MPI_Request *request)
  ```

- Fortran:

  ```
  MPI_IREDUCE(SENDBUF, RECVBUF, COUNT, DATATYPE, OP,
  ROOT, COMM, REQUEST, IERROR)
  TYPE(*), DIMENSION(..) :: sendbuf, recvbuf; INTEGER :: count, root
  TYPE(MPI_Datatype) :: datatype; TYPE(MPI_Comm) :: comm;
  TYPE(MPI_Op) :: op; INTEGER, OPTIONAL :: ierror
  TYPE(MPI_Request) :: request
  ```

- Reduces values on all processes to a single value in a non-blocking way
- MPI_Ireduce_... variants are available.

MPI_Probe, MPI_Iprobe

- C:
  int MPI_Iprobe(int source, int tag, MPI_Comm comm, int *flag*, MPI_Status *status*)
- Fortran:
  MPI_IPROBE(source, tag, comm, flag, status, ierror)

      INTEGER :: source,tag; INTEGER, OPTIONAL :: ierror
      TYPE(MPI_Comm) :: comm; TYPE(MPI_Status) :: status
      LOGICAL :: flag

- Checks for the message with source, tag and comm
- flag = true if there is a message that can be received and that matches the pattern specified by the arguments source, tag, and comm.
- MPI_ANY_SOURCE: messages from an arbitrary source
- MPI_ANY_TAG: messages with an arbitrary tag

Example – MPI Iprobe

```
int main(int argc, char* argv[]){
  int myRank, ierror, a[5], i, flag=0;
  MPI_Status status;
  MPI_Request request;

  ierror=MPI_Init(&argc, &argv);
  ierror=MPI_Comm_rank(MPI_COMM_WORLD, &myRank);

  if(myRank ==0){
    a[0]=2345; a[1]=654; a[2]=96574; a[3]=-12; a[4]=7676;
    int tag=myRank;
    printf("Process %d: sending the message.\n", myRank);
    ierror=MPI_Issend(a, 5, MPI_INT, 1, tag, MPI_COMM_WORLD,&request);
    ierror=MPI_Wait(&request,&status);
    }
  else if(myRank == 1){
    while (flag == 0){
      ierror=MPI_Iprobe(MPI_ANY_SOURCE, MPI_ANY_TAG, MPI_COMM_WORLD, &flag, &status);
      printf("After MPI_Iprobe, flag = %d\n", flag);
    }
    ierror=MPI_Recv(a, 5, MPI_INT, status.MPI_SOURCE, status.MPI_TAG, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
    printf("Process %d: message received.\n", myRank);
    for(i=0; i<5; i++) printf("a[%d]=%d\n", i, a[i]);
  }

    ierror=MPI_Finalize();
    return ierror;}
```

Practical

- Practical 2: communication in a ring
- Practical 3: array increment