High-Performance Mathematics

Collective communications

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1 Collective Communications

Collective Communications

A collective communication is a communication that involves a group (or groups) of processes.

- the group of processes is represented as always as a communicator that provides a context for the operation,
- Syntax and semantics of the collective operations are consistent with the syntax and semantics of the point-to-point operations,
- For collective operations, the amount of data sent must exactly match the amount of data specified by the receiver.

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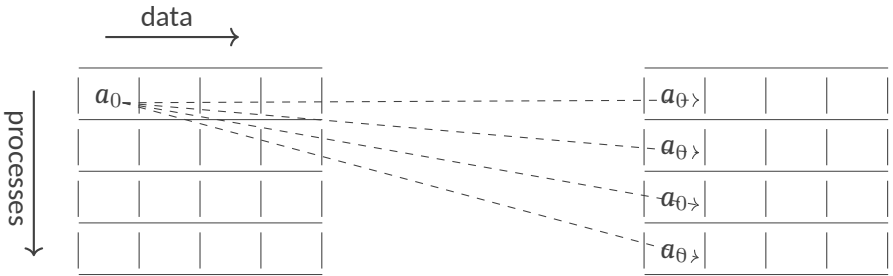
Mixing type of calls

Collective communication calls may use the same communicators as point-to-point communication; Any (conforming) implementation of MPI messages guarantees that calls generated on behalf of collective communication calls will not be confused with messages generated by point-to-point communication.

Taxonomy of collective communications

- The broadcast operation



In the broadcast, initially just the first process contains the data a_0, but after the broadcast all processes contain it.

- This is an example of a **one-to-all** communication, i.e., only one process contributes to the result, while all processes receive the result.

Taxonomy of collective communications: Broadcast


```
int MPI_Bcast(void* buffer, int count, MPI_Datatype datatype, int root,
  MPI_Comm comm)
```

Broadcasts a message from the process with rank `root` to all processes of the group, itself included.

`void* buffer` on return, the content of root's buffer is copied to all other processes.

`int count` size of the message

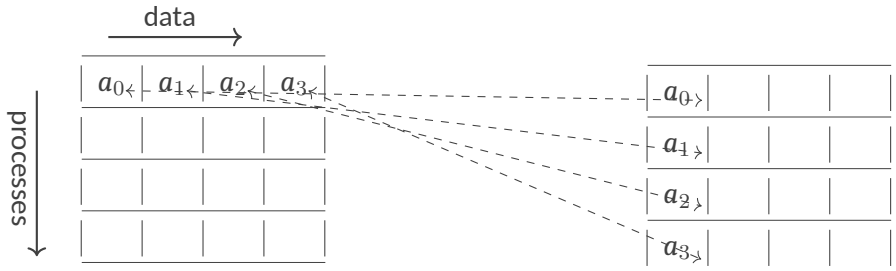
`MPI_Datatype datatype` type of the `buffer`

`int root` `rank` of the process broadcasting the message

`MPI_Comm comm` communicator grouping the processes involved in the broadcast operation

Taxonomy of collective comm‘s: Scatter and Gather

- The scatter and gather operations



- In the **scatter**, initially just the first process contains the data $a_0, \ldots, a_3$, but after the **scatter** the jth process contains the a_j data.
- In the **gather**, initially the jth process contains the a_j data, but after the **gather** the first process contains the data $a_0, \ldots, a_3$

Taxonomy of collective communications: Gather

Each process (root process included) sends the contents of its send buffer to the root process. The latter receives the messages and stores them in rank order.

```
int MPI_Gather(const void* sendbuf, int sendcount, MPI_Datatype sendtype,
 void* recvbuf, int recvcount, MPI_Datatype recvtype, int root, MPI_Comm comm)
```

`const void* sendbuf` starting address of send buffer

`int sendcount` number of elements in send buffer

`MPI_Datatype sendtype` data type of send buffer elements

`void* recvbuf` address of receive buffer

`int recvcount` number of elements for any single receive (and not the total number of items!)

`MPI_Datatype recvtype` data type of received buffer elements

`int root` rank of receiving process

`MPI_Comm comm` communicator

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These are significant only at `root`!

Taxonomy of collective communications: Gather

Observe that

- The type signature of `sendcount`, `sendtype` on each process must be equal to the type signature of `recvcount`, `recvtype` at all the processes.
- The amount of data sent must be equal to the amount of data received, pairwise between each process and the root.

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- The amount of data sent must be equal to the amount of data received, pairwise between each process and the root.

Therefore, if we need to **have a varying count of data** from each process, we need to use instead

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

where

`const int recvcounts[]` is an array (of length group size) containing the number of elements that are received from each process,

`const int displs[]` is an array (of length group size). Entry `i` specifies the displacement relative to `recvbuf` at which to place the incoming data from process `i`.

Taxonomy of collective communications: Gather

If we need to have the result of the *gather* operation on every process involved in the communicator we can use the variant

```
int MPI_Allgather(const void* sendbuf, int sendcount,
 MPI_Datatype sendtype, void* recvbuf, int recvcount,
 MPI_Datatype recvtype, MPI_Comm comm)
```

- All processes in the communicator `comm` receive the result. The block of data sent from the *j*th process is received by every process and placed in the *j*th block of the buffer `recvbuf`.
- The type signature associated with `sendcount`, `sendtype`, at a process must be equal to the type signature associated with `recvcount`, `recvtype` at any other process.

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- The type signature associated with `sendcount`, `sendtype`, at a process must be equal to the type signature associated with `recvcount`, `recvtype` at any other process.

This function has also the version for gathering messages with different sizes:

```
int MPI_Allgatherv(const void* sendbuf, int sendcount,
 MPI_Datatype sendtype, void* recvbuf, const int recvcounts[],
 const int displs[], MPI_Datatype recvtype, MPI_Comm comm)
```

and works in a way analogous to the `MPI_Gatherv`.

Taxonomy of collective communications: Scatter

This is simply the *inverse* operation of `MPI_Gather`

```
int MPI_Scatter(const void* sendbuf, int sendcount,
 MPI_Datatype sendtype, void* recvbuf, int recvcount,
 MPI_Datatype recvtype, int root, MPI_Comm comm)
```

`const void* sendbuf` address of send buffer

`int sendcount` number of elements sent to each process

`MPI_Datatype sendtype` type of send buffer elements

`void* recvbuf` address of receive buffer

`int recvcount` number of elements in receive buffer

`MPI_Datatype recvtype` data type of receive buffer elements

`int root` rank of sending process

`MPI_Comm comm` communicator

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- The amount of data sent must be equal to the amount of data received, pairwise between each process and the root.

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```
int MPI_Scatterv(const void* sendbuf, const int sendcounts[],
 const int displs[], MPI_Datatype sendtype, void* recvbuf,
 int recvcount, MPI_Datatype recvtype, int root, MPI_Comm comm)
```

where

`const int sendcounts[]` is an array (of length group size) containing the number of elements that are sent to each process,

`const int displs[]` is an array (of length group size). Entry `i` specifies the displacement relative to `recvbuf` from which to take the outgoing data to process `i`.

Modifying the 1st derivative code

Let us perform the following modification to our first derivative code:

1. Taking from input the number of points to use in each interval,
2. Collecting the whole result on one process and print it on file.

For the first step we use the `MPI_Bcast` function,

```
if(mynode == 0){
if(argc != 2){
 n = 20;
}else{
 n = atoi(argv[1]);
}
}
MPI_Bcast(&n,1,MPI_INT,
 0,MPI_COMM_WORLD);
```

- We read on `rank` 0 the number `n` from command line,
- Then we broadcast it with `MPI_Bcast`, pay attention to the fact that the broadcast operations happens on all the processes!

Modifying the 1st derivative code

Then we *gather* all the derivatives from the various processes and collect them on process `0`.

```
if(mynode == 0)
globalderiv = (double *)
 malloc(sizeof(double)
 *(n*totalnodes));
MPI_Gather(fx,n,MPI_DOUBLE,
 globalderiv,n,MPI_DOUBLE,
 0,MPI_COMM_WORLD);
```

- we allocate on `rank 0` the memory that is necessary to store the whole derivative array,
- then we use the `MPI_Gather` to gather all the array `fx` (of `double`) inside the `globalderiv` array.

Modifying the 1st derivative code

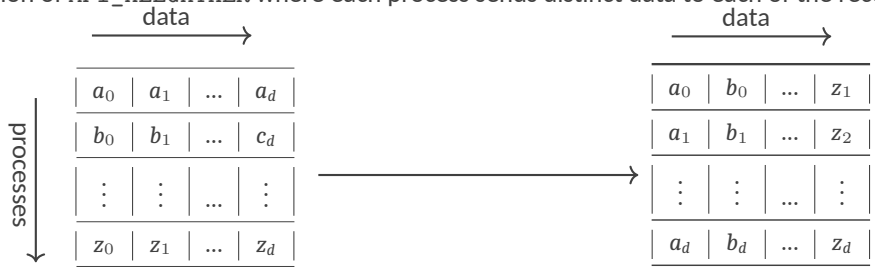
At last we print it out on file on `rank 0`

```
if(mynode == 0){
FILE *fptr;
fptr = fopen("derivative", "w");
for(int i = 0; i < n*totalnodes; i++)
 fprintf(fptr,"%f %f\n",globala+i*dx,globalderiv[i]);
fclose(fptr);
free(globalderiv);
}
```

File is now formatted in such a way that you can use MATLAB/Octave or Gnuplot to get a figure.

All-to-All

Extension of `MPI_ALLGATHER` where each process sends distinct data to each of the receivers.




```
int MPI_Alltoall(const void* sendbuf, int sendcount, MPI_Datatype sendtype,
 void* recvbuf, int recvcount, MPI_Datatype recvtype, MPI_Comm comm)
```

- The jth block sent from process i is received by process j and is placed in the ith block of `recvbuf`.
- The type signature for `sendcount`, `sendtype`, at a process must be equal to the type signature for `recvcount`, `recvtype` at any other process.

All-to-All different data size

If we need to send data of different size between the processes

```
int MPI_Alltoallv(const void* sendbuf, const int sendcounts[],
 const int sdispls[], MPI_Datatype sendtype, void* recvbuf,
 const int recvcounts[], const int rdispls[],
 MPI_Datatype recvtype, MPI_Comm comm);
```

`const void* sendbuf` starting address of send buffer

`const int sendcounts[]` array specifying the number of elements to send to each rank

`const int sdispls[]` entry j specifies the displacement (relative to `sendbuf`) from which to take the outgoing data destined for process j

`void* recvbuf` array specifying the number of elements that can be received from each rank

`const int recvcounts[]` integer array. Entry i specifies the displacement (relative to `recvbuf`) at which to place the incoming data from process i

`const int rdispls[]` entry i specifies the displacement (relative to `recvbuf`) at which to place the incoming data from process i

The reduce operation

The reduce operation for a given operator takes a data buffer from each of the processes in the communicator group and combines it according to operator rules.

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

`const void* sendbuf` address of send buffer

`void* recvbuf` address of receive buffer

`int count` number of elements in send buffer

`MPI_Datatype datatype` data type of elements of send buffer

`MPI_Op op` reduce operation

`int root` rank of root process

`MPI_Comm comm` communicator

The reduce operation

The value of `MPI_Op op` for the reduce operation can be taken from any of the following operators.

`MPI_MAX`	Maximum	`MPI_MAXLOC`	Max value and location
`MPI_MIN`	Minimum	`MPI_MINLOC`	Minimum value and location
`MPI_SUM`	Sum	`MPI_LOR`	Logical or
`MPI_PROD`	Product	`MPI_BOR`	Bit-wise or
`MPI_LAND`	Logical and	`MPI_LXOR`	Logical exclusive or
`MPI_BAND`	Bit-wise and	`MPI_BXOR`	Bit-wise exclusive or

The reduce operation

Moreover, **if a different operator is needed**, it is possible to create it by means of the function

```
int MPI_Op_create(MPI_User_function* user_fn, int commute,
 MPI_Op* op)
```

In C the prototype for a `MPI_User_function` is

```
typedef void MPI_User_function(void* invec, void* inoutvec,
 int *len, MPI_Datatype *datatype);
```

Global reduce operation – All-Reduce

As for other collective operations we may want to have the result of the reduction available on every process in a group.
The routine for obtaining such result is

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

`const void* sendbuf` address of send buffer

`void* recvbuf` address of receive buffer

`int count` number of elements in send buffer

`MPI_Datatype datatype` data type of elements of send buffer

`MPI_Op op` reduce operation

`MPI_Comm comm` communicator

This instruction behaves like a combination of a *reduction* and *broadcast* operation.

Global reduce operation – All-Reduce-Scatter

This is another variant of the reduction operation in which the result is *scattered* to all processes in a group on return.

```
int MPI_Reduce_scatter_block(const void* sendbuf,
 void* recvbuf, int recvcount, MPI_Datatype datatype,
 MPI_Op op, MPI_Comm comm);
```

- The routine is called by all group members using the same arguments for `recvcount`, `datatype`, `op` and `comm`.
- The resulting vector is treated as `n` consecutive blocks of `recvcount` elements that are scattered to the processes of the group `comm`.
- The *i*th block is sent to process *i* and stored in the receive buffer defined by `recvbuf`, `recvcount`, and `datatype`.

Global reduce operation – All-Reduce-Scatter

Of this function also a variant with variable block-size is available

```
int MPI_Reduce_scatter(const void* sendbuf, void* recvbuf,
 const int recvcounts[], MPI_Datatype datatype, MPI_Op op,
 MPI_Comm comm);
```

- This routine first performs a global element-wise reduction on vectors of $\texttt{count} = \sum_{i=0}^{n-1} \texttt{recevcounts[i]}$ elements in the send buffers defined by `sendbuf`, `count` and `datatype`, using the operation `op`, where `n` is the size of the communicator.
- The routine is called by all group members using the same arguments for `recvcounts`, `datatype`, `op` and `comm`.
- The resulting vector is treated as `n` consecutive blocks where the number of elements of the *i*th block is `recvcounts[i]`.
- The *i*th block is sent to process *i* and stored in the receive buffer defined by `recvbuf`, `recvcounts[i]` and `datatype`.

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2 Some computations using collective communications

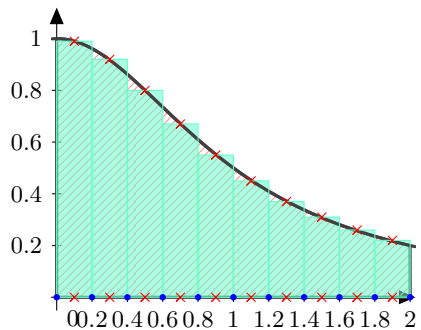
Integrals with parallel midpoint quadrature rule

Given $f : [a, b] \to \mathbb{R}$ the *midpoint* rule (sometimes *rectangle* rule) is given by

$$\int_a^b f(x)dx \approx I_1 = (b-a)f\left(\frac{a+b}{2}\right),$$

This is a very crude approximation, to make it more accurate we may break up the interval $[a, b]$ into a number n of non-overlapping subintervals $[a_k, b_k]$ such that $[a, b] = \cup_k [a_k, b_k]$,

$$I_n = \sum_{k=0}^{n} (b_k - a_k) f\left(\frac{a_k + b_k}{2}\right)$$



Integrals with parallel midpoint quadrature rule

If we want to transform this computation in a parallel computation we can adopt the following sketch:

1. `if (mynode == 0)` get number of intervals for quadrature
2. broadcast number of intervals to all the processes
3. assign the non-overlapping intervals to the processes
4. sum function values in the center of each interval
5. reduce with operator sum the integral on process 0.

As a test function for the parallel integration routine we can use

$$f(x) = \frac{4}{1+x^2}; \qquad I = \int_0^1 \frac{4}{1+x^2} dx = \pi.$$

To evaluate the error we can use the value :

```
double PI25DT = 3.14159265358979323846264 3;
```

Computing integrals with parallel midpoint quadrature rule

2 Some computations using collective communications

```
h   = 1.0 / ((double) n*totalnodes);
sum = 0.0;
for (i = 1+mynode*n;
i <= n*(mynode+1);
i++){
 x = h * ((double)i - 0.5);
 sum += f(x);
}
mypi = h * sum;
MPI_Reduce(&mypi, &pi, 1,
MPI_DOUBLE,
MPI_SUM, 0,
MPI_COMM_WORLD);
```

- We assume that all the intervals have the same size, thus the scaling `h = 1.0 / (double) n`,
- We compute all the value x that are in the local process and increment the local sum,
- in conclusion we perform an `MPI_Reduce` to sum together all the local sums.

Computing integrals with parallel midpoint quadrature rule

You can then print out the obtained value of π and the error with respect to `PI25DT` as

```
if (mynode == 0){
 printf("pi is approximately %.16f, Error is %e\n",
 pi, fabs(pi - PI25DT));
}
```

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3 Timers and Synchronization

Timers and Synchronization

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- the timer returns a floating-point number of seconds, representing elapsed wall-clock time since *some time in the past*:

  ```
  double MPI_Wtime(void);
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  ```
  double MPI_Wtime(void);
  ```
  the *time in the past* is guaranteed not to change during the life of the process.
- the usual application of a timer is something of the form:
  ```
  double starttime, endtime;
  starttime = MPI_Wtime();
  < --- foolish things happen here --- >
  endtime = MPI_Wtime();
  printf("That took %f seconds\n",endtime-starttime);
  ```

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  ```
  double MPI_Wtime(void);
  ```

  the *time in the past* is guaranteed not to change during the life of the process.
- There exists a tag `MPI_WTIME_IS_GLOBAL` that is `1` if clocks at all processes in `MPI_COMM_WORLD` are synchronized, `0` otherwise.

Timers and Synchronization

- MPI offers a *barrier* function that blocks the caller until all processes in the communicator have called it

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

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- It can be used together with the `MPI_Wait` function to force a synchronization point in the program.

- It can be used to regulate the access to an external resource (e.g., a file) in such a way that every processor accesses it in an order way: if you are interested in writing file in parallel you can look at Chapter 13 of the MPI guide[1]

[1] Message Passing Interface Forum. MPI: A Message-Passing Interface Standard, Version 3.1. `https://www.mpi-forum.org/docs/mpi-3.1/mpi31-report.pdf`, High Performance Computing Center Stuttgart (HLRS).

Evaluating performances

3 Timers and Synchronization

You can use the `MPI_Wtime()` to give a simple evalaution of the performances of your program.

Consider, e.g., the two programs for the computation of the π constant. You can evaluate the weak scalability of your code by looking at the time spent in doing the whole computation for growing size of processor numbers and samples.

We can compute the efficiency of the code by measuring:

$$E = t(1)/t(N) \in [0, 1]$$

where

- $t(1)$ is the amount of time to complete a work unit with 1 processing element,
- $t(N)$ is the amount of time to complete N of the same work units with N processing elements.

Further modifications

3 Timers and Synchronization

For the derivative program:

- In every case the function `void firstderiv1Dp_vec` wants to exchange information between two adjacent processes, i.e., every process wants to “swap” is halo with its adjacent process. We can rewrite the whole function by using the `MPI_Sendrecv_replace` point-to-point communication routine.
- We can rewrite the entire program in an “embarrassing parallel” way, if every process has access to f, and are assuming that all the interval are partitioned the same way, by using the knowledge of our `rank` we can compute what are the boundary elements at the previous and following process. Thus, no communication at all!

For the π programs,

- Make a graph of the timings to evaluate the weak scaling efficiency.

– Try this at home! (Maybe here, if there is still time...) –