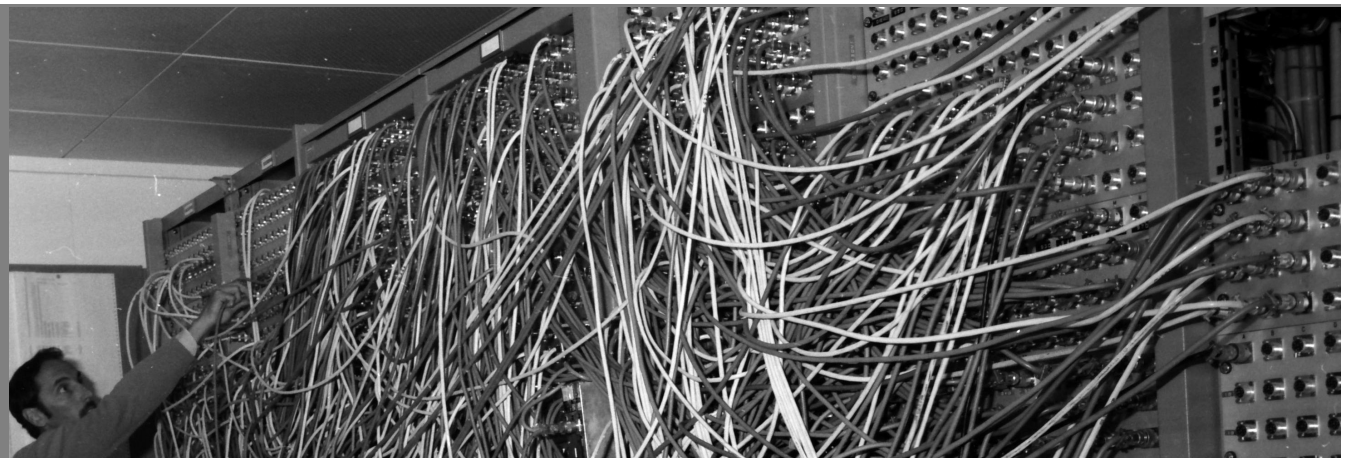

Calcolo Parallelo : Lezione 2

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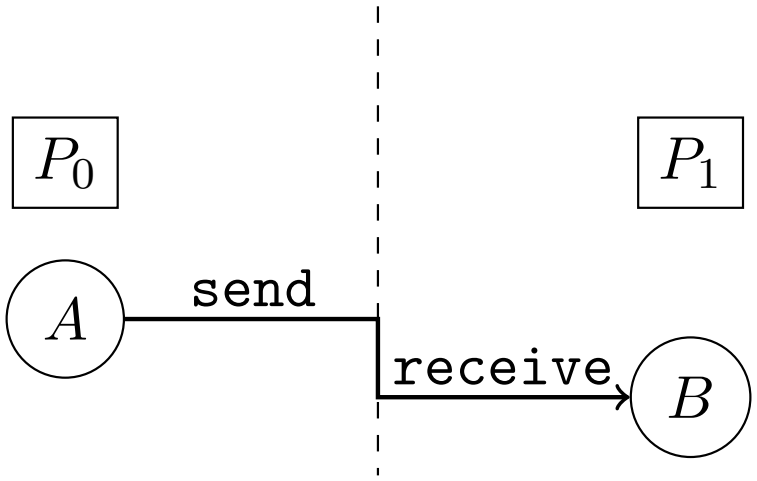
Master in Scienze e Tecnologie Spaziali, 2020

1. Point-to-Point Communications
   - Deadlock
   - Nonblocking communications
   - Sendreceive
   - Things left out

2. A First Scientific Computation

Sending and Receiving Messages

We have seen that each process within a *communicator* is identified by its *rank*, how can we exchange data between two processes?



We need to posses several information to have a meaningful message

- Who is sending the data?
- To whom the data is sent?
- What type of data are we sending?
- How does the receiver can identify it?

The blocking send and receive

```
int MPI_Send(void *message, int count,
        MPI_Datatype datatype, int dest, int tag,
        MPI_Comm comm)
```

`void *message` points to the message content itself, it can be a simple scalar or a group of data,

`int count` specifies the number of data elements of which the message is composed,

`MPI_Datatype datatype` indicates the data type of the elements that make up the message,

`int dest` the rank of the destination process,

`int tag` the user-defined tag field,

`MPI_Comm comm` the communicator in which the source and destination processes reside and for which their respective ranks are defined.

The blocking send and receive

```
int MPI_Recv (void *message, int count,
        MPI_Datatype datatype, int source, int tag,
        MPI_Comm comm, MPI_Status *status)
```

`void *message` points to the message content itself, it can be a simple scalar or a group of data,

`int count` specifies the number of data elements of which the message is composed,

`MPI_Datatype datatype` indicates the data type of the elements that make up the message,

`int dest` the rank of the source process,

`int tag` the user-defined tag field,

`MPI_Comm comm` the communicator in which the source and destination processes reside,

`MPI_Status *status` is a structure that contains three fields named `MPI_SOURCE` , `MPI_TAG`, and `MPI_ERROR`.

Basic MPI Data Types

Of the inputs in the previous slides the only one that is specific to MPI is the `MPI_Datatype`, these corresponds to a C data type

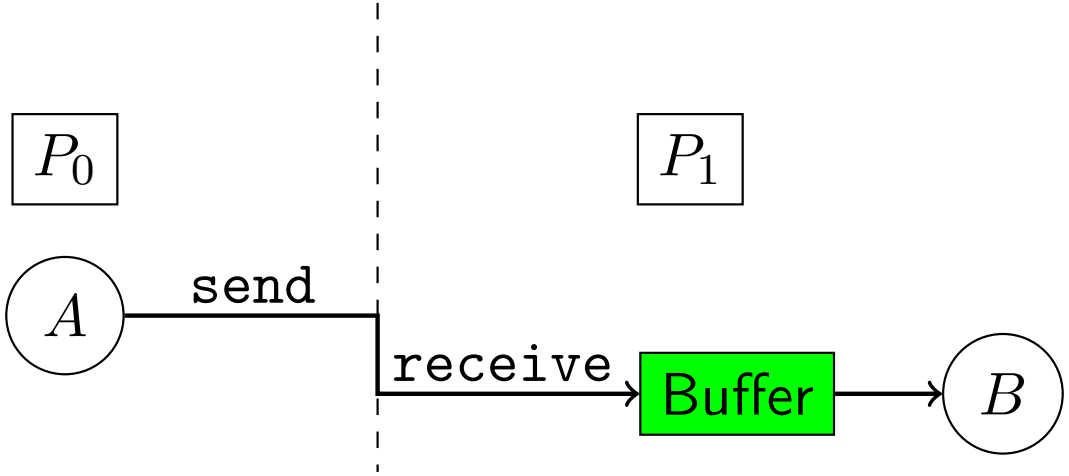
`MPI_CHAR`	`signed char`
`MPI_SHORT`	`signed short int`
`MPI_INT`	`signed int`
`MPI_LONG`	`signed long int`
`MPI_FLOAT`	`float`
`MPI_DOUBLE`	`double`
`MPI_LONG_DOUBLE`	`long double`
`MPI_UNSIGNED_CHAR`	`unsigned char`
`MPI_UNSIGNED_SHORT`	`unsigned short int`
`MPI_UNSIGNED`	`unsigned int`
`MPI_UNSIGNED_LONG`	`unsigned long int`

Note: we will see in the following how to `send`/`receive` user–defined data structures.

Why "blocking" send and receive?

For the `MPI_Send` to be blocking means that it does not return until the message data and envelope have been safely stored away so that the sender is free to modify the send buffer: it is a *non local* operation.

Note: The message might be copied directly into the matching receive buffer (as in the first figure), or it might be copied into a temporary system buffer.



Why "blocking" send and receive?

For the `MPI_Send` to be blocking means that it does not return until the message data and envelope have been safely stored away so that the sender is free to modify the send buffer: it is a *non local* operation.

The `MPI_Receive`, on the other hand returns only after the receive buffer contains the newly received message. A receive can complete before the matching send has completed, but, of course, it can complete only after the matching send has started.

A simple send/receive example

```
#include "mpi.h"
#include <string.h>
#include <stdio.h>
int main( int argc, char **argv){
 char message[20];
 int myrank;
 MPI_Status status;
 MPI_Init( &argc, &argv );
 MPI_Comm_rank( MPI_COMM_WORLD, &myrank );
 if (myrank == 0){  /* code for process zero */
  strcpy(message,"Hello, there");
  MPI_Send(message, strlen(message)+1, MPI_CHAR, 1, 99, MPI_COMM_WORLD);
 }
 else if (myrank == 1){ /* code for process one */
  MPI_Recv(message, 20, MPI_CHAR, 0, 99, MPI_COMM_WORLD, &status);
  printf("received :%s:\n", message);
 }
 MPI_Finalize();
 return 0;
}
```

A simple send/receive example

We can compile our code by simply adding to our `Makefile`

```
easysendrecv: easysendrecv.c
  $(MPICC) $(CFLAGS) $(LDFLAGS) $? $(LDLIBS) -o $@
```

then, we type `make`, and we run our program with

```
mpirun -np 2 easysendrecv
```

getting as answer

```
received :Hello, there:
```

So, what have we done?

```
MPI_Send(message, strlen(message)+1, MPI_CHAR, 1, 99, MPI_COMM_WORLD);
```

Process 0 sends the content of the `char` array `message[20]`, whose size is `strlen(message)+1` size of `char` (`MPI_CHAR`) to processor 1 with tag 99 on the communicator `MPI_COMM_WORLD`.

```
MPI_Recv(message, 20, MPI_CHAR, 0, 99, MPI_COMM_WORLD, &status);
```

on the other side process 1, receives into the buffer `message[20]` an array with size 20 size of `MPI_CHAR`, from process 0 with tag 99 on the same communicator `MPI_COMM_WORLD`.

A simple send/receive example : programmer smash!

It is a good exercise to try and mess things up, so let us see some damaging suggestions:

- What happens if we have a mismatch in the tags?
- What happens if we have a mismatch in the ranks of the sending and receiving processes?
- What happens if we use the wrong message size?
- What happens if we have a mismatch in the type?

A simple send/receive example : programmer smash!

It is a good exercise to try and mess things up, so let us see some damaging suggestions:

- What happens if we have a mismatch in the tags?

A: The process stays there hanging waiting for a message with a tag that will never come...

- What happens if we have a mismatch in the ranks of the sending and receiving processes?

- What happens if we use the wrong message size?

- What happens if we have a mismatch in the type?

A simple send/receive example : programmer smash!

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A: The process stays there hanging waiting for a message with a tag that will never come...

- What happens if we have a mismatch in the ranks of the sending and receiving processes?

A: The process stays there hanging trying to match messages that will never come...

- What happens if we use the wrong message size?

- What happens if we have a mismatch in the type?

A simple send/receive example : programmer smash!

It is a good exercise to try and mess things up, so let us see some damaging suggestions:

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- What happens if we have a mismatch in the ranks of the sending and receiving processes?

A: The process stays there hanging trying to match messages that will never come...

- What happens if we use the wrong message size?

A: If the size of the arriving message is longer than the expected we get an error of `MPI_ERR_TRUNCATE: message truncated`, note that there are combinations of wrong sizes for which things still works

- What happens if we have a mismatch in the type?

A simple send/receive example : programmer smash!

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- What happens if we have a mismatch in the ranks of the sending and receiving processes?

A: The process stays there hanging trying to match messages that will never come...

- What happens if we use the wrong message size?

A: If the size of the arriving message is longer than the expected we get an error of `MPI_ERR_TRUNCATE: message truncated`, note that there are combinations of wrong sizes for which things still works

- What happens if we have a mismatch in the type?

A: There are combinations of instances in which things seems to work, but the code is erroneous, and the behavior is not deterministic.

Dealing with more than one send and receive

We have now two processes that needs to exchange some data

- Solution 1:

```
MPI_Comm_rank(comm, &myrank);
if (myrank == 0){
 MPI_Send(sendbuf, count, MPI_DOUBLE, 1, tag, comm);
 MPI_Recv(recvbuf, count, MPI_DOUBLE, 1, tag, comm, status);
}else if(myrank == 1){
 MPI_Send(sendbuf, count, MPI_DOUBLE, 0, tag, comm);
 MPI_Recv(recvbuf, count, MPI_DOUBLE, 0, tag, comm, status);
}
```

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 MPI_Send(sendbuf, count, MPI_DOUBLE, 0, tag, comm);
 MPI_Recv(recvbuf, count, MPI_DOUBLE, 0, tag, comm, status);
}
```

- Solution 2:

```
MPI_Comm_rank(comm, &myrank);
if (myrank == 0){
 MPI_Recv(recvbuf, count, MPI_DOUBLE, 1, tag, comm, status);
 MPI_Send(sendbuf, count, MPI_DOUBLE, 1, tag, comm);
}else if(myrank == 1){
 MPI_Recv(recvbuf, count, MPI_DOUBLE, 0, tag, comm, status);
 MPI_Send(sendbuf, count, MPI_DOUBLE, 0, tag, comm);
}
```

Dealing with more than one send and receive

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 MPI_Recv(recvbuf, count, MPI_DOUBLE, 1, tag, comm, status);
 MPI_Send(sendbuf, count, MPI_DOUBLE, 1, tag, comm);
}else if(myrank == 1){
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 MPI_Send(sendbuf, count, MPI_DOUBLE, 0, tag, comm);
}
```

- Solution 3:

```
MPI_Comm_rank(comm, &myrank);
if (myrank == 0){
 MPI_Send(sendbuf, count, MPI_DOUBLE, 1, tag, comm);
 MPI_Recv(recvbuf, count, MPI_DOUBLE, 1, tag, comm, status);
}else if(myrank == 1){
 MPI_Recv(recvbuf, count, MPI_DOUBLE, 0, tag, comm, status);
 MPI_Send(sendbuf, count, MPI_DOUBLE, 0, tag, comm);
}
```

Dealing with more than one send and receive

In the case of Solution 1:

```
MPI_Comm_rank(comm, &myrank);
if (myrank == 0){
 MPI_Send(...);
 MPI_Recv(...);
}else if(myrank == 1){
 MPI_Send(...);
 MPI_Recv(...);
}
```

- The call `MPI_Send` is blocking, therefore the message sent by each process has to be copied out before the send operation returns and the receive operation starts.
- For the call to complete successfully, it is then necessary that at least one of the two messages sent be buffered, otherwise ...
- a deadlock situation occurs: both processes are blocked since there is no buffer space available!

Dealing with more than one send and receive

Here what happens to your program when you encounter Deadlock

In the case of Solution 1:

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MPI_Comm_rank(comm, &myrank);
if (myrank == 0){
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- a deadlock situation occurs: both processes are blocked since there is no buffer space available!

Dealing with more than one send and receive

In the case of Solution 2:

```
MPI_Comm_rank(comm, &myrank);
if (myrank == 0){
 MPI_Recv(...);
 MPI_Send(...);
}else if(myrank == 1){
 MPI_Recv(...);
 MPI_Send(...);
}
```

- The receive operation of process 0 must complete before its send. It can complete only if the matching send of processor 1 is executed.
- The receive operation of process 1 must complete before its send. It can complete only if the matching send of processor 0 is executed.
- This program will always deadlock.

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Dealing with more than one send and receive

In the case of Solution 3:

```
MPI_Comm_rank(comm, &myrank);
if (myrank == 0){
 MPI_Send(...);
 MPI_Recv(...);
}else if(myrank == 1){
 MPI_Recv(...);
 MPI_Send(...);
}
```

- This program will succeed even if no buffer space for data is available.

Dealing with more than one send and receive

This way you can beat Deadlock!

In the case of Solution 3:

```
MPI_Comm_rank(comm, &myrank);
if (myrank == 0){
 MPI_Send(...);
 MPI_Recv(...);
}else if(myrank == 1){
 MPI_Recv(...);
 MPI_Send(...);
}
```

- This program will succeed even if no buffer space for data is available.

Deadlock Issues

We can try to salvage what the situation in the case of Solution 1 by allocating the buffer space for the send calls

```
if (myrank == 0){
 MPI_Send(...);
 MPI_Recv(...);
}else if(myrank == 1){
 MPI_Send(...);
 MPI_Recv(...);
}
```

We can substitute the MPI_Send operation with a Send in buffered mode

```
int MPI_Bsend(const void* buf, int count,
  MPI_Datatype datatype, int dest,
  int tag, MPI_Comm comm)
```

- A buffered mode send operation can be started whether or not a matching receive has been posted;
- It may complete before a matching receive is posted;
- This operation is *local*!

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We can substitute the MPI_Send operation with a Send in buffered mode

```
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```

```
if (myrank == 0){
 MPI_Send(...);
 MPI_Recv(...);
}else if(myrank == 1){
 MPI_Send(...);
 MPI_Recv(...);
}
```

- A buffered mode send operation can be started whether or not a matching receive has been posted;
- It may complete before a matching receive is posted;
- This operation is *local*!
- The bad news is that if the buffer space is not enough we have exchanged the deadlock error with a buffer overflow condition;

Deadlock Issues

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- A buffered mode send operation can be started whether or not a matching receive has been posted;
- It may complete before a matching receive is posted;
- This operation is *local*!
- The good news is that buffer overflow condition are easier to detect than deadlock.

Allocating buffer space

To actually use the MPI_Bsend we need also to allocate the space for the buffer, therefore we need to use the two functions

```
int MPI_Buffer_attach(void* buffer, int size)
```

```
int MPI_Buffer_detach(void* buffer_addr, int* size)
```

- MPI_Buffer_attach provides a buffer in the user's memory to be used for buffering outgoing messages, where buffer is the starting address of a memory region
- MPI_Buffer_detach detaches the buffer currently associated with MPI. The call returns the address and the size of the detached buffer. This operation will block until all messages currently in the buffer have been transmitted.

Allocating buffer space

To actually use the MPI_Bsend we need also to allocate the space for the buffer, therefore we need to use the two functions

```
int MPI_Buffer_attach(void* buffer, int size)
```

```
int MPI_Buffer_detach(void* buffer_addr, int* size)
```

```
#define BUFFSIZE 10000
int size; char *buff;
// Buffer of 10000 bytes for MPI_Bsend
MPI_Buffer_attach( malloc(BUFFSIZE), BUFFSIZE);
// Buffer size reduced to zero
MPI_Buffer_detach( &buff, &size);
// Buffer of 10000 bytes available again
MPI_Buffer_attach( buff, size);
```

Note: a pointer to the buffer is passed to MPI_Buffer_attach while the address of the pointer is passed to MPI_Buffer_detach and these are both void *.

Nonblocking communications

As we have seen the use of blocking communications ensures that

- the send and receive buffers used in the `MPI_Send` and `MPI_Recv` arguments are safe to use or reuse after the function call,
- but it also means that unless there is a simultaneously matching send for each receive, the code will deadlock.

There exists a version of the point-to-point communication that returns immediately from the function call before confirming that the send or the receive has completed, these are the nonblocking send and receive functions.

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There exists a version of the point-to-point communication that returns immediately from the function call before confirming that the send or the receive has completed, these are the nonblocking send and receive functions.

- To verify that the data has been copied out of the send buffer a separate call is needed,
- To verify that the data has been received into the receive buffer a separate call is needed,
- The sender should not modify any part of the send buffer after a nonblocking send operation is called, until the send completes.
- The receiver should not access any part of the receive buffer after a nonblocking receive operation is called, until the receive completes.

Nonblocking communications: MPI_Isend and MPI_Irecv

The two nonblocking point-to-point communication call are then

```
int MPI_Isend(void *message, int count,
   MPI_Datatype datatype, int dest, int tag,
   MPI_Comm comm, MPI_Request *send_request);

int MPI_Irecv(void *message, int count,
   MPI_Datatype datatype, int source, int tag,
   MPI_Comm comm, MPI_Request *recv_request);
```

- The MPI_Request variables substitute the MPI_Status and store information about the status of the pending communication operation.
- The way of saying when this communications must be completed is by using the

  ```
  int MPI_Wait(MPI_Request *request, MPI_Status *status)
  ```

  when is called, the nonblocking request originating from MPI_Isend or MPI_Irecv is provided as an argument.

Nonblocking communications: an example

```
int main(int argc, char **argv) {
 int a, b, size, rank, tag = 0;
 MPI_Status status;
 MPI_Request send_request, recv_request;
 MPI_Init(&argc, &argv);
 MPI_Comm_size(MPI_COMM_WORLD, &size);
 MPI_Comm_rank(MPI_COMM_WORLD, &rank);
if (rank == 0) {
 a = 314159;
 MPI_Isend(&a, 1, MPI_INT, 1, tag, MPI_COMM_WORLD, &send_request);
 MPI_Irecv (&b, 1, MPI_INT, 1, tag, MPI_COMM_WORLD, &recv_request);
 MPI_Wait(&send_request, &status);
 MPI_Wait(&recv_request, &status);
 printf ("Process %d received value %d\n", rank, b);
} else {
 a = 667;
 MPI_Isend (&a, 1, MPI_INT, 0, tag, MPI_COMM_WORLD, &send_request);
 MPI_Irecv (&b, 1, MPI_INT, 0, tag, MPI_COMM_WORLD, &recv_request);
 MPI_Wait(&send_request, &status);
 MPI_Wait(&recv_request, &status);
 printf ("Process %d received value %d\n", rank, b);
}
 MPI_Finalize();
 return 0;
}
```

A simple send/receive example

We can compile our code by simply adding to our `Makefile`

```
nonblockingsendrecv: nonblockingsendrecv.c
  $(MPICC) $(CFLAGS) $(LDFLAGS) $? $(LDLIBS) -o $@
```

then, we type `make`, and we run our program with

```
mpirun -np 2 nonblockingsendrecv
```

getting as answer

```
Process 0 received value 667
Process 1 received value 314159
```

A simple send/receive example

We can compile our code by simply adding to our `Makefile`

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nonblockingsendrecv: nonblockingsendrecv.c
  $(MPICC) $(CFLAGS) $(LDFLAGS) $? $(LDLIBS) -o $@
```

then, we type `make`, and we run our program with

```
mpirun -np 2 nonblockingsendrecv
```

getting as answer

```
Process 0 received value 667
Process 1 received value 314159
```

Another useful instruction for the case of nonblocking communication is represented by

```
int MPI_Test(MPI_Request *request, int *flag, MPI_Status *status);
```

A call to `MPI_TEST` returns `flag = true` if the operation identified by request is complete. In such a case, the status object is set to contain information on the completed operation.

Send-Receive

The send-receive operations combine in one call the sending of a message to one destination and the receiving of another message, from another process.

- Source and destination are possibly the same,
- Send-receive operation is very useful for executing a shift operation across a chain of processes,
- A message sent by a send-receive operation can be received by a regular receive operation

```
int MPI_Sendrecv(const void *sendbuf, int sendcount,
  MPI_Datatype sendtype, int dest, int sendtag,
  void *recvbuf, int recvcount, MPI_Datatype recvtype,
  int source, int recvtag, MPI_Comm comm,
  MPI_Status *status);
```

Send-Receive-Replace

A slight variant of the MPI_Sendrecv operation is represented by the MPI_Sendrecv_replace operation

```
int MPI_Sendrecv_replace(void* buf, int count,
        MPI_Datatype datatype, int dest, int sendtag,
        int source, int recvtag,
        MPI_Comm comm, MPI_Status *status)
```

as the name suggests, the same buffer is used both for the send and for the receive, so that the message sent is replaced by the message received.

Clearly, if you confront its arguments with the one of the MPI_Sendrecv, the arguments `void *recvbuf, int recvcount` are absent.

Things left out

We are leaving out from this presentation some variants of the point-to-point communication:

- Both for blocking and nonblocking communications we have left out the **synchronous** and **ready** mode,
- For nonblocking communications we have also the **buffered** variants,
- Instead of waiting/testing for a single communication at the time we could wait for the completion of some, or all the operations in a list. There are specific routines for achieving this.

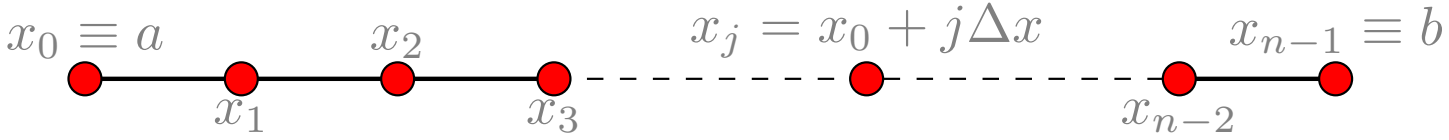
You can read about this on the manual:

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).

The 1st derivative of a function with finite differences

Given a function $f(x) : [a, b] \to \mathbb{R}$ we want to approximate $f'(x)$ on a (uniform) grid on the $[a, b]$ interval by using a finite difference scheme in parallel.

- Given an integer $n \in \mathbb{N}$ we can subdivide the interval $[a, b]$ into intervals of length $\Delta x = {}^{(b-a)}/_{n-1}$ with grid points $\{x_j\}_{j=0}^{n} = \{x_j = a + j\Delta x\}_{j=0}^{n-1}$:



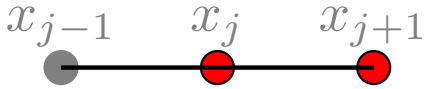
,

- and consider the values $\{f_j\}_{j=0}^{n-1} = \{f(x_j)\}_{j=0}^{n-1}$
- We can approximate the values of $f'(x_j)$, for $j = 1, \ldots, n-2$, by using only the values of f at the knots $\{f_j\}_{j=0}^{n-1}$

The 1st derivative of a function with finite differences

- The first derivative of f at $x = x_j$ can be expressed by using knots for $j' > j$

$$f'(x_j) \triangleq \lim_{\Delta x \to 0} \frac{f_{j+1} - f_j}{\Delta x} \approx \frac{f_{j+1} - f_j}{\Delta x} \triangleq D_+ f_j,$$



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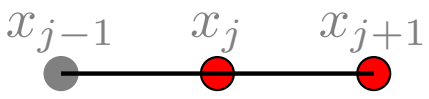
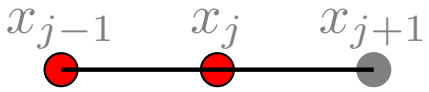


- or equivalently by using knots for $j' < j$

$$f'(x_j) \triangleq \lim_{\Delta x \to 0} \frac{f_j - f_{j-1}}{\Delta x} \approx \frac{f_j - f_{j-1}}{\Delta x} \triangleq D_- f_j,$$



The 1st derivative of a function with finite differences

- The first derivative of f at $x = x_j$ can be expressed by using knots for $j' > j$

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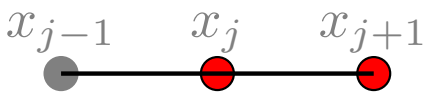

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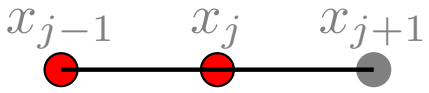
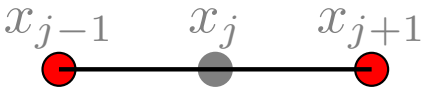


- at last we can consider the arithmetic mean of previous two:

$$f'(x_j) \approx D_0 f_j \triangleq \frac{1}{2}(D_- f_j + D_+ f_j) = \frac{f_{j+1} - f_{j-1}}{2\Delta x},$$



Writing the sequential algorithm

The sequential algorithms needs to break the approximation process into three parts

1. evaluate the derivative $f'(x_i)$ for $i = 1, \ldots, n-2$,
2. evaluate the derivative at the left–hand side $f'(x_0)$,
3. evaluate the derivative at the right–hand side $f'(x_{n-1})$.

To have the same *order of approximation* at each point of the grid we need to use a one–sided formula for the steps 2. and 3., specifically

$$f'(x_0) \approx \frac{-3f_0 + 4f_1 - f_2}{2\Delta x}, \quad f'(x_{n-1}) \approx \frac{3f_{n-1} - 4f_{n-2} + f_{n-3}}{2\Delta x}$$

Writing the sequential algorithm

Then the sequential algorithm can be written as

```
void firstderiv1D_vec(int n, double dx, double *f, double *fx){
double scale;
scale = 1.0/(2.0*dx);
for (int i = 1; i < n-1; i++){
 fx[i] = (f[i+1] - f[i-1])*scale;
}
 fx[0] = (-3.0*f[0] + 4.0*f[1] - f[2])*scale;
 fx[n-1] = (3.0*f[n-1] - 4.0*f[n-2] + f[n-3])*scale;
 return;
}
```

The function takes as input

- the number of grid points is n,
- the amplitude of such intervals Δx,
- the array containing the evaluation of f (intent: input),
- the array that will contain the value of the derivative (intent: output)

Writing the parallel algorithm

To implement the sequential differencing functions in parallel with MPI, we have to perform several steps

1. partition our domain $[a, b]$ among the processors,
2. each processor then computes the finite differences for all the points contained on that processor

Writing the parallel algorithm

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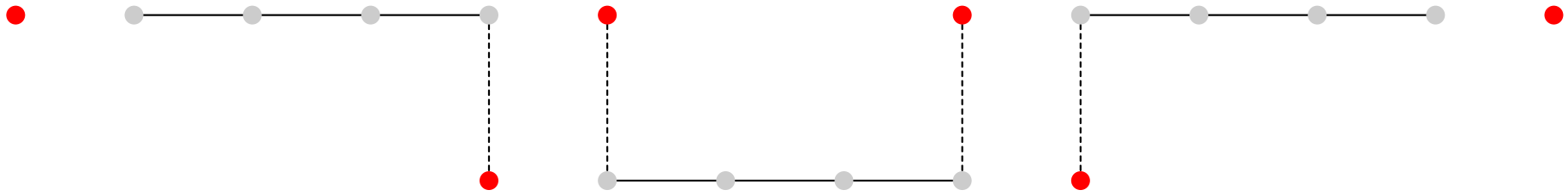
2. each processor then computes the finite differences for all the points contained on that processor

To actually perform the second step, we need to observe that the end-points on each subdomain needs information that is not contained on the processor, but that resides on a different one, we need to communicate boundary data!



Red dots are *halo* data, the one we need to communicate, while gray dots are data owned by the process.

Writing the parallel algorithm

The prototype of the function we want to write can be, in this case,

```
void firstderiv1Dp_vec(int n, double dx, double *f,
  double *fx, int mynode, int totalnodes)
```

where

- `int n` is the number of points per process,
- `double dx` the amplitude of each interval,
- `double *f, double *fx` the local portions with the values of $f(x)$ (input) and $f'(x)$ (output),
- `int mynode` the rank of the current process,
- `int totalnodes` the size of the communicator

We declare then the variables

```
double scale = 1.0/(2.0*dx);
double mpitemp;
MPI_Status status;
```

Writing the parallel algorithm

Then we can treat the case in which we are at the beginning or at the end of the global interval

```
if(mynode == 0){
 fx[0] = (-3.0*f[0] + 4.0*f[1] - f[2])*scale;
}
if(mynode == (totalnodes-1)){
 fx[n-1] = (3.0*f[n-1] - 4.0*f[n-2] + f[n-3])*scale;
}
```

this approximate the derivative at the first and last point of the global interval.

Writing the parallel algorithm

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}
```

this approximate the derivative at the first and last point of the global interval.

Then, we can compute the inner part (the gray points) of the local interval by doing:

```
for(int i=1;i<n-1;i++){
 fx[i] = (f[i+1]-f[i-1])*scale;
}
```

Writing the parallel algorithm

The other case we need to treat is again the particular case in which we are in the first, or in the last interval. In both cases we have only one communication to perform

```
if(mynode == 0){
 mpitemp = f[n-1];
 MPI_Send();
 MPI_Recv();
 fx[n-1] = (mpitemp - f[n-2])*scale;
}
else if(mynode == (totalnodes-1)){
 MPI_Recv();
 fx[0] = (f[1]-mpitemp)*scale;
 mpitemp = f[0];
 MPI_Send();
}
```

Writing the parallel algorithm

The other case we need to treat is again the particular case in which we are in the first, or in the last interval. In both cases we have only one communication to perform

```
if(mynode == 0){
 mpitemp = f[n-1];
 MPI_Send(&mpitemp,1,MPI_DOUBLE,1,1,MPI_COMM_WORLD);
 MPI_Recv(&mpitemp,1,MPI_DOUBLE,1,1,MPI_COMM_WORLD,&status);
 fx[n-1] = (mpitemp - f[n-2])*scale;
}
else if(mynode == (totalnodes-1)){
 MPI_Recv(&mpitemp,1,MPI_DOUBLE,mynode-1,1,MPI_COMM_WORLD,
   &status);
 fx[0] = (f[1]-mpitemp)*scale;
 mpitemp = f[0];
 MPI_Send(&mpitemp,1,MPI_DOUBLE,mynode-1,1,MPI_COMM_WORLD);
}
```

Writing the parallel algorithm

Finally, the only remaining case is the one in which we need to communicate both the extremes of the interval

```
else{
 MPI_Recv();
 fx[0] = (f[1]-mpitemp)*scale;
 mpitemp = f[0];
 MPI_Send();
 mpitemp = f[n-1];
 MPI_Send();
 MPI_Recv();
 fx[n-1] = (mpitemp-f[n-2])*scale;
}
```

Writing the parallel algorithm

Finally, the only remaining case is the one in which we need to communicate both the extremes of the interval

```
else{
 MPI_Recv(&mpitemp,1,MPI_DOUBLE,mynode-1,1,MPI_COMM_WORLD,
   &status);
 fx[0] = (f[1]-mpitemp)*scale;
 mpitemp = f[0];
 MPI_Send(&mpitemp,1,MPI_DOUBLE,mynode-1,1,MPI_COMM_WORLD);
 mpitemp = f[n-1];
 MPI_Send(&mpitemp,1,MPI_DOUBLE,mynode+1,1,MPI_COMM_WORLD);
 MPI_Recv(&mpitemp,1,MPI_DOUBLE,mynode+1,1,MPI_COMM_WORLD,
   &status);
 fx[n-1] = (mpitemp-f[n-2])*scale;
}
```

And the routine is complete!

Writing the parallel algorithm

A simple (and not very useful) principal program for this routine can be written by first initializing the parallel environment, and discovering who we are.

```
MPI_Init( &argc, &argv );
MPI_Comm_rank( MPI_COMM_WORLD, &mynode );
MPI_Comm_size( MPI_COMM_WORLD, &totalnodes );
```

Then we build the local values of the f function

```
globala = 0;
globalb = 1;
a = globala + ((double) mynode)*(globalb - globala)
        /( (double) totalnodes);
b = globala + ((double) mynode+1)*(globalb - globala)
        /( (double) totalnodes);
f  = (double *) malloc(sizeof(double)*(n));
fx = (double *) malloc(sizeof(double)*(n));
dx = (b-a)/((double) n);
for( int i = 0; i < n; i++){
 f[i] = fun(a+((double) i)*dx);
}
```

Finally we invoke our parallel computation

```
firstderiv1Dp_vec( n, dx, f, fx, mynode, totalnodes);
```

Writing the parallel algorithm

To check if what we have done makes sens we evaluate the error in the $\|\cdot\|_2$ norm on the grid, i.e., $\sqrt{\Delta x}\|\mathbf{f}' - \mathbf{fx}\|_2$ on every process

```
error = 0.0;
for(int i = 0; i < n; i++){
 error += pow( fx[i]-funprime(a+((b-a)*((double) i))
         /((double) n)),2.0);
}
error = sqrt(dx*error);
printf("Node %d ||f' - fx||_2 = %e\n",mynode,error);
```

Then we clear the memory and close the parallel environment

```
free(f);
free(fx);
MPI_Finalize();
```

Further modifications

- 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!

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