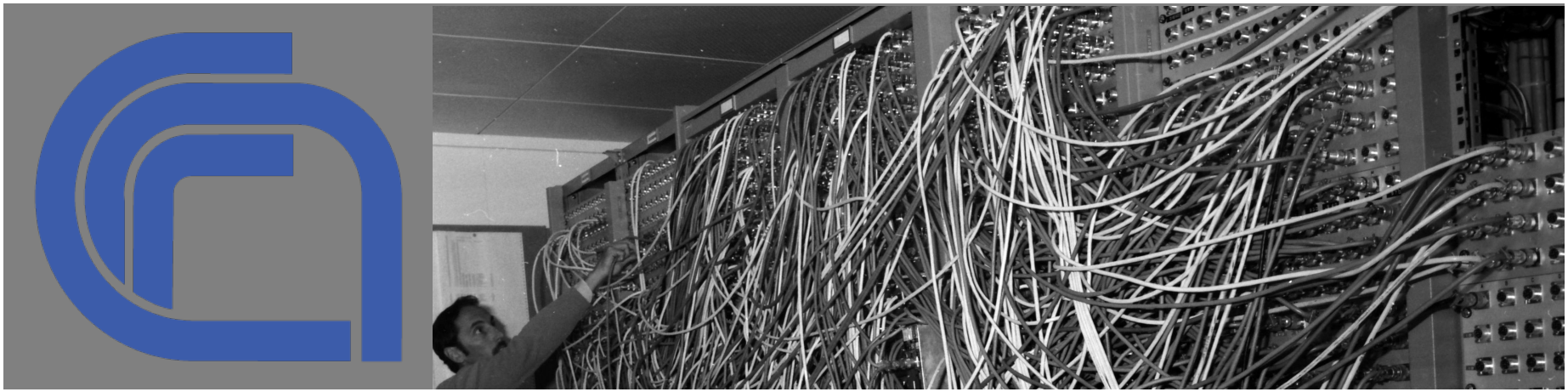

# Calcolo Parallelo : Lezione 3

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Master in Scienze e Tecnologie Spaziali, 2020

1. Collective Communications
   - Broadcast, Gather and Scatter
   - Modifying the $1^{st}$ derivative code
   - All-to-All Scatter/Gather
   - Global reduce operation

2. Some computations using collective communications
   - Computing Integrals
   - Random number generation: Montecarlo type algorithms

# 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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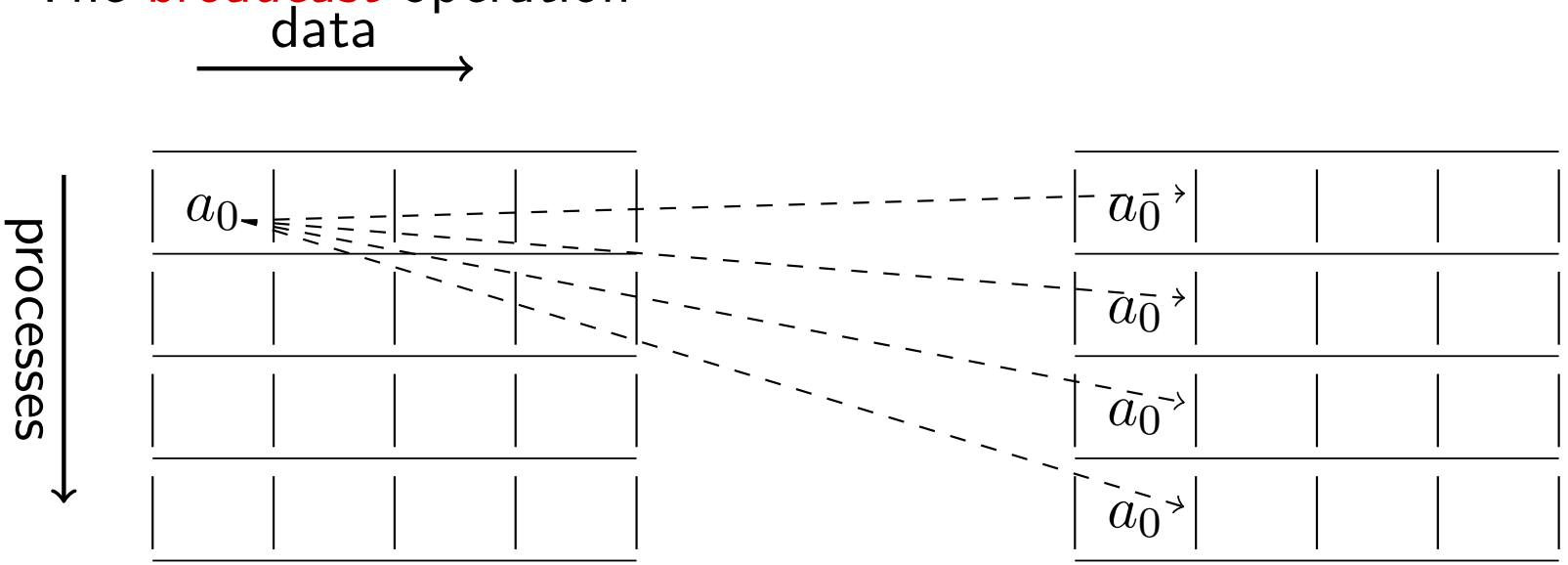
## Mixing type of calls

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

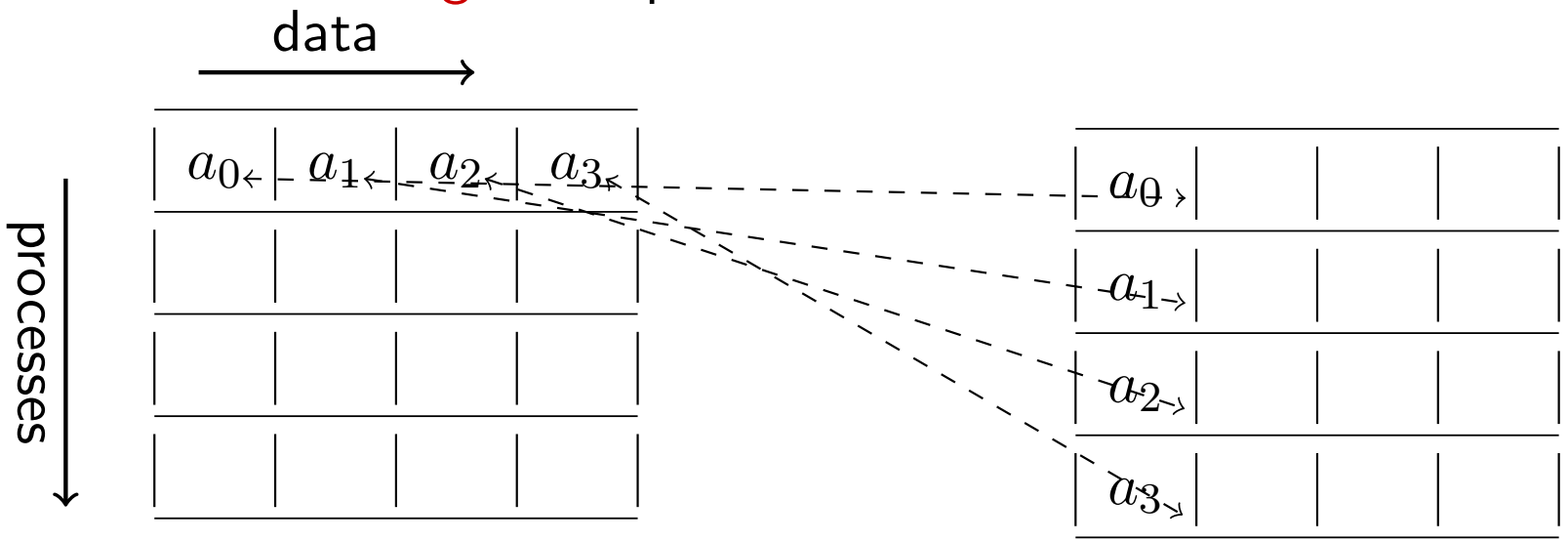
`MPI_Datatype datatype` type of the `buffer`

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

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

# Taxonomy of collective communications: 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 $j$th process contains the $a_j$ data.
- In the **gather**, initially the $j$th 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

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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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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

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Observe that

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

```
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);
```

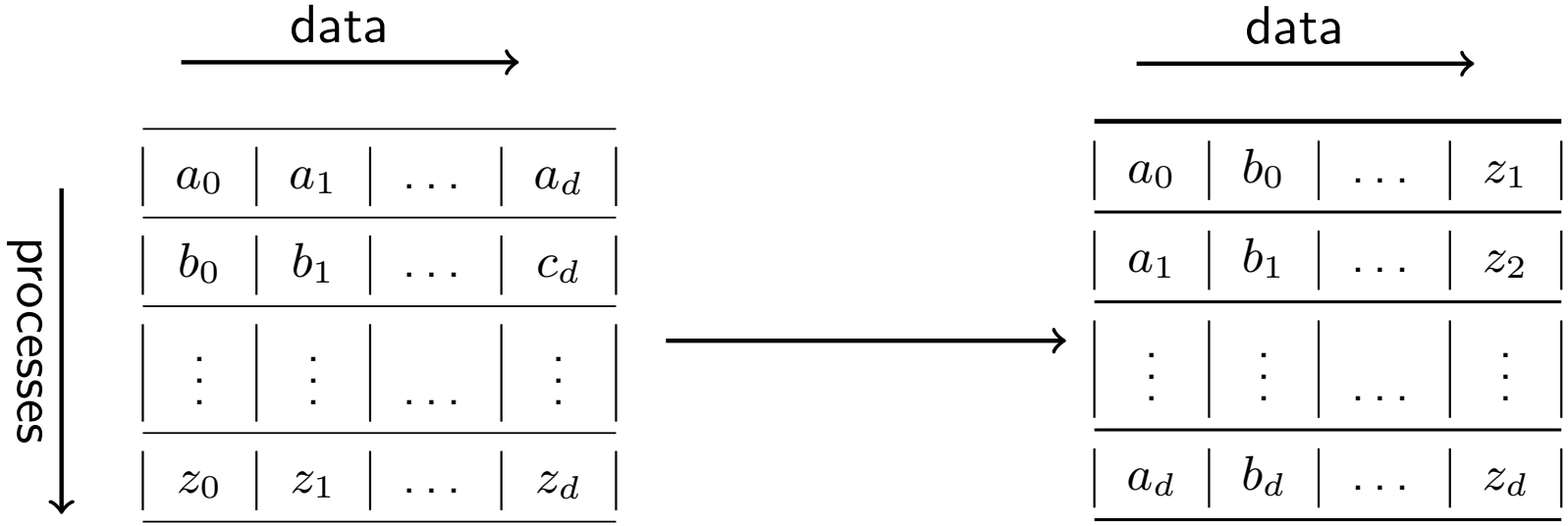
- we allocate on `rank 0` the memory that is necessary to store the whole derivative array,
- then we use the `MPI_Gather` to gather all the array `fx` (of `double`) inside the `globalderiv` array.

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);}
```

# All-to-All

`MPI_ALLTOALL` is an extension of `MPI_ALLGATHER` to the case 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 $j$th block sent from process $i$ is received by process $j$ and is placed in the $i$th 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 |

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| `MPI_LAND` | Logical and | `MPI_LXOR` | Logical exclusive or |
| `MPI_BAND` | Bit-wise and | `MPI_BXOR` | Bit-wise exclusive or |

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 `count` $= \sum_{i=0}^{n-1}$ `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`.

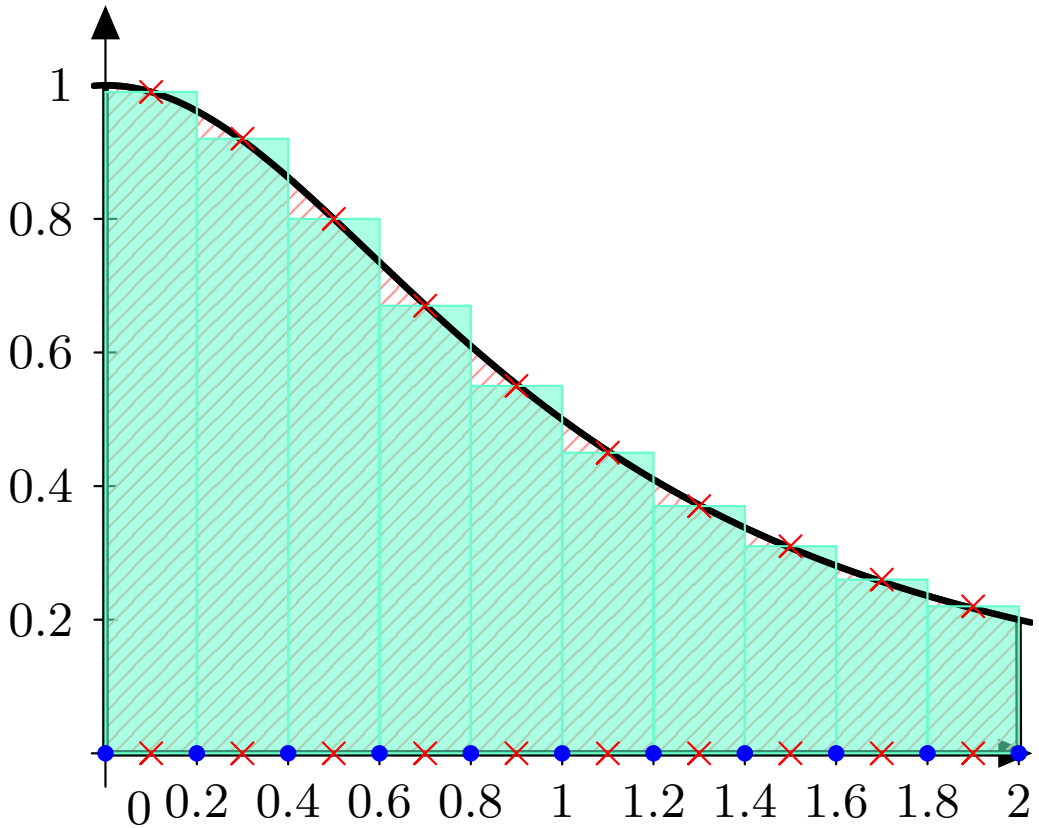
# Computing integrals with parallel midpoint quadrature rule

For an integrable function $f : [a, b] \to \mathbb{R}$ 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 $[a, b] = \cup_k [a_k, b_k]$,

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



# Computing 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 = 3.14159265358979323846264338;
```

# Computing integrals with parallel midpoint quadrature rule

```
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.

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

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

# Computing $\pi$ Montecarlo Style

Montecarlo methods are algorithms that rely on a procedure of repeated random sampling to obtain numerical results[1].

A generic Montecarlo algorithm can be described by the following 4 steps

1. define a domain of possible samples
2. generate the samples from a probability distribution over such domain
3. perform a deterministic computation on the inputs
4. aggregate the results

[1] For some historical information about this idea: http://shorturl.at/mAWY8

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4. aggregate the results

Let us use it to approximate $\pi$

1. we consider the square $S = [-1, 1] \times [-1, 1]$,
2. we generate samples in $S$ from a uniform probability distribution
3. we count the number of points $(x, y)$ that are such that $x^2 + y^2 \leq 1$,
4. the approximation of $\pi$ is given by the ratio

$$\pi \approx |\{(x,y): x^2+y^2 \leq 1\}| / |\{(x,y) \in S\}|$$

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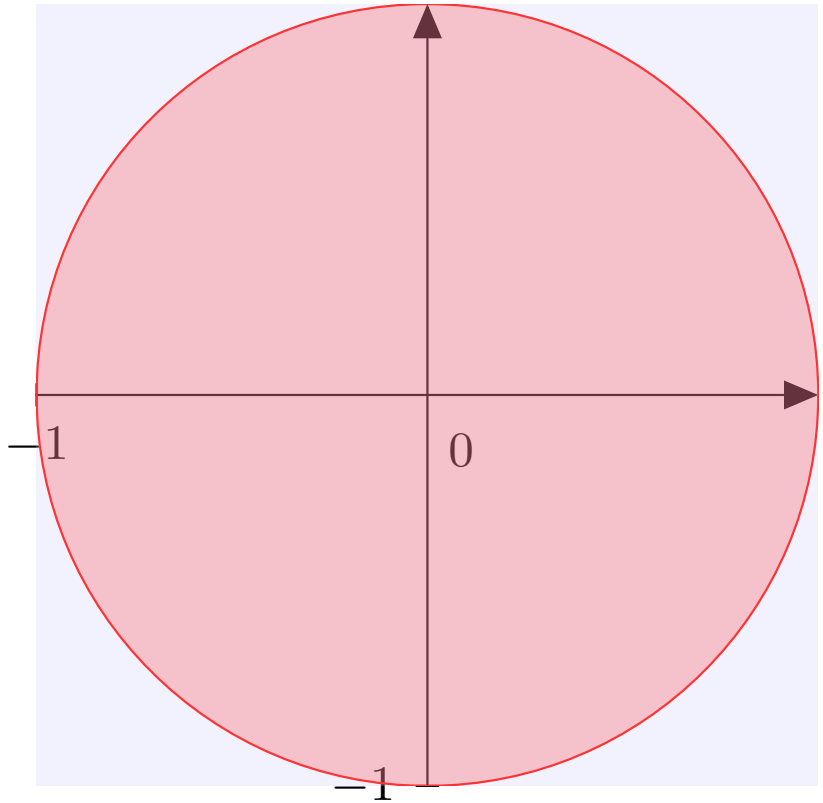
# Computing $\pi$ Montecarlo Style

We can write the parallel version of such algorithm in the following way



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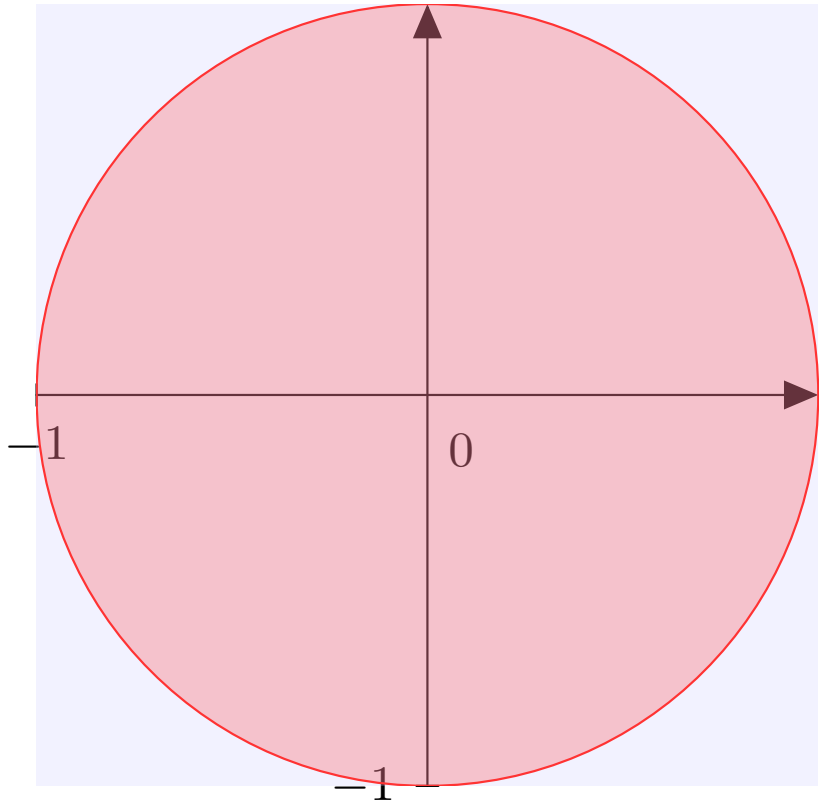

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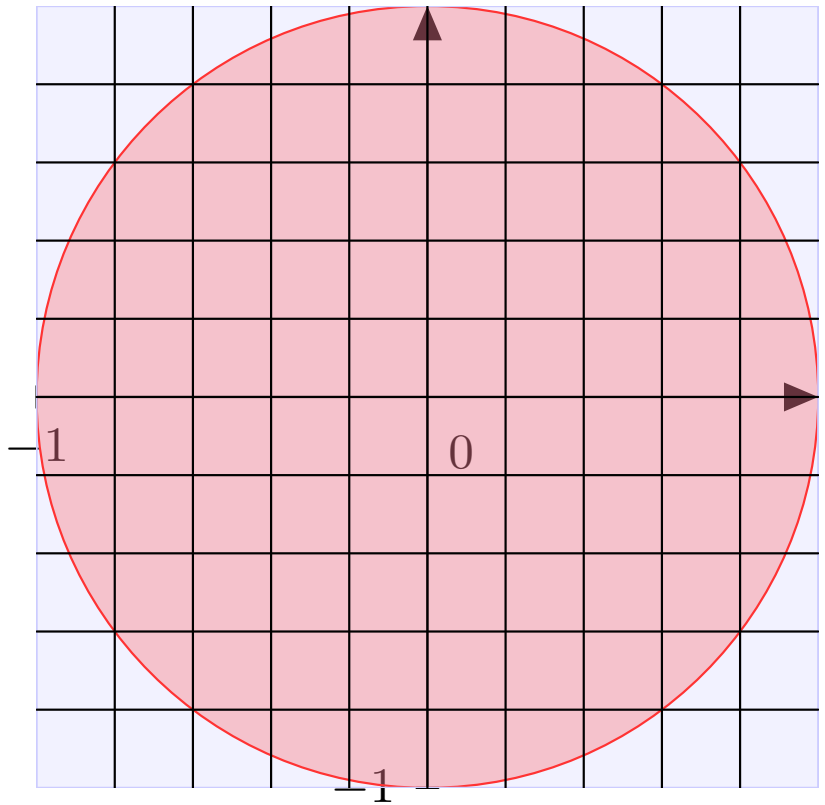

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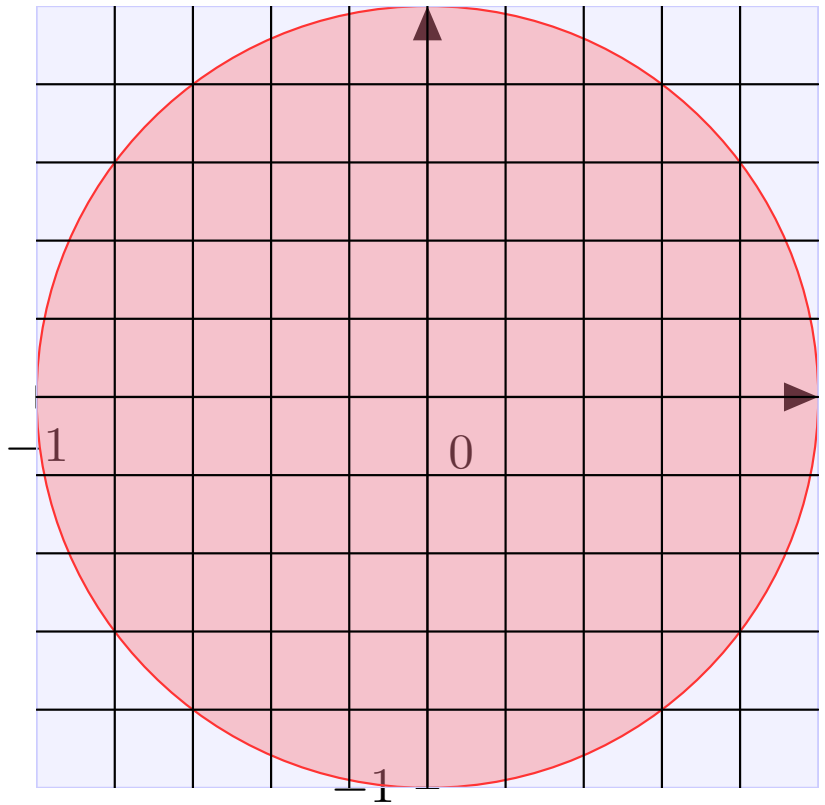

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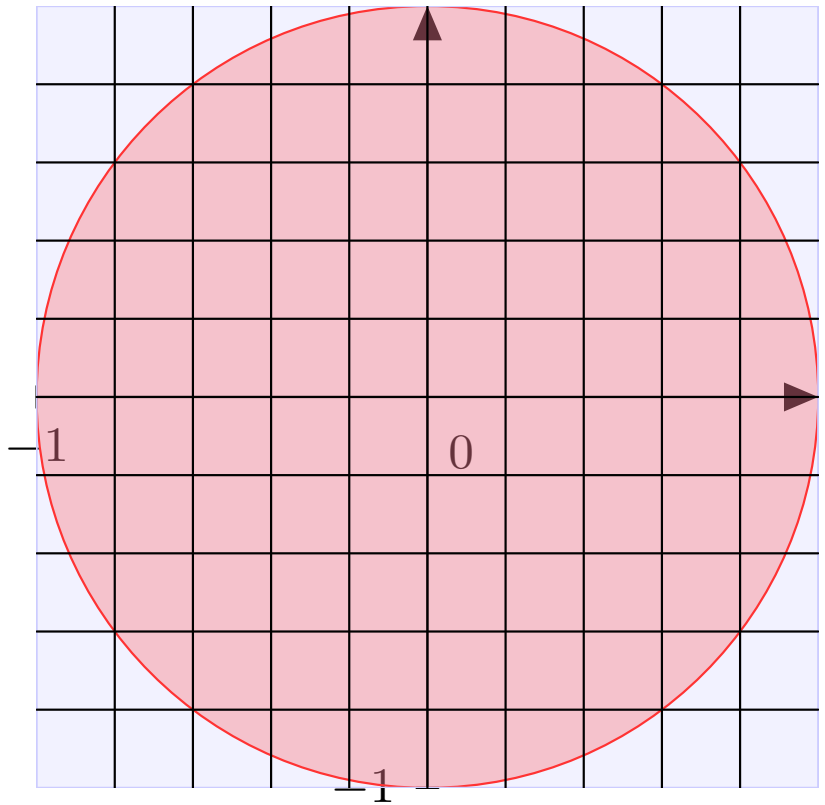
4. sum-reduce the number of points in the square and in the circle



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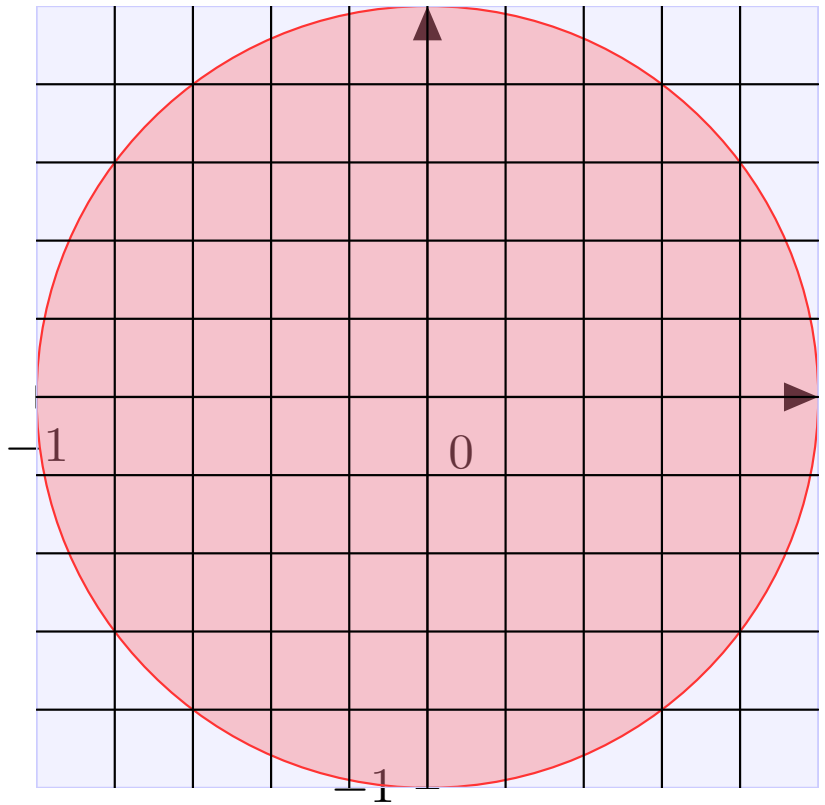
3. we compute how many points fall in the circle
4. sum-reduce the number of points in the square and in the circle
5. divide the two numbers on process 0 to get the approximation



# Computing $\pi$ Montecarlo Style

We can generate on each node the sampling on the reference square by

```
h  = 2.0 / (double) totalnodes;
x1 = -1.0 + mynode * h;
x2 = x1 + h;
y1 = -1.0;
y2 = 1.0;
my_SqPoints  = 0;
my_CiPoints  = 0;

for (i = 1; i <= n; i += totalnodes){
 x = rand(); x = x / RAND_MAX; x = x1 + x * (x2 - x1);
 y = rand(); y = y / RAND_MAX; y = y1 + y * (y2 - y1);
 my_SqPoints++;
 if ( ( x*x + y*y ) <= 1.0 ) my_CiPoints++;
}
```

# Computing $\pi$ Montecarlo Style

Then we perform the reduction by doing

```
SqPoints = 0;
CiPoints = 0;
MPI_Reduce(&my_SqPoints, &SqPoints, 1, MPI_INT, MPI_SUM, 0,
        MPI_COMM_WORLD);
MPI_Reduce(&my_CiPoints, &CiPoints, 1, MPI_INT, MPI_SUM, 0,
        MPI_COMM_WORLD);
```

and print the approximation

```
if (mynode == 0){
pi = 4.0 * (double)CiPoints / (double)SqPoints;
printf("Pi is approximately %.16f, Error is %e\n"
        ,pi, fabs(pi - PI25DT));
}
```