

Calcolo Parallelo: Lezione 2

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- A First Scientific Computation
- Collective Communications
 - Broadcast, Gather and Scatter
 - Modifying the 1st derivative code
 - All-to-All Scatter/Gather
 - Global reduce operation
- Some computations using collective communications
 - Computing Integrals
 - Random number generation: Montecarlo type algorithms

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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 $\{x_j\}_{j=0}^n = \{x_j = a + j\Delta x\}_{j=0}^{n-1}$:

$$x_0 \equiv a \qquad x_2 \qquad x_j = x_0 + j\Delta x \qquad x_{n-1} \equiv b$$

- ▶ 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

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

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

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

 \blacktriangleright or equivalently by using knots for j' < j

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

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The 1st derivative of a function with finite differences

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

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

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

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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, ..., 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;
}</pre>
```

The function takes as input

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

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

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

- 1. partition our domain $\left[a,b\right]$ among the processors,
- 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.

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;
```

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.

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}
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.

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;
}</pre>
```

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();
}
```

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);
}
```

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;
}
```

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!

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);
```

```
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{f}\mathbf{x}\|_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();
```

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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Collective Communications

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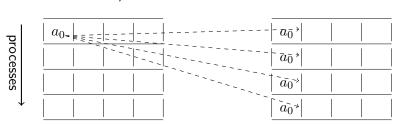
- the group of processes is represented as always as a communicator that provides a context for the operation,
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Mixing type of calls

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.

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► The broadcast operation data



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.

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```
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

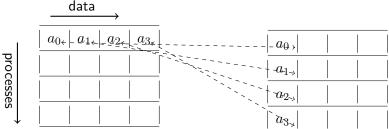
int root rank of the process broadcasting the message

MPI_Comm communicator grouping the processes involved in the broadcast operation

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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 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

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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 recytype, 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* recybuf address of receive buffer
int recycount number of elements for any single receive (and not the total
             number of items!)
MPI Datatype recytype data type of received buffer elements
   int root rank of receiving process
```

MPI_Comm comm communicator

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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

MPI_Datatype recvtype data type of received buffer elements

int root rank of receiving process

MPI_Comm comm communicator

These are significant only at root!

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 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.

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,

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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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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.

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.

```
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 recytype, 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* recybuf address of receive buffer
int recycount number of elements in receive buffer
MPI_Datatype recytype data type of receive buffer elements
  int root rank of sending process
MPI_Comm comm communicator
```

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```
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 recytype, 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* recybuf address of receive buffer
int recycount number of elements in receive buffer
MPI_Datatype recytype data type of receive buffer elements
  int root rank of sending process
MPI Comm comm communicator
This choices are significant only at root!
```

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Observe that

- ► The type signature of sendcount, sendtype on each process must be equal to the type signature of recvcount, recvtype at the root.
- ► 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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Observe that

- ► The type signature of sendcount, sendtype on each process must be equal to the type signature of recvcount, recvtype at the root.
- ► 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_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,

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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,
  O, MPI COMM WORLD);
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++)</pre>

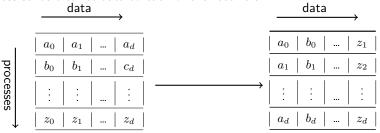
fclose(fptr); free(globalderiv);}

- 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.

fprintf(fptr, "%f %f\n", globala+i*dx, globalderiv[i]);

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

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All-to-All different data size

each rank

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
```

- 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

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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* recybuf 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
```

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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_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

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,
^^Iint *len, MPI_Datatype *datatype);
```

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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.

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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.

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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 $= \sum_{i=0}^{n-1} \texttt{recevcounts[i]}$ 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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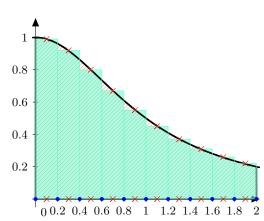
Computing integrals with parallel midpoint quadrature rule

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 = 3.141592653589793238462643;

Computing integrals with parallel midpoint quadrature rule

```
h = 1.0 / ((double) n*totalnodes);
sum = 0.0;
for (i = 1+mynode*n;
                                We assume that all the intervals have the
^^Ii <= n*(mynode+1);
                                   same size, thus the scaling
^^Ii++){
                                   h = 1.0 / (double) n
 x = h * ((double)i - 0.5);
                                ▶ We compute all the value x that are in the
 sum += f(x):
}
                                   local process and increment the local sum,
mvpi = h * sum;
                                in conclusion we perform an MPI_Reduce
MPI_Reduce(&mypi, &pi, 1,
                                   to sum together all the local sums.
^^IMPI DOUBLE,
^^IMPI SUM, 0,
^^IMPI COMM WORLD);
 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",
  ^^Ipi, fabs(pi - PI25DT));
```

Montecarlo methods are algorithms that rely on a procedure of repeated random sampling to obtain numerical results¹.

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

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

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

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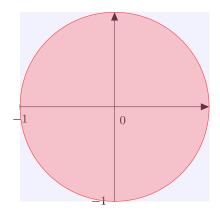
Let us use it to approximate π

- 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 π is given by the ratio

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

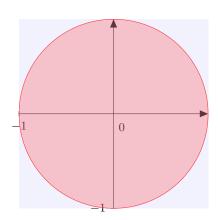
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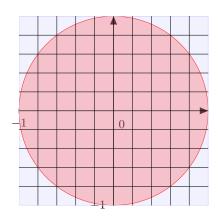


We can write the parallel version of such algorithm in the following way

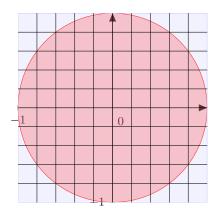
 we divide a square in an number of parts equal to the number of processes we have,



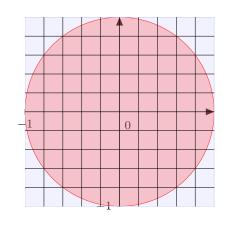
- we divide a square in an number of parts equal to the number of processes we have,
- 2. we generate a number of random points (x,y) in the area owned by each process,



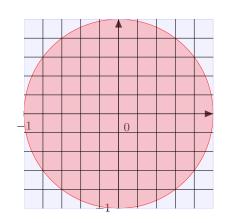
- we divide a square in an number of parts equal to the number of processes we have,
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- we divide a square in an number of parts equal to the number of processes we have,
- 2. we generate a number of random points (x,y) in the area owned by each process,
- 3. we compute how many points fall in the circle
- sum-reduce the number of points in the square and in the circle
- divide the two numbers on process 0 to get the approximation



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;
v1 = -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) \le 1.0 ) my_CiPoints++;
```

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));
```