High Performance Computing

Autumn, 2018

Lecture 16

Imperial College
London

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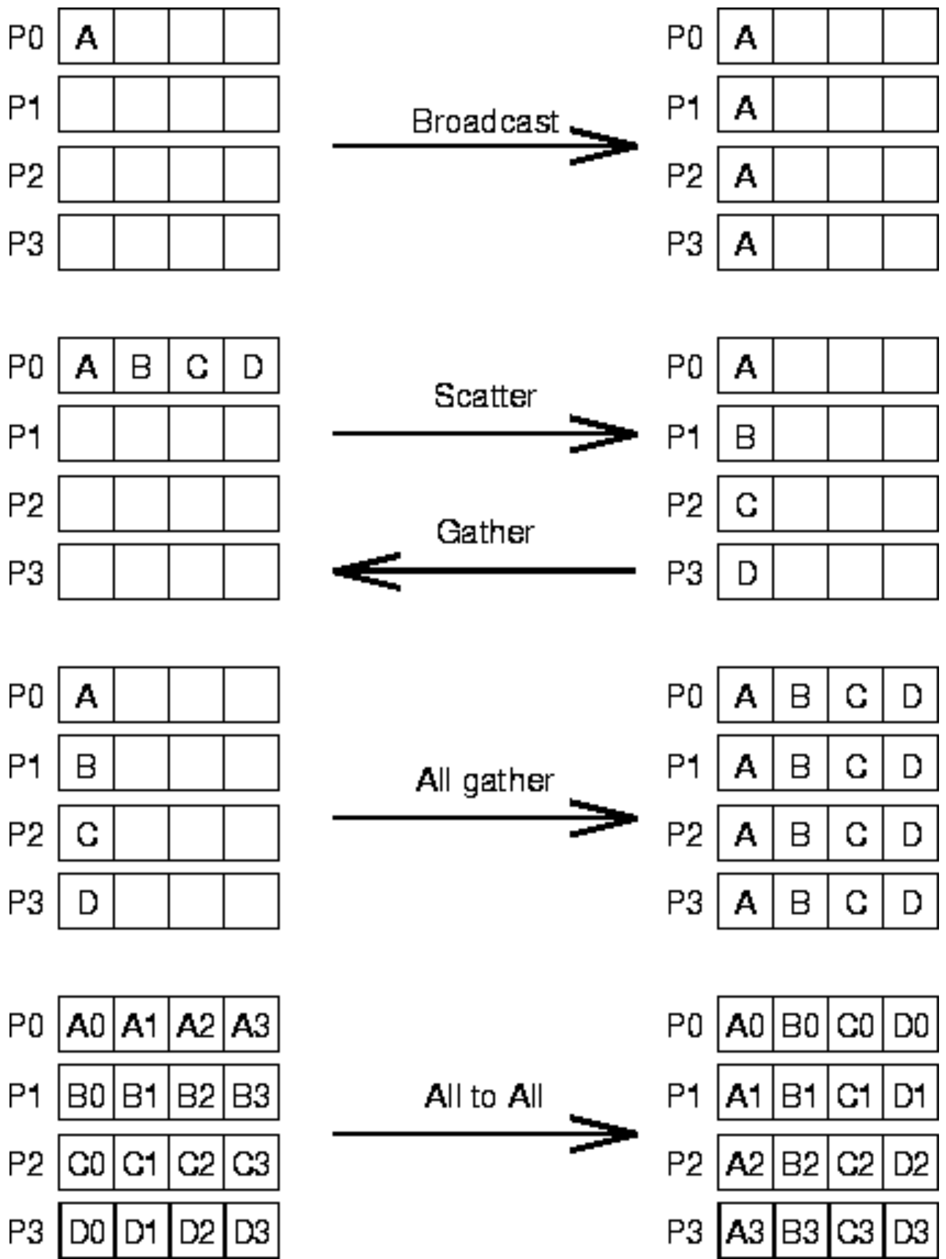
27 November 2018

Last time: MPI collective data movement



From *Using MPI*

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Today

- **Coarse grain parallelization**
- **Send and Receive**
- **Domain Decomposition**
- **Using** gather **and** gatherv

Coarse-grain vs fine-grain parallelism

- With OpenMP, we've used fine-grain approach
  - Look for a code segment (e.g. a loop) that can be parallelized
  - Let OpenMP do the rest (just for that segment)

Coarse-grain vs fine-grain parallelism

- With OpenMP, we've used fine-grain approach
  - Look for a code segment (e.g. a loop) that can be parallelized
  - Let OpenMP do the rest (just for that segment)

- With MPI, typically take a coarse-grain approach
  - At beginning of simulation, distribute data and tasks to processes
  - Each process works on its own problem
  - Occasionally communicating when necessary

- Can also use coarse-grain approach in OpenMP!

Coarse-grain approach

- **We have already seen a “sort-of” coarse grain approach with quadrature:**

```
 !set number of intervals per processor
    Nper_proc =  (N + numprocs - 1)/numprocs

!starting and ending points for processor
    istart = myid * Nper_proc + 1
    iend = (myid+1) * Nper_proc
    if (iend>N) iend = N
```

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    if (iend>N) iend = N

!loop over intervals computing each interval's contribution to
integral
    do i1 = istart,iend
        xm = dx*(i1-0.5) !midpoint of interval i1
        call integrand(xm,f)
        sum_i = dx*f
        sum_proc = sum_proc + sum_i !add contribution from interval
to total integral
    end do
```

Coarse-grain approach

- **More generally, at start of program we will:**

  1. **Obtain *myid* and total number of processes, *numprocs*:**

     ```
     call MPI_COMM_RANK(MPI_COMM_WORLD, myid, ierr)
     call MPI_COMM_SIZE(MPI_COMM_WORLD, numprocs, ierr)
     ```

  2. **Use this information to distribute *Ntotal* points (or pieces of data) across *numprocs* processors**

Coarse-grain approach

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     ```

  2. **Use this information to distribute *Ntotal* points (or pieces of data) across *numprocs* processors**

  3. **We will use a simple fortran subroutine, *MPE_DECOMP1D*:**

     ```
     call MPE_DECOMP1D( Ntotal, numprocs, myid, istart, iend)

     Nlocal = iend – istart + 1
     ```

     - **Simple subroutine which assigns** istart **and** iend **to each process**

     - **If Ntotal=100, numprocs = 2:**
       - ***myid* = 0 →** istart **= 1,** iend **= 50**
       - ***myid* = 1 →** istart **= 51,** iend **= 100**

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Complex parallelization

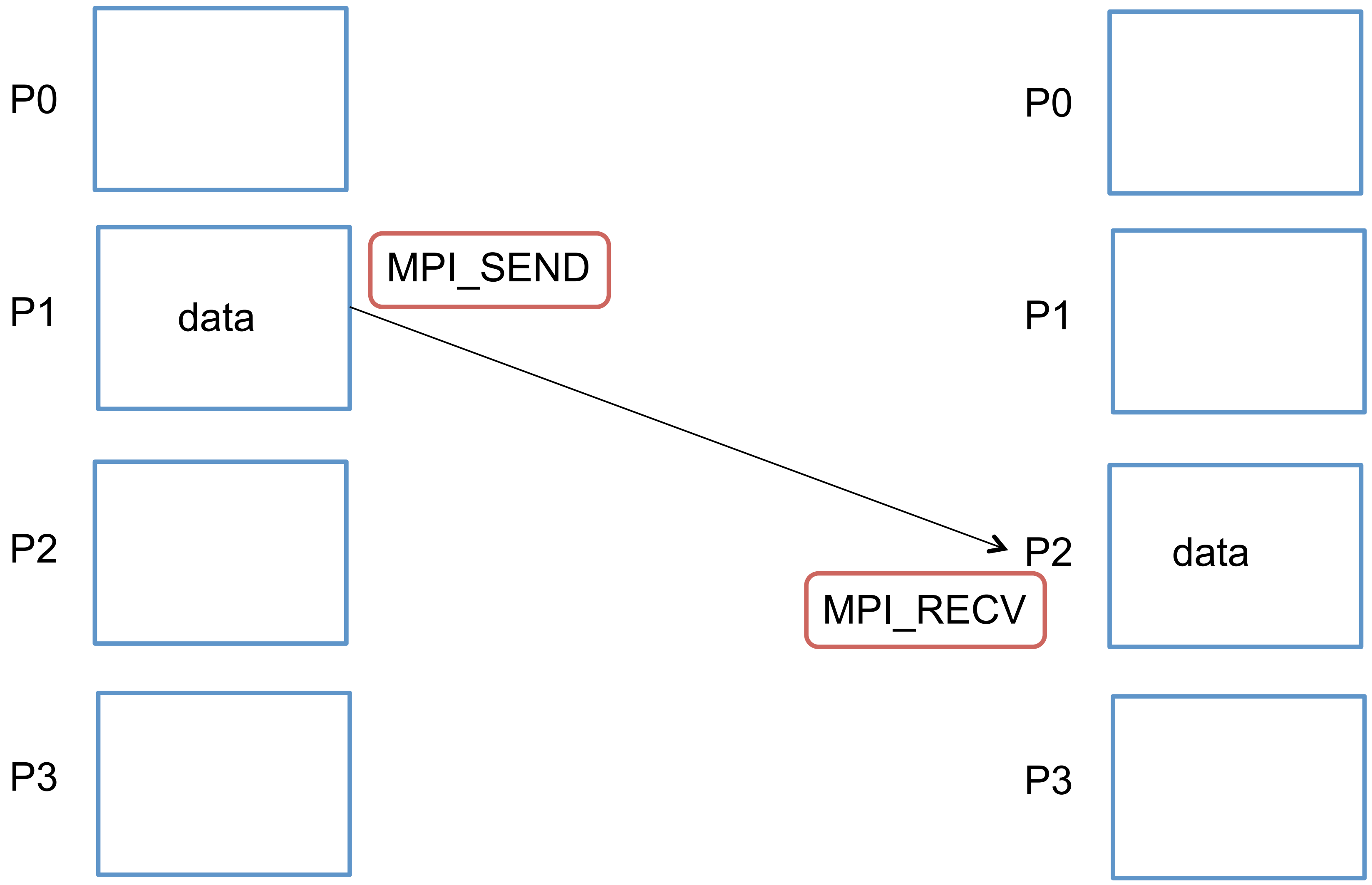
- **MPE_DECOMP1D partitions data on a ‘line’**
- **What about more complicated topologies or networks?**
  - **e.g. simulation of 1e7 air molecules?**
  - **Advanced tools exist to do the partitioning for you**
  - **E.g. *ParMETIS:***

ParMETIS is an MPI-based parallel library that implements a variety of algorithms for partitioning unstructured graphs, meshes, and for computing fill-reducing orderings of sparse matrices. ParMETIS extends the functionality provided by METIS and includes routines that are especially suited for parallel AMR computations and large scale numerical simulations. The algorithms implemented in ParMETIS are based on the parallel multilevel k-way graph-partitioning, adaptive repartitioning, and parallel multi-constrained partitioning schemes developed in our lab.

MPI Send/Recv

- Bcast and Reduce are examples of *collective* communication
- *Point-to-point* communication carried out by send and recv
- Probably the most basic and most important MPI commands

MPI send/recv



MPI Send/Recv

- **Bcast and Reduce are examples of *collective* communication**
- ***Point-to-point* communication carried out by send and recv**
- **Probably the most basic and most important MPI commands**

- **Can send data between any two processors.**
- **Both send and recv are needed for data transfer.**
- **E.g. for previous figure need:** if myid==1, send data to P2 *and* If myid==2 receive data from P1

MPI Send/Recv

```
If (myid==1) call MPI_SEND(n, 1, MPI_INTEGER,0, tag, MPI_COMM_WORLD,ierr)

If (myid==0) call MPI_RECV(n, 1, MPI_INTEGER,1,
                                        tag, MPI_COMM_WORLD, status, ierr)
```

These will send the integer n which has size 1 from processor 1 to processor 0.

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MPI Send/Recv

If (myid==1) call MPI_SEND(n, 1, MPI_INTEGER,0, **tag**, MPI_COMM_WORLD,ierr)

If (myid==0) call MPI_RECV(n, 1, MPI_INTEGER,1,
tag, MPI_COMM_WORLD, *status,* ierr)

These will send the integer n which has size 1 from processor 1 to processor 0.

tag: an integer label which can contain information about the data (*e.g.* which molecule the data belongs to or which row in a matrix)

status: **provides information about the received message (source, tag, length)**

MPI Send/Recv: example

- **f90example2.f90: compute** array1 = sin(i1), i1=1,2,…
- **New code: *sendExample.f90***
- **Now,** array1 **is only computed on P0, and we want to send the 3rd component to P1 and store it in P1's (empty) array1**

MPI Send/Recv: example

- **f90example2.f90: compute** array1 = sin(i1), i1=1,2,…
- **New code: *sendExample.f90***
- **Now,** array1 **is only computed on P0, and we want to send the 3rd component to P1 and store it in P1's (empty) array1**
- **Compute array1 on P0 and send it to P1:**

```fortran
if (myid==0) then
    i1 = 3
    call calculations(N,array1) !fill in array1
    call MPI_SEND(array1(i1),1,MPI_DOUBLE_PRECISION,1,i1,MPI_COMM_WORLD,
                                                                  ierr)
```

Destination

Tag

MPI Send/Recv: example

Compute array1 on P0, and send it to P1:

Destination

Tag

```
if (myid==0) then
    i1 = 3
    call calculations(N,array1) !fill in array1
    call MPI_SEND(array1(i1),1,MPI_DOUBLE_PRECISION,1,i1,MPI_COMM_WORLD,
                                                                   ierr)
```

Source

Must **also have MPI_RECV on P1:**

```
elseif (myid==1) then
   call MPI_RECV(var1,1,MPI_DOUBLE_PRECISION,0,MPI_ANY_TAG,
                                              MPI_COMM_WORLD,status,ierr)
   j1 = status(MPI_TAG) !location where var1 will be stored in array1
   array1(j1) = var1
```

Notes:

- MPI_ANY_TAG: **The destination will accept a message with any tag**
- status(MPI_TAG) = 3; **we have used the tag to send/set the array index**

Comments on send/recv

- Send/Recv are *blocking* operations
  - Code waits at send until the data has “left”?
  - But what if all processes are trying to send data to each other?
    - Can degrade performance or freeze the code

Comments on send/recv

- Send/Recv are *blocking* operations
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    - Can degrade performance or freeze the code

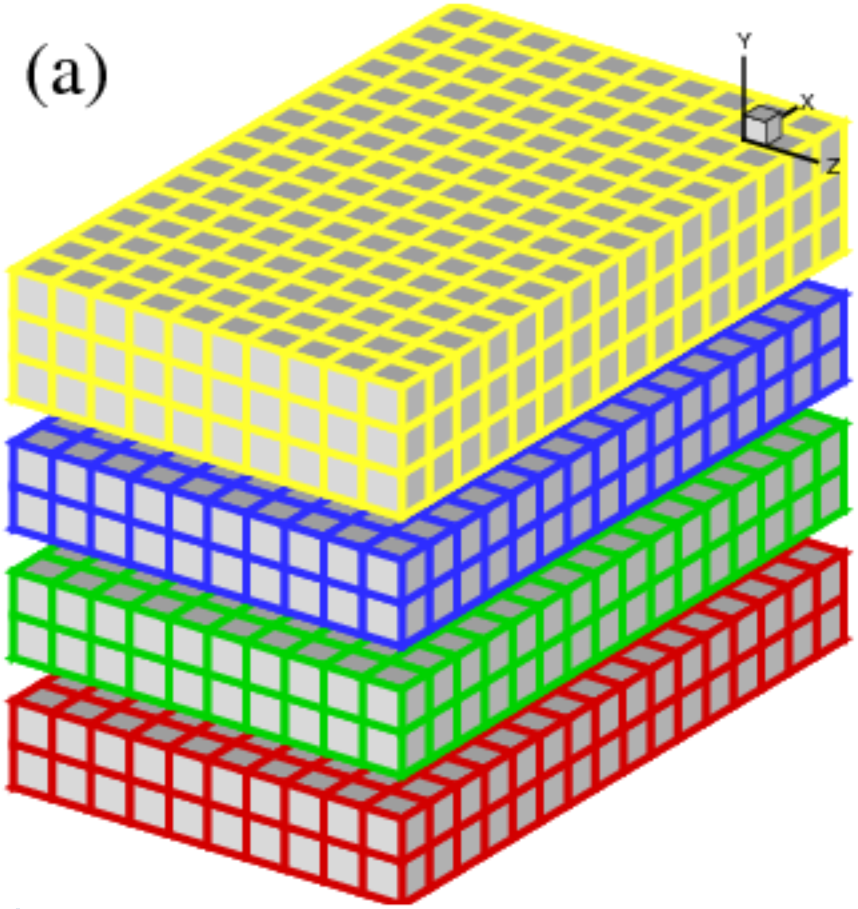
- Solutions:
  - Combined send/recv: MPI_SENDRECV
  - Non-blocking send/recv: MPI_ISEND, MPI_IRECV

    - Usually used with MPI_WAIT or MPI_TEST

  - Buffered send: MPI_BSEND
    - Sender sends message and moves on
    - Message is stored in buffer until receiver is ready

Send/Recv and domain decomposition

A parallel computation computes a potential field, *f(x,y,z,t)* on four processors.
P0, P1, P2, P3 solve for *f* in separate subdomains



How would you compute the gradient?

$$\nabla f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}\right)$$

Computation of derivative

Equispaced grid: $x = x_1, x_2, x_3, \ldots$

$x_{i+1} - x_i = h = \text{constant}$

Then, $$\frac{df_i}{dx} \approx \frac{f_{i+1} - f_{i-1}}{2h}$$

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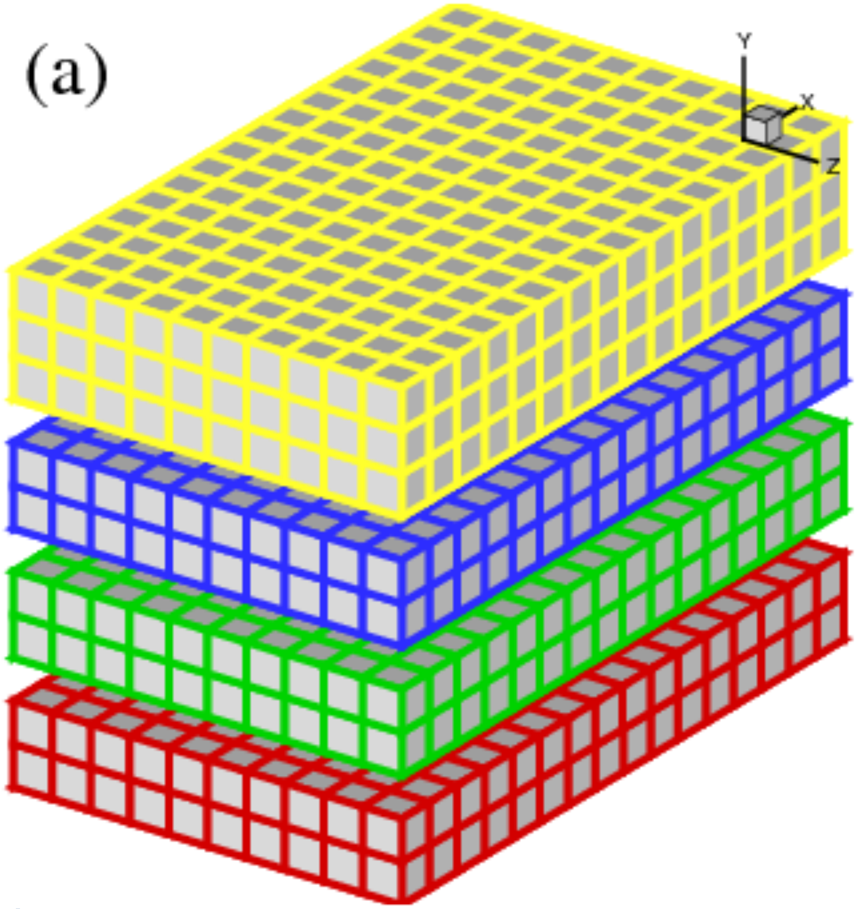


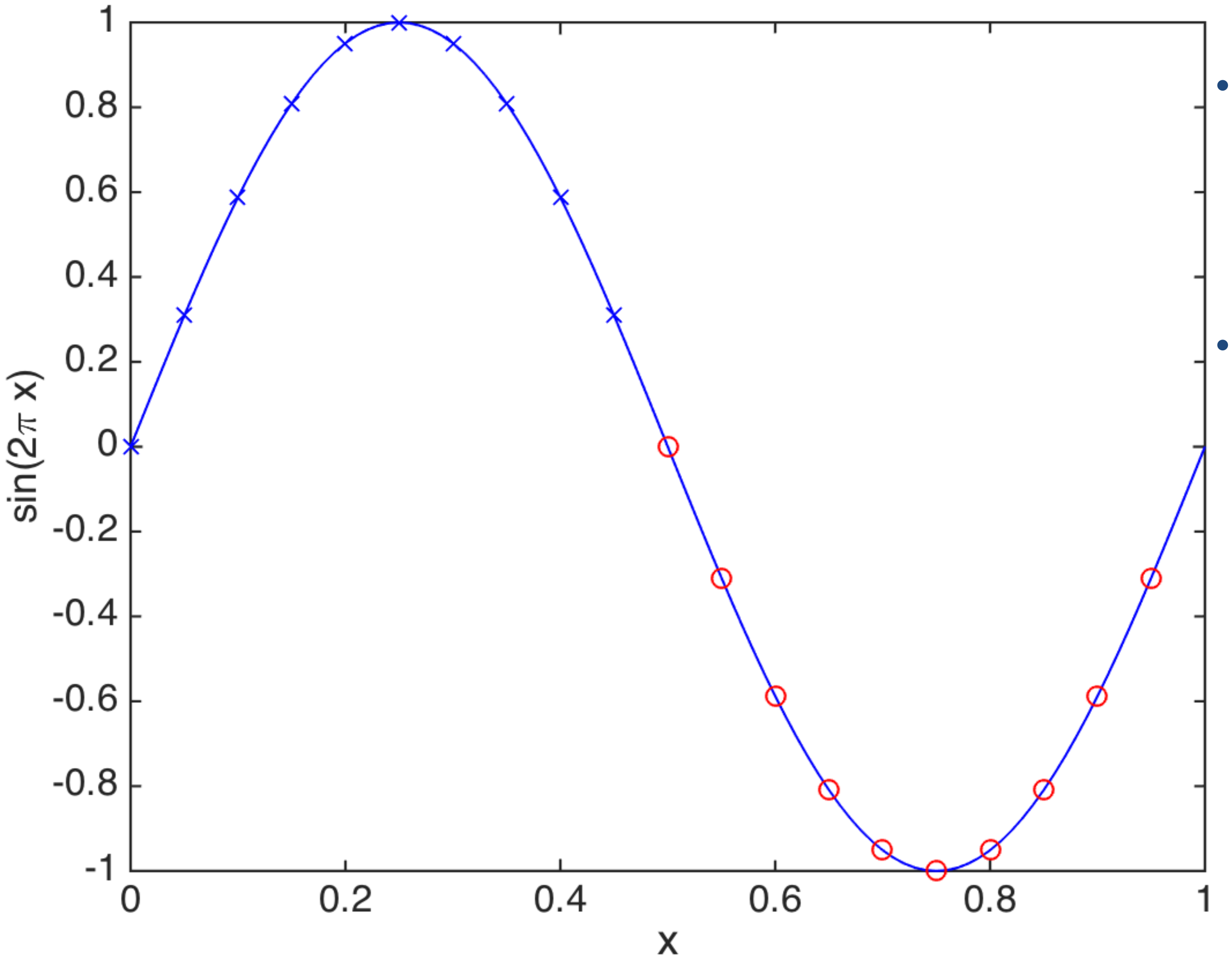
- **How would you compute the gradient?**

$$\nabla f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z} \right)$$

- **No problems with x and z directions**
- **But what about y?**

Send/Recv and domain decomposition

Let's look at a simpler 1-D problem



- 10 points on P0, 10 points on P1
- To compute df/dx for i=10 on P0, need to recv f(i=11) from P1

- On P0, f will have 12 points:
  - The ten points shown
  - and 2 points received from each neighbor

Parallel differentiation example

- **gradient_p.f90: compute** df/dx **given** f=sin(2πx) **distributed across processors**

Code outline:

1. Initialize MPI

2. Read Ntotal **from *data.in***

3. Construct domain decomposition – assign Nlocal **points from** istart **to** iend **to each processor.**

4. Make grid and field, f=sin(2*pi*x), in the local subdomain

5. Compute derivative

6. Output error

Parallel differentiation example

Key parts:

- **Domain decomposition (subroutine from MPE library)**

```
 !construct decomposition
    call MPE_DECOMP1D( Ntotal, numprocs, myid, istart, iend)
    Nlocal = iend - istart + 1
```

Parallel differentiation example

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- **Domain decomposition (subroutine from MPE library)**

```
 !construct decomposition
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    Nlocal = iend - istart + 1
```

- **Make *local* grid and field**

```
 !make grid and field
    call make_grid(Ntotal,Nlocal,istart,iend,x)
    dx = x(2)-x(1)
    print *, 'proc', myid, ' has been assigned the interval x=', 
x(1),x(Nlocal)

    call make_field(Nlocal,x,f(2:Nlocal+1)) !note: f(1) and 
f(Nlocal+2) must be obtained from neighboring processors
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Parallel differentiation example

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- **Compute derivative (with send/recv at subdomain boundaries)…**

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Parallel differentiation example

```
!-------------------------------------------------------------
!Send data at top boundary up to next processor
!i.e. send f(nlocal+1) to myid+1 and store it there as f(1)
!data from myid=numprocs-1 is sent to myid=0
!-------------------------------------------------------------
    if (myid<numprocs-1) then
        receiver = myid+1
    else
         receiver = 0
    end if

    if (myid>0) then
        sender = myid-1
    else
        sender = numprocs-1
    end if

    call MPI_ISEND(f(Nlocal+1),1,MPI_DOUBLE_PRECISION,receiver,0,
                                    MPI_COMM_WORLD,request,ierr)
    call MPI_RECV(f(1) 1,MPI_DOUBLE_PRECISION,sender,MPI_ANY_TAG,
                                    MPI_COMM_WORLD,status,ierr)
```

Parallel differentiation example

- **At end of computation, each process has it's own part of df/dx**
- **The code uses** MPI_ISEND **rather than** MPI_SEND **(why?)**
- **It is sometimes useful to *gather* the data onto one process (*e.g.* for writing data to a file)**
- **Easy to do if gathering ten numbers from ten processors and storing them in an an array**

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```
!gather Nlocal from each proc to array Nper_proc on myid=0
call MPI_GATHER(Nlocal,1,MPI_INT,Nper_proc,1,MPI_INT 0,MPI_COMM_WORLD,
                                                                  ierr)
```

- Nlocal **(size 1, type int) is sent into** Nper_proc **(rank 1 array, type int) on *myid* = 0**

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Parallel differentiation example

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- Nlocal **(size 1, type int) is sent into** Nper_proc **(rank 1 array, type int) on *myid* = 0**

- **Trickier to do when gathering arrays into larger array. Then need array of locations where to place sub-arrays**
  - **e.g., disps = [0, Nper_proc(1), Nper_proc(1)+Nper_proc(2), …]**

Parallel differentiation example

- **Trickier to do when gathering arrays into larger array. Then need array of locations where to place sub-arrays**
  - **e.g.**, disps = [0, Nper_proc(1), Nper_proc(1)+Nper_proc(2), …]

  - **Then use *mpi_gatherv* with** disps **as input:**