AMath 483/583 — Lecture 19 — May 9, 2011

Today:

- MPI send and receive
- Heat equation and discretization

Wednesday:

- Iterative methods

Read: Class notes and references

MPI — Simple example

```
program test1
    use mpi
    implicit none
    integer :: ierr, numprocs, proc_num,

    call mpi_init(ierr)
    call mpi_comm_size(MPI_COMM_WORLD, numprocs, ierr)
    call mpi_comm_rank(MPI_COMM_WORLD, proc_num, ierr)

    print *, 'Hello from Process ', proc_num, &
             ' of ', numprocs, ' processes'

    call mpi_finalize(ierr)

end program test1
```

Always need to: `use mpi`,

Start with `mpi_init`,

End with `mpi_finalize`.

mpi module

The mpi module includes:

Subroutines such as `mpi_init, mpi_comm_size, mpi_comm_rank, ...`

Global variables such as

`MPI_COMM_WORLD`: a communicator,

`MPI_INTEGER`: used to specify the type of data being sent

`MPI_SUM`: used to specify a type of reduction

Remember: Fortran is case insensitive:

`mpi_init` is the same as `MPI_INIT`.

MPI functions

There are 125 MPI functions.

Can write many program with these 8:

- `MPI_INIT(ierr)` Initialize
- `MPI_FINALIZE(ierr)` Finalize
- `MPI_COMM_SIZE(...)` Number of processors
- `MPI_COMM_RANK(...)` Rank of this processor
- `MPI_SEND(...)` Send a message
- `MPI_RCV(...)` Receive a message
- `MPI_BCAST(...)` Broadcast to other processors
- `MPI_REDUCE(...)` Reduction operation

MPI Reduce for vectors

Compute: $\|A\|_1 = \max_{1 \le j \le n} \sum_{i=1}^{m} |a_{ij}|$ for an $m \times n$ matrix A.

Suppose there are m processes and the ith process has a vector `arow(1:n)` containing the ith row of A.

Sum the row vectors (using Reduce) and then take maximum of resulting vector...

```
real(kind=8) :: arow(n), arow_abs(n), colsum(n)
...
arow_abs = abs(arow)

call MPI_REDUCE(arow_abs(1), colsum, n, &
                MPI_DOUBLE_PRECISION,MPI_SUM,0, &
                MPI_COMM_WORLD,ierr)

if (proc_num == 0) then
    anorm = 0.d0
    do j=1,n
       anorm = max(anorm, colsum(j))
       enddo
    print "1-norm of A = ", anorm
    endif
```

MPI AllReduce

To make a reduction available to *all* processes:

```
call MPI_REDUCE(xnorm_proc, xnorm, 1, &
                MPI_DOUBLE_PRECISION,MPI_SUM, 0, &
                MPI_COMM_WORLD,ierr)
! only Process 0 has the value of xnorm

call MPI_BCAST(xnorm, 1, &
                MPI_DOUBLE_PRECISION, 0, &
                MPI_COMM_WORLD,ierr)
```

Or: simpler and perhaps more efficient...

```
call MPI_ALLREDUCE(xnorm_proc, xnorm, 1, &
                MPI_DOUBLE_PRECISION,MPI_SUM, &
                MPI_COMM_WORLD,ierr)
```

MPI Send and Receive

`MPI_BCAST` sends from one process to all processes.

Often want to send selectively from Process i to Process j.

Use `MPI_SEND` and `MPI_RECV`.

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Use `MPI_SEND` and `MPI_RECV`.

Need a way to tag messages so they can be identified.

The parameter `tag` is an integer that can be matched to identify a message.

Tag can also be used to provide information about what is being sent, for example if a Master process sends rows of a matrix to other processes, the `tag` might be the row number.

MPI Send

Send value(s) from this Process to Process `dest`.

General form:

```
call MPI_SEND(start, count, &
              datatype, dest, &
              tag, comm, ierr)
```

where:

- `start`: starting address (variable, array element)
- `count`: number of elements to send
- `datatype`: type of each element
- `dest`: destination process
- `tag`: identifier tag (integer between 0 and 32767)
- `comm`: communicator

MPI Receive

Receive value(s) from Process `source` with label `tag`.

General form:

```
call MPI_RECV(start, count, &
              datatype, source, &
              tag, comm, status, ierr)
```

where:

- `source`: source process
- `tag`: identifier tag (integer between 0 and 32767)
- `comm`: communicator
- `status`: integer array of length `MPI_STATUS_SIZE`.

MPI Receive

Receive value(s) from Process `source` with label `tag`.

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              datatype, source, &
              tag, comm, status, ierr)
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where:

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- `tag`: identifier tag (integer between 0 and 32767)
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- `status`: integer array of length `MPI_STATUS_SIZE`.

source could be `MPI_ANY_SOURCE` to match any source.

tag could be `MPI_ANY_TAG` to match any tag.

MPI Send and Receive — simple example

```
if (proc_num == 4) then
    i = 55
    call MPI_SEND(i, 1, MPI_INTEGER, 3, 21, &
                  MPI_COMM_WORLD, ierr)
    endif
if (proc_num == 3) then
    call MPI_RECV(j, 1, MPI_INTEGER, 4, 21, &
                  MPI_COMM_WORLD, status, ierr)
    print *, "j = ", j
    endif
```

Processor 3 will print `j = 55`

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The tag is 21. (Arbitrary integer between 0 and 32767)

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Blocking Receive: Processor 3 won't return from `MPI_RECV` until message is received.

MPI Send and Receive — simple example

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Run-time error if `num_procs <= 4` (Procs are 0,1,2,3)

Send/Receive example

Pass value of `i` from Processor 0 to 1 to 2 ... to `num_procs-1`

```
if (proc_num == 0) then

    i = 55
    call MPI_SEND(i, 1, MPI_INTEGER, 1, 21, &
                  MPI_COMM_WORLD, ierr)
    endif

else if (proc_num < num_procs - 1) then

    call MPI_RECV(i, 1, MPI_INTEGER, proc_num-1, 21, &
                  MPI_COMM_WORLD, status, ierr)

    call MPI_SEND(i, 1, MPI_INTEGER, proc_num+1, 21, &
                  MPI_COMM_WORLD, ierr)

else if (proc_num == num_procs - 1) then

    call MPI_RECV(i, 1, MPI_INTEGER, proc_num-1, 21, &
                  MPI_COMM_WORLD, status, ierr)
    print *, "i = ", i
    endif
```

MPI Receive

Receive value(s) from Process `source` with label `tag`.

General form:

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call MPI_RECV(start, count, &
              datatype, source, &
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source could be `MPI_ANY_SOURCE` to match any source.

tag could be `MPI_ANY_TAG` to match any tag.

MPI Receive — `status` argument

```
call MPI_RECV(start, count, &
              datatype, source, &
              tag, comm, status, ierr)
```

Elements of the `status` array give additional useful information about the message received.

In particular,

`status(MPI_SOURCE)` is the source of the message,
May be needed if `source = MPI_ANY_SOURCE`.

`status(MPI_TAG)` is the tag of the message received,
May be needed if `tag = MPI_ANY_TAG`.

Another Send/Receive example

Master (Processor 0) sends jth column to Worker Processor j, gets back 1-norm to store in `anorm(j)`, $j = 1, \ldots,$ `ncols`

```
! code for Master (Processor 0):
if (proc_num == 0) then

   do j=1,ncols
     call MPI_SEND(a(1,j), nrows, MPI_DOUBLE_PRECISION,&
                   j, j, MPI_COMM_WORLD, ierr)
     enddo

   do j=1,ncols
     call MPI_RECV(colnorm, 1, MPI_DOUBLE_PRECISION, &
                   MPI_ANY_SOURCE, MPI_ANY_TAG, &
                   MPI_COMM_WORLD, status, ierr)
     jj = status(MPI_TAG)
     anorm(jj) = colnorm
     enddo
   endif
```

Note: Master may receive back in any order!

`MPI_ANY_SOURCE` will match first to arrive.

The tag is used to tell which column's norm has arrived (`jj`).

Send and Receive example — worker code

Master (Processor 0) sends jth column to Worker Processor j, gets back 1-norm to store in `anorm(j)`, $j = 1, \ldots,$ `ncols`

```
! code for Workers (Processors 1, 2, ...):

if (proc_num /= 0) then

   call MPI_RECV(colvect, nrows, MPI_DOUBLE_PRECISION,&
                    0, MPI_ANY_TAG, &
                    MPI_COMM_WORLD, status, ierr)

   j = status(MPI_TAG)    ! this is the column number

   colnorm = 0.d0
   do i=1,nrows
       colnorm = colnorm + abs(colvect(i))
       enddo

   call MPI_SEND(colnorm, 1, MPI_DOUBLE_PRECISION, &
                  0, j, MPI_COMM_WORLD, ierr)

   endif
```

Note: Sends back with tag j.

Send may be blocking

```
if (proc_num == 4) then
    i = 55
    call MPI_SEND(i, 1, MPI_INTEGER, 3, 21, &
                  MPI_COMM_WORLD, ierr)
    call MPI_RECV(j, 1, MPI_INTEGER, 3, 22, &
                  MPI_COMM_WORLD, status, ierr)
    endif

if (proc_num == 3) then
    j = 66
    call MPI_SEND(j, 1, MPI_INTEGER, 4, 22, &
                  MPI_COMM_WORLD, ierr)
    call MPI_RECV(i, 1, MPI_INTEGER, 4, 21, &
                  MPI_COMM_WORLD, status, ierr)
    endif
```

Both processors might get stuck in `MPI_SEND`!

Implementation-dependent: waits for send buffer to be free.

Blocking send: `MPI_SSEND`. See documentation

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if (proc_num == 4) then
    i = 55
    call MPI_SEND(i, 1, MPI_INTEGER, 3, 21, &
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    call MPI_RECV(j, 1, MPI_INTEGER, 3, 22, &
                  MPI_COMM_WORLD, status, ierr)
    endif

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    j = 66
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                  MPI_COMM_WORLD, ierr)
    call MPI_RECV(i, 1, MPI_INTEGER, 4, 21, &
                  MPI_COMM_WORLD, status, ierr)
    endif
```

Both processors might get stuck in `MPI_SEND`!

Implementation-dependent: waits for send buffer to be free.

Blocking send: `MPI_SSEND`. See documentation

There are also non-blocking sends and receives:

`MPI_ISEND, MPI_IRECV`

Heat Equation / Diffusion Equation

Partial differential equation for $u(x,t)$ in one space dimension and time.

u represents temperature in a 1-dimensional metal rod, for example.

Or concentration (density) of a chemical diffusing in a tube of water.

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Or concentration (density) of a chemical diffusing in a tube of water.

The PDE is

$$u_t(x,t) = Du_{xx}(x,t) + f(x,t)$$

where subscripts represent partial derivatives,

$D =$ diffusion coefficient,

$f(x,t) =$ source term.

Steady state diffusion

If $f(x,t) = f(x)$ does not depend on time and if the boundary conditions don't depend on time, then $u(x,t)$ will converge towards steady state distribution satisfying

$$0 = Du_{xx}(x) + f(x)$$

(by setting $u_t = 0$.)

This is now an ordinary differential equation (ODE) for $u(x)$.

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This is now an ordinary differential equation (ODE) for $u(x)$.

We can solve this on an interval, say $0 \le x \le 1$ with

Boundary conditions:

$$u(0) = \alpha, \qquad u(1) = \beta.$$

Steady state diffusion

More generally: Take $D = 1$ or absorb in f,

$$u_{xx}(x) = -f(x) \qquad \text{for } 0 \le x \le 1,$$

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Can be solved exactly if we can integrate f twice and use boundary conditions to choose the two constants of integration.

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Example: $f(x) = 0, \quad \alpha = 20, \quad \beta = 60$:

Solution: $u(x) = \alpha + x(\beta - \alpha)$.

No heat source $\implies$ linear variation in steady state ($u_{xx} = 0$).

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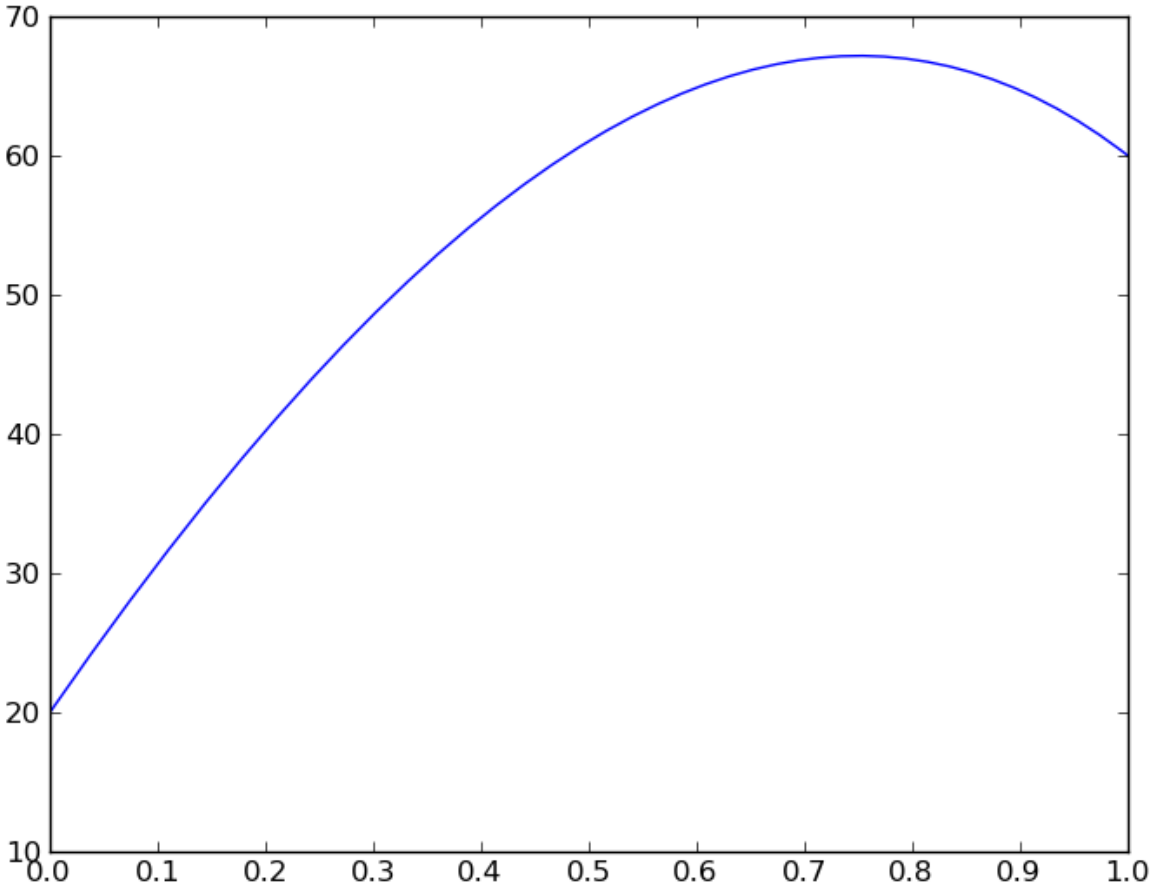
More interesting example:

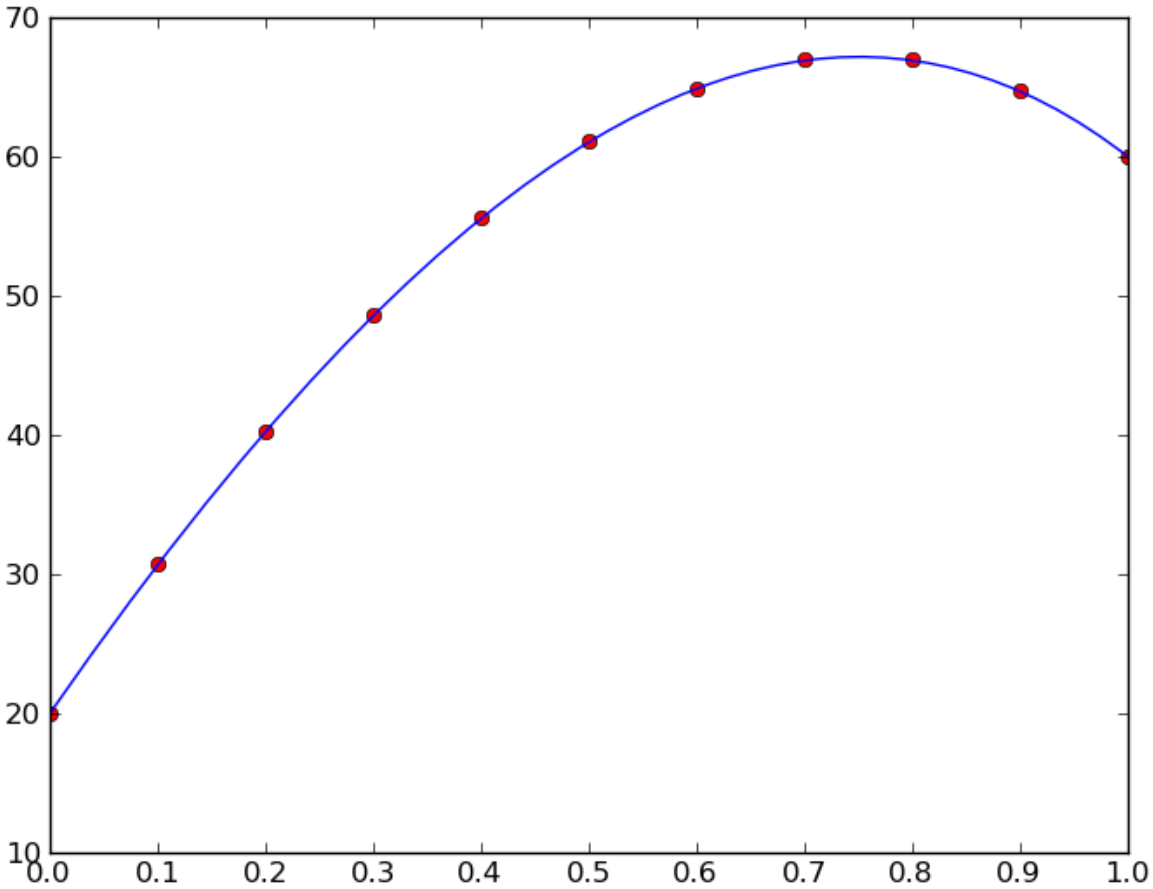
Example: $f(x) = 100e^x, \quad \alpha = 20, \quad \beta = 60$:

Solution: $u(x) = -100e^x + (100e - 60)x + 120.$

Steady state diffusion



Steady state diffusion



For more complicated equations, numerical methods must generally be used, giving approximations at discrete points.

Finite difference method

Define grid points $x_i = i\Delta x$ in interval $0 \le x \le 1$, where

$$\Delta x = \frac{1}{n+1}$$

So $x_0 = 0,\ x_{n+1} = 1$, and the n grid points $x_1,\ x_2,\ \ldots,\ x_n$ are equally spaced inside the interval.

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Let $U_i \approx u(x_i)$ denote approximate solution.

We know $U_0 = \alpha$ and $U_{m+1} = \beta$ from boundary conditions.

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Idea: Replace differential equation for $u(x)$ by system of n algebraic equations for U_i values ($i = 1,\ 2,\ \ldots,\ n$).

Finite difference method

$$U_i \approx u(x_i)$$

$$u_x(x_{i+1/2}) \approx \frac{U_{i+1} - U_i}{\Delta x}$$

$$u_x(x_{i-1/2}) \approx \frac{U_i - U_{i-1}}{\Delta x}$$

Finite difference method

$U_i \approx u(x_i)$

$u_x(x_{i+1/2}) \approx \frac{U_{i+1}-U_i}{\Delta x}$

$u_x(x_{i-1/2}) \approx \frac{U_i-U_{i-1}}{\Delta x}$

So we can approximate second derivative at x_i by:

$$u_{xx}(x_i) \approx \frac{1}{\Delta x}\left(\frac{U_{i+1}-U_i}{\Delta x} - \frac{U_i-U_{i-1}}{\Delta x}\right)$$

$$= \frac{1}{\Delta x^2}\left(U_{i-1} - 2U_i + U_{i+1}\right)$$

Finite difference method

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$u_x(x_{i+1/2}) \approx \frac{U_{i+1}-U_i}{\Delta x}$

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$$= \frac{1}{\Delta x^2}\left(U_{i-1} - 2U_i + U_{i+1}\right)$$

This gives coupled system of n linear equations:

$$\frac{1}{\Delta x^2}\left(U_{i-1} - 2U_i + U_{i+1}\right) = -f(x_i)$$

for $i = 1,\ 2,\ \ldots,\ n$. With $U_0 = \alpha$ and $U_{m+1} = \beta$.

Tridiagonal linear system

For $n = 5$:

$$\begin{bmatrix} -2 & 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 1 & -2 \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \\ U_4 \\ U_5 \end{bmatrix} = -\Delta x^2 \begin{bmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \\ f(x_4) \\ f(x_5) \end{bmatrix} - \begin{bmatrix} \alpha \\ 0 \\ 0 \\ 0 \\ \beta \end{bmatrix}.$$

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General $n \times n$ system requires $O(n^3)$ flops to solve.

Tridiagonal $n \times n$ system requires $O(n)$ flops to solve.

Could use LAPACK routine `dgtsv`.