Introduction to High Performance Scientific Computing

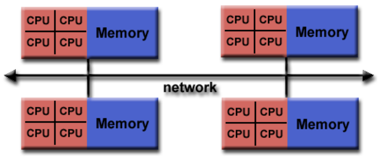
Autumn, 2016

Lecture 15

Imperial College London

Prasun Ray
28 November 2016

Parallel computing paradigms

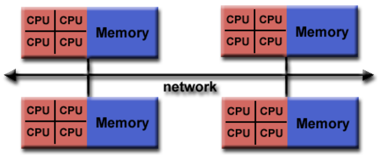


Distributed memory

- Each (4-core) chip has its own memory
- The chips are connected by network 'cables'
- MPI coordinates communication between two or more CPUs

Imperial College London

Parallel computing paradigms



Related approaches:

- Hybrid programming: mix of shared-memory (OpenMP) and distributed-memory (MPI) programming
- GPU's: Shared memory programming (CUDA or OpenCL)
- Coprocessors and co-array programming

Imperial College London

MPI intro

- MPI: *Message Passing Interface*
- Standard for exchanging data between processors
- Supports Fortran, c, C++
- Can also be used with Python

Imperial College London

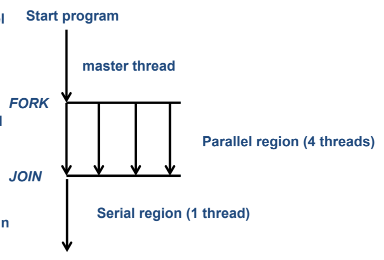
OpenMP schematic

Program starts with single *master thread*

Then, launch parallel region with multiple threads.

Each thread has access to all variables introduced previously

Can end parallel region if/when desired and launch parallel regions again in future as needed

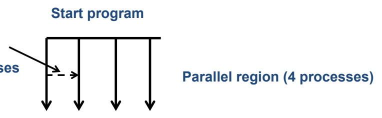


Imperial College London

MPI schematic

Program starts with all processes running

MPI controls communication between processes



Imperial College London

MPI intro

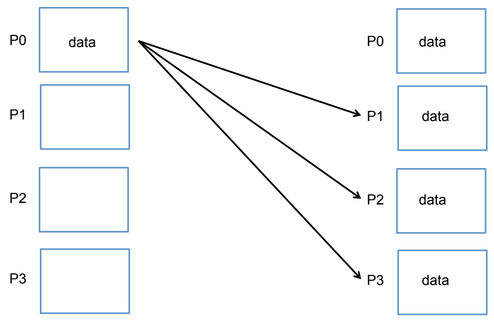
- Basic idea: calls to MPI subroutines control data exchange between processors
- Example:

```
call MPI_BCAST(n, 1, MPI_INTEGER,0,MPI_COMM_WORLD,ierr)
```

This will send the integer n which has size 1 from processor 0 to all of the other processors.

Imperial College
London

MPI broadcast



Imperial College
London

MPI intro

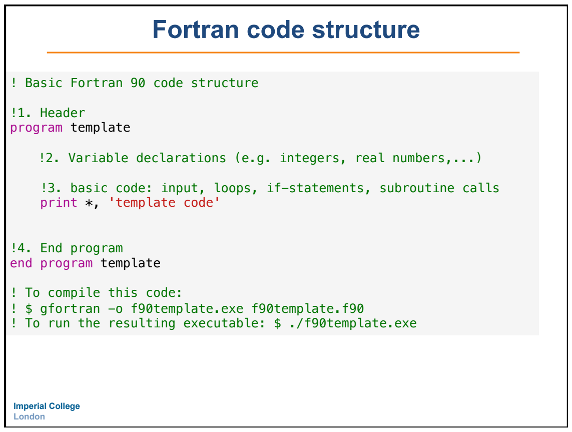
- Basic idea: calls to MPI subroutines control data exchange between processors
- Example:

```
call MPI_BCAST(n, 1, MPI_INTEGER,0,MPI_COMM_WORLD,ierr)
```

This will send the integer n which has size 1 from processor 0 to all of the other processors.

Generally, need to specify:
- source and/or destination of message
- size of data contained in message
- type of data contained in message (integer, double precision, …)
- the data itself (or its location)

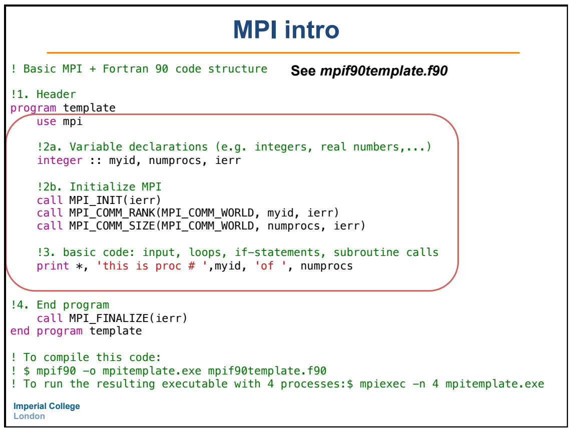
Imperial College
London



Fortran code structure

```
! Basic Fortran 90 code structure

!1. Header
program template

    !2. Variable declarations (e.g. integers, real numbers,...)

    !3. basic code: input, loops, if-statements, subroutine calls
    print *, 'template code'


!4. End program
end program template

! To compile this code:
! $ gfortran -o f90template.exe f90template.f90
! To run the resulting executable: $ ./f90template.exe
```

Imperial College London

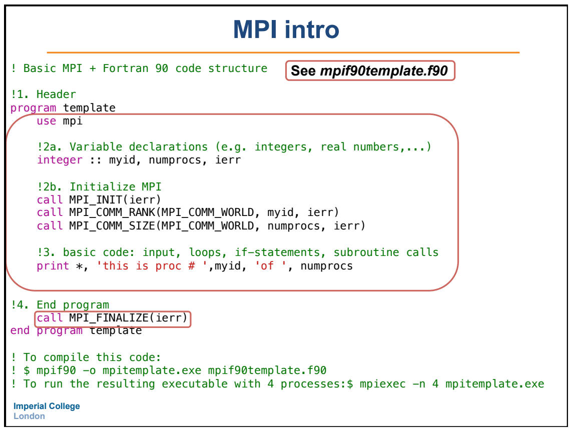


MPI intro

See *mpif90template.f90*

```
! Basic MPI + Fortran 90 code structure

!1. Header
program template
    use mpi

    !2a. Variable declarations (e.g. integers, real numbers,...)
    integer :: myid, numprocs, ierr

    !2b. Initialize MPI
    call MPI_INIT(ierr)
    call MPI_COMM_RANK(MPI_COMM_WORLD, myid, ierr)
    call MPI_COMM_SIZE(MPI_COMM_WORLD, numprocs, ierr)

    !3. basic code: input, loops, if-statements, subroutine calls
    print *, 'this is proc # ',myid, 'of ', numprocs

!4. End program
    call MPI_FINALIZE(ierr)
end program template

! To compile this code:
! $ mpif90 -o mpitemplate.exe mpif90template.f90
! To run the resulting executable with 4 processes:$ mpiexec -n 4 mpitemplate.exe
```

Imperial College London



MPI intro

See *mpif90template.f90*

```
! Basic MPI + Fortran 90 code structure

!1. Header
program template
    use mpi

    !2a. Variable declarations (e.g. integers, real numbers,...)
    integer :: myid, numprocs, ierr

    !2b. Initialize MPI
    call MPI_INIT(ierr)
    call MPI_COMM_RANK(MPI_COMM_WORLD, myid, ierr)
    call MPI_COMM_SIZE(MPI_COMM_WORLD, numprocs, ierr)

    !3. basic code: input, loops, if-statements, subroutine calls
    print *, 'this is proc # ',myid, 'of ', numprocs

!4. End program
    call MPI_FINALIZE(ierr)
end program template

! To compile this code:
! $ mpif90 -o mpitemplate.exe mpif90template.f90
! To run the resulting executable with 4 processes:$ mpiexec -n 4 mpitemplate.exe
```

Imperial College London

MPI intro

See *mpif90template.f90*

```
! Basic MPI + Fortran 90 code structure

!1. Header
program template
    use mpi

    !2a. Variable declarations (e.g. integers, real numbers,...)
    integer :: myid, numprocs, ierr

    !2b. Initialize MPI
    call MPI_INIT(ierr)
    call MPI_COMM_RANK(MPI_COMM_WORLD, myid, ierr)
    call MPI_COMM_SIZE(MPI_COMM_WORLD, numprocs, ierr)

    !3. basic code: input, loops, if-statements, subroutine calls
    print *, 'this is proc # ',myid, 'of ', numprocs

!4. End program
    call MPI_FINALIZE(ierr)
end program template

! To compile this code:
! $ mpif90 -o mpitemplate.exe mpif90template.f90
! To run the resulting executable with 4 processes:$ mpiexec -n 4 mpitemplate.exe
```

Imperial College
London

MPI intro

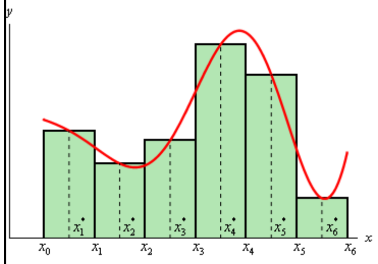
- **Compile + run:**

```
$ mpif90 -o mpif90template.exe mpif90template.f90

$ mpiexec -n 4 mpif90template.exe
 this is proc #           0 of           4
 this is proc #           3 of           4
 this is proc #           1 of           4
 this is proc #           2 of           4
```

Note: The number of processes specified with mpiexec can be larger than the number of cores on your machine, but then tasks are run sequentially.

Imperial College
London

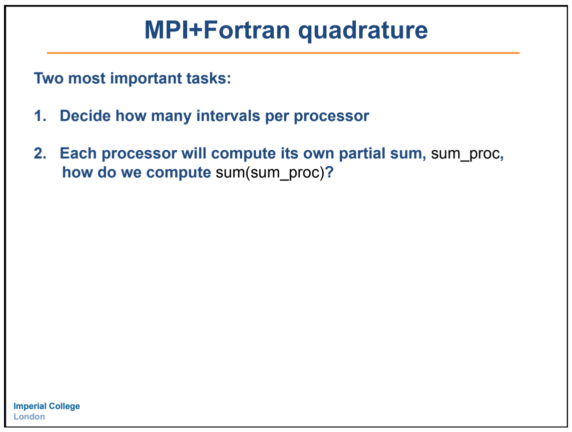
MPI+Fortran example: computing an integral



- **Estimate integral with midpoint rule,**

$$I = \int_0^1 \frac{4}{1+x^2} dx$$

Imperial College
London

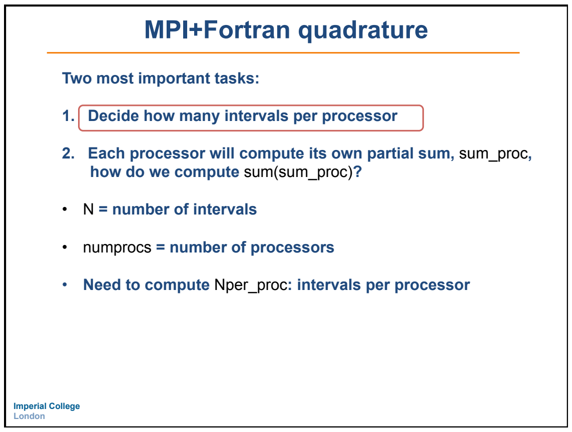


MPI+Fortran quadrature

Two most important tasks:

1. Decide how many intervals per processor
2. Each processor will compute its own partial sum, sum_proc, how do we compute sum(sum_proc)?

Imperial College London



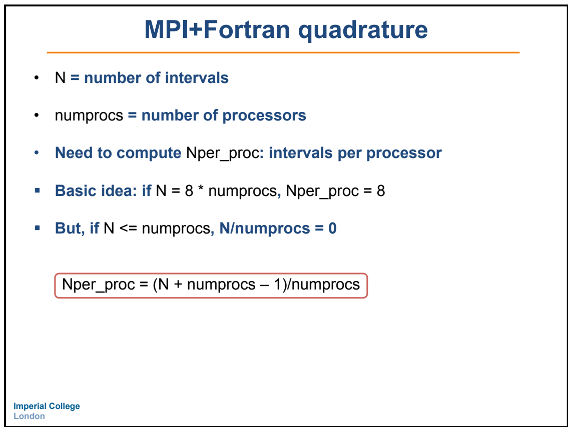
MPI+Fortran quadrature

Two most important tasks:

1. Decide how many intervals per processor
2. Each processor will compute its own partial sum, sum_proc, how do we compute sum(sum_proc)?

- N = number of intervals
- numprocs = number of processors
- Need to compute Nper_proc: intervals per processor

Imperial College London

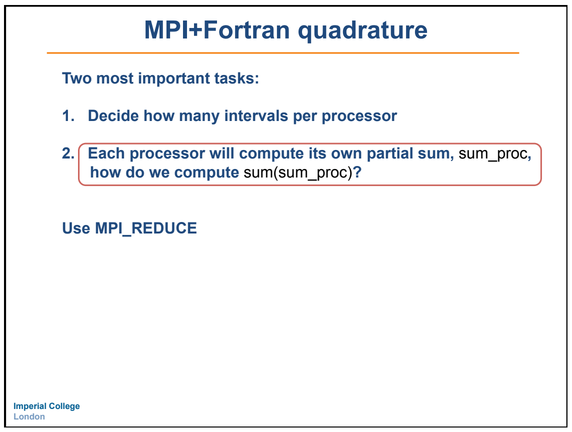


MPI+Fortran quadrature

- N = number of intervals
- numprocs = number of processors
- Need to compute Nper_proc: intervals per processor
- Basic idea: if N = 8 * numprocs, Nper_proc = 8
- But, if N <= numprocs, N/numprocs = 0

Nper_proc = (N + numprocs – 1)/numprocs

Imperial College London



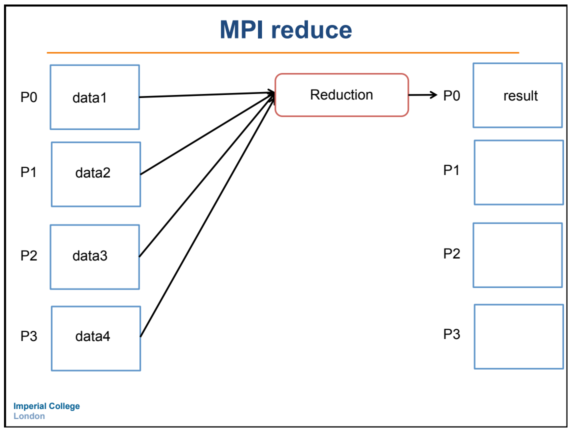
MPI+Fortran quadrature

Two most important tasks:

1. Decide how many intervals per processor
2. Each processor will compute its own partial sum, sum_proc, how do we compute sum(sum_proc)?

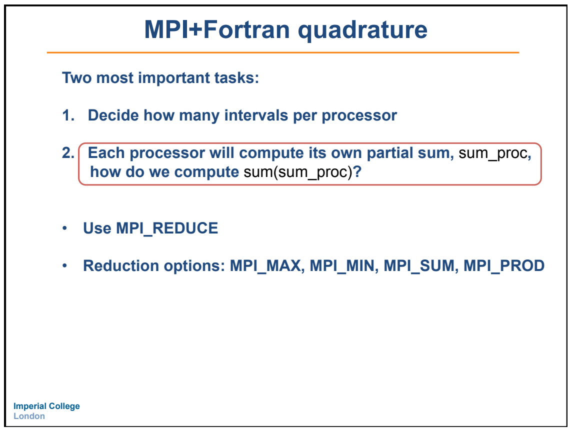
Use MPI_REDUCE

Imperial College London



MPI reduce

Imperial College London



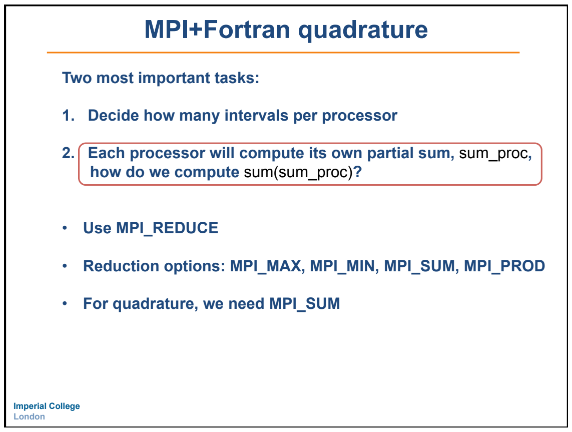
MPI+Fortran quadrature

Two most important tasks:

1. Decide how many intervals per processor
2. Each processor will compute its own partial sum, sum_proc, how do we compute sum(sum_proc)?

- Use MPI_REDUCE
- Reduction options: MPI_MAX, MPI_MIN, MPI_SUM, MPI_PROD

Imperial College London



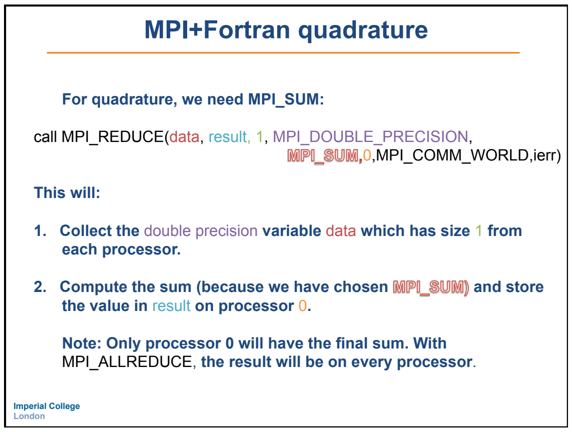
MPI+Fortran quadrature

Two most important tasks:

1. Decide how many intervals per processor
2. Each processor will compute its own partial sum, sum_proc, how do we compute sum(sum_proc)?

- Use MPI_REDUCE
- Reduction options: MPI_MAX, MPI_MIN, MPI_SUM, MPI_PROD
- For quadrature, we need MPI_SUM

Imperial College London



MPI+Fortran quadrature

For quadrature, we need MPI_SUM:

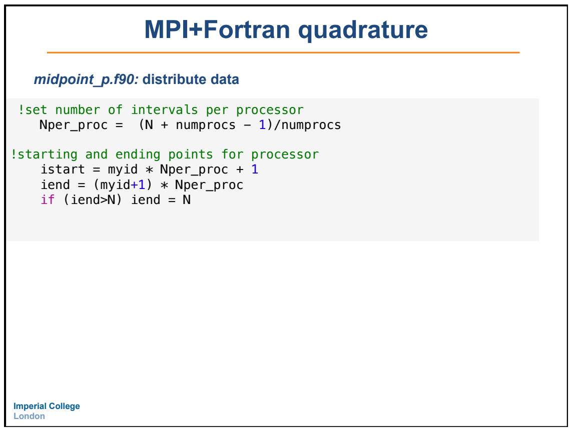
```
call MPI_REDUCE(data, result, 1, MPI_DOUBLE_PRECISION,
                                   MPI_SUM,0,MPI_COMM_WORLD,ierr)
```

This will:

1. Collect the double precision variable data which has size 1 from each processor.
2. Compute the sum (because we have chosen MPI_SUM) and store the value in result on processor 0.

   Note: Only processor 0 will have the final sum. With MPI_ALLREDUCE, the result will be on every processor.

Imperial College London



MPI+Fortran quadrature

midpoint_p.f90: distribute data

```
 !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
```

Imperial College London

MPI+Fortran quadrature

***midpoint_p.f90:* 1. distribute data, 2. compute** sum_proc

```
 !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

!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
```

Imperial College
London

MPI+Fortran quadrature

***midpoint_p.f90:* 1. distribute data, 2. compute** sum_proc, **3. reduction**

```
 !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

!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
!collect double precision variable, sum, with size 1 on process 0 using
the MPI_SUM option
    call MPI_REDUCE(sum_proc,sum,1,MPI_DOUBLE_PRECISION,MPI_SUM,
0,MPI_COMM_WORLD,ierr)
```

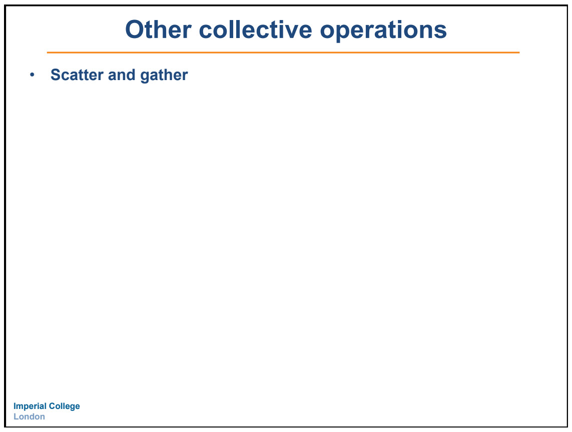
London

MPI+Fortran quadrature

Compile and run:

```
$ mpif90 -o midpoint_p.exe midpoint_p.f90

$ mpiexec -n 2 midpoint_p.exe
 number of intervals =         1000
 number of procs =            2
 Nper_proc=          500
 The partial sum on proc #           0 is:   1.8545905426699112
 The partial sum on proc #           1 is:   1.2870021942532193
 N=        1000
 sum=   3.1415927369231307
 error=   8.3333337563828991E-008
```

Imperial College
London

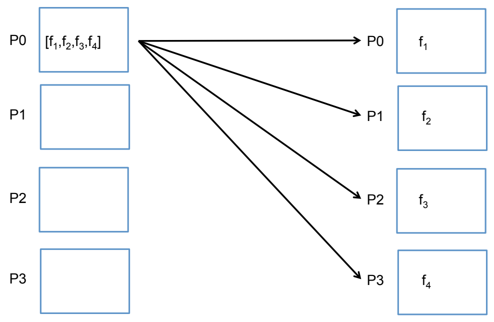


Other collective operations

- Scatter and gather

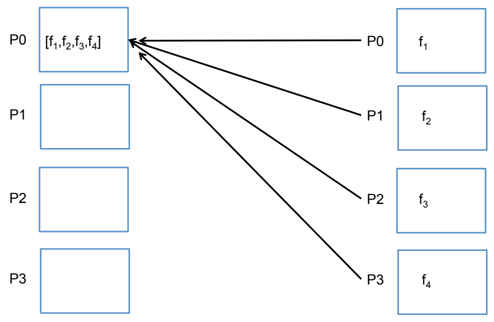
Imperial College London

MPI scatter



Imperial College London

MPI gather



Imperial College London

Other collective operations

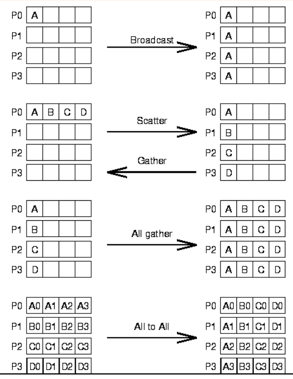
- Scatter and gather
  - *Gather* all particles on processor
  - Compute interaction forces for particles on that processor

$$\frac{d^2\mathbf{x}_i}{dt^2} = \sum_{j=1}^{N} f(|\mathbf{x_i} - \mathbf{x_j}|),\ i = 1, 2, ..., N$$

- Avoid for big problems (why?)

Imperial College London

MPI collective data movement



Imperial College London

From *Using MPI*