High Performance Technical Computing: Lab Sessions

Irene Moulitsas

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1 Working with the `Delta/Crescent` cluster

In order to use MPI and run on an HPC cluster, you will be working with Delta/Crescent, Cranfield University-wide research HPC facility. Delta has a 60 TFlops CPU performance, 1920 user-accessible CPU cores available, interconnected with Mellanox EDR Infiniband 100 GB/s network, 120TB of GPFS scratch storage and 1.2 TB application storage area. It can be accessed through two login nodes (front-ends), known as `delta`, each connected to the outside network by 10 GB/s ethernet.

You will have access to the Delta/Crescent for the duration of your MSc CSTE studies.

Figure 1: `Delta` HPC Cluster at Cranfield University

When developing and testing Message Passing Interface (MPI) programs, some users tend to run small MPI programs interactively on the front node. This is *not* good practice and should be avoided. In order to run computations which measure execution time, it is only advisable that you use `PBS` - a batch system which manages jobs on Delta and ensures that each of your MPI processes gets allocated to a separate CPU.

1.1 Accessing Delta

A substantial amount of information regarding research computing at Cranfield University can be found at the IT managed website: https://intranet.cranfield.ac.uk/it/Pages/HighPerformance.aspx

In order to login to Delta from the command line of your local Linux machine:

```
ssh -X s123456@delta.central.cranfield.ac.uk
```

replacing s123456 with your Cranfield University username.

Once logged on, you have a single storage area, your home folder, with 250GB storage space. Your home folder is located at /mnt/gpfs0/home/$USER.

If you are accessing Delta from a Windows machine you can use putty, or some other similar program.

1.2 Some useful commands

Transferring files

To copy a file, for example test.c, from directory X on Delta, to the current directory on the local machine:

```
scp s123456@delta.central.cranfield.ac.uk:~/X/test.c ./.
```

To copy all files, from directory X on Delta, to the current directory on the local machine:

```
scp s123456@delta.central.cranfield.ac.uk:~/X/* ./
```

To copy a file, for example test.c, from the current directory on the local machine, to directory X on Delta:

```
scp ./test.c s123456@delta.central.cranfield.ac.uk:~/X/
```

To copy all files, from current directory on the local machine, to directory X on Delta:

```
scp ./* s123456@delta.central.cranfield.ac.uk:~/X/
```

If you are accessing Delta from a Windows machine you can use winscp3, or some other similar program.

Standard Commands

Some Unix commands you might find useful:

- `ls` - list the files in the current directory
- `ls -laF` - list the files in the current directory including details such as modification date and file size
- `cd A` - change directory to A
- `cd ..` - change directory - go one level up
- `mkdir` - create a directory
- `cp pathA/file.A pathB` - copy file.A from directory given by pathA to directory given by pathB

- `rm file.A` - remove file file.A
- `rmdir` A - remove directory A
- `cat file.A` - print the contents of file.A on the screen
- `less file.A` - open file.A in a viewer (q to exit the viewer)
- `history` - print last commands executed
- `pwd` - print working directory

In general you have access to further information and the arguments of a Unix command by:

- `man command_name`

Editing files on `Delta`

You can either run the editor on `Delta` remotely, i.e. after logging in via ssh:

```
nedit &
```

or edit files locally and copy to `Delta` using `scp`.
Please issue a `module load NEdit` to load the appropriate module, before issuing the command.

There are more advanced editors for Unix based environments, such as `vi` or `vim`, but one needs to get acquainted to the command interface of such editors.

2 MPI

2.1 Compiling MPI programs

In order to use MPI one first needs to set their environment variables accordingly.

To use Intel MPI

```
module load intel
```

In order to compile an MPI C or FORTRAN program, run:

```
mpicc <intel c options> file_name.c
```

or

```
mpif90 <intel fortran options> file_name.f90
```

mpicc and mpif90 are in fact wrappers for Intel's icc or ifort compiler, so all options which you can specify for icc or ifort are applicable. For more details

```
man icc
```

or

```
man ifort
```

2.2 Running MPI programs

To run an mpi program, say `a.out`, the command is:

```
mpirun -np <number of processes to start> ./a.out
```

As discussed earlier, the scheduling system should be used in order to run a program. To submit an MPI program to the scheduler you will need to use:

```
qsub script_name
```

where `script_name` is the job submission script which may correspond to the following template:

```
#!/bin/bash
##
## MPI submission script for PBS on DELTA
## ---------------------------------------
##
## Follow the 6 steps below to configure your job. If you edit this from Windows,
## *before* submitting via "qsub" run "dos2unix" on this file - or you will
## get strange errors. You have been warned.
##
## STEP 1:
## Enter a job name after the -N on the line below:
##
#PBS -N mpi_example
##
## STEP 2:
## Select the number of cpus/cores required by modifying the #PBS -l select line below
##
## Normally you select cpus in chunks of 16 cpus
## The maximum value for ncpus is 16 and mpiprocs MUST be the same value as ncpus.
##
## If more than 16 cpus are required then select multiple chunks of 16
## e.g. 16 CPUs: select=1:ncpus=16:mpiprocs=16
##      32 CPUs: select=2:ncpus=16:mpiprocs=16
##      48 CPUs: select=3:ncpus=16:mpiprocs=16
##      ..etc..
##
#PBS -l select=1:ncpus=16:mpiprocs=16
##
## STEP 3:
## Select the correct queue by modifying the #PBS -q line below
##
## half_hour    -  30 minutes
## one_hour     -   1 hour
## half_day     -  12 hours
## one_day      -  24 hours
## two_day      -  48 hours
## five_day     - 120 hours
## ten_day      - 240 hours (by special arrangement)
##
```

```
#PBS -q half_hour
##
## STEP 4:
## Replace the a.bcdefg@cranfield.ac.uk email address
## with your Cranfield email address on the #PBS -M line below:
## Your email address is NOT your username
##
#PBS -m abe
#PBS -M a.bcdefg@cranfield.ac.uk
##
## ====================================
## DO NOT CHANGE THE LINES BETWEEN HERE
## ====================================
#PBS -j oe
#PBS -W sandbox=PRIVATE
#PBS -k n
ln -s $PWD $PBS_O_WORKDIR/$PBS_JOBID
## Change to working directory
cd $PBS_O_WORKDIR
## Calculate number of CPUs
cpus=‘cat $PBS_NODEFILE | wc -l‘
## set some MPI tuning parameters to use the correct transport
export I_MPI_FABRICS=shm:dapl
export I_MPI_DAPL_UD=enable
export I_MPI_PLATFORM=bdw
export I_MPI_ADJUST_ALLREDUCE=5
## ========
## AND HERE
## ========
##
## STEP 5:
##  Load the default application environment
##  For a specific version add the version number, e.g.
##  module load intel/2016b
##  To load the latest version
##  module load intel
##
##
module load intel
##
##
## STEP 6:
##
## Run MPI code
##
## The main parameter to modify is your mpi program name
## - change ./a.out to your own filename
##
```

```
mpirun -machinefile $PBS_NODEFILE -np ${cpus} ./a.out

## Tidy up the log directory
## DO NOT CHANGE THE LINE BELOW
## ============================
rm $PBS_O_WORKDIR/$PBS_JOBID
```

Where you specify your values for the job name, number of processors and executable name. Once the job has been submitted you can use `qstat` command to show the status of the queue and your job's position.

Sample PBS scripts can be found at `/apps/examples/pbs`

3 Tasks

In these lab sessions you will write four MPI programs:

- Simple Hello World Send-Receive test
- Parallel Dot Product computation
- Parallel Pi computation
- Parallel Ping-Pong network timing

You may find the following online MPI references useful:

`http://www.netlib.org/utk/papers/mpi-book/mpi-book.html`
`http://www.llnl.gov/computing/tutorials/mpi/`

3.1 Hello World

- Write an MPI program which:
  - Initialises MPI
  - Obtains the rank of the process
  - For each process prints "Hello World" message and the rank of the process
  - Do not forget to check the return value of every MPI operation to detect errors
- Run this program interactively on 2 processors.
- Run the program through the scheduler on 16 processors

3.2 Send-Receive Test

- Modify your Hello World program so that:
  - Process 0 Sends each process a message with a real array with n variables, where n is the user input
  - Each of the other processes receives the array and prints "Hello World" message, rank of the process and the first element of the array received
  - Process 0 measures the **overall send** time using MPI_WTIME function
  - Do not forget to check the return value of every MPI operation to detect errors
- Run this program interactively on 2 processors.
- Run the program through the scheduler on 16 processors

3.3 Dot Product Computation

Based on the following serial implementation of the dot product computation, write an MPI program to implement the same tasks. Vectors will be distributed among the processes and use MPI_Allreduce when necessary.

```
c  serial_dot.f -- compute a dot product
c                  serially -- on a single processor.
c
c  Input:
c      n: vector size
c      x, y: vectors
c
c  Output:
c      the dot product of x and y.
c
       PROGRAM serial_dot
       implicit none
       integer MAX_ORDER, i, n
       parameter (MAX_ORDER = 20000)
       real dot, x(MAX_ORDER), y(MAX_ORDER)
       double precision t1, t2
c
       real serial_dot_product
c
       call timing(t1)

       print *, 'Enter the vector size'
       read *, n
       call read_vector('the first vector', x, n)
       call read_vector('the second vector', y, n)

       do i=1, 1000000
         dot = serial_dot_product(x, y, n)
       enddo
       write (*,*) 'The dot product is ', dot

       call timing(t2)
       write (*,*) 'user+system time=',t2-t1

       stop
       end
c
c ****************************************************************
       subroutine read_vector(prompt, v, n)
       implicit none
       integer i, n
       character *20  prompt
       real  v(n)
c
       print *, 'Enter ', prompt, 'data (return after each entry): '
       do i = 1, n
         read (*,*) v(i)
       enddo
```

```
      return
      end
c
c ************************************************************
      real function serial_dot_product(x, y, n)
      implicit none
      integer i, n
      real  x(n), y(n)
      real  sum
c
      sum = 0.0
      do i = 1, n
        sum = sum + x(i)*y(i)
      enddo
      serial_dot_product = sum

      return
      end
c
c ************************************************************
      subroutine timing (tnow)
      double precision tnow
      real*4 d(2)

      rtnow=etime(d)
      tnow=d(1)+d(2)

c     write (*,*) 'rtnow=', rtnow

      return
      end
```

3.4 Computation of PI

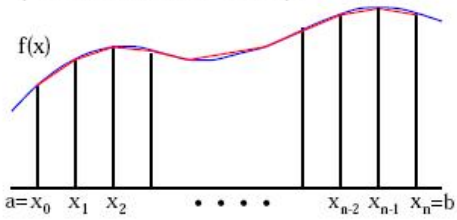
Parallelisation can be achieved based on the split of the integration interval into sub-intervals with each processor computing its part of the integral sum and returning it to the master processor which gathers the result. The sequential code is given by (or you can use the code which you have written during the introduction week) :

```
program compute_pi
      integer n, i
      double precision w, x, sum, pi, f, a
! function
      f(a) = 4.d0 / (1.d0 + a*a)
      print *,‘ Enter number of intervals: ’
      read *,n
! interval size
      w = 1.0d0/n
      sum = 0.0d0
      do i = 1, n
            x = w * (i - 0.5d0)
            sum = sum + f(x)
      end do
```

- Well-known formula:

$$\int_0^1 \frac{4}{1+x^2}\,dx = \pi.$$

- Numerical integration (Trapezoidal rule):



$$\int_a^b f(x)\,dx \approx h[\frac{1}{2}f(x_0) + f(x_1) + \cdots + f(x_{n-1}) + \frac{1}{2}f(x_n)].$$

$$x_i = a + ih, \quad h = (b-a)/n, \quad n = \#\text{ of subintervals.}$$

Figure 2: Computation of π

```
      pi = w * sum
      print *, 'computed pi = ', pi
      stop
end program compute_pi
```

- Time the execution of the sequential code using `CPU_TIME FORTRAN` subroutine (see Intel's FORTRAN reference on the Blackboard).
- Parallelise the algorithm based on the split of the integration interval into n subintervals where n is the number of processes
- Write the following two parallel versions of this program:
  - Version based on the reduction operation `MPI_REDUCE`.
  - Version based on point-to-point communications `MPI_SEND, MPI_RECV`.
  - Each version should calculate the execution using using `MPI_WTIME` function.
- Run these programs interactively on 2 processors.
- Run these programs through the scheduler on 16 processors

3.5 Ping-Pong

- Generate a ping-pong code which exchanges 1000 messages of double arrays of size n, where n is user input, between two processes and measures the total communication time.
- Run the program locally on the Astral master node
- Run the program through the scheduler

- Run the program using explicit hosts specification:

  `mpirun -np <number of processors> <executable>`

- Based on the comparison of the communication time difference between different nodes and on the same node comment on the network speed versus the memory speed.