UBDA Platform

Example for FORTRAN with MPI

User Guide

Version 1.0

16 July 2018

Revision History

Version	Date	Prepared By	Summary of Changes
1.0	Jul 16, 2018		Initial release

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1. Introduction

This document is shown a FORTRAN example by using MPI method running on the UBDA platform.

Note: User should first register a user account through UBDA website at: https://www.polyu.edu.hk/pfs/index.php/177729 to access the UBDA Platform

2. Perform the test

2.1 Login to ubdaplatform.polyu.edu.hk via SSH

2.2 Create the testing directory

```
$ mkdir -p $HOME/mpi_pi_fortran
$ cd $HOME/mpi_pi_fortran
```

2.3 Prepare the FORTRAN program (Filename: mpi_pi.f)

```
program main
      include "mpif.h"
      double precision  PI25DT
      parameter        (PI25DT = 3.14159265358979323846264338327950288419716939937510d0)
      double precision  mypi, pi, h, sum, x, f, a
      integer n, myid, numprocs, i, ierr
      f(a) = 4.d0 / (1.d0 + a*a)

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

 10   if ( myid .eq. 0 ) then
         print *, 'Enter the number of intervals: (0 quits) '
         read(*,*) n
      endif
      call MPI_BCAST(n,1,MPI_INTEGER,0,MPI_COMM_WORLD,ierr)
      if ( n .le. 0 ) goto 30
      h = 1.0d0/n
      sum = 0.0d0
      do 20 i = myid+1, n, numprocs
         x = h * (dble(i) - 0.5d0)
         sum = sum + f(x)
 20   continue
      mypi = h * sum
      call MPI_REDUCE(mypi,pi,1,MPI_DOUBLE_PRECISION,MPI_SUM,0,
     $MPI_COMM_WORLD,ierr)
      if (myid .eq. 0) then
         print *, 'pi is ', pi, ' Error is', abs(pi - PI25DT)
      endif
      goto 10
 30   call MPI_FINALIZE(ierr)
      stop
      end
```

2.4 Load the MPI user environment. You can select OpenMPI with gcc.

For select OpenMPI, use the following:

```
$ module available
----------------- /ubda/apps/modules/modules-
4.1.2/modulefiles -----------------
anaconda3-5.2.0    cuda-9.1                  perl-5.26.1
ansys-17.2-fluent  fsl-5.0.11                python-2.7.15
atlas-3.10.3       gcc-5.5.0                 python-3.6.6
autodock-4.2.6     ips_xe_2018_u3            quantum-
espresso-6.2.1
cmake-3.12.1       mpich-3.2.1-gcc-5.5.0     R-3.5.0
cuda-9.0           openmpi-3.0.1-gcc-5.5.0   singularity-
2.6.0

$ module load openmpi-3.0.1-gcc-5.5.0
$ module list
Currently Loaded Modulefiles:
     1) openmpi-3.0.1-gcc-5.5.0
$ which mpicc
/ubda/apps/openmpi/openmpi-3.0.1-gcc-5.5.0/bin/mpicc
```

For select MPICH, use the following:

```
$ module available
----------------- /ubda/apps/modules/modules-
4.1.2/modulefiles -----------------
anaconda3-5.2.0    cuda-9.1                  perl-5.26.1
ansys-17.2-fluent  fsl-5.0.11                python-2.7.15
atlas-3.10.3       gcc-5.5.0                 python-3.6.6
autodock-4.2.6     ips_xe_2018_u3            quantum-
espresso-6.2.1
cmake-3.12.1       mpich-3.2.1-gcc-5.5.0     R-3.5.0
cuda-9.0           openmpi-3.0.1-gcc-5.5.0   singularity-
2.6.0

$ module load mpich-3.2.1-gcc-5.5.0
$ module list
Currently Loaded Modulefiles:
     1) mpich-3.2.1-gcc-5.3.0
$ which mpicc
/ubda/apps/mpich/mpich-3.2.1-gcc-5.5.0/bin/mpicc
```

2.5 Build the executable binary by using the selected MPI

```
$ mpif90 -o mpi_pi mpi_pi.f
$ file mpi_pi
mpi_pi: ELF 64-bit LSB executable, x86-64, version 1 (SYSV),
dynamically linked (uses shared libs), for GNU/Linux 2.6.18, not
stripped
```

2.6 Prepare the input data file (Filename: input.dat)

```
19
299
3999
49999
599999
6999999
79999999
899999999
0
```

2.7 Prepare the job script file.

For select OpenMPI, use the following (Filename: mpi_pi_f_openmpi.pbs)

```
#!/bin/sh
#PBS -N mpi_pi_fortran_test
#PBS -l nodes=1:ppn=8
#PBS -l walltime=12:00:00
#PBS -q q2s01
#PBS -V
#PBS -S /bin/bash

module load openmpi-3.0.1-gcc-5.5.0

EXEC=mpi_pi
#############################################################
NP=`cat $PBS_NODEFILE | wc -l`
NN=`cat $PBS_NODEFILE | sort | uniq | tee /tmp/nodes.$$ | wc -l`
cat $PBS_NODEFILE > /tmp/nodefile.$$
echo "process will start at : "
date
echo "++++++++++++++++++++++++++++++++++++++"
cd $PBS_O_WORKDIR

mpirun -n $NP --mca blt self,openib $EXEC < input.dat >
result.out


echo "++++++++++++++++++++++++++++++++++++++"
echo "processs will sleep 5 minutes"
#sleep 300
echo "process end at : "
date
rm -f /tmp/nodefile.$$
rm -f /tmp/nodes.$$
module unload openmpi-3.0.1-gcc-5.5.0
```

For select MPICH, use the following (Filename: mpi_pi_f_mpich.pbs)

```
#!/bin/sh
#PBS -N mpi_pi_fortran_test
#PBS -l nodes=1:ppn=8
#PBS -l walltime=12:00:00
#PBS -q q2s01
#PBS -V
#PBS -S /bin/bash

module load mpich-3.2.1-gcc-5.5.0

EXEC=mpi_pi_mpich
#############################################################
NP=`cat $PBS_NODEFILE | wc -l`
NN=`cat $PBS_NODEFILE | sort | uniq | tee /tmp/nodes.$$ | wc -l`
cat $PBS_NODEFILE > /tmp/nodefile.$$
```

```
echo "process will start at : "
date
echo "++++++++++++++++++++++++++++++++++++++++"
cd $PBS_O_WORKDIR

mpiexec -genvall -launcher-exec
"/ubda/apps/tsce/tsce4.1/torque6/bin/pbsdsh_host" -rmk pbs $EXEC
< input.dat > result.out

echo "++++++++++++++++++++++++++++++++++++++++"
echo "processs will sleep 5 minutes"
#sleep 300
echo "process end at : "
date
rm -f /tmp/nodefile.$$
rm -f /tmp/nodes.$$
module unload mpich-3.2.1-gcc-5.5.0
```

Please remind to change the values for your application.

```
#PBS -N mpi_pi_fortran_test {your job name}
#PBS -l nodes=1:ppn=8 {your requested resource;nodes and
processors per node}
#PBS -q q2s01 {the job queue}
EXEC=mpi_pi/ mpi_pi_mpich {your execute file name}
```

Example files can be found at:
/ubda/apps/examples/FORTRAN/

input.dat
mpi_pi.f
mpi_pi_f_openmpi.pbs
mpi_pi_f_mpich.pbs

3 Job submission

3.1 Submit the script (***mpi_pi_c_openmpi.sbatch***) to job queue.
A job ID number will be returned.

```
$ qsub mpi_pi_f_openmpi.pbs
1185.ubda-mgt01
```

3.2 Enquiry the submitted job status.

```
$ qstat -na

ubda-mgt01:
                                                                  Req'd       Req'd       Elap
Job ID                  Username    Queue    Jobname           SessID  NDS   TSK   Memory      Time      S   Time
----------------------- ----------- -------- ----------------  ------ ----- ------ --------- --------- - --------
--
1185.ubda-mgt01         ubdademo9   q2s01    mpi_pi_fortran_test 219882       1      8    --   12:00:00 R
00:00:01
   ubda-d050/0-7
```

Job status field name	Explanation	Example
JOB ID	Unique Job id.	1185.ubda-mgt01
Job name	Name for the job allocation	mpi_pi_fortran_test
Queue name	Name of the job queue that the job has assigned.	q2s01
Username	Your NetID	ubdademo9
S	Job current status. Q = queued R = Job is executing C = Job was completed	Running
ELAP TIME	Time for the job executed	
Req'd Time	The maximum execution time	12:00:00 (1 day)
NDS	Total number of nodes assigned	1
TSK	Total number of cores assigned	8
NODELIST(REASON)	Name of nodes has assigned	ubda-d050/0-7

4 How to check the result

4.1 Check for any error messages for JobID

```
$ more mpi_pi_fortran_test.e1185
Host key verification failed.(know error message can be ignored)

$ more mpi_pi_fortran_test.o1185
Wed Jul 11 15:46:03 HKT 2018
++++++++++++++++++++++++++++++++++++++
++++++++++++++++++++++++++++++++++++++
processs will sleep 5 minutes
process end at :
Wed Jul 11 15:46:04 HKT 2018
```

4.2 Check for result

```
$ wc -l result.out
17 result.out

$ cat result.out
Enter the number of intervals: (0 quits)
pi is   3.1418234938074781     Error is   2.3084021768493557E-004
Enter the number of intervals: (0 quits)
pi is   3.1415935857195603     Error is   9.3212976715051354E-007
Enter the number of intervals: (0 quits)
pi is   3.1415926588007332     Error is   5.2109401238453756E-009
Enter the number of intervals: (0 quits)
pi is   3.1415926536231282     Error is   3.3335112448185100E-011
Enter the number of intervals: (0 quits)
pi is   3.1415926535900298     Error is   2.3669954885008337E-013
Enter the number of intervals: (0 quits)
pi is   3.1415926535897869     Error is   6.2172489379008766E-015
Enter the number of intervals: (0 quits)
pi is   3.1415926535897092     Error is   8.3932860661661834E-014
Enter the number of intervals: (0 quits)
pi is   3.1415926535897700     Error is   2.3092638912203256E-014
Enter the number of intervals: (0 quits)
```

5 Useful Reference

- Manpage for OpenMPI - mpif90
  URL: https://www.open-mpi.org/doc/v3.0/man1/mpif90.1.php

- Manpage for OpenMPI - mpirun
  URL: https://www.open-mpi.org/doc/v3.0/man1/mpirun.1.php

- Manpage for MPICH
  URL: https://www.mpich.org/static/docs/v3.2/

- Command reference for qstat
  URL: http://docs.adaptivecomputing.com/torque/6-0-0/help.htm#topics/torque/commands/qstat.htm?Highlight=qstat