Posted Date: July 7, 2010

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HOW TO COMPILE/EXECUTE ODU TERAFLOPS CLUSTERS "ZORKA"
(in serial and/or parallel modes) ?

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1. From any UNIX computer at ODU (such as stjohn computer), at the system prompt, type:

   ssh -x go-zorka.hpc.odu.edu

   then

   ENTER user's MIDAS password

2. In the user's ZORKA main/root directory, please make sure that you have the .tcshrc file, which contains the following 3 statements:

   source /usr/local/Modules/3.2.6/init/tcsh

   source /opt/intel/fce/10.1.015/bin/ifortvars.csh
   source /opt/intel/impi/3.1/bin64/mpivars.csh

3. go to the following user's SCRATCH directory:

   cd /scratch/nfs/<username>/

   and make sure to have the following 2 "script" files

   submit_mpi ..... for submitting a PARALLEL fortran job
   which contains the following statements:

```
#!/bin/tcsh

#$ -cwd
#$ -pe  impi-smp8x4 4

source /opt/intel/fce/10.1.015/bin/ifortvars.csh
source /opt/intel/impi/3.1/bin64/mpivars.csh

sort $TMPDIR/machines|uniq > ./mpd.hosts

mpirun -r ssh -n $NSLOTS ./a.out
```

Notes: By default, the above " submit_mpi " script file will be submitted with 4 processors (see the above 3-rd statement). However, the user can easily overides this defaul by specifying different number of processors, as will be shown later !

submit_serial ..... for submitting a SERIAL fortran job
which contains the following statements:

```
#!/bin/tcsh

#$ -cwd
#$ -pe  impi-smp8x4 1

source /opt/intel/fce/10.1.015/bin/ifortvars.csh
# urce /opt/intel/impi/3.1/bin64/mpivars.csh

# rt $TMPDIR/machinesluniq > ./mpd.hosts

# irun -r ssh -n $NSLOTS ./a.out
                ./a.out >&! out1
```

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To emphasize, the "&" MUST NOT be used (for example "out1 &") inside submit_serial.
Applications MUST run in the foreground in compute node.
The "&" will result in disassociation of the job/application from its SGE job,
and thus, violate the second policy statement above.

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4. To COMPILE an mpi FORTRAN code (should be done in SCRATCH directory), type:
mpiifort simple_mpi.f

To EXECUTE an mpi FORTRAN code (should be done in SCRATCH directory),
with the default 2 processors, just type:
qsub submit_mpi

To check the MPI job status, type:
qstat

The output of simple_mpi.f will be stored under the fn "submit_mpi.oxxxxxx";
where xxxxxx represents the job ID# (which can be obtained right after
executing the job via the command qsub submit_mpi, or through the command
qstat)

To EXECUTE an mpi FORTRAN code (should be done in SCRATCH directory),
with the user's specified # processors (say, 3 processors), just type:
qsub -pe impi 3 submit_mpi

5. "BEFORE" executing an MPI-fortran parallel job, it may be a good idea
to find out how many processors are still available for you ??, by
typing the following command:

qstat -f -pe impi -U <username>

then observe (as an example) on the computer screen, under column labled "used/tot"

4/4
4/4
0/4
4/4
2/4
3/4
4/4
3/4
4/4

From the above statistical data, we knew that out of a maximum 36 (= 4*9)
processors, there are still 0 + 0 + 4 + 0 + 2 + 1 + 0 + 1 + 0 = 8 processors
available for you !!

6. To COMPILE a SERIAL FORTRAN code (should be done in SCRATCH directory), type:
ifort serial_fortran.f

To EXECUTE a SERIAL FORTRAN code (should be done in SCRATCH directory), type:
(note: the output file will be stored at / redirected to file out1)
qsub submit_serial

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To emphasize, the "&" MUST NOT be used (for example "out1 &") inside submit_serial.
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and thus, violate the second policy statement above.

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7. To be SAFE, your FORTRAN source codes should be stored in your main directory,
with small/limited of space, such as:

cd ~

and, to be EXTRA SAFE, your FORTRAN source codes should be stored
(as backed-up) in the mass storage directory, such as:

cd /ms/<username>/

NOTE: You canNOT submit/execute a (serial, or mpi) fortran job from the
mass storage directory. This should be done in your SCRATCH directory !

8. IF YOU HAVE ANY QUESTIONS ABOUT "ZORKA" COMPUTER CLUSTERS, PLEASE CONTACT:

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For questions related to SERIAL and/or PARALLEL "numerical algorithms", please contact:

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