Practical session with BlueGene / P

The purpose of this exercise is starting a test job with the program NAMD using 512 cores of the IBM BlueGene / P.
Most software packages at the supercomputer of the National Supercomputing Center can be conveniently accessed via a shell variable and using modules.

List of available modules can be obtained by command

module avail

Consider an example of using the program NAMD. From the output of the above command it can be seen that there are three available versions of the program, namely

namd2/2.6 namd2/2.7b1 namd2/cvs20110219 namd2/cvs20110504
Executing:

module help namd2/2.6

one can obtain help about how to use the module. In this case, it is stated that the executable program NAMD2 version 2.6 is available via the shell variable NAMD2_EXE.

Let's run a sample problem with this program. Untar the benchmark case that we downloaded from http://www.ks.uiuc.edu/Research/namd/utilities/apoa1.tar.gz in a directory name of your choice.

For example <dir name> can be $HOME/<number>/test

export TESTDIR=$HOME/<number>/test
mkdir –p $TESTDIR
cd $TESTDIR/
tar zxvf $HOME/apoa1.tar.gz

Change to the apoa1 directory and obtain list of files:

cd $TESTDIR/apoa1
ls

From **$HOME** directory copy the file **namd.jcf,** which describes how to run the task with LoadLeveler (the IBM batch system).
Load modules for namd2/2.6:

module load namd/2.6

Now the path to the program namd2, version 2.6 is in the shell variable NAMD2_EXE.
If you execute the command

echo $NAMD2_EXE

you will see the location of this file, which in this case is in **/bgusr/namd2/2.6/namd2**.
To edit text files we can use text editors nano, jpico, vi or emacs for example. Below we will use the text editor nano. To edit the file named **namd.jcf**, execute:

nano namd.jcf

```
#!/bin/bash
#@ job_type = bluegene
#@ class = n0128
# one of  n0128,n0256,n0512,n1024,n2048
#@ environment = COPY_ALL
#@ wall_clock_limit = 01:00:00
#maximum execution time
#@ error = apoa1.$(jobid).err
#standard output
#@ output = apoa1.$(jobid).out
#standard error
#@ bg_size = 128
#Number of CPUs - 128,256,512,1024, 2048
#@ queue

/bgsys/drivers/ppcfloor/bin/mpirun –exe $NAMD2_EXE –env BG_MAPPING=TXYZ –env COREDUMPDISABLED=1 –np 512 –mode VN -args 'apoa1.namd'
```

Take account of the following:
– lines beginning with *#@* are directives of LoadLeveler, those starting with # are commentaries
– through the command */bgsys/drivers/ppcfloor/bin/mpirun* the parallel application is started on computational nodes of the supercomputer IBM BlueGene / P.
The environment variables are copied from the user's environment. It is important that $NAMD2_EXE be defined.

Options of **mpirun**:
-exe - executable file path
-env - define shell variables that should be visible to the executable
-mode - mode of the use of IBM BlueGene/P nodes - VN, DUAL or SMP (Virtual Node, Dual, SMP).
-args - list of arguments to the executable
-np - number of requested cores –
- from 1 to 4xbg_size (VN mode);
- 2xbg_size (DUAL mode);
- bg_size (SMP mode)

The most important commands of LoadLeveler are:
– **llsubmit <jcf file>** - send a job to the queue
– **llq** - list jobs and their status
– **llcancel <job id>** - delete a job from the queue

For this test we can submit the job:
llsubmit namd.jcf

and check the status:
llq

For the purposes of this practical session we stop the job with **llcancel**, using the JobID that we received from **llsubmit**.

Useful information can be found at: http://www.redbooks.ibm.com/redbooks/pdfs/sg247287.pdf
and http://www.redbooks.ibm.com/redbooks/pdfs/sg246038.pdf