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SUN README

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File name: USING CHPC SUN FUSION

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FILE INFORMATION

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Sunstudio provides compilers and tools for C, C++, and Fortran develpment. Located in >> /opt/gridware/sunstudio12.1/

To set your environment to use sun compilers and MPI that is compiled to run over the infiniband please do the following:

```
module add sunstudio
module add clustertools
```

To set up the environment on use the intel compiler and the MPI compiled to run over the infiniband please do the following:

```
module add intel
```

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LOGIN DETAILS FOR LINUX OPERATING SYSTEM

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```
ssh username@sun.chpc.ac.za (from anywhere in the internet)
ssh username@41.193.29.30(from anywhere in the internet)
ssh username@10.128.15.16 (from e1350 cluster)
ssh username@chpcsun.csir.co.za (from CSIR)
ssh username@146.64.21.24 (from CSIR)
ssh username@196.13.250.16 (from University of Cape Town)
```

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LOGIN DETAILS FOR WINDOWS OPERATING SYSTEM

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USING PUTTY.EXE

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1.open Putty.exe
2.Category: Session
3.Under Host Name or IP address:

sun.chpc.ac.za (from anywhere in the internet)
41.193.29.30 (from anywhere in the internet)
10.128.15.16 (from e1350 cluster)
chpcsun.csir.co.za (from CSIR)
146.64.21.24 (from CSIR)
196.13.250.16 (from University of Cape Town)

4.Port: 22
5.Connection Type: SSH
6.Saved Session: e.g CHPC-SUN
7.Close window on exit: Only on clean exit

8.Click Open
9.login as: your username
10.Password: your password

NB:We will still have to confirm the login details from UCT via SANRen temporaly you can use the internet or first login to the e1350 (ssh username@196.13.250.16) then to the SUN cluster.

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SUN FUSION INFRASTRUSTURE

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1.HARPERTOWN

48x Sun Blade X6250 (2 x Intel Xeon quad core 3.0 Ghz/16GB RAM) Compute blade (48 nodes) running SLES 10 64 bit

2.NEHALEM

144 x Sun Blade X6275 (2 x Intel Xeon quad core 2.93 Ghz/12GB RAM) Compute blades (288 nodes) running SLES 10 64 bit

3.SUN SPARC M9000 [SMP]

M9000-64 SPARC64 VII: Up to 64 CPUs (512 Cores) with each CMU having 128GB RAM running SOLARIS 10

4.VISUALISATION SERVER (VIZ01)

1x Sun Fire X4600 Visualization Node with nVidia QuadroPlex running RHEL 5.1

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SUBMITTING A JOB USING MOAB

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Create a test job

vi test (job name)

include the following in your script (for more info check http://www.clusterresources.com)

To get the defination and more flags of MSUB do a "man msub"

```
=========================================================================================
************************************************
###These lines are for Moab
#MSUB -l nodes=4:ppn=8
#MSUB -l walltime=2:00:00
#MSUB -m be
#MSUB -o /export/home/username/scratch/test/dlpoly.3.07.out
#MSUB -e /export/home/username/scratch/test/dlpoly.3.07.err
#MSUB -d /export/home/username/scratch/test
#MSUB -mb
#MSUB -M username@csir.co.za

##### Running commands
NP=`cat $PBS_NODEFILE | wc -l`
mpirun -np $NP -machinefile $PBS_NODEFILE DLPOLY_3
************************************************
```

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SCRIPT	Description/Notes
#MSUB -a	Declares the time after which the job is eligible for execution. Syntax: (brackets delimit optional items with the default being current date/time):
#MSUB -A account	Defines the account associated with the job.
#MSUB -e	Defines the file name to be used for stderr.
#MSUB -d path	Specifies the directory in which the job should begin executing.
#MSUB -h	Put a user hold on the job at submission time.
#MSUB -j oe	Combine stdout and stderr into the same output file
#MSUB -l string	Defines the resources that are required by the job
#MSUB -m options	Defines the set of conditions (a=abort,b=begin,e=end) when the server will send a mail message about the job to the user
#MSUB -N name	Gives a user specified name to the job
#MSUB -o filename	Defines the file name to be used for stdout.
#MSUB -p priority	Assigns a user priority value to a job
#MSUB -q queue	Run the job in the specified queue (short.q,long.q,graphics.q,serial.q and interactive.q)
#MSUB -r y	Automatically rerun the job is there is a system failure
#MSUB -S path	Specifies the shell which interprets the job script. The default is your login shell.
#MSUB -v list	Specifically adds a list (comma separated) of environment variables that are exported to the job
#MSUB -V	Declares that all environment variables in the msub environment are exported to the batch job.
#MSUB -W	This option has been deprecated and should be ignored.

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submit test:

msub test -q x (where x=nehalem, sparc)

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POST AND PRE PROCESSING

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Please use the following node for post and pre processing:
chpcsp01
chpcsp02

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BG/P README*

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Revision 2 Monday, August 2010
Author: CHPC

Table of Contents:

Overview of the System

The CHPC systems consists of IBM Blue Gene/P:

IBM BlueGeneP

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* Loadlever scheduler.
* 1024 compute nodes + 16 I/O nodes.
* Each compute node contains 2 GB of memory

Logging into the System

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Please make sure you have read and signed the CHPC Use Policies (The file is located in this directory and is named "CHPC Use Policies v0.1.pdf). These policy has to be signed and fax to 021 658-2744.
Chances are you have already done so to get to this point.

LOGIN TO BLUEGENE/P

```
ssh username@bgp.chpc.ac.za
```

A 'df -h' command the following filesystem layout and mount points. For example:

```
          # df -h

Size  Used Avail Use% Mounted on

2.8T  1.7T  1.1T  62% /CHPC/home          :repository for source code, binaries, libraries and small applications
310G   27G  284G   9% /CHPC/usr/local     :repository for system software
91T   85T  6.5T  93% /CHPC/work           :temporary repository , where application are executed and can manage
                                           large files and processing.
```

As per the CHPC agreements, please keep your password private and change it if you suspect it has become know to anyone else.

To change password:

```
#ssh chpcfen (supply your password)
 #username@chpcms:~> passwd
  Changing password for username.
  Old Password:

 New password:
 Re-enter new password:
 Password changed
```

Compiling and Linking

The primary compiler on the Cluster system is the IBM Pathscale compiler which provides methods for 'C', 'C++' and various specifications of Fortran.

IBM BlueGeneP

- Based on GCC 4.1.2: gcc, g++, gfortran
- IBM XL C/C++ Advanced Edition for Blue Gene/P, V9.0.
- IBM Fortran: mpixlf77, mpixlf2003, mpixlf90, mpixlf95

Useful Compiler switches include:

- Optimisation: -O3
- Pre-processor: -F
- Profiling: -g and -gp
- Loop Nest Optimizer: e.g. -LNO:opt=1

A special note for programmers mixing 'C' and Fortran code where the main() function is written in 'C' to link against the pathfortran library using the '-lpathfortran' switch in the link flags.

In general BEST PRACTICE for the cluster system is to use the following:

```
# export FC=pathf90
# export CC=pathcc
# export FFLAGS=□-fno-underscoring□
```

If you run into a problem with double underscoring then use the mvapich*_nsu (no second underscore) library.

[NOTE: see Compiler_Pathscale_C_Fortran_Name_Mangling_Policy.txt for details]

Running Jobs

```
=============================================================================================
=======================================================================
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```

Jobs on the Sun are scheduled by Moab$Torque

Example script for Sun

```
-----------------------

#/usr/bin/ksh
##These lines are for Moab
#MSUB -l nodes=2:ppn=4
#MSUB -l walltime=01:00:00
#MSUB -m be
#MSUB -o /export/home/username/moabtes.out
#MSUB -e /export/home/username/moabtest/moabtes.err
#MSUB -d /export/home/username/moabtest
#MSUB -mb
#MSUB -M user@e-mail.co.za

##### Running commands
nproc=`cat $PBS_NODEFILE | wc -l`
cd /CHPC/work/username/moabtest
/CHPC/usr/local/mpiexec-0.83/bin/mpiexec -n $nproc /CHPC/usr/local/e1350/dlpoly/DLPOLY2.18.X
(EXECUTABLE)

*************************************************************************************************
```

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	Syntax: (brackets delimit optional items with the default being current date/time):
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#MSUB -d path	Specifies the directory in which the job should begin executing.
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#MSUB -N name	Gives a user specified name to the job
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