HPCC - Hrothgar
Getting Started User Guide –
User's Environment

High Performance Computing Center
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User Guide

1. Login Shell

The most important component of a user's environment is the login shell that interprets text on each interactive command line and statements in shell scripts. Each user's login information has a line entry in the /etc/passwd file, and the last field contains the shell launched at login. To determine your login shell, execute:

> *echo $SHELL {to see your login shell}*

Bash is the default and recommended shell. A user can choose to use sh, csh, tcsh and ksh instead. The chsh command is used to change the login shell; instructions are in the man page. Available shells are listed in the /etc/shells file with their full-path. To change your login shell, execute:

> *cat /etc/shells   {select a <shell> from list}*

> *chsh -s <shell> <username> {use full path of the shell}*

Note: We **do not encourage** users to change the default shell, it may cause inconsistency of the user information throughout the cluster.

2. Environment Variables

The next most important component of a user's environment is the set of environment variables. Many of the LINUX commands and tools, such as the compilers, debuggers, profilers, editors, and just about all applications that have GUIs (Graphical User Interfaces), look in the environment for variables that specify information they may need to access. To see the variables in your environment execute the command:

> *env*

The variables are listed as keyword/value pairs separated by an equal (=) sign, as illustrated below by the HOME and PATH variables.

> *HOME=/home/users/*

> *PATH=/bin:/usr/bin:/usr/local/apps:/opt/intel/bin*

PATH has a colon (:) separating list of paths of executables. It is important to realize that variables set in the environment (with command "setenv" for C shells and "export" for Bourne shells) are called "environment variables", and they are "carried" to the environment of shell scripts and new shell invocations, while normal "shell" variables (created with the "set" command) are useful only in the present shell. Only environment

variables are seen in the "env" (or "printenv") command. To see normal shell variables, execute "set" command:

> *set*

Command "export" is used to create environment variables in Bourne shells (bash). For example,

> *export PATH=$PATH:~/bin*

This command adds the directory "bin" in current user's home directory to the variable PATH. The environment variable setting is valid till the user logs out.

3.   Startup Scripts

All LINUX systems set up a default environment and provide administrators and users with the ability to execute additional LINUX commands to alter the environment. These commands are "sourced"; that is, they are executed by your login shell, and the variables (both normal and environmental) as well as aliases and functions are included in the present environment.

Basic site environment variables and aliases are set in

> */etc/cshrc.cshrc* **{C-shell (csh, tcsh), non-login specific}**
>
> */etc/login.csh* **{C-shell (csh, tcsh), specific to login}**
>
> */etc/profile* **{Bourne-type shells (sh, bash, ksh)}**

HPCC has to coordinate the environments on platforms of several systems. In order to efficiently maintain and create a common environment among these systems, HPCC uses its own startup files in /etc/profile.d/. A corresponding file in this etc directory is sourced by the .profile file that resides in your home directory. Please do not remove these files and the sourcing commands in them, even if you are a LINUX guru.
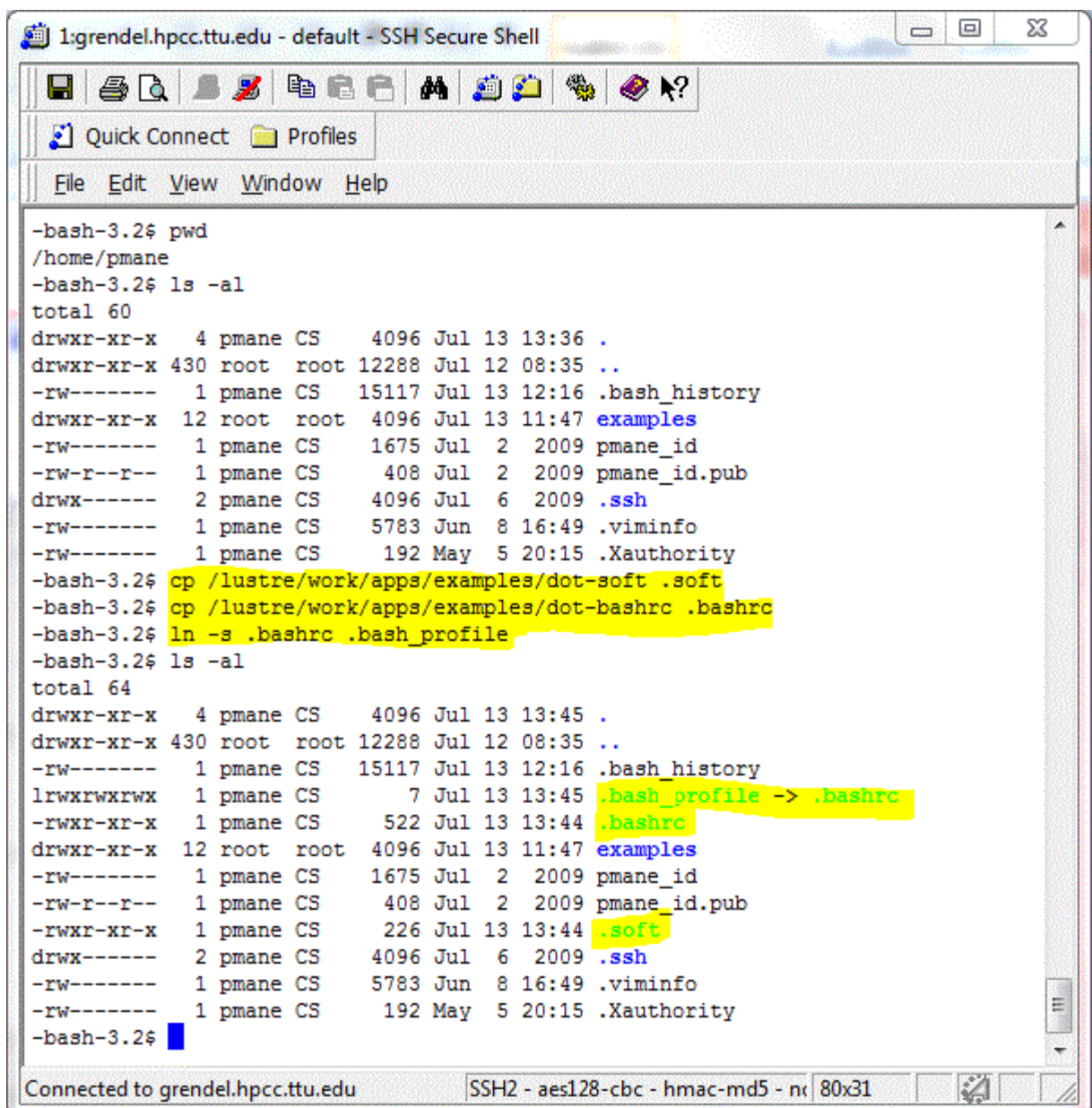
4.   Softenv

HPCC uses the softenv system to set user environments. It is used by Teragrid (https://www.teragrid.org/web/user-support/softenv) and is conceptually similar to the "modules" software used by Ranger and Lonestar. It frees the user from complex and often-changing environment setup in .bashrc, .cshrc, .profile, etc. Its usage is optional but highly recommended. It works for both Bourne shell (sh/bash) and C-shell (tcsh) environments. Custom commands can also be added to both environments outside of softenv.

The major purpose is to set up the execution path $PATH and dynamic link path $LD_LIBRARY_PATH for your choice of compilers, MPI, and applications.

There are example scripts dot-bashrc and dot-soft in Htothgar at: /lustre/work/apps/examples to illustrate the usage. These files are copied to your home directory when your account is created. If they are obsolete due to system upgrade, or messed up, you may copy these to your $HOME/.bashrc and $HOME/.soft respectively:

$ cp /lustre/work/apps/examples/dot-bashrc .bashrc

$ cp /lustre/work/apps/examples/dot-soft .soft

```
1:grendel.hpcc.ttu.edu - default - SSH Secure Shell
 Quick Connect    Profiles
 File  Edit  View  Window  Help
-bash-3.2$ pwd
/home/pmane
-bash-3.2$ ls -al
total 60
drwxr-xr-x    4 pmane CS    4096 Jul 13 13:36 .
drwxr-xr-x 430 root  root 12288 Jul 12 08:35 ..
-rw-------    1 pmane CS   15117 Jul 13 12:16 .bash_history
drwxr-xr-x  12 root  root  4096 Jul 13 11:47 examples
-rw-------    1 pmane CS    1675 Jul  2  2009 pmane_id
-rw-r--r--    1 pmane CS     408 Jul  2  2009 pmane_id.pub
drwx------    2 pmane CS    4096 Jul  6  2009 .ssh
-rw-------    1 pmane CS    5783 Jun  8 16:49 .viminfo
-rw-------    1 pmane CS     192 May  5 20:15 .Xauthority
-bash-3.2$ cp /lustre/work/apps/examples/dot-soft .soft
-bash-3.2$ cp /lustre/work/apps/examples/dot-bashrc .bashrc
-bash-3.2$ ln -s .bashrc .bash_profile
-bash-3.2$ ls -al
total 64
drwxr-xr-x    4 pmane CS    4096 Jul 13 13:45 .
drwxr-xr-x 430 root  root 12288 Jul 12 08:35 ..
-rw-------    1 pmane CS   15117 Jul 13 12:16 .bash_history
lrwxrwxrwx    1 pmane CS       7 Jul 13 13:45 .bash_profile -> .bashrc
-rwxr-xr-x    1 pmane CS     522 Jul 13 13:44 .bashrc
drwxr-xr-x  12 root  root  4096 Jul 13 11:47 examples
-rw-------    1 pmane CS    1675 Jul  2  2009 pmane_id
-rw-r--r--    1 pmane CS     408 Jul  2  2009 pmane_id.pub
-rwxr-xr-x    1 pmane CS     226 Jul 13 13:44 .soft
drwx------    2 pmane CS    4096 Jul  6  2009 .ssh
-rw-------    1 pmane CS    5783 Jun  8 16:49 .viminfo
-rw-------    1 pmane CS     192 May  5 20:15 .Xauthority
-bash-3.2$
Connected to grendel.hpcc.ttu.edu    SSH2 - aes128-cbc - hmac-md5 - n 80x31
```

Softenv only sets environment variables, not executes commands, so there are still some things that should go in .bashrc. An example of the .bashrc file is shown below. The scripts *softenv-load.sh* and *softenv-aliases.sh* tell the system to use softenv. The *ulimit* commands set the proper limits for large parallel program. The optional *PS1* sets your bash command prompt. The *resoft* command makes sure that the system softenv commands, some of which are recursive to cover the permutations of compiler/MPI, get executed. If you don't want to use softenv, omit the first two lines and the "resoft" line. Lines starting with # are comments.

```
. /share/apps/softenv/etc/softenv-load.sh
. /share/apps/softenv/etc/softenv-aliases.sh
 ulimit -s unlimited 1>/dev/null 2>/dev/null
 ulimit -l unlimited 1>/dev/null 2>/dev/null
#set prompt
PS1='`/bin/hostname -s`:`echo $PWD | sed "s=$HOME=="`$ '
#properly set recursive softenv scripts
 resoft
```

The $HOME/.soft file controls the usage of softenv and is identical for bash and csh. Use "+" and the name to load a softenv component. Everyone should load the "+sge" component at the first, and the "@default" at the last. Next, load one of the two compilers and one of the MPI versions. If you don't use MPI at all, you may (unsupported) load more than one compiler as the compiler link name space generally doesn't overlap. You can't effectively load more than one MPI version at all, as they all have the same link name space. Last, load any application software, such as "+nwchem". Like in bash and csh, "#" in the first space is a comment.

```
        #Don't change the first line
        +sge
        #Choice of compilers: intel, gnu
        +intel
        #Choice of mpi versions: openmpi, mvapich2-ge, mvapich2-ib
        +openmpi
        #optional programs: run command soft-list.sh for the complete application list
        +nwchem-5.1
        #Don't change the last line
        @default
```

5. Additional notes

There are some dependencies among the applications and the MPI versions, and some applications have more than one version installed. Users should pay more attention if they are going to use the following applications.

1. The default Intel compile option "+intel" points to the 64-bit 11.1.064 version. If users need 32-bit Intel compiler, use option "+intel-11.1-32" instead.
2. If +gromacs, +nwchem, or +amber are selected, the only mpi option should be +openmpi.
3. If multiple versions of the same applications are installed, the option without a version number points to the latest version. If a user needs to use the version that is not the latest, the option with the version number should be selected. For example, there are two versions of Amber installed, Amber10 and Amber 8. The default option "+amber" and "+amber10" both point to Amber10. Amber 8 users should use the option "+amber8".
4. Some applications require licenses. Users should be responsible for their own licenses. These applications include: Abaqus, Ansoft, Ansys, Cplex, Eclips, FEAP, Fluent, Endyn, HFSS, IDL, LSYNA, Petrel, Schrondinger, Silvaco, VASP etc. For license information, please consult HPCC.
5. For a full list of applications, run command "soft-list.sh".

We also recommend that you link your .bashrc to .profile and source .bashrc in your sge scripts to make sure you get the same environment regardless of login method:

$ cd ~
$ ln -is .bashrc .profile

In SGE script, add this line: . $HOME/.bashrc

There is a script soft-list.sh to list the currently defined softenv environments (execute the actual script for the current list). The environments without a version number (such as +amber) are pointers to a default version (such as +amber10), so version updates are automatic if you use the non-versioned pointers. If you need a particular version, you can specify it. Defaults should only change over system outages unless there is a compelling reason to upgrade.

Soft-list.sh

(@teragrid)
(@default)

(+user_paths)
(+os_paths)
(+sge)
(+sge-6.1u4)
(+intel)
(+intel-11.1-64)
(+intel-11.1-32)
(+gnu)
(+gnu-4.1)
(+matlab)
(+matlab-r2011b)
(+matlab-r2010a)
(+matlab-math)
(+matlab-cs)
(+matlab-bio)
(+nco)
(+nco-3.9.7)
(+starp)
(+starp-2.7.0)
(+fluent)
(+lsdyna)
(+cplex)
(+amplcplex)
(+ansys)
(+ansys12)
(+gromacs)
(+gromacs-mvapich)
(+gromacs-mal)
(+gromacs-4.5.3)
(+END)
(+mpi)
(+openmpi)
(+openmpi-lustre)
(+mvapich)
(+mvapich2-ge)
(+mvapich2-ib)
(+netcdf)
(+nwchem)
(+nwchem-6)

(+nwchem-5.1)
(+nwchem-5.1.1)
(+gnuplot)
(+grace)
(+abaqus)
(+unafold)
(+amber)
(+amber10)
(+amber8)
(+vtk)
(+vtk-5.2.1)
(+mkl)
(+namd)
(+Namd-2.7-b1)
(+Namd-2.7)
(+blast)
(+cluster)
(+java-treeview)
(+espresso)
(+abinit)
(+xanim)
(+lammps)
(+ansoft)
(+gamess)
(+totalview)
(+soap)
(+phylokmer)
(+abyss)
(+R)
(+bowtie)
(+tcoffee)
(+mpiblast)
(+SOAPdenovo)
(+SAMTOOLS)
(+imagemagick)
(+hfss)
(+feap)
(+qiime)
(+vasp)

(+svn)
(+ncl)
(+vapor)
(+cm1)
(+grads)
(+idl81)
(+python)
(+ncview)
(+saga)
(+boost)
(+gams)
(+java)
(+sratoolkit)

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