

Introduction to Unix

Remote Access

- Telnet/SSH/rlogin
 - Telnet software on PC's usually has a 'Connect' option in the menu
 - Telnet software on Unix systems may run from the command line
 - telnet hostname
 - You will need to provide your username and password
 - SSH – secure shell, may be required for some systems
- X terminal emulation
 - Allows graphical windows to be displayed on the local machine (moe -X11 can be used to run moe this way)

Exercise 1

- Find telnet software on the PC you are sitting at and login to one a unix system (ours if you have accounts, UT systems if they allow remote access)
- Our systems should all require SSH access – you may need to download software – I use PuTTY (easily found by most internet search engines)

File Transfer

- Network File System (NFS)
 - Our SGI's are interconnected by NFS – files can be directly copied between mounted drives
 - Several PC's in my lab run NFS Maestro Solo, which allows the SGI drives to be associated with a free drive letter on the PC – files can be directly copied
- File Transfer Protocol (FTP)
 - On PC's, FTP software is usually menu-driven. You connect to a remote host and can copy files in either direction
 - On Unix systems, FTP software is generally run from the command line
 - ftp hostname
 - get file
 - mget files* } from remote host to local host
 - put file
 - mput files* } from local host to remote host
 - In either case you will provide your username and password
 - Computers that require secure logins may also require secure ftp (sftp) – available with PuTTY

Unix Commands (file manipulation)

- ls – file listing (current directory by default)
- more xx – file display
- cat xx – file display (not graceful with binary files)
- cp xx1 xx2 – copy file xx1 to xx2
- mv xx1 xx2 – move file xx1 to xx2 (basically rename)
- rm xx – remove file xx
- grep y xx – find pattern y in file xx
- tar xx – tape archiver (rolls multiple files into 1 for easy compression/backup)
- compress xx – compress file xx to make xx.Z
- uncompress xx.Z – uncompress file xx.Z to make xx

Unix Commands (directory structure)

- cd xx – change directory to xx
 - relative path: xx=subdirectory of current working directory (example, I have subdirectory EDG5 in /usr/people/aparrill/EDG5 so xx can be EDG5 if I am in my home directory)
 - absolute path: xx=path from root (example, I would let xx be /usr/people/aparrill/EDG5 if I were not in my home directory)
- mkdir xx – make directory xx
- rmdir xx – remove directory xx
- ~ - refers to your own home directory
- ~user – refers to the home directory of user

Unix Commands (system information)

- pwd – print working directory
- top - continuous display of most CPU-intensive processes currently running (q to quit)
- ps – list active processes
- du xx – disk usage for file/directory xx
- df – directory of filesystems
- who – who is logged in to system
- whoami – user logged in to session
- man xx – manual pages

Exercise 2

- How many processors are in use on your remote system?
- How many processors are available to run new jobs?

Unix Commands (miscellaneous)

- * - wildcard character
- > - redirect standard output
 - ls > directory.log will put listing of directory contents in file called directory.log
- >& - redirect standard output and standard error messages (required when using MOE in batch mode)
- & - run command in background
- | - pipe results of one command through another
 - ps | grep user will list only processes that include user
- chmod – change file permissions (see man page for details)

Personalizing the Unix Environment

- Important Files
 - .login – viewed by system at login, allows some personalization of the system
 - .cshrc – viewed by system when new shell is invoked, also allows some personalization of the system
- Common Changes
 - alias com command – make a long command shorter
 - setenv XXX xx – define environment variables used by various software packages

Editing Text Files

- User-friendly text editors
 - nedit
 - jot
 - MOE's text editor
- High-functionality text editors
 - vi
 - emacs

Exercise 3

- Define an alias in your .cshrc file (if you don't know one you want, define mine so that you get a listing of processes you are running)

Shell Scripting

- Shell scripts are executable files (use `chmod +x file` to make executable) containing shell commands
- Example:

```
starts a new c shell      #!/bin/csh
starts loop, defines variable called file  foreach file (*.gpf)
runs a command, :r removes extension     autogrid -p $file -l $file:r.glg
ends loop                  end
```

- Shell scripts are run by typing their names at the command line

MOE Scripting

- Moe can be run interactively (as we have done in class) or in batch mode
 - Interactive invoked by `moe`
 - Batch invoked by `moebatch`
 - default is to allow typed commands
 - `-script` option allows commands to be read from moe script file

Example MOE Script

```
pot_Load '/usr/local/moe/lib/mmff94.ff':
PotSetup [solEnable:1, solDielectric: 80.0];

Open 'EDG5Frot_S1P18.moe':
MM [sd_maxit:100, sd_gtest:1000, cg_maxit:100, cg_gtest:100, maxit:1000,
gtest:0.001, maxstep:1, tetherWeight:0 ];
SaveAs 'EDG5Frot_S1P18_min.moe';
Close [];

Open 'EDG5Frot_S1P31.moe':
MM [sd_maxit:100, sd_gtest:1000, cg_maxit:100, cg_gtest:100, maxit:1000,
gtest:0.001, maxstep:1, tetherWeight:0 ];
SaveAs 'EDG5Frot_S1P31_min.moe';
Close [];
```

Finding Other MOE Commands

- MOE → Help → Function Index
 - Provides listing of MOE functions
 - `aXX` refers to operations on atoms
 - `rXX` refers to operations on residues
 - `cXX` refers to operations on chains
 - Others often common sense
 - Selecting a MOE function will give details on expected arguments and syntax

Exercise 4

- Identify a computation in MOE that you might want to perform repetitively (other than minimization)
- Find the function associated with that computation in the help pages
- Compare the listing of arguments to the dialog box that interactive MOE provides when you run the command
- Type the command as you might want to use it (you only need to include arguments if you don't want to use their default value)
- Ask me to check it for you