

Brief Introduction to Facility Workstations

Files and Directories:

- File names are case sensitive and the characters " ' ` ? < > () { } [] * & \$: ; | \ / and space should be avoided.
- One dot (.) corresponds to the current directory, two (..) to the parent directory.
- All directories are somewhere under the root directory "/", and are hierarchical: /bin is in the root directory, /usr/local/bin is another directory two levels down.
- User home directories are mounted from the facility file server over the network, and can be accessed from any of the workstations.

Simple Commands:

(all file and directory names below can also include the path to the file e.g. "<dir>" can be "../calcs/gauss/water" or "/usr/bin/X11")

pwd = print working directory, displays current directory

cd <dir> = change working directory to <dir>, if <dir> is blank, change to user home directory.

ls [name] = list contents of current directory, or optionally the directory or file [name].
Several useful arguments: -l = long list; -a = show all files including hidden (.something)

man <command> = shows the user's manual for <command>

cat <file1> [file2] ... = concatenate and show file1 [and file2 ...] contents

cp [-r] <infile> <outfile> = copy <infile> to <outfile>, works recursively on directories with -r option

mv [-r] <infile> <outfile> = move or rename a file [or directory with -r]

rm [-r] <file> = remove a file [or directory with -r]

mkdir <dir> = makes new directory <dir>

rmdir <dir> = removes directory <dir>, but only if empty

grep "some text" <file> = finds lines in <file> that contain "some text"

Utilities:

less <file> = file viewer, type "q" to quit

gvim = graphical version of vim, the text editor

bc = calculator in terminal

xcalc = calculator in window

top = shows process list and system info, type "q" to quit

Applications:

gv = starts GaussView interface to Gaussian03

spartan = starts Spartan interface

vmd = starts VMD

maestro = starts Macromodel interface

ebuilder = graphical molecule builder