Introduction to Computational Quantum Chemistry

Introduction to Unix

Martin Novák, simplified by JN (NCBR)

Very brief introduction to Unix

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- Developped in 1970s in C language
- Open source code
- Multiuser system

Case-sensitive system

- Many distributions developped since:
 - Ubuntu
 - Debian
 - BSD
 - Fedora
 - ...

Cluster Wolf

• Scientific software administrator: RNDr. Petr Kulhánek, PhD.

https://einfra.ncbr.muni.cz/whitezone/root/index.php?lang=enaction=ncbr show=wolf



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Superuser

- Administrative privileges
- Can edit system files
- User
 - Cannot edit system files
 - Only selected items are editable/accessible
 - Belongs to certain groups with respective rights (hardware/software access...)

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- No "Windows-like" discs
- Everything mounted under "/" (root) directory
- Slash sign is used as separator between directories
- Important paths:
 - /home/username/ or "~": Quota 1.5 GB, backed-up
 - /scratch/username/: No quota, NOT backed-up
 - /media/filesystem/: USB sticks, DVD discs...
- Everything is either *file* or *process*
- Arbitrary suffixes for files

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General advices aka "Good-To-Follow" rules:

- Case-sensitive system
- Do NOT use spaces in filenames (use underscore or dash)
- Good characters:
 - Alphanumerics

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- Forbidden characters:
 - Any kind of diacritics
 - Quotation marks
 - Brackets

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- Found in Applications \rightarrow Accessories \rightarrow Terminal
- Shell interpreter translating written commands into actions
- Cygwin, PuTTY: Terminal emulators for Windows machines
- Pros:
 - Fast and effective way of work
 - Directly visible output from operation
 - Error tracking
 - No GUI needed
- Cons:
 - Need of memorizing commands

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Command	Action			
cd foo	Change current working directory to "foo"			
ls	List files in directory			
<i>cp</i> source target	Copy source file to target file			
cp -r source target	Copy source directory recursively into target			
mv source target	Move source file to target file			
mkdir foo	Create "foo" directory			
<i>rmdir</i> foo	Remove ^a "foo" directory (only if empty)			
<i>rm</i> foo	Remove ^a "foo" file			
<i>rm</i> -r foo	Remove ^a "foo" directory recursively			
<i>cat</i> foo	Print content of a "foo" file into terminal			
<i>grep</i> foo file	Print only line containing "foo" keyword in "file"			
top	See currently running processes			
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^a Removing means deleting from the disc. **NOT** moving into trash.

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Command	Action
head -n number foo	Print first "number" rows of "foo" file
<i>tail</i> -n number foo	Print last "number" rows of "foo" file
<i>echo</i> foo	Prints "foo" into terminal
printf	Similar to echo but handles formatted text
chmod switch foo	Changes rights of "foo" file according to switch
quota	Prints current quota of user and disc usage
<i>ssh</i> user@host	Remote access to host machine
exit	Logout from the terminal
who	Prints all users logged into machine
passwd	Change current pasword
kill PID	Kill the process with number "PID"
ps	Print all current processes running in terminal
module	Accessing the scientific software

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- Use ArrowUp and ArrowDown for searching the command history
- Use Tabulator for word completion
- Copy/Paste from terminal using mouse (CTRL+c/CTRL+v does NOT work here)

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Wild characters

Notation	Matches
*	Any string of characters including empty string
?	Any single character
[jklm.]	Single character j, k, l, m or a dot
[a-m]	Single character from range a to m
[2-9]	Single number from range of 2 to 9

- Example:
- \$ *ls* a*[0-2].??[df] This command will print all files which:
 - Start with "a"
 - Then they have any string of characters
 - Then there is either 0, 1, or 2
 - Followed by a dot
 - Then any two characters
 - Last character is either "d" or "f"
- All conditions must be satisfied

Listing and killing processes

- Once command is run, it obtains a unique process ID (PID)
- \$ top
 # Displays currently running jobs in real time
- \$ kill PID # Kills process with a given PID
- \$ kill -9 PID # Kills process (Signal cannot be blocked)

martin@debian: ~/Documents _ 💷 🗙										
File I	Edit View	Search	Terminal	Help						
mnovak	<@wolf15:~,	/test\$	top							
top -16:40:23 up 9:09, 1 user, load average: 0.00, 0.01, 0.05 Tasks: 119 total, 1 running, 118 sleeping, 0 stopped, 0 zombie Cpu(s): 0.0%us, 0.3%sy, 0.0%ni, 99.7%id, 0.0%wa, 0.0%hi, 0.0%si, 0.0%st Mem: 2032876k total, 1035056k used, 997820k free, 89876k buffers Swap: 4194300k total, 0k used, 4194300k free, 716420k cached										
PID	USER	PR N	I VIRT	RES	SHR	S %CPU	%MEM	TIME+	COMMAND	
	mnovak							0:00.08		
7678		20 (9128	1136	852			0:00.07	top	

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- With graphical interface:
 - gedit
 - kate
 - kwrite
 - gvim
- Without graphical interface (editing in terminal):
 - vi / vim
- Programmed to highlight keywords of many languages/source codes

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- Fast and effective way to edit files in remote machine
- 3 modes:
 - Command mode
 - Edit mode
 - Visual mode
- Enter command mode via ESC key
- Enter edit mode via Insert or "i" key
- Visual mode for editing blocks of text:

http://vimdoc.sourceforge.net/htmldoc/visual.html#Visual

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Commands of editor vi

Command	Action
:w	Save document
:w filename	Save document as "filename"
:q	Quit document
:q!	Quit without saving
:wq	Save and quit
:u	Undo
i / insert	Enter edit mode
R	Enter replace mode
gg	Go to the beginning of the document
G	Go to the end of the document
dd	Delete current line
25D	Delete next 25 lines
dG	Delete all lines starting from cursor
/keyword	Search for keyword

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• Writing a plain text file:

- \$ vi test.dat Open 'test.dat' file for editing
- i / insert Enter editing mode

Write some text

- ESC exit editing mode and enter command mode
- :w Write text to file
- gg Go to first line
- 2D Delete two lines
- :u Undo last change
- :wq Write and quit
- \$ rm test.dat Remove file

- Accessing remote machine via ethernet or internet
- *ssh* command:
- \$ ssh [username@]hostmachine
- username does not have to be specified if same as current login
- If X applications should be exportable, use "-X" switch

- Access the wolf node next to yours with X server export enabled
- Find out who is logged in there
- Exit from this computer
- Help: here

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Passwordless authentication within cluster

- No password required for access the host machine
- Should be used with great care only on local networks
- Procedure:
 - \$ cd .ssh
 \$ ssh-keygen
 <enter>
 <enter>
 \$ cat id rsa.pub » authorized keys
- Try to remotely access the same machine

Copying files between machines

• \$ scp source target

- Source and/or target can be on remote machine:
- mnovak@wolf12:~\$ scp text.dat wolf13:/scratch/mnovak/
- mnovak@wolf12:~\$ scp -r wolf13:/scratch/mnovak/ directory/

• \$ mc

- Midnight commander same as in Windows/Mac machines
- "Graphical interface"
- \$ gftp
 - "Real" graphical interface

Absolute versus Relative paths

- Absolute path:
 - Total path from the root directory
 - /scratch/mnovak/test
 - ~/Documents/
- Relative path:
 - ./ # Current directory
 - ../ # Parent directory
 - ../../../data/test/

Access permissions

- Each file has permissions for Owner, Group and Others
- drwxrwxrwx
 - d Directory
 - r Read
 - w Write
 - x Execute
 - Permission not granted

martin@debian: "/Documents U ×						
File Edit	View Search	Terminal	Help			
total 56K drwxr-xr- drwxr-xr- -rw-rr- -rwxrr- -rw-rr- -rwxr-xr-	x 2 mnovak x 73 mnovak - 1 mnovak - 1 mnovak - 1 mnovak x 1 mnovak	nmr 4.0K nmr 12K nmr 201 nmr 1.1K nmr 74 nmr 17K n <u>m</u> r 5.2K	Mar Mar Mar Mar Mar Mar	4 15:09 4 15:09 4 15:09 4 15:09 4 15:09 4 15:09	 aimextractor.awk beta_master.sh	

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- \$ *chmod* switch file
- examples of switches:
 - u+x User can execute file
 - go+w Group members and others can write to file
 - a-r Remove right to read for all users
 - o-rwx Remove right to read, write and execute to others

- Create in your home folder directory folder01
- Copy current pdf presentation and *.tex from address wolf01:/share/ivavik/novotnyj/teaching to your newly created directory, try to open it from terminal using evince, make it readable for all users
- Using vi editor create a plain text file called **prop.txt** and insert inside complete info about the pdf file based on Is output
- please store all subsequent working commands in this prop.txt file (use another terminal window for easier copying)

- Study the manual info about *pdfjam* tool for manipulating pdf files and generate a new pdf file containing first 4 slides in landscape orientation (**pres4.pdf**)
- run simple command in terminal and inspect its function: for ((i=1; i<30; i++)); do head -n\$i 01.tex | tail -1 > \$i.tex; done
- remove all .tex files whose index ends 0 or 5
- create folder your_username a move there .tex files and prop.txt with inserted commands for the entire excercise
- copy recursively the folder your_username to wolf01:/share/ivavik/novotnyj/teaching