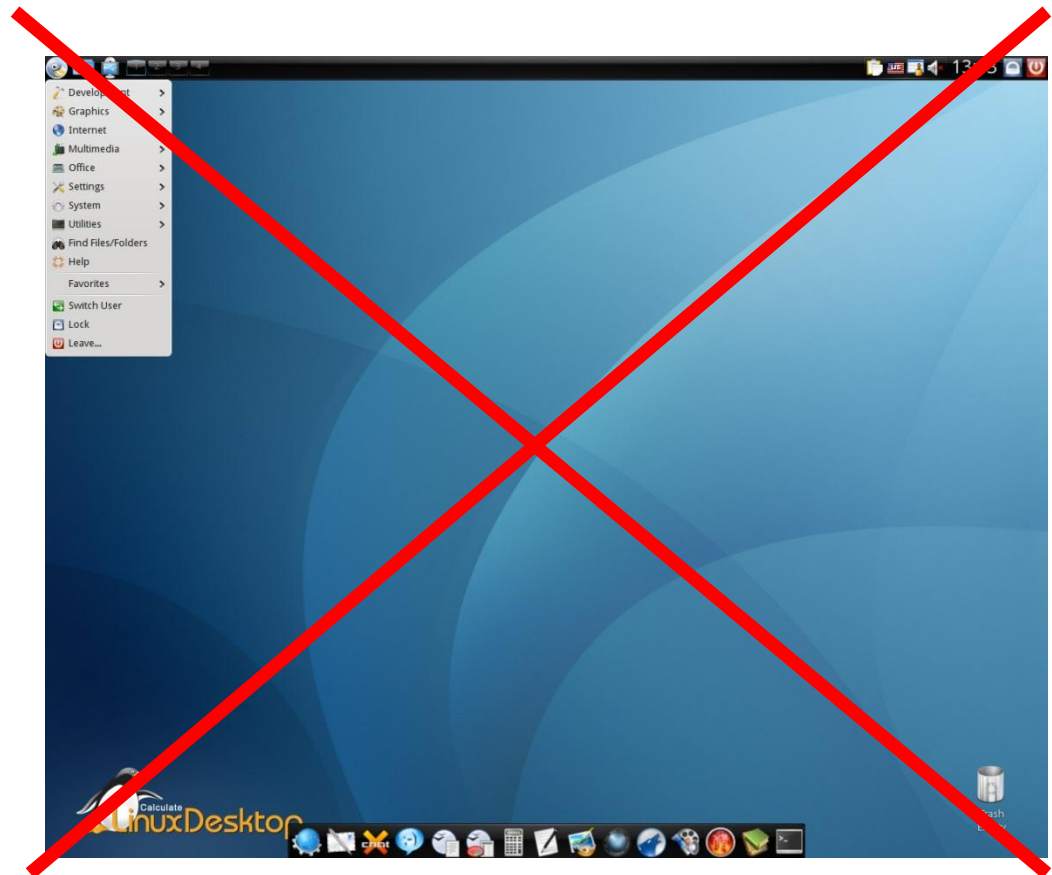
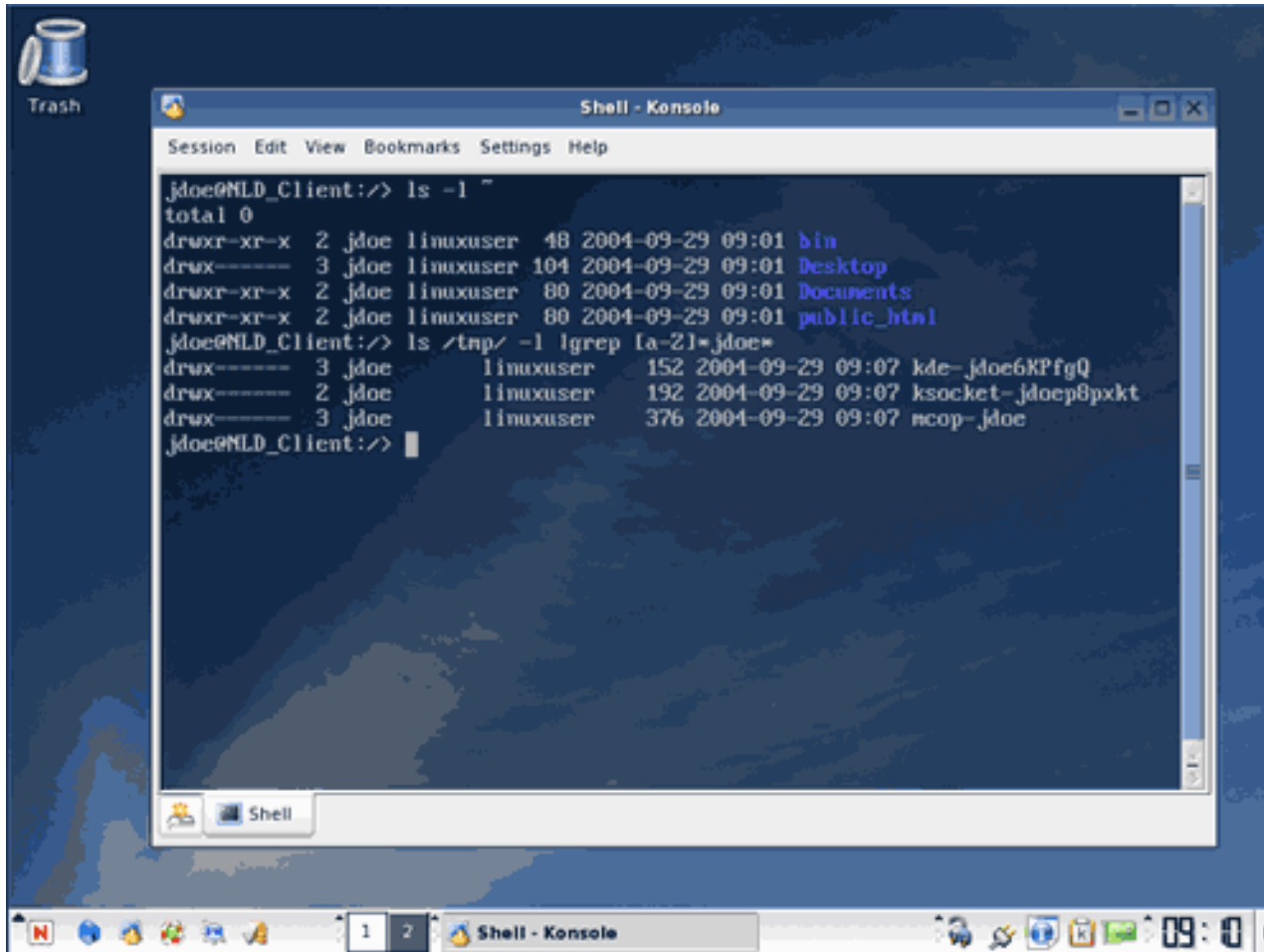


# Introduction to Linux Environment

Yun-Wen Chen



# The Text (Command) Mode in Linux Environment



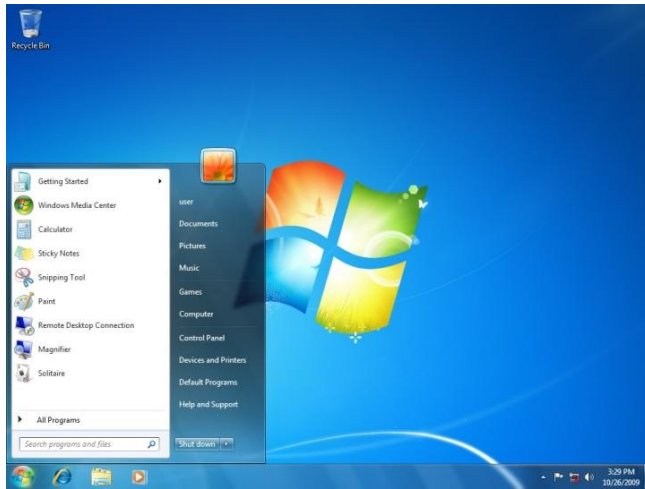
The screenshot shows a Linux desktop environment with a blue background. In the top-left corner, there is a 'Trash' icon. A terminal window titled 'Shell - Konsole' is open, displaying the following commands and output:

```
jdock@MLD_Client:~$ ls -l ~
total 0
drwxr-xr-x  2 jdock linuxuser  48 2004-09-29 09:01 bin
drwx----- 3 jdock linuxuser 104 2004-09-29 09:01 Desktop
drwxr-xr-x  2 jdock linuxuser  80 2004-09-29 09:01 Documents
drwxr-xr-x  2 jdock linuxuser  80 2004-09-29 09:01 public_html
jdock@MLD_Client:~$ ls /tmp/ -l |grep [a-zA-Z]*jdock*
drwx----- 3 jdock linuxuser 152 2004-09-29 09:07 kde-jdock6KPfgQ
drwx----- 2 jdock linuxuser 192 2004-09-29 09:07 ksocket-jdock8pxkt
drwx----- 3 jdock linuxuser 376 2004-09-29 09:07 ncop-jdock
jdock@MLD_Client:~$
```

The terminal window has a menu bar with 'Session', 'Edit', 'View', 'Bookmarks', 'Settings', and 'Help'. The desktop taskbar at the bottom shows several icons, including a network icon, a clock showing 09:00, and a 'Shell - Konsole' window icon.

# The Main Operating Systems We May Meet

## 1. Windows



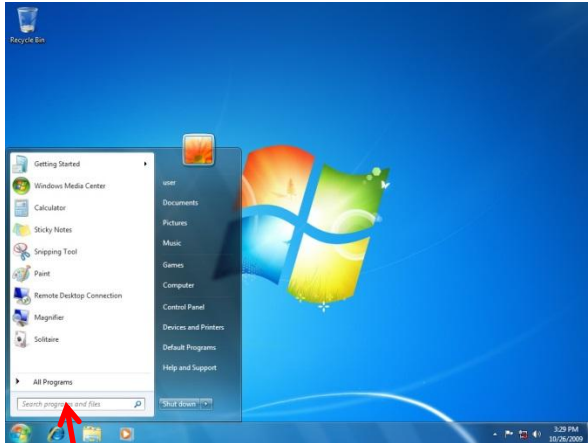
## 2. Mac



### 3. Linux (Unix)



# Windows Command Mode and DOS



Type "cmd" at here



```
Administrator: cmd
Microsoft Windows [Version 6.2.9200]
(c) 2012 Microsoft Corporation. All rights reserved.

C:\Windows\system32>sfc /scannow

Beginning system scan. This process will take some time.

Beginning verification phase of system scan.
Verification 100% complete.

Windows Resource Protection did not find any integrity violations.

C:\Windows\system32>_
```

# Windows Command Mode and DOS

DOS (before 1992)

```
A:\>dir /w

Volume in drive A has no label
Volume Serial Number is B83C-98D8
Directory of A:\

AM2100.DO_   AVEXTRA.TXT   COMDEV.IN_   DEPCA.DO_   E20ND.DO_
E21ND.DO_   ELNK.DO_      ELNK16.DO_   ELNK3.DO_   ELNK11.DO_
ELNKMC.DO_   ELNKPL.DO_    EXP16.DO_    EXPAND.EXE   I82593.DO_
IBMTOK.DO_   IFSHLP.SY_    LICENSE.TXT   LM21DRV.UP_  MSDLC.EX_
NDIS39XR.DO_ NDISHLP.SY_    NE1000.DO_   NE2000.DO_   NET.EX_
NET.MS_      NETBIND.COM    NETH.MS_     NI6510.DO_   NWLINK.EXE
OEMDLC.INF   OEMODI.IN_     OEMRAS.IN_    OEMTCPIP.INF OLITOK.DO_
PE2NDIS.DO_  PENDIS.DO_     PRO4.DO_      PRORAPM.DW_  PROTMAN.DO_
PROTMAN.EX_  RASCOPY.BA_    README.TXT    SETUP.EXE     SMCMAC.DO_
SMC_ARC.DO_  STRN.DO_       TLNK.DO_      WCNET.INF     WCSETUP.INF
WCSYS.INI    WORKGRP.SY_

          52 file(s)          1,130,630 bytes
                                   312,832 bytes free

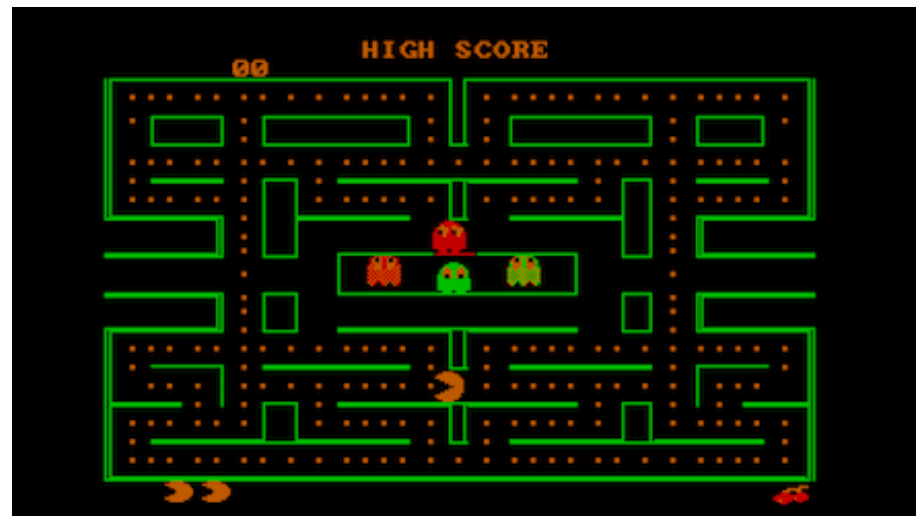
A:\>
A:\>
A:\>
A:\>
```

Common command:

dir, cd, del, rd, erase, format, fdisk, print, ren, chkdsk

Of course, you can run programs, games in it...

Like...



# Mac Command Mode



However, I am not a Mac user, I can not introduce you the great details of command mode in Mac.

But I know Mac can open a command mode window (terminal) to login into a remote workstation. (usually in linux)

```
jim — bash — 102x19
Last login: Tue Sep 25 12:52:00 on console
Jim-Hoskinss-iMac:~ jim$ ls -l ~
total 0
drwx-----+ 7 jim  staff   238 Sep 25 12:57 Desktop
drwx-----+ 4 jim  staff   136 Sep 25 12:50 Documents
drwx-----+ 4 jim  staff   136 Sep 25 12:50 Downloads
drwx-----+ 31 jim  staff  1054 Sep 25 12:53 Library
drwx-----+ 3 jim  staff   102 Sep 25 12:50 Movies
drwx-----+ 3 jim  staff   102 Sep 25 12:50 Music
drwx-----+ 4 jim  staff   136 Sep 25 12:50 Pictures
drwxr-xr-x+ 5 jim  staff   170 Sep 25 12:50 Public
Jim-Hoskinss-iMac:~ jim$
```

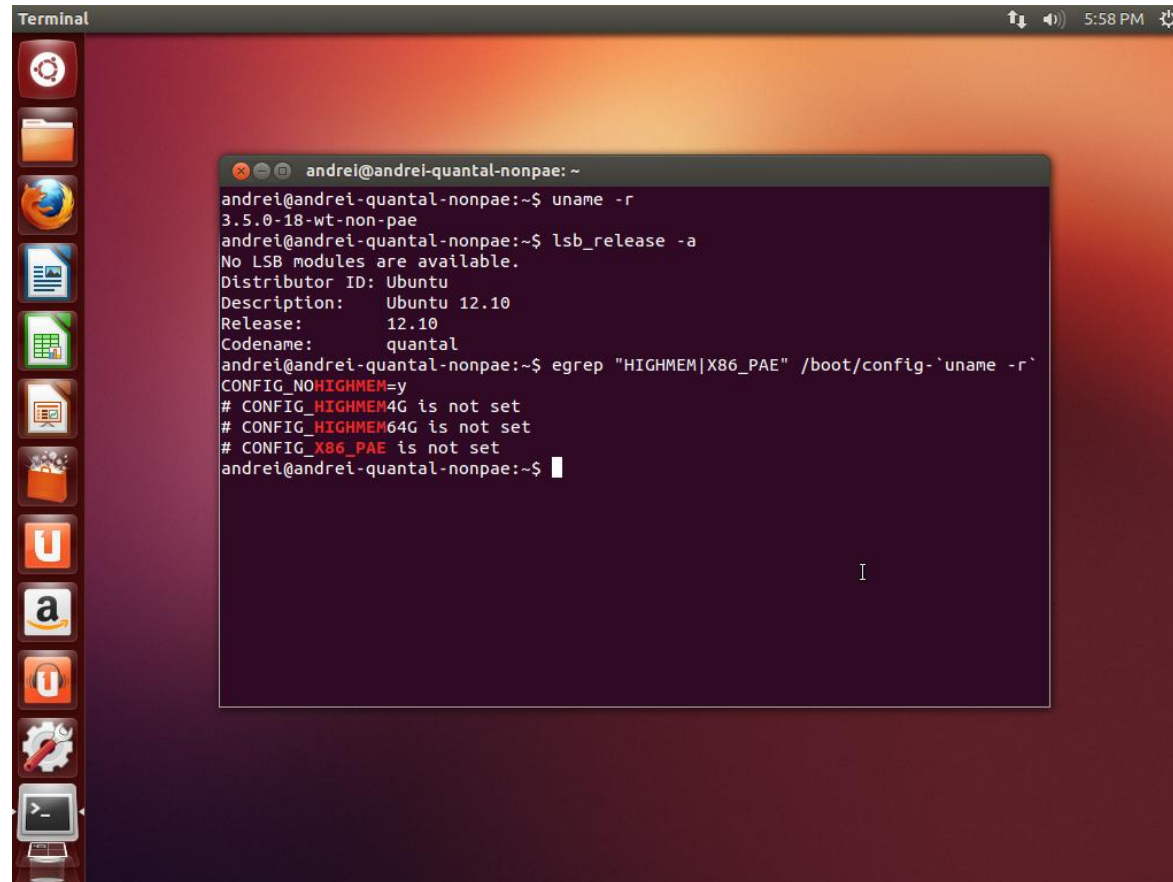


# Linux Command Mode

If you are a Linux user, you will be very familiar with the Linux commands in work station.

Many computational scientists install Linux on their PC. However, the library and drivers are much harder to be found for executables than in windows and Mac.

Example  
(Ubuntu)

A screenshot of an Ubuntu desktop environment. The desktop background is a dark red gradient. On the left side, there is a vertical dock with several application icons: Dash, Home Folder, Firefox, LibreOffice Writer, LibreOffice Calc, LibreOffice Impress, LibreOffice Draw, LibreOffice Base, LibreOffice Math, LibreOffice Remote, LibreOffice Template Gallery, LibreOffice Start Center, and the Dash icon. A terminal window is open in the center of the screen, displaying the following text:

```
Terminal
andrei@andrei-quantal-nonpae: ~
andrei@andrei-quantal-nonpae:~$ uname -r
3.5.0-18-wt-non-pae
andrei@andrei-quantal-nonpae:~$ lsb_release -a
No LSB modules are available.
Distributor ID: Ubuntu
Description:    Ubuntu 12.10
Release:        12.10
Codename:       quantal
andrei@andrei-quantal-nonpae:~$ egrep "HIGHMEM|X86_PAE" /boot/config-`uname -r`
CONFIG_NOHIGHMEM=y
# CONFIG_HIGHMEM4G is not set
# CONFIG_HIGHMEM64G is not set
# CONFIG_X86_PAE is not set
andrei@andrei-quantal-nonpae:~$
```

Click here 



# Linux Commands

Linus Commands		DOS Counterpart
ls	List directory contents	dir
cd	Change directory	cd
mkdir	Make a new directory	md
rmdir, rm -r	Remove a directory	Rd
pwd	Display directory location	chdir
rm	Remove a file	del
cp	Copy a file	Copy
mv	Rename/move a file	rename, move
grep	Look for a word in files given in command line	Find
cat	Dump contents of a file to users screen	type
more	Pipe output a single page at a time	more

More you can find on website:

[http://www.yolinux.com/TUTORIALS/unix\\_for\\_dos\\_users.html](http://www.yolinux.com/TUTORIALS/unix_for_dos_users.html)

<http://www.linuxdevcenter.com/cmd/>

# How to Login into a Linux System (Workstation)

## 1. Linux and Mac

Open a terminal and then type :

```
ssh (-l -X) username@workstation
```



You may need

Username:

Workstation:

Password:

## 2. Windows (7)

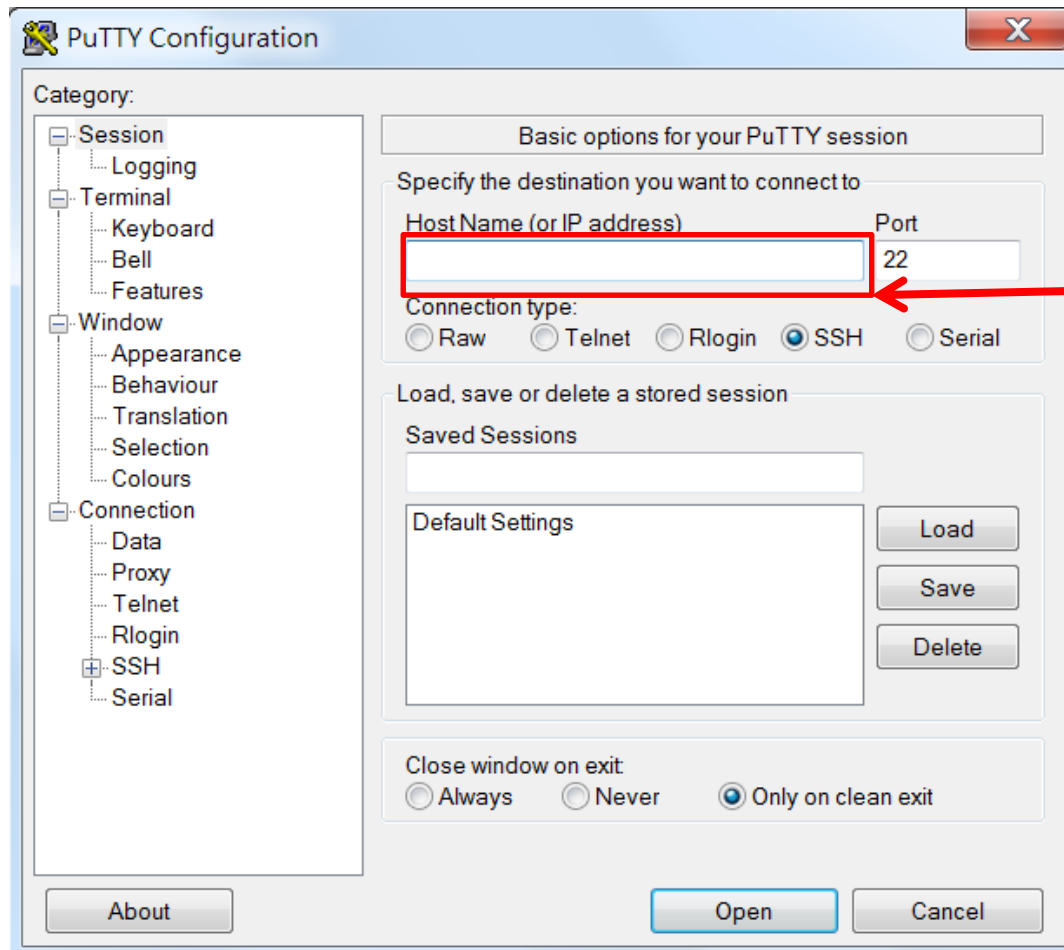
You need to install a windows interface to login  
And also type the same (similar) command of above

Two windows interface you may install:

1. Putty (<http://www.chiark.greenend.org.uk/~sgtatham/putty/download.html>) (smaller, but without X-window)
2. MobaXterm (<http://mobaxterm.mobatek.net/>) (larger, with X-window)

In the following, I am going to use putty to introduce something in Linux.

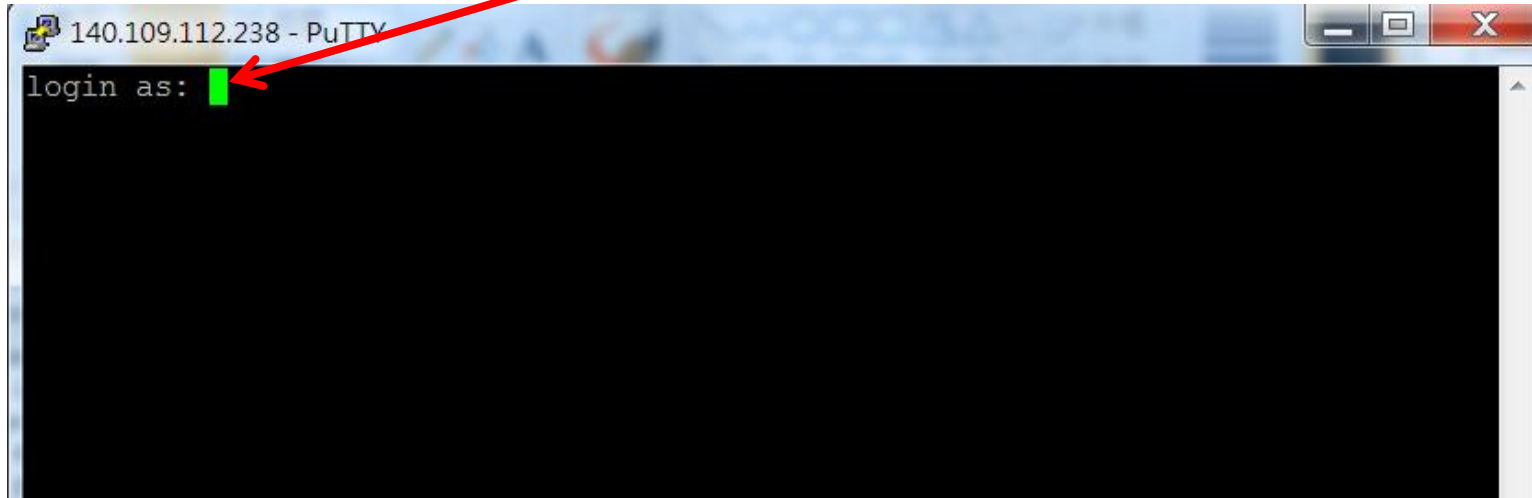
# How to Login into a Linux System (Workstation)



Here type in the  
workstation name

# How to Login into a Linux System (Workstation)

Here type in the user name, and then type in the password



# More Things about Linux

- In Linux, you also can run programs, games like in Windows. Of course, we are not going to talk about games here. The program we are going to run in the next few weeks is VASP. Other simulation programs like gaussian, Siesta, could also be run in Linux.
- However, as mentioned, before you install some software, you may need to find proper libraries for installing it (like VASP) by yourself.
- In Linux, you can also install C++, Fortran (and others) compilers to compile the codes you have.
- Why we need to use Linux? Because: 1. In workstations, the computational jobs can run in parallel to shorten the time needed for large jobs. 2. In Linux, you need to (can) deal with the input, output files directly; you don't get blind by the convenient windows interface.

# Practice in Linux System

`cd /lustre/lwork/tigp/Teach-2015-spring/`

Please don't go to User0 and change things inside.

`mkdir name` Create a practice directory with the **name** you like

`cp -r /User0/* name` Copy the files to your practice directory.

`cd name` or `Go to your practice directory.`  
`/lustre/lwork/tigp/Teach-2015-spring/name/`

`ls` List directory contents

`cd VASP-Graphene`

`pwd` Display directory location

# File System in Linux System

Type "ls -l"

```
[tigp@c238-1 lwork]$ cd tigp/Teach-2015-spring/
[tigp@c238-1 Teach-2015-spring]$ ls
User0
[tigp@c238-1 Teach-2015-spring]$ cd User0/
[tigp@c238-1 User0]$ ls
codes VASP-Graphene
[tigp@c238-1 User0]$ cd VASP-Graphene/
[tigp@c238-1 VASP-Graphene]$ ls -l
total 152
drwxr-xr-x 2 tigp kaito 4096 May 6 16:44 Band
-rw-r--r-- 1 tigp kaito 203 May 6 16:44 INCAR
-rw-r--r-- 1 tigp kaito 61 May 6 16:44 KPOINTS
-rw-r--r-- 1 tigp kaito 380 May 6 17:09 POSCAR
-rw-r--r-- 1 tigp kaito 134016 May 6 16:44 POTCAR
-rw-r--r-- 1 tigp kaito 678 May 6 16:44 VASP5.2_openmpi.job
[tigp@c238-1 VASP-Graphene]$ pwd
/lustre/lwork/tigp/Teach-2015-spring/User0/VASP-Graphene
```

There are 10 indexes for each file:

- The 1<sup>st</sup> one could be "d" or "-". "d" means it is a directory
- The first 3 indexes indicate the file could be "read", "wrote", or "executed" by user.
- The second 3 indexes are for the group you belong to.
- The third 3 indexes are for the whole users registered in this workstation.
- The files may be readable with vi or emacs, but also can be in unreadable format (ASCII)



# Practice in Linux System

more INCAR

cat INCAR

more POTCAR

cat POTCAR | more

cp INCAR temp

mv temp ../

cd ../

ls

rm temp

You can stop the  
displaying by  
"Ctrl-C"

cd VASP-Graphene

grep NPAR INCAR

# Editor

Like in Windows (and also Mac, DOS), you need editor software to edit some documents (files).

In Windows, "Word", "Notepad" are the famous editor. "Excel", "Paint", and other office software are also editors for different types of files.

In Mac, Linux Ubuntu should also offer some editor software.

In Linux command mode (terminal), the most popular editors are

**vi** (most popular) (<http://www.cs.colostate.edu/helpdocs/vi.html>)  
(<http://www.lagmonster.org/docs/vi.html>)

**emacs** (I use this one) (<http://www.cs.colostate.edu/helpdocs/emacs.html>)  
(<http://www.linuxhelp.net/guides/emacs/>)

It is depending on you which one you like to be familiar with.

# Practice in Linux System

**cp INCAR temp**

**vi temp**            or            **emacs temp**

Basic vi commands ([ESC] returns the editor to command mode)

:x	Exit, saving changes	dd	Delete current line
:q	Exit as long as there have been no changes	:d	Delete current line
ZZ	Exit and save changes if any have been made	b	Move to the beginning of the word
:q!	Exit and ignore any changes	B	Move to the beginning of blank delimited word
i	Insert before cursor	e	Move to the end of the word
I	Insert before line	E	Move to the end of Blank delimited word
a	Append after cursor	(	Move a sentence back
A	Append after line	)	Move a sentence forward
o	Open a new line after current line	{	Move a paragraph back
O	Open a new line before current line	}	Move a paragraph forward
r	Replace one character		
R	Replace many characters	Ctrl F	Move one page down (forward)
x	Delete character to the right of cursor	Ctrl B	Move one page up (backward)
X	Delete character to the left of cursor	gg	Move to the begining of the file
D	Delete to the end of the line	G	Move to the end of the file

# Practice in Linux System

## Basic emacs commands (C- = Ctrl)

C-x C-c	<i>save-buffers-kill-emacs</i>	C-b	<i>move cursor backward one character</i>
C-g	keyboard-quit	C-n	<i>move cursor to next line</i>
C-x u	undo	C-p	<i>move cursor to previous line</i>
ESC x	execute-extended-command	C-v	<i>scroll file forward by one screenful</i>
C-s	isearch-forward	ESC v	<i>scroll file backward by one screenful</i>
C-r	<i>isearch-backward</i>		
ESC %	<i>query-replace</i>	C-x C-s	<i>save-buffer</i>
C-d	<i>delete-char</i>		
ESC d	<i>delete-word</i>		
C-k	<i>kill-line</i>		
C-w	<i>kill-region</i>		
ESC w	<i>copy-region-as-kill</i>		
C-a	<i>move cursor to (at) beginning-of-line</i>	C-h a	<i>command-apropos</i>
C-e	<i>move cursor to end-of-line</i>	C-h i	<i>information</i>
C-f	<i>move cursor forward one character</i>	C-h t	<i>help-with-tutorial</i>

# Practice in Linux System

Compile Fortran, C codes

`cd /lustre/lwork/tigp/Teach-2015-spring/User0/codes`

`ifort Fortran_code.f90`  `./a.out`

`gcc C_code.c`  `./a.out`

<http://www.chem.ox.ac.uk/fortran/fortran1.html>

<http://www.cplusplus.com/>

Run VASP

`cd /lustre/lwork/tigp/Teach-2015-spring/User0/VASP-Graphene/`

`qsub VASP5.2_openmpi.job`

`qstat -u tigp`

`tail log`

<http://cms.mpi.univie.ac.at/vasp/vasp/vasp.html>

# Bash Shell Script

```
#!/bin/bash
# bash trap command
trap bashtrap INT
# bash clear screen command
clear;
# bash trap function is executed when CTRL-C is pressed:
# bash prints message => Executing bash trap subroutine !
bashtrap()
{
    echo "CTRL+C Detected !...executing bash trap !"
}
# for loop from 1/10 to 10/10
for a in `seq 1 10`; do
    echo "$a/10 to Exit."
    sleep 1;
done
echo "Exit Bash Trap Example!!!"
```

Shell Script also can perform some program for you. But the efficiency will be low.

<http://linuxconfig.org/bash-scripting-tutorial>