C2110 UNIX and programming

1. lesson

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czech republic

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INVESTMENTS IN EDUCATION DEVELOPMENT

CZ.1.07/2.2.00/15.0233

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Motivation

Supercomputing

MetaCentrum a CERIT-SC

- National grid environment
- OS Debian
- cca **8500 CPU cores**
- **CEITEC/NCBR own resources cca 850** CPU cores
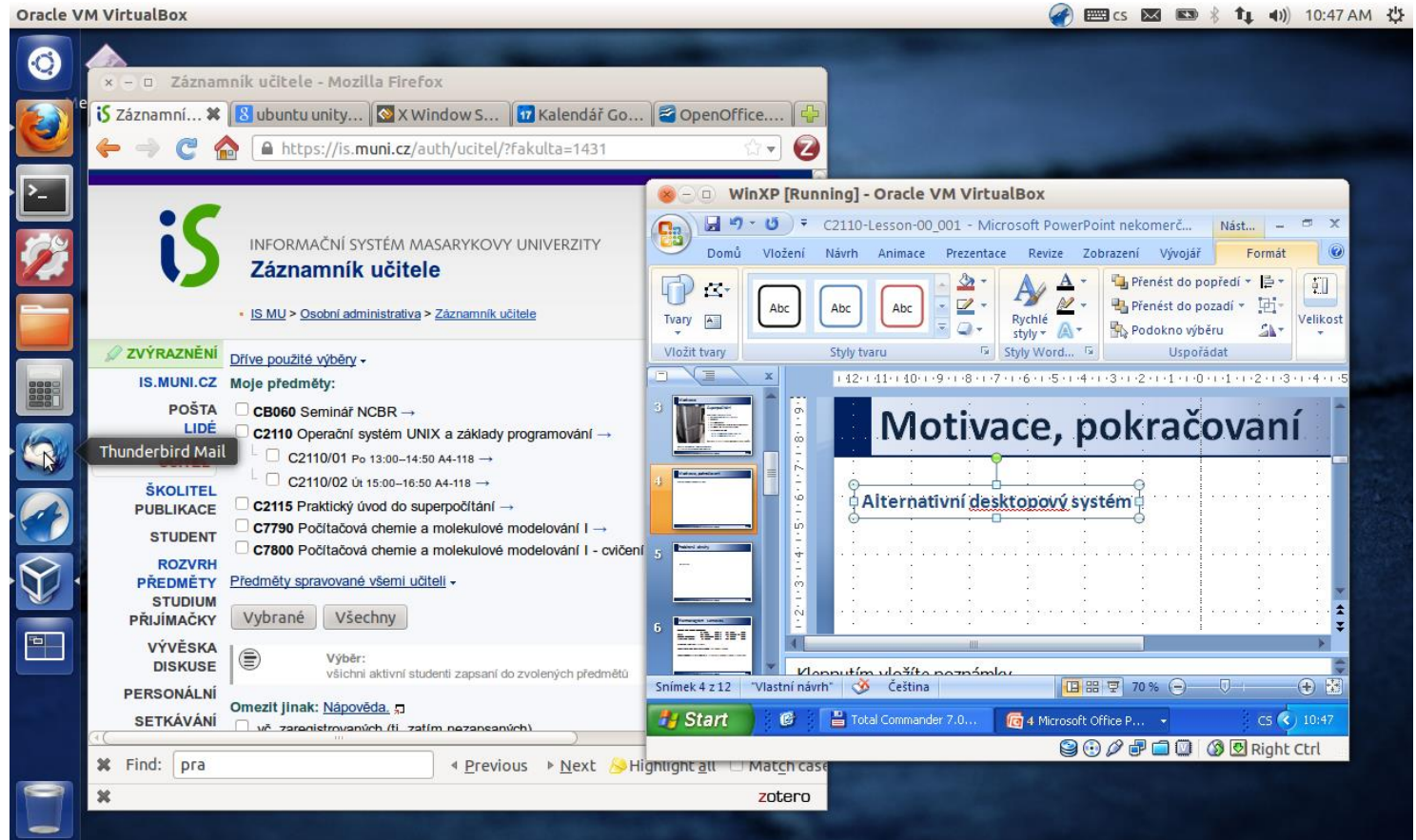- Total **1000 TB** storage capacity
- cca **10 TB per user**

http://www.metacentrum.cz/
http://www.cerit-sc.cz/

Free access maybe provided to any CZ university member.

Follow-up course (autumn semester – block lectures in January)
C2115 Practical Introduction to Supercomputing

Motivation, continue..

Alternative desktop system

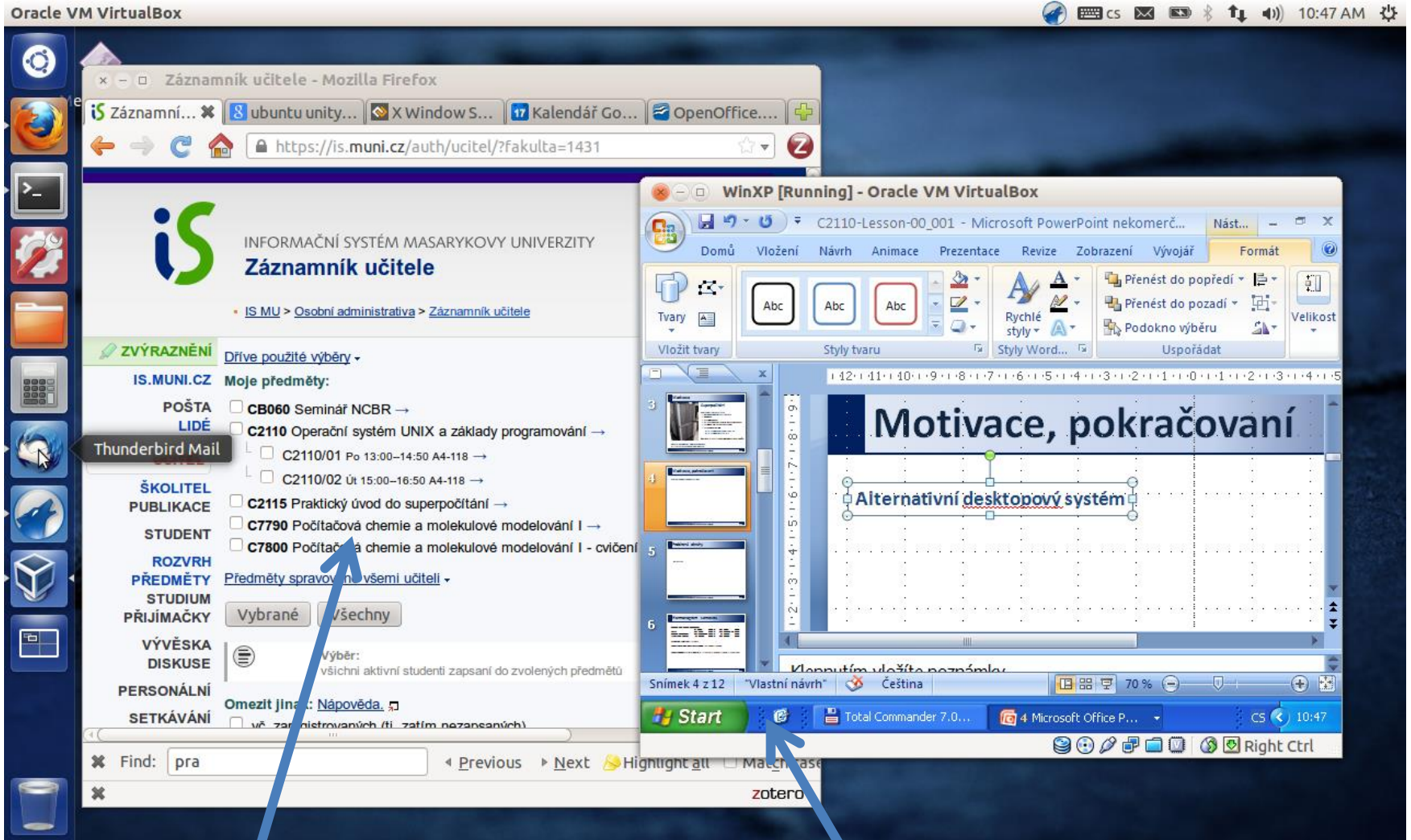**Advantages:** free, flexible, extensible, scriptable.

Syllabus

➢ **Basic OS usage**
➢ **Virtualization**
➢ **Command line work**
➢ **Scripting languages**
  bash
  gnuplot
  awk

Virtualization

Host: Ubuntu 12.04   **Guest:** Windows XP (virtual machine)

Text file analysis

```
.............
.............
NSTEP =       6000  TIME(PS) =        206.000  TEMP(K) =   291.69  PRESS =        0.0
Etot    =        160.8627  EKtot    =        18.5486  EPtot      =        142.3142
BOND    =          7.2673  ANGLE    =        17.6964  DIHED      =         13.5633
1-4 NB =           4.8403  1-4 EEL =        199.3739  VDWAALS    =          1.5430
EELEC  =         -101.9700  EHBOND   =         0.0000  RESTRAINT  =          0.0000
.............
.............
```
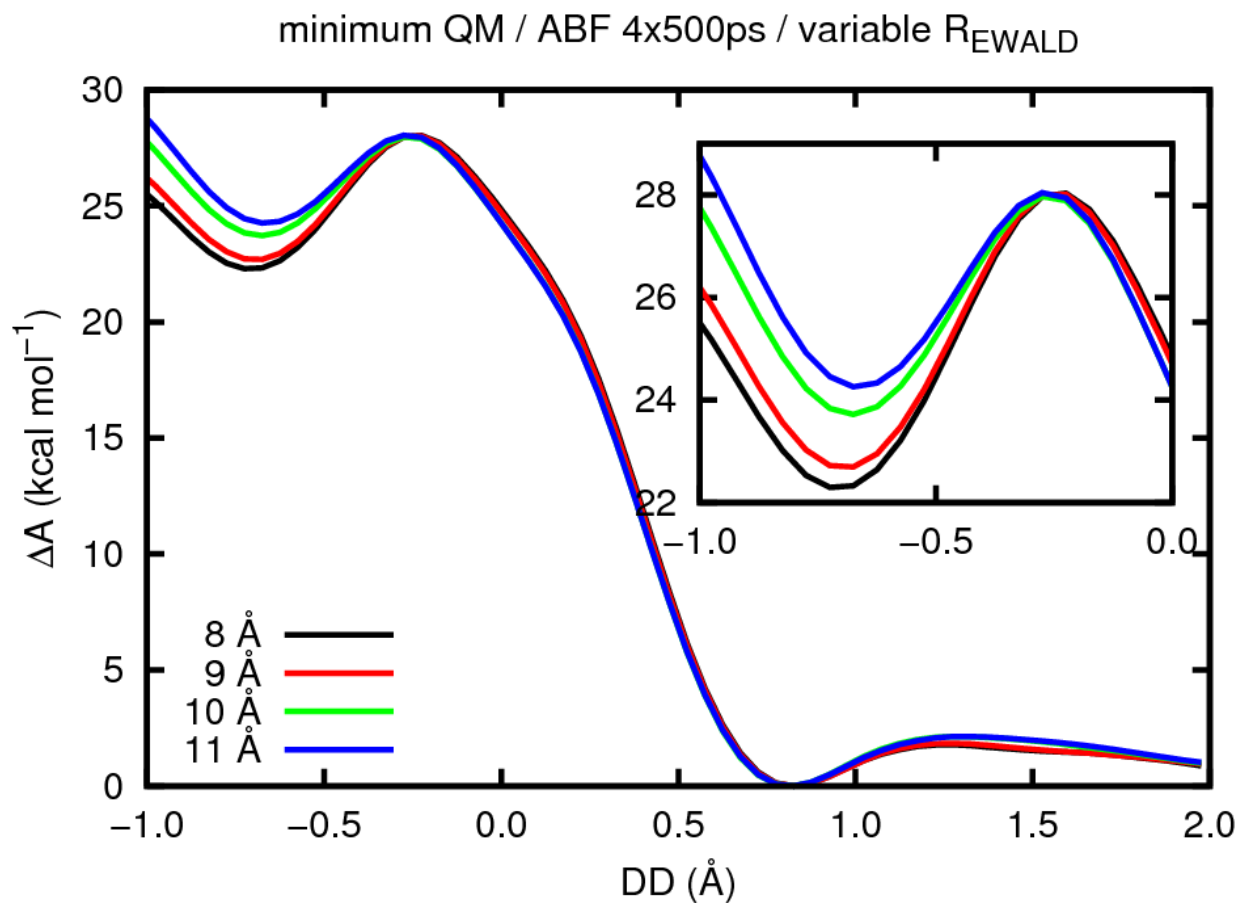
Easy data extraction using AWK language
(analyzing scientific program output).

```
.............
.............
206.000  291.69
.............
.............
```

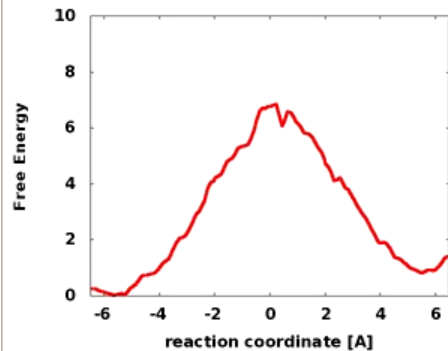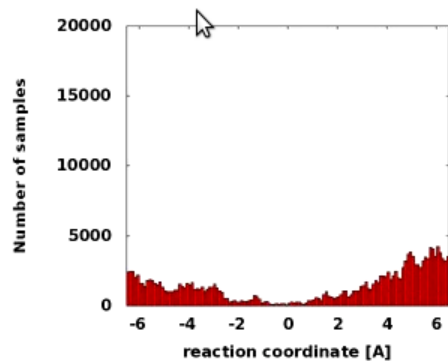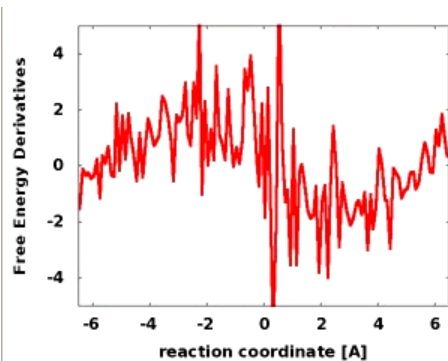**Data:** /home/kulhanek/Documents/2013/C2110_UNIX/data/rst.out

```
$ grep TIME rst.out | awk '{ print $6, $9 }'
$ awk '/TIME/{ print $6, $9 }' rst.out
```

Results Visualization

Creating graphs from extracted values (gnuplot).
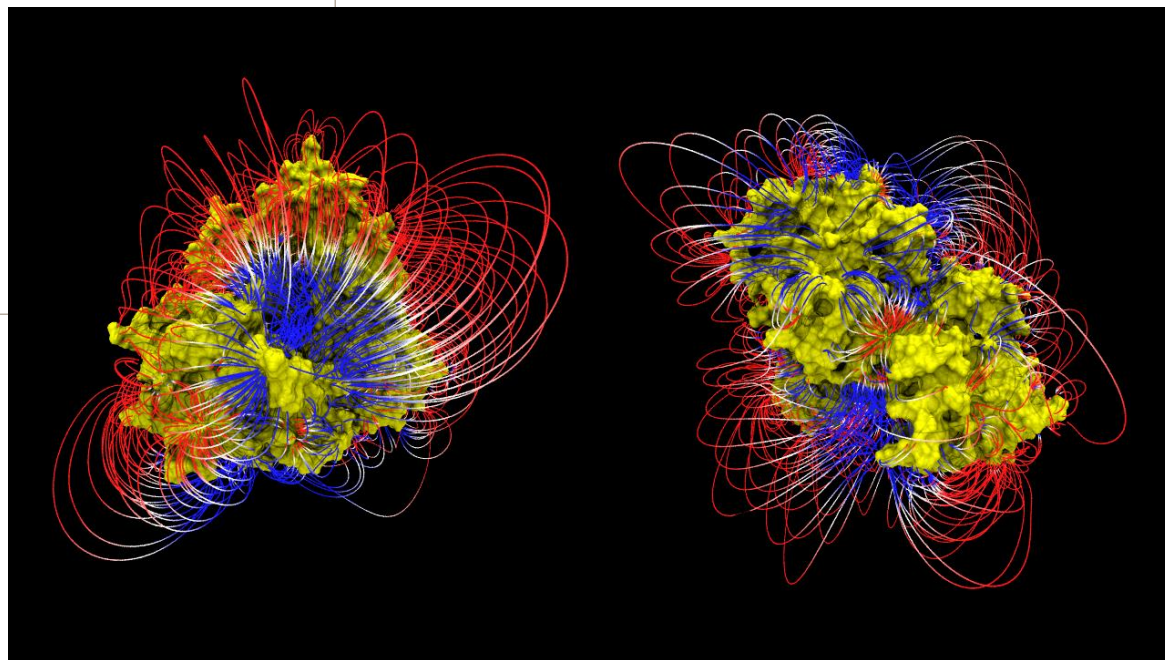
Automation

Show video

ABF: Petr Kulhánek

BsoBI: Ivo Kabelka

Course organization

- ➢ **Time schedule, teaching methods**
- ➢ **Knowledge evaluation, final test**

Time schedule, teaching

Course enrollment period:	2. 9. 2013	-	29. 9. 2013
Teaching:	16. 9. 2013	-	20. 12. 2013
Vacations:	21. 12. 2013	-	1. 1 2014
Examinations:	2. 1. 2013	-	14. 2. 2014

Extent: colloquium (2 credits)

Total lecture time: 14 x 2 hours = 28 hours

Total course time demands:

> 1 ECTS credit -> 26 hours of studies (see ECTS Label)

> 2 credits -> 2x 26 hours = **52 hours of studies**

Voluntary exercise tests via e-learning:
> 1x per 2 weeks, accessible only 2 weeks from release
> unlimited opening and evaluations
> random generated questions set

Absence two times is permitted, apologize in advance!
(either by e-mailem or by IS)

Knowledge evaluation, final test

Two tests in-semester: (20 minut)   2x10 points

Final testing:
        - final test (1 hour)   50 points
        - script task (1 hour)   30 points
==
Total: 100 points
Passed: **>= 80 points**

Cluster WOLF

- ➢ **Room 1.18**
- ➢ **Structure**
- ➢ **Rules**
- ➢ **Administrators**

Room 1.18

- 23 PC
- 3D visualization
- Computing cluster organization

Safety rules!

PC room is accessible to students of LCC group, and students of any course taught in same semester in room 1.18.

WOLF cluster structure

University network
wolf.ncbr.muni.cz

Local network
wolf.wolf.inet

Private network: *wolf.inet*
(not accessible directly)

switch

wolf

wolf01 wolf02 wolf03 wolf04 wolf05

wolf06 wolf07 wolf08 ■ ■ ■ ■ ■ wolf23
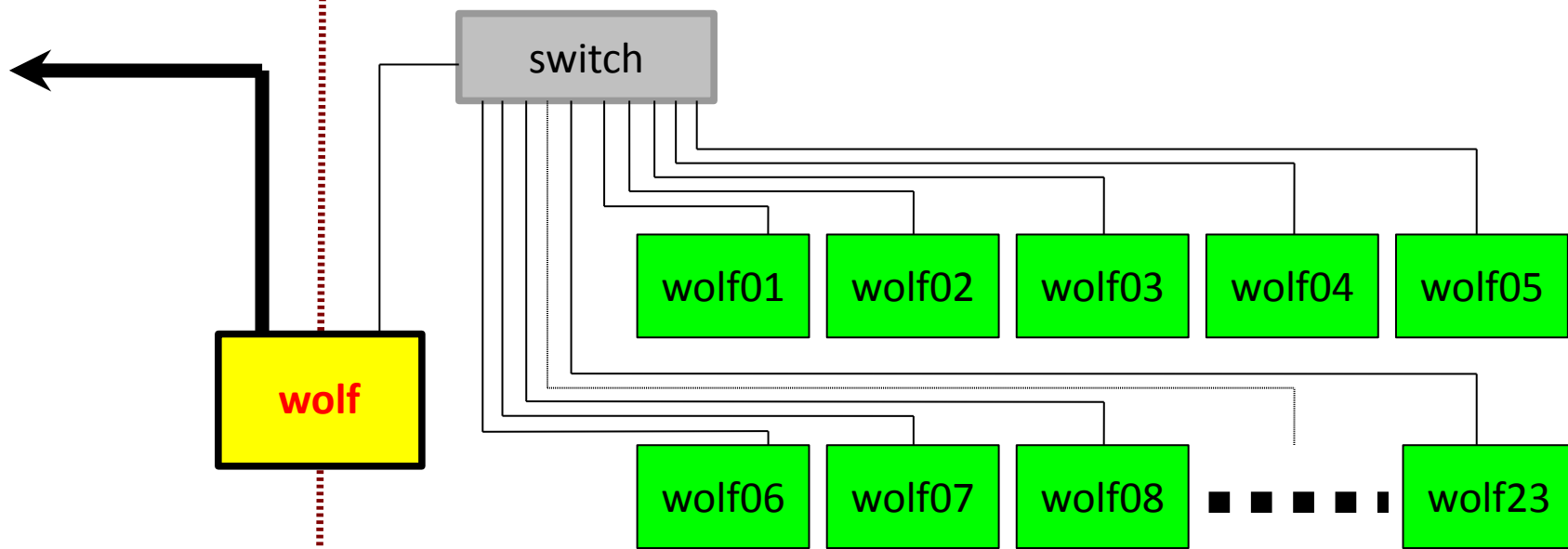
server

Work nodes (computational nodes)

Operating system: Ubuntu 12.04 (Precise) LTS

http://www.ubuntu.com/

Rules

WOLF cluster is strictly dedicated to teaching purposes or scientific work within National Centre for Biomolecular Research.

It is strictly forbidden to:

> download data with illegal contents (author protected work etc.)
>
> virus and spam distribution
>
> system hacking

Removing or changes to unprotected content of other users

Obligatory are rules of Masaryk University network:
https://is.muni.cz/auth/do/rect/normy/smernicerektora/Smernice_MU_9-2013.pdf

Login name and password is user identity. Do never give it to any other person, send (e.g. by e-mail) or save unencrypted.

Cluster administrators - problems

Before contacting administrators, **consult** your problem with colleagues, teacher or supervisor. If you do not solve problem, **please report to administrators by e-mail**.

support@lcc.ncbr.muni.cz

In message state:
- ➢ Problem description, command name
- ➢ User name, machine name
- ➢ Copy error output from command line

Main WOLF cluster administrator:

Jakub Štěpán

Account management, hardware, system and software administrator

Scientific applications (modules) administrator:

Petr Kulhánek

First login

- ➤ **Local login**
- ➤ **Desktop environment**
- ➤ **Standard applications**

Local login

Local terminals:

- Six **text terminals** (F1 … F6)
- One **graphical terminal** (F7, F8, …)
- Switching between them by keys **Ctrl+Alt+F1 … Ctrl+Alt+F7**

Login:

- Needed input **user name** (login) and **password**

Linux operating system is very flexible and enables various ways of local login, for example by ID cards or cryptographic keys. More can be found in PAM (Pluggable Authentication Modules) system manual.

$ man 8 pam

Local login

Text terminal (F1-F6):

➢ Access to CLI – command line interface

➢ Start directory is **/home/your_login** (home directory)

➢ Graphical applications (X11) can be run only by **display export** to remote graphical interface

➢ Logout by command **exit**

Graphical terminal (F7):

➢ Runs X11 server and desktop environment in it (KDE, Unity, GNOME, atd.)

➢ Desktop environment **can be selected** before actual login

➢ Enables direct GUI – graphical user interface applications running

➢ Command line is accessible through special applications

 ➢ xterm

 ➢ **konsole**
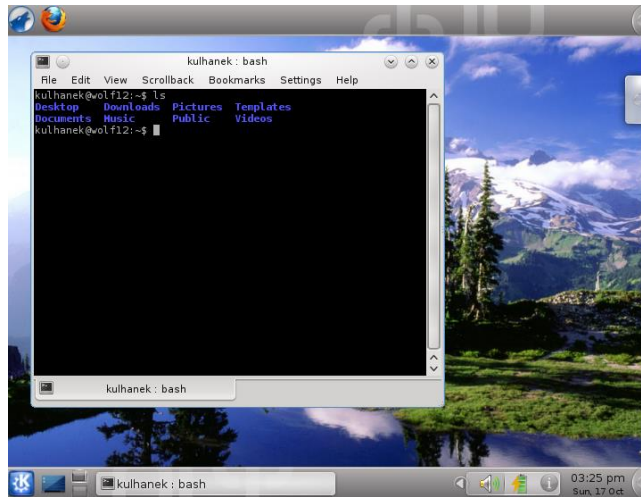
➢ Logout **using GUI menu** in desktop environment.

Login – LightDM X manager

Desktop environment choice

Login

Username

Login name (Enter)
Password (Enter)
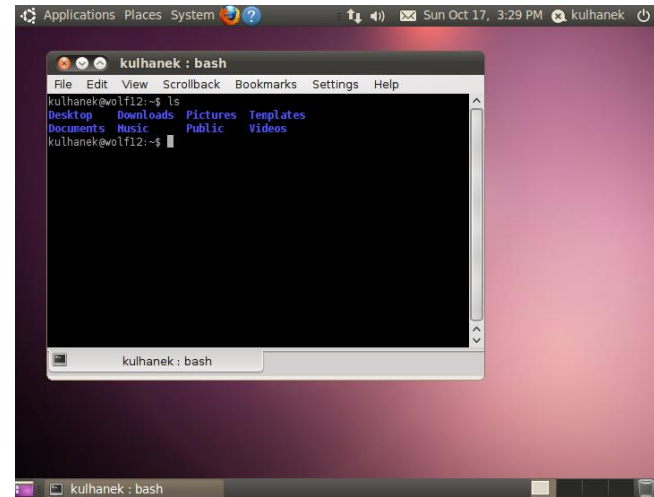
ubuntu® 12.04 LTS
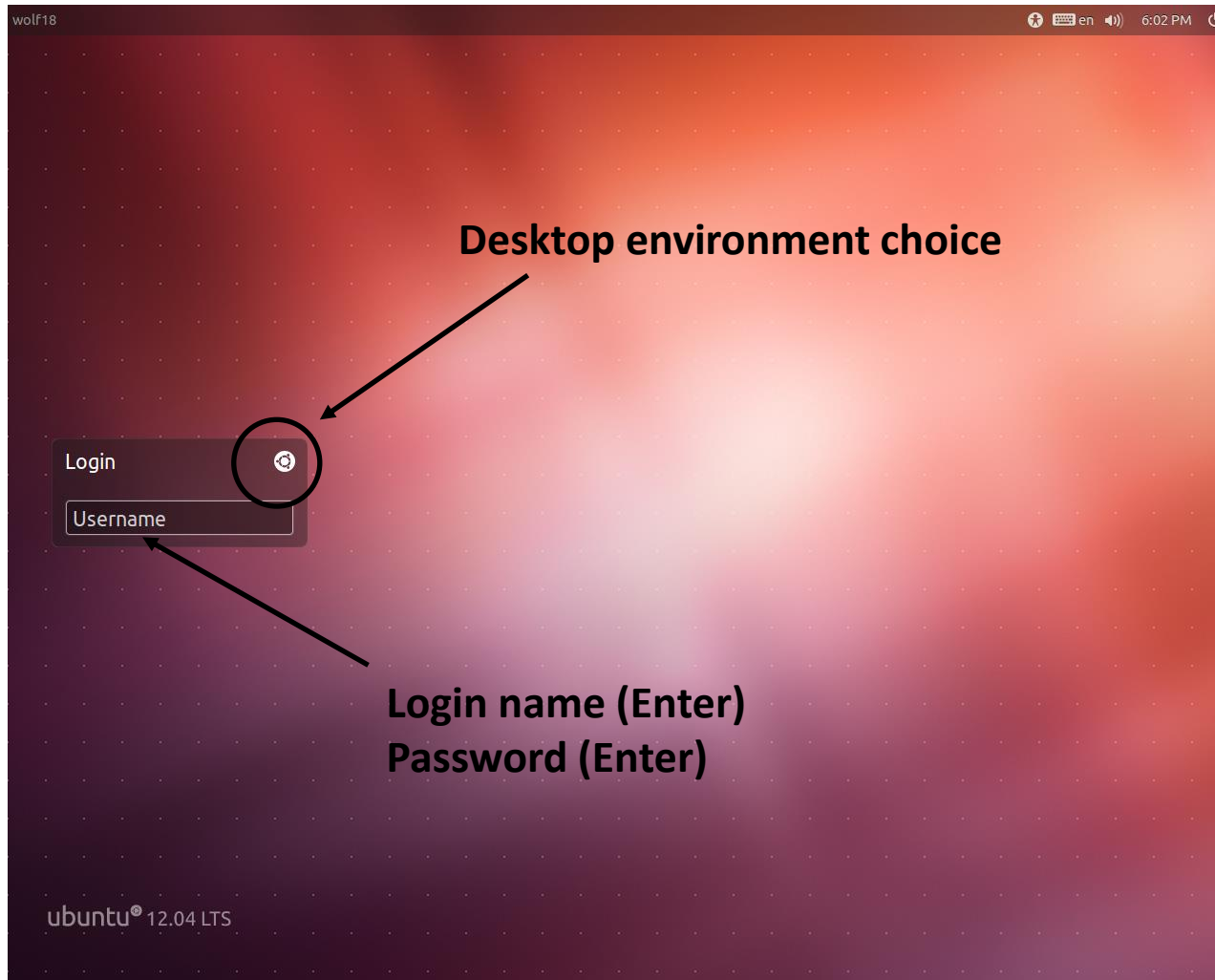
Default keyboard layout is English (**EN**).
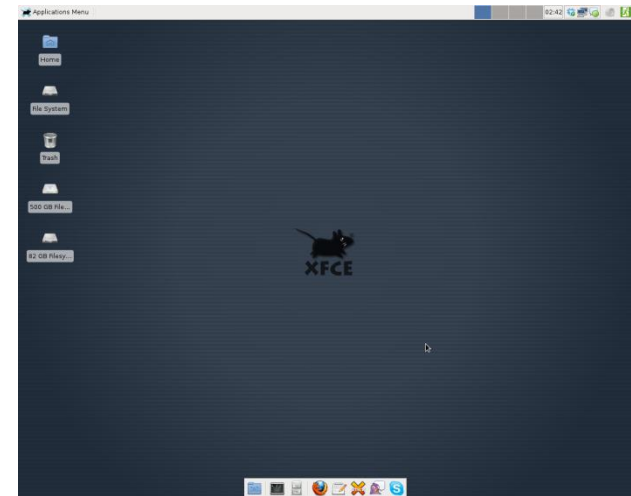When using numeric keyboard check **NumLock**.

Desktop Environments

KDE

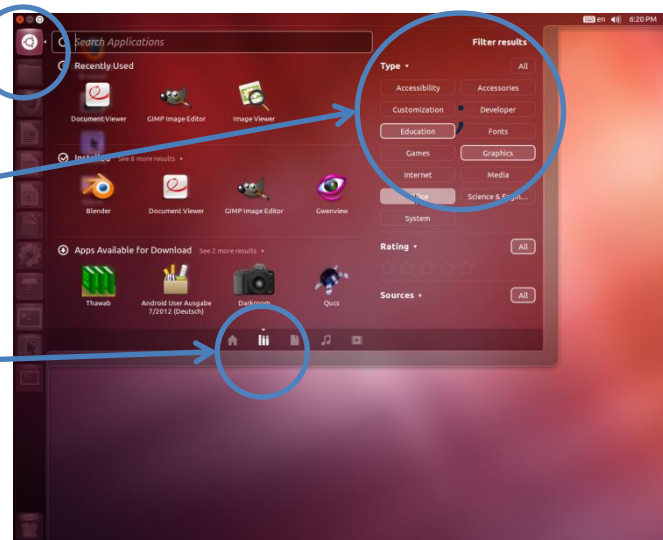GNOME
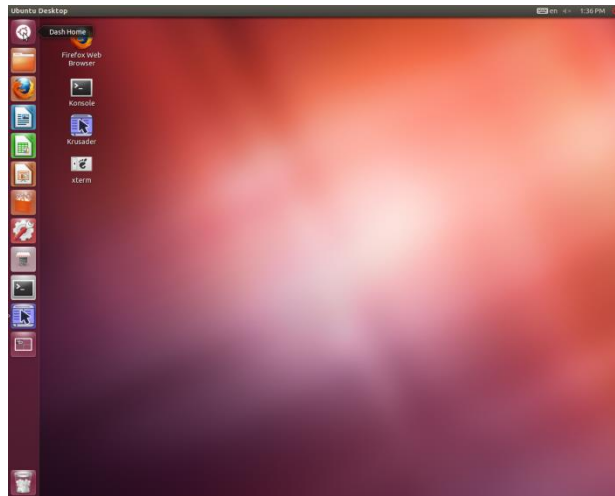
Unity (menu item Ubuntu)

Xfce

Standard applications

Main menu

Results filter

Submenu

Firefox	web browser
OpenOffice/LibreOffice	text editor (Writer)
	tab editor (Calc)
	presentations (Impress)
Gimp	raster graphics editor
Inkscape	vector graphics editor
Okular	PDF documents reader

Exercise

1. Login to desktop environment Unity (menu item Ubuntu). Login name is **guestXX,** where **XX** is PC number 01 – 23. Password will be given by teacher.

2. Try system applications (Gimp, Libre Office Writer, Inkscape)

3. Try login to other desktop environments (Xfce, Gnome, KDE), try to find application menu in them and run system applications.

Password change
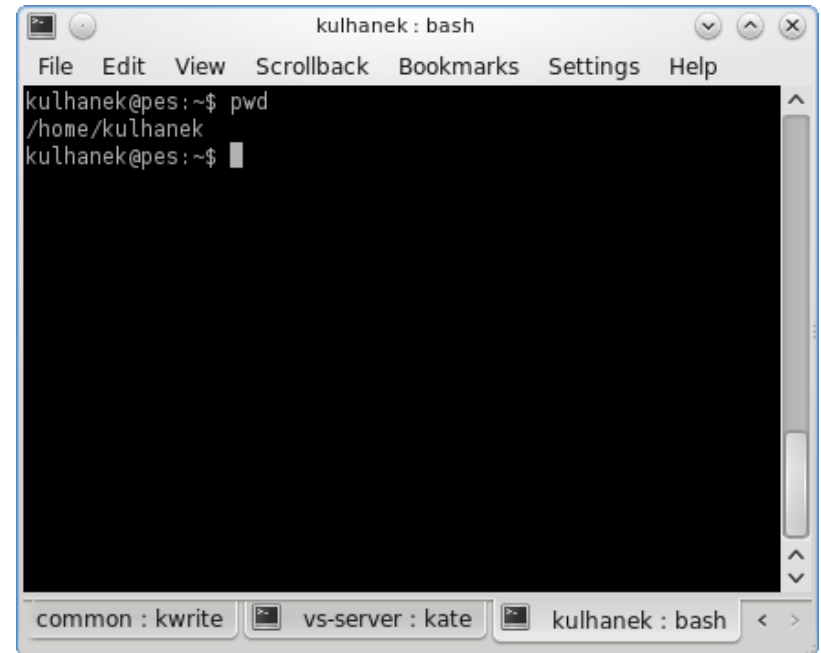
> **Terminals**
> **Command passwd**

Terminals

Command line is accessible on text terminals. In graphics terminal X11 terminal emulator is needed.
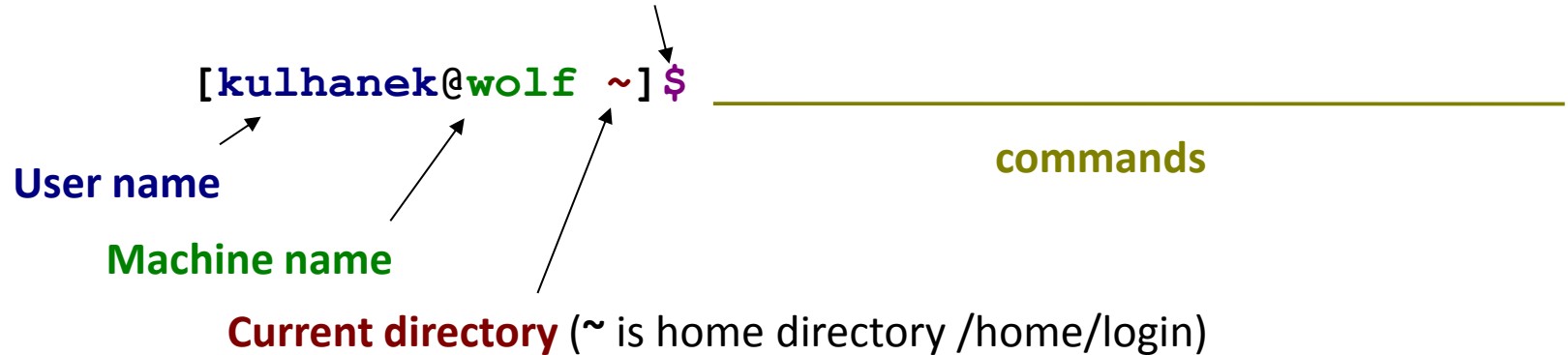
xterm

konsole

Easy, standard on all systems   configurable

Default directory is: **/home/vas_login**

Command line

`[kulhanek@wolf ~]$` _____

commands

User name

Machine name

Current directory (**~** is home directory /home/login)

Command is given by key **Enter**.

History: by arrow keys (up, down) list of recently used commands can be searched. Any command can be re-used or edited and used. Full list of recorded commands can be printed by command **history**.

Auto complete: Tab key makes command line interpreter to try complete started word. Completed can be command names, paths, file names (if one click does not complete word, there is more possibilities to complete, another click shows list of them).

Text copy: Do not use Ctrl+C! Mouse text select automatically adds text to clipboard, press mouse wheel to paste on cursor place.

Password change, command passwd

- ➤ Password can be changed after login to system by command **passwd**.
- ➤ Running command **passwd** asks user for **current password**, and **new password.** To avoid typo retype is requested.
- ➤ Change is automatic for **all WOLF** cluster computers.
- ➤ Password needs to be strong enough. It should contain combination of upper, lower case, numbers and other characters.
- ➤ Type password on main keyboard part, do not use numeric keyboard and special keys. You avoid possible problems with password input.
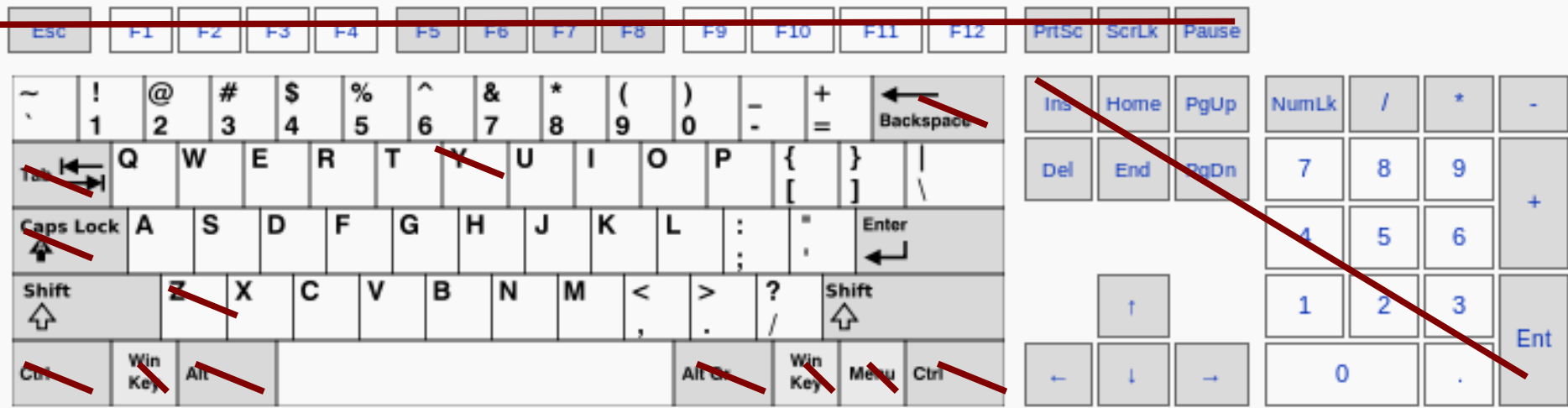
Default keyboard is English (**EN**).

Password

A valid password should be a mix of upper and lower case letters, digits, and other characters. You can use an 8 character long password with characters from at least 3 of these 4 classes, or a 7 character long password containing characters from all the classes. An upper case letter that begins the password and a digit that ends it do not count towards the number of character classes used.

Password change - passwd

No signs appears when writing

```
kulhanek@wolf:~$ passwd
Enter login(LDAP) password:

You can now choose the new password or passphrase.

A valid password should be a mix of upper and lower case letters,
digits, and other characters.  You can use an 8 character long
password with characters from at least 3 of these 4 classes, or
a 7 character long password containing characters from all the
classes.  An upper case letter that begins the password and a
digit that ends it do not count towards the number of character
classes used.

A passphrase should be of at least 3 words, 11 to 40 characters
long, and contain enough different characters.

Alternatively, if no one else can see your terminal now, you can
pick this as your password:

Enter new password:
Re-type new password:
LDAP password information changed for kulhanek
passwd: password updated successfully
kulhanek@wolf:~$
```

Exercise

1. Logout from active session.

2. Login with your log name and start password.

3. Open terminal.

4. Change your password by command **passwd**.

5. Logout.

6. Login wit your log name and new password.