

C2110 *UNIX operating system and programming basics*

1st lesson

Getting Started

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Content

➤ Aims of the course

- Motivation, discussed topics, practical examples

➤ Organization

- Schedule, form of teaching
- Assessment, completing a course

➤ Cluster WOLF

- Room 1.18, structure, usage rules, administrators

➤ Getting started

- Local login, standard applications, command line, scientific and technical applications, desktop environments

Aims of the course

- **Motivation**
- **Discussed topics**

Motivation - Supercomputing

MetaCentrum a CERIT-SC (<http://metavo.metacentrum.cz>)

Valid in 2016

- National Grid infrastructure, OS Debian
- ca **11000 CPU** cores, **1100 TiB** disk array, **17 PiB** hierarchical storage

Any college student in the Czech Republic can get access.

IT4Innovations (<http://it4i.cz>)

- National Supercomputing Centre, OS CentOS and Bullx
- salomon (cca 24192 CPU cores, 129TB RAM, Intel Xeon Phi MIC)
 - 40th place (TOP500, **139th place in 06/2018**))
- anselm (approximately 3000 CPU cores, RAM 15Tb)

The machine time is sought through grant competitions.

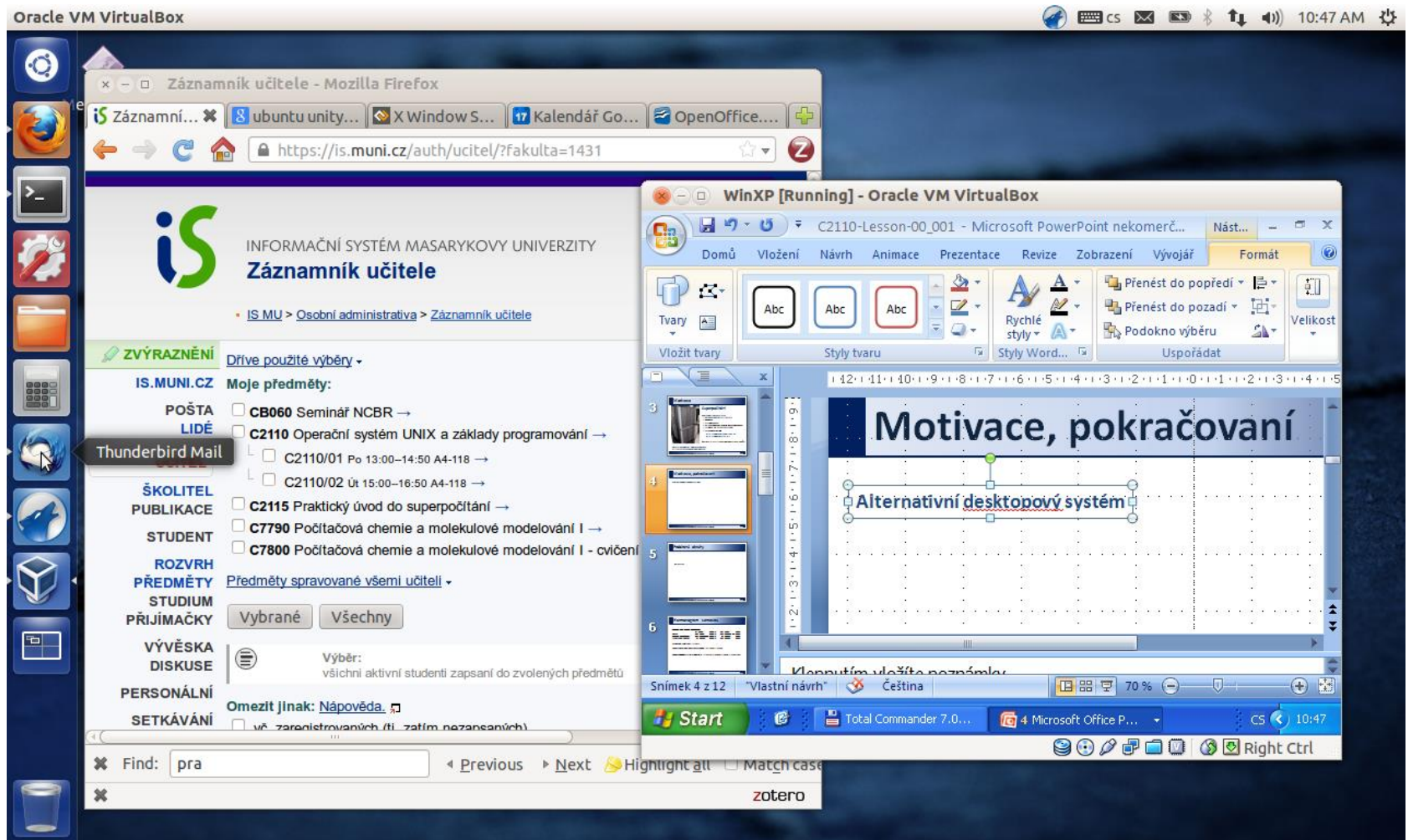
Local computing clusters at NCBR and CEITEC-MU

Follow-Up Course (fall semester - block lectures):

C2115 Practical Introduction to Supercomputing



Motivation - desktop system



Advantages: free, flexible and extensible, scripting capabilities

Discussed topics

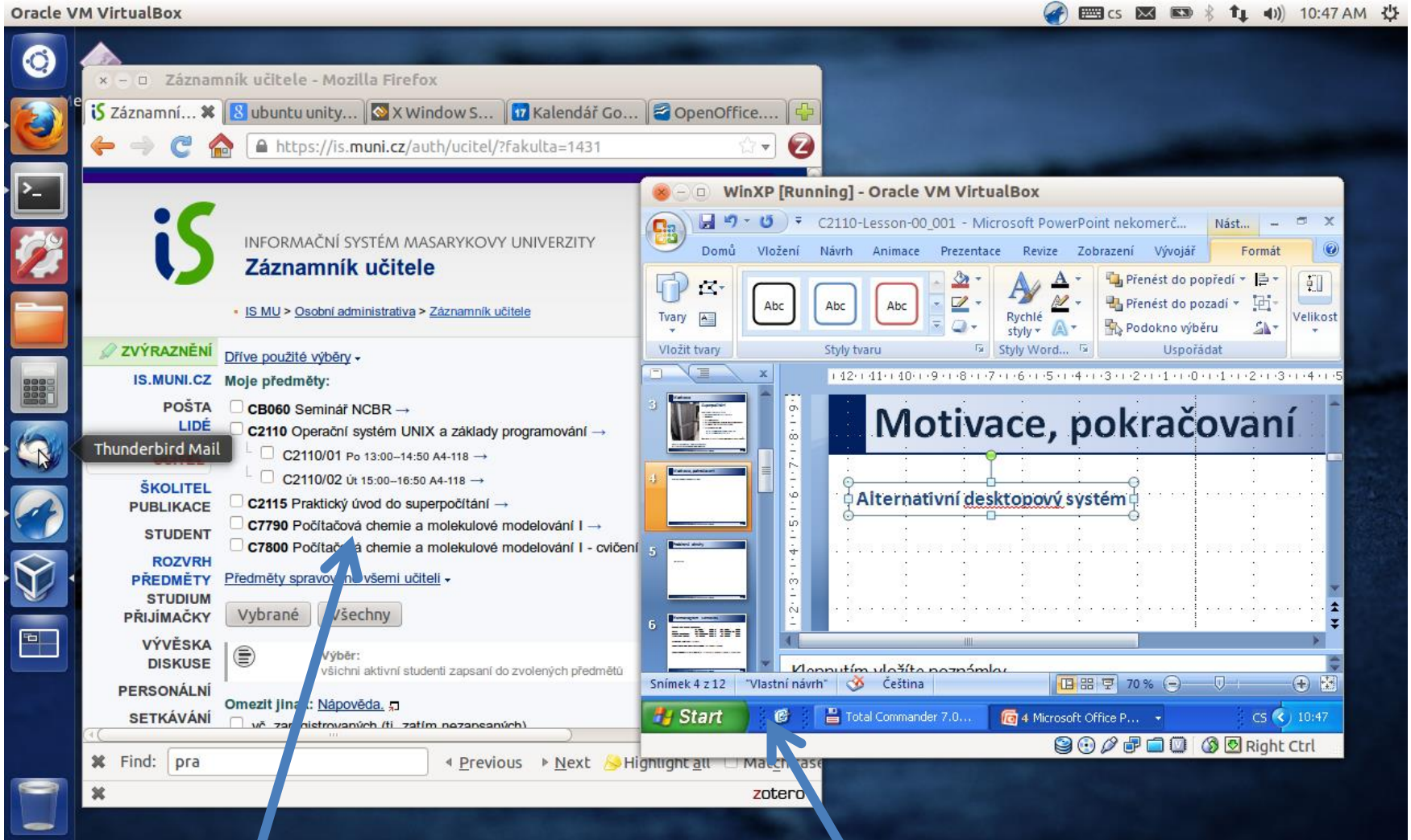
- **Basic work with OS**
- **Virtualization**
- **Using the command line**
- **Scripting language**

bash

gnuplot

awk

Virtualization



Host: Ubuntu 12.04

Guest: Windows XP (virtual machine)

Processing of text files

```
.....  
.....  
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  
.....  
.....
```

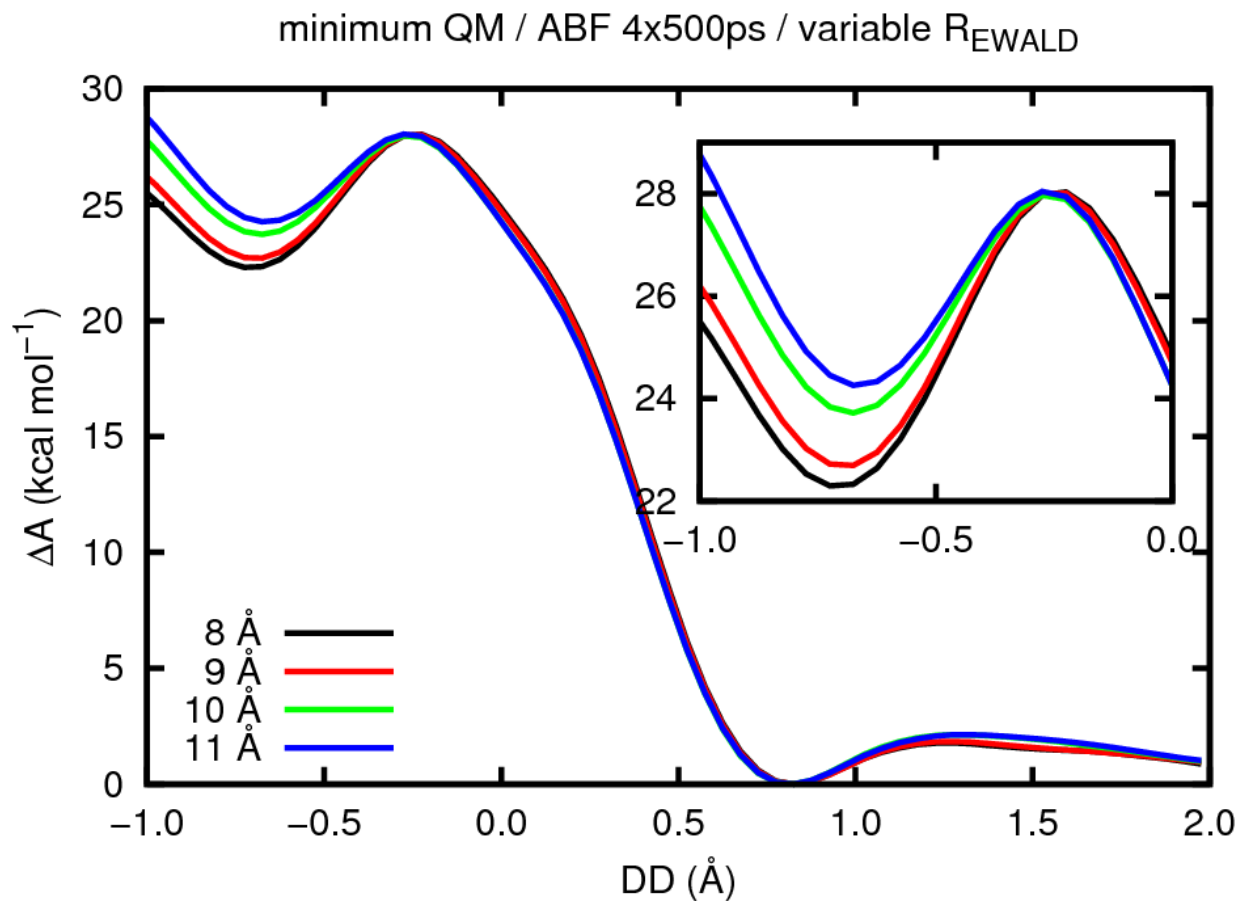
easy data extraction using AWK language
(outputs of computational programmes)

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

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

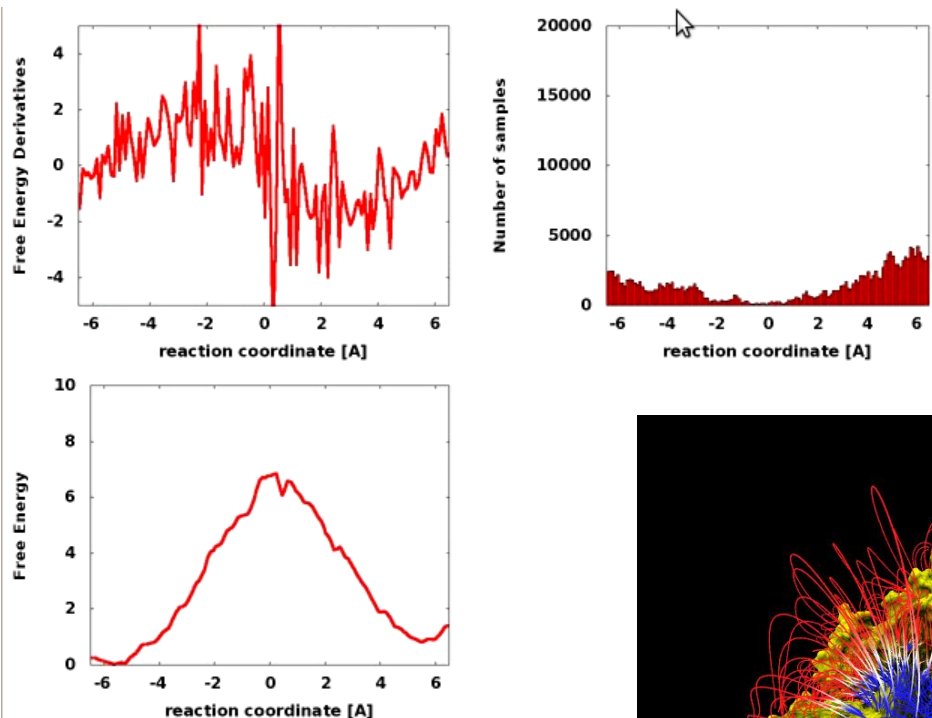
```
$ grep TIME rst.out | awk '{ print $6, $9 }'  
$ awk '/TIME/{ print $6, $9 }' rst.out
```


Visualization of results

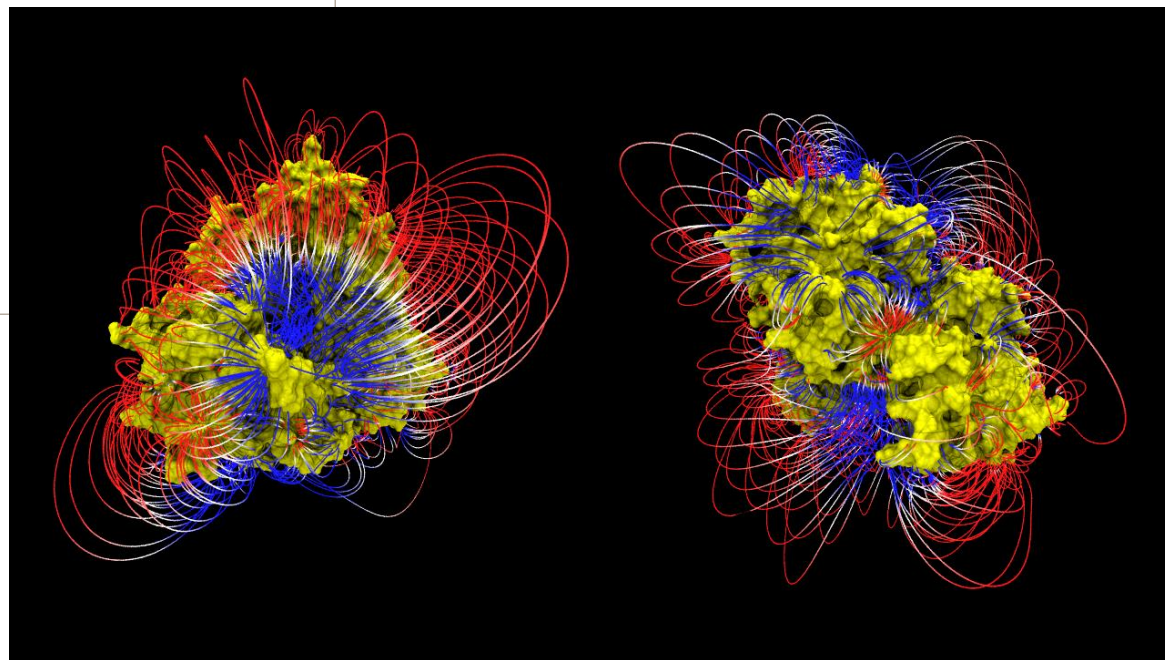


Displaying of the extracted data in graphs (gnuplot).

Automation



Show video



ABF: Petr Kulhánek

Data: /home/kulhanek/Documents/2013/C2110_UNIX/video

BsoBI: Ivo Kabelka

Organization of lectures

- **Schedule, form of teaching**
- **Assessment, completing a course**

Schedule, form of teaching

Lesson: September 17, 2018 - December 17, 2018

Examination period: January 2, 2019 - February 12, 2019

Completion: colloquium (2 credits)

Total number of presented hours: 13 x 2 hours = 26 hours

total hourly load of the course:

1 ECTS credit -> 26 hours workload

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



Self, homework, exam preparations: 26 hours

Voluntary practice:

ROPOT once per 14 days, open two weeks after the publication
unlimited number of opening and evaluation
randomly generated set of questions

two excused absences in advance are allowed!

(via mail or via the information system)

Completion - knowledge assessment

Two written tests: (20 minutes) 2x10 points

Completion:

- final test (1 hodina) 50 points

- Script by assignment (1 hour) 30 points

=====

Total: 100 points

Passed: >= 80 points

You are allowed to use all study materials, any books and the Internet. When writing a test or script creation and will be allowed to use a computer, you can use scripts from exercises or from homeworks. However, you are not allowed to cooperate with other people (Facebook, mobile, etc.).

Cluster WOLF

- **Classroom 1.18**
- **Structure**
- **Terms of Use**
- **Administrators**

Room 1.18



- Room with 23 PCs
- 3D Visualization
- Organized as computational cluster

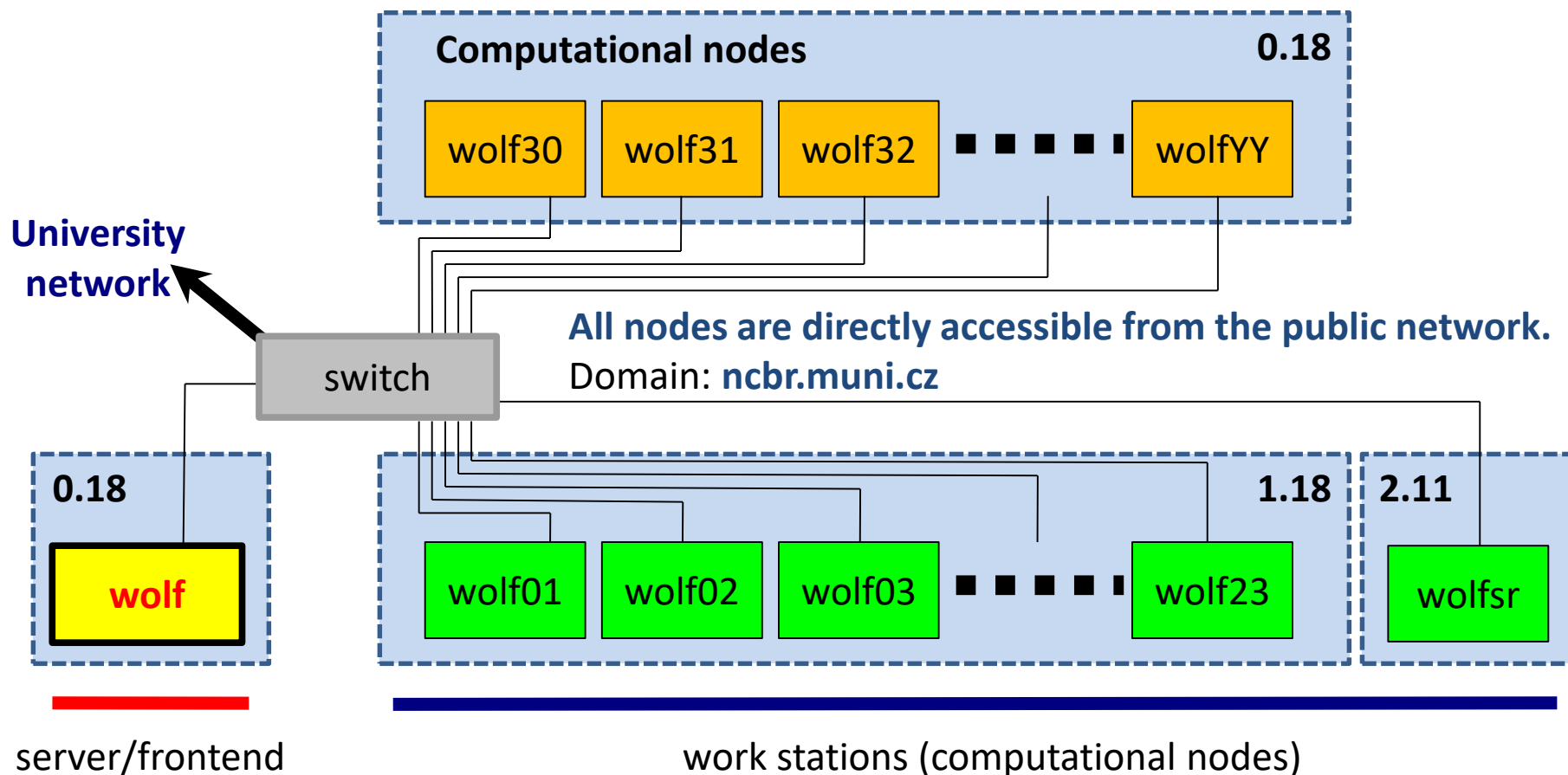
Safety rules

Basic information:

<http://wolf.ncbr.muni.cz>

The room is freely accessible to students who are working on projects at NCBR, and students who have lectures in the semester take place in the room.

Cluster WOLF - structure



Místnosti:

- 0.18 Server room A4/UKB
- 1.18 Computer lab A4/UKB
- 2.11 Seminar room A4/UKB

Operation system: **Ubuntu 16.04 (Xenial) LTS**
(<http://www.ubuntu.com/>)

Terms of use

The cluster WOLF is exclusively intended for educational purposes and/or for scientific work within National Centre for Biomolecular Research.

The cluster WOLF is explicitly forbidden to use for:

- downloading of illegal content (copyrighted works, etc.).
- sending out viruses, spam and similar materials
- breaking protection of other computers
- reading, deleting or changing unprotected contents of other users

Binding rules for the use of computer network of Masaryk University:

https://is.muni.cz/auth/do/mu/Uredni_deska/Predpisy_MU/Masarykova_univerzita/Smernice_MU/SM10-17/

The login name and password form your identity and, therefore, it is fundamental to keep it safe and hidden from third parties. Do not store or send it (by e-mail) in unencrypted form!

Terms of use ...

The cluster WOLF is also explicitly forbidden to use for:

- executing computational jobs on the frontend (wolf.ncbr.muni.cz)
- running jobs anywhere in your home directory (especially data-intensive tasks)
- executing tasks on work stations during the lesson (if a teacher does not say otherwise)

Time demanding jobs must be run through a batch system:

More information in C2115 Practical introduction to Supercomputing.

Cluster administrators - problems

Before contacting administrator, consult your problem with your colleagues, teacher or supervisor. If the problem is not resolved, report the problem to the administrators via e-mail

support@lcc.ncbr.muni.cz

In your report:

- Describe the problem, the command name
- Your user name, name of the machine
- Copy error output (from the award of the entire command)

Getting started

- **Local login**
- **Standard applications**
- **Command line**
- **Scientific and technical applications**
- **Desktop environments**
- **Change of your password**

Local sessions

Local terminals:

- six **text terminals** (F1 ... F6)
- **graphical terminal** (F7, F8, ...)
- switching between them by **Ctrl + Alt + F1 ... Ctrl + Alt + F7**

Login:

- you have to enter your **username** and the **password** to log in

Linux operating system is very flexible and allows other ways of local login, eg. by identification cards or cryptographic keys. More can be found in the help of system PAM (Pluggable Authentication Modules).

```
$ man 8 pam
```

Local sessions

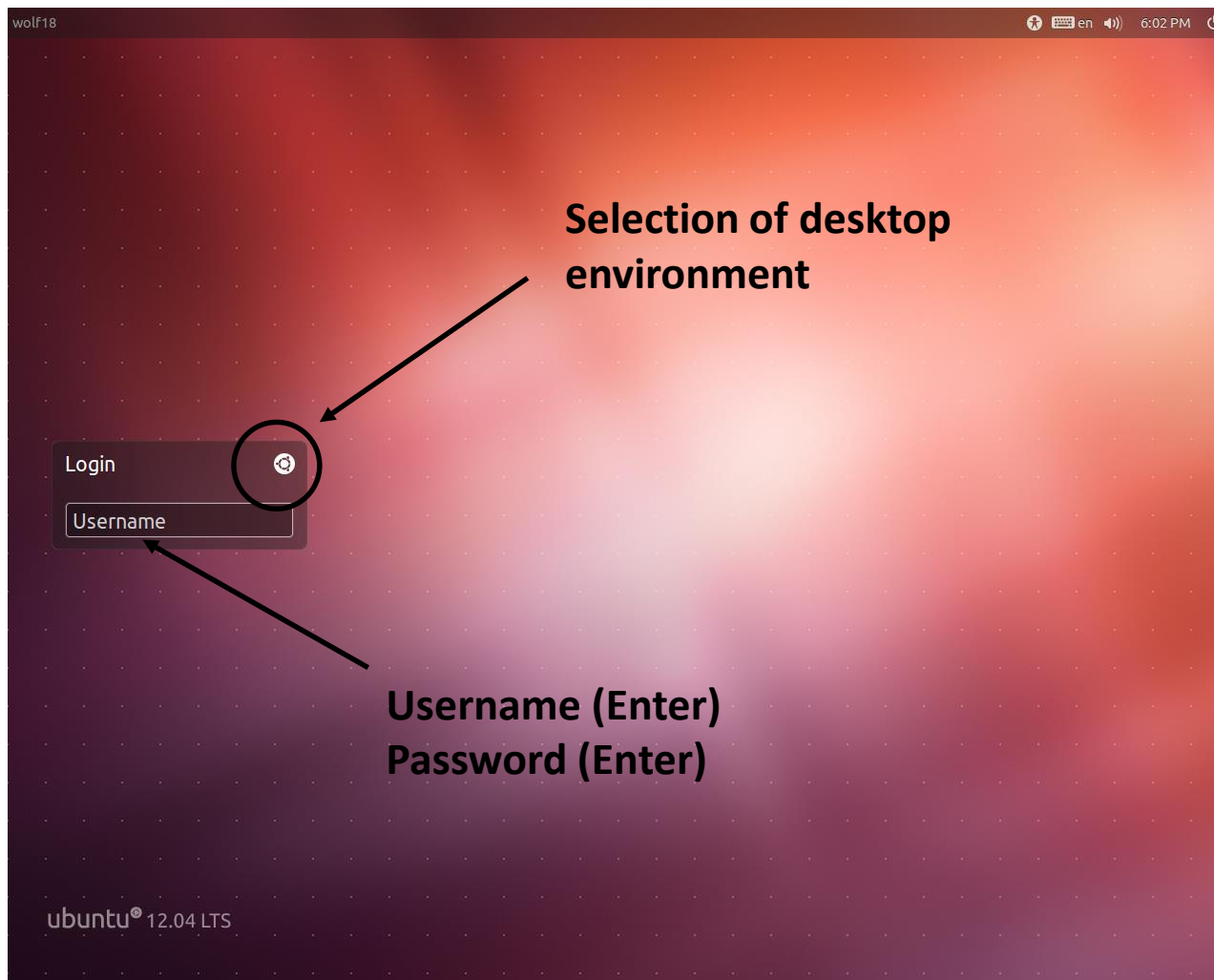
Text terminals (F1-F6):

- these terminals provide a command-line interface (CLI - Command Line Interface)
- the default directory is **/home/username** (home directory)
- graphics applications (X11) are possible to run only by **exporting display** to a remote graphic terminal
- session termination: **exit**

Graphical terminal (F7):

- this terminal starts an X11 server and with a window manager (KDE, Unity, GNOME, etc.)
- a window manager (desktop environment) can be selected before login
- it allows to run directly graphical programs (GUI - Graphical User Interface)
- a command line is available by special applications
 - **xterm**
 - **konsole**
 - **gnome-terminal**
- session termination: use **an option from the menu** of a windows manager

Log in - lightdm X manager



Default keyboard is **English (EN)**.

Check if the **Num Lock** is activated when using a numeric keypad.

Exercise

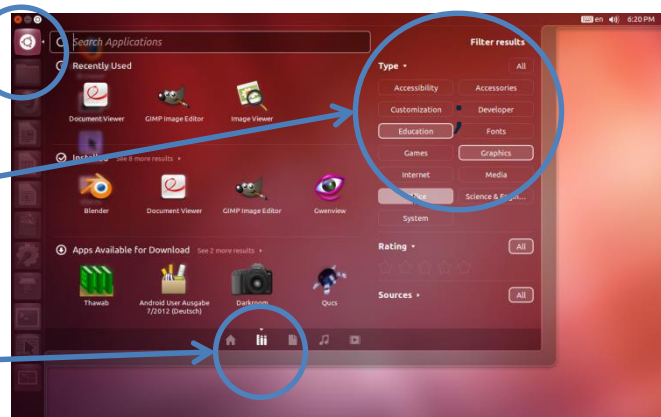
1. Log in to the desktop environment Unity (Ubuntu option in the menu environment option)
2. Log in to the text terminal number 03
3. Enter the command `ls` in it. Guess what is a purpose of the command
4. Log off from the text terminal and go back to the graphical terminal.
5. Open your Web browser and portal cluster WOLF in it. Log into the inner part. Display occupancy of the cluster.
6. Log in to the Information System and open this presentation in the study materials.

Standard Applications

Main menu

Results filtering

Submenu



Firefox	firefox	web browser
LibreOffice	libreoffice	text processor (Writer), spreadsheet (Calc), presentation (Impress)
Gimp	gimp	editor of raster graphics
Inkscape	inkscape	editor of vector graphics
Okular	okular	PDF viewer



name of command that launches the application

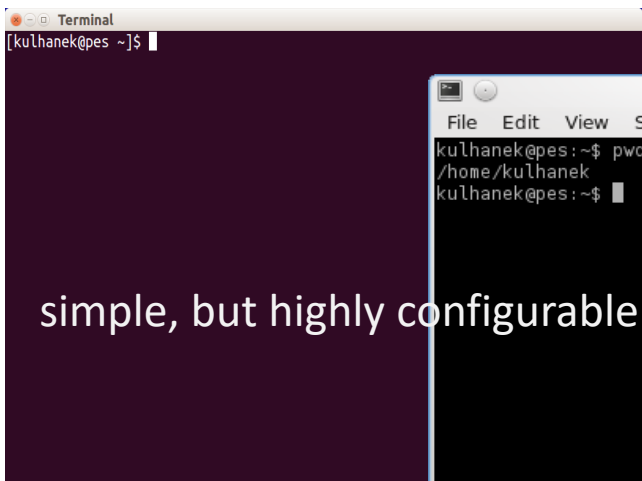
Terminals

Command line is accessible directly from text terminals. In a graphical environment X11 must be run in the appropriate application emulating a text terminal:

- **gnome-terminal (Terminal)**
- **konsole**
- **xterm**

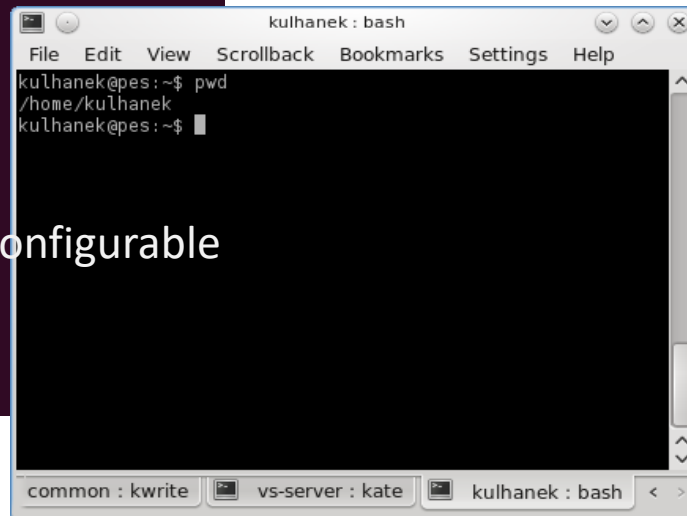
Default directory is: **/home/username**

gnome-terminal

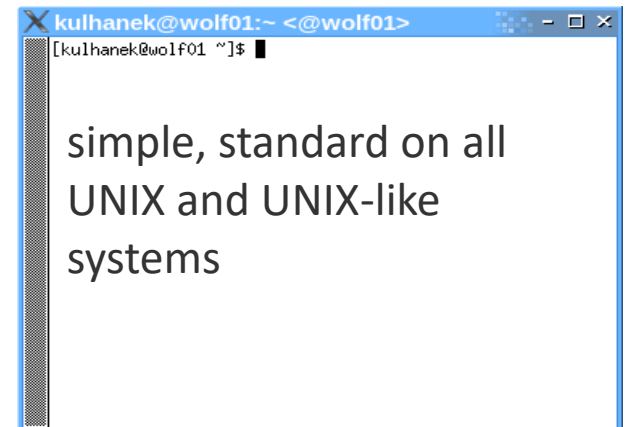


simple, but highly configurable

konsole



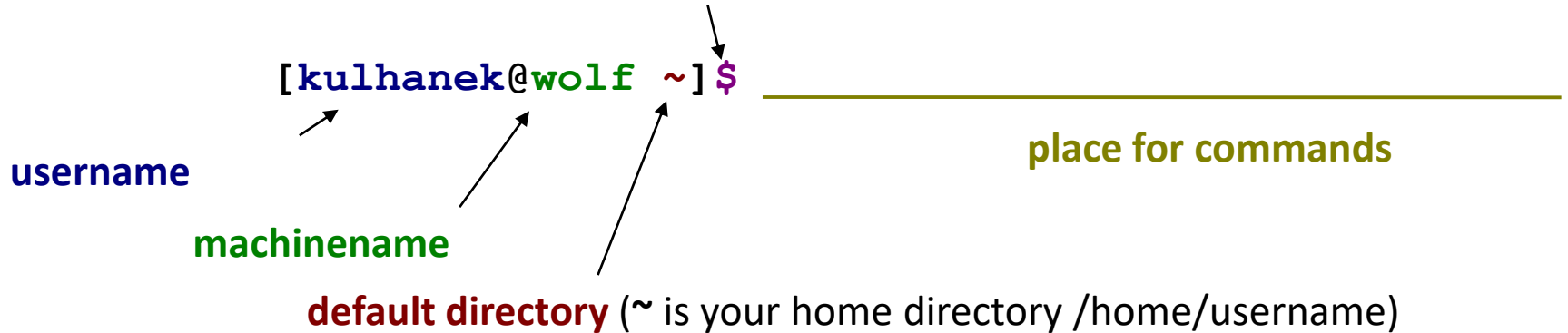
xterm



simple, standard on all
UNIX and UNIX-like
systems

Command line

Prompt - user type / calls (\$ normal user, # super user, other possibilities %, >)



command is executed by hitting **Enter**.

History: using the arrow keys up and down is possible to scroll through the list of previously used commands. The command from history can be reused or modified to use. History is also accessible by command **history**.

Autocompletion: hitting Tab (TAB) is a command line interpreter trying to complete itemized word. It can be use for completion of command names, paths and filenames (if one press does not cause anything, there are more options additions are displayed by repeated press).

Text copying: Not using Ctrl + C! To copy text from the terminal just mark a text, for subsequent insertion press the mouse wheel (the middle button).

Scientific and technical applications

Scientific and technical applications, that are installed in several versions (version, compilation type, parallel versions) are available as **modules**. Before using it is necessary to active appropriate module.

List of available applications:

`$ module`

in the command line, the text is written without the \$

List of available versions of the application:

`$ module versions vmd`

Version number and the name of module is separated by colon

Activation of application:

`$ module add vmd`

`$ module add vmd:1.9.0`

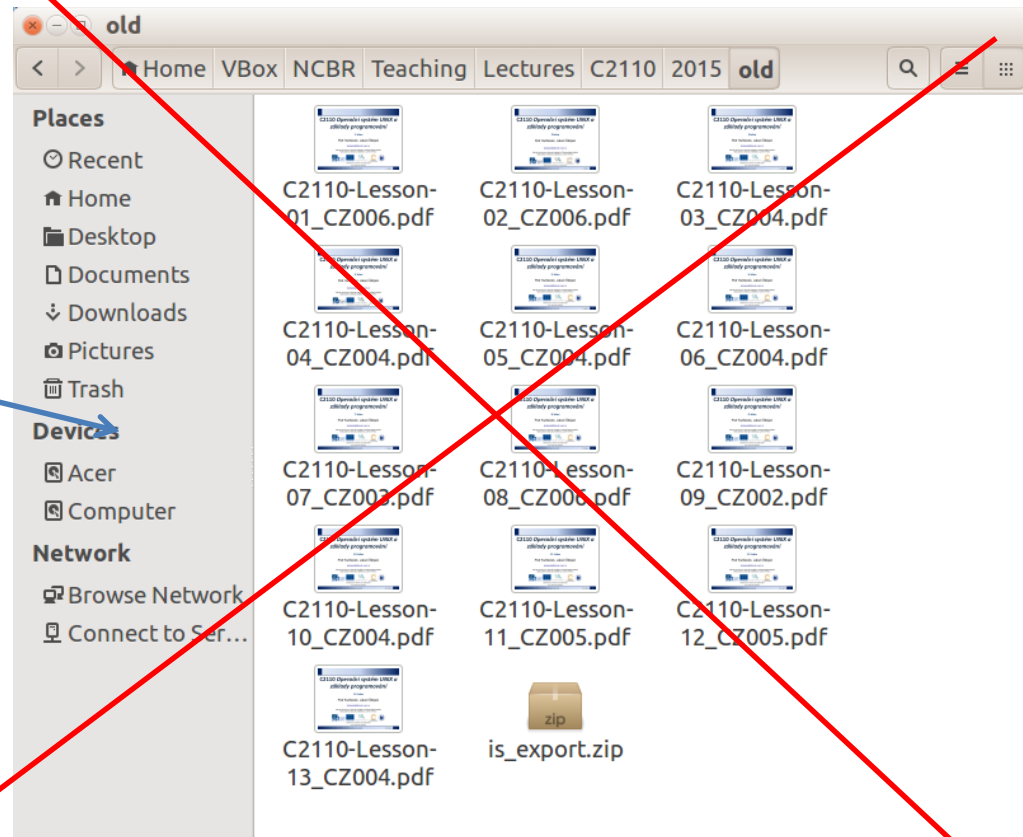
Launch vmd:

`$ vmd`

activate default version of module

name of module and application can differs.

File managers



!!!! Do not use!!!!

At supercomputer centers, there is mostly graphical interface not available
During exercise, unless otherwise stated, **use only command line.**

Prior preparation prevents poor performance

Exercise

1. Start **gimp** using Unity menu. In the program, draw a house with one pen line. The resulting triangles fill by various colors.
2. Start **Inkscape** from the command line. In a program, draw the flag of Czech Republic. Try to estimate the fundamental difference between this two programs.
3. Start **nemesis** by adding **nemesis** from the modules. Model the molecule of acetic acid and run geometry optimization in the program.
4. Start **LibreOffice**. In spreadsheet, shows the course of the sine function in the range of 0-360 °.

More in C2150 Information processing and visualization in chemistry

Conclusions

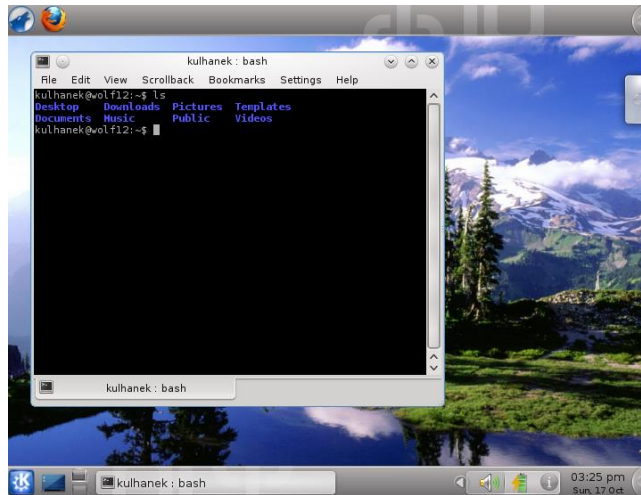
Conclusions

- Ubuntu is a **modern desktop environment** (this also applies to other distributions based on OS Unix).
- Ubuntu **includes alternatives of standard applications**: office packages (Writer, Calc, Impress), programs for creating vector (Inkscape) or raster (Gimp) graphics, programs for viewing web pages (Firefox).
- It has native support for **command line**.

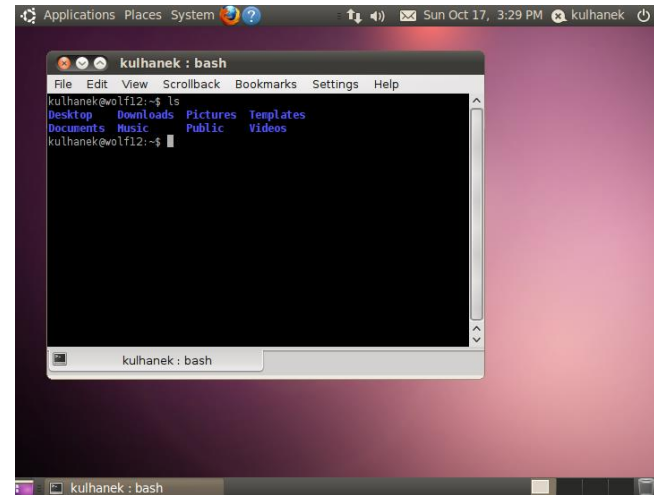
Desktop environments



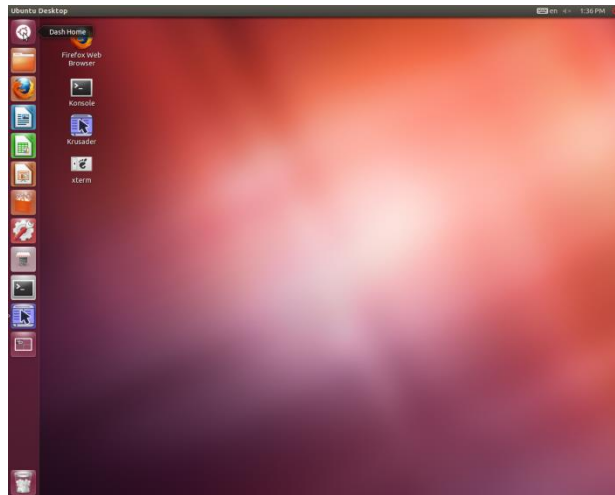
Desktopová prostředí



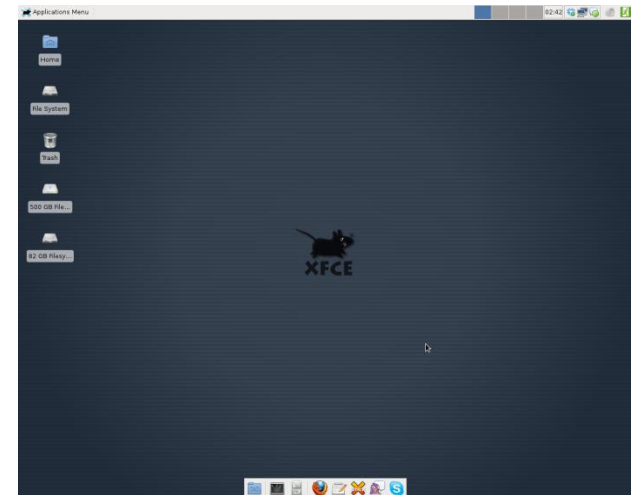
KDE



GNOME



Unity (in menu option Ubuntu)



Xfce

Homeworks

1. Gradually, log in to different desktop environments, which are available on workstations of cluster WOLF.
2. When you choose to work in any other desktop environment than Unity. Get familiar with it.
3. If you are used to work with Czech keyboard, install it into desktop environment of your choice.

Acknowledgement

On course preparation participated:

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