

C2110 UNIX and programming

3.lekce

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INVESTICE DO ROZVOJE VZDĚLÁVÁNÍ

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Scientific-technical applications

➤ module

Scientific – technical applications

Scientific-technical applications are installed in multiple versions (application version, compilation type, parallel version), these are available through **module** system. Before running application, particular module has to be activated.

Available modules list:

```
$ module
```

Available versions of module:

```
$ module versions vmd
```

Module activation:

```
$ module add vmd
```

```
$ module add vmd:1.9.0
```

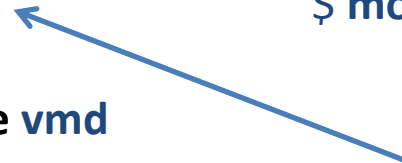
Module version is separated
by colon



Running application from module vmd

```
$ vmd
```

Activates default version



Exercise

1. List all applications accessible in module system.
2. Which versions are accessible for module **vmd** and **nemesis**.
3. Activate module **vmd** version **1.9.0** and run program **vmd**.
4. Activate module **nemesis** in default version and run program **nemesis**.

Remote file transfer

➤ `scp`

➤ `wget`

Remote copy

For remote copy there is command **scp**.

Syntax:

[] – maybe omitted

```
$ scp [-r] source destination
```

Source and destination can be file or directory. In case of directory copy option **-r** (recursive) has to be used.

Remote source or destination is identified by machine hostname separated by colon.

```
[user@]hostname: [path/] file
```

Usage examples:

```
$ scp pokus.txt wolf01.wolf.inet:/scratch/kulhanek
```

```
$ scp wolf01.wolf.inet:/scratch/kulhanek/pokus.txt .
```

Web file download


For file download from web command **wget** can be used. Remote machines has to provide files using protocol **ftp**, **http** or **https**.

```
$ wget [-O output_name] url
```

Upper case O



url (uniform resource locator)
www file identification



Usage examples:

```
$ wget http://www.rcsb.org/pdb/files/1SS9.pdb
```

PDB structure code



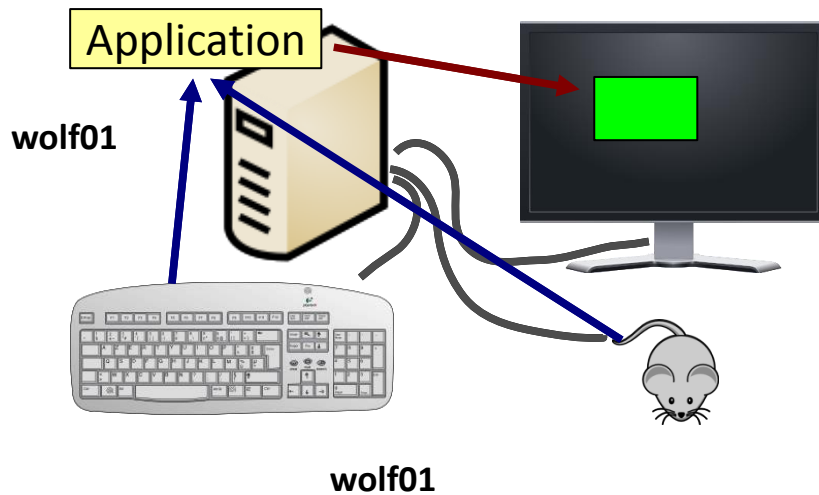
Remote graphical applications

- **Display export**

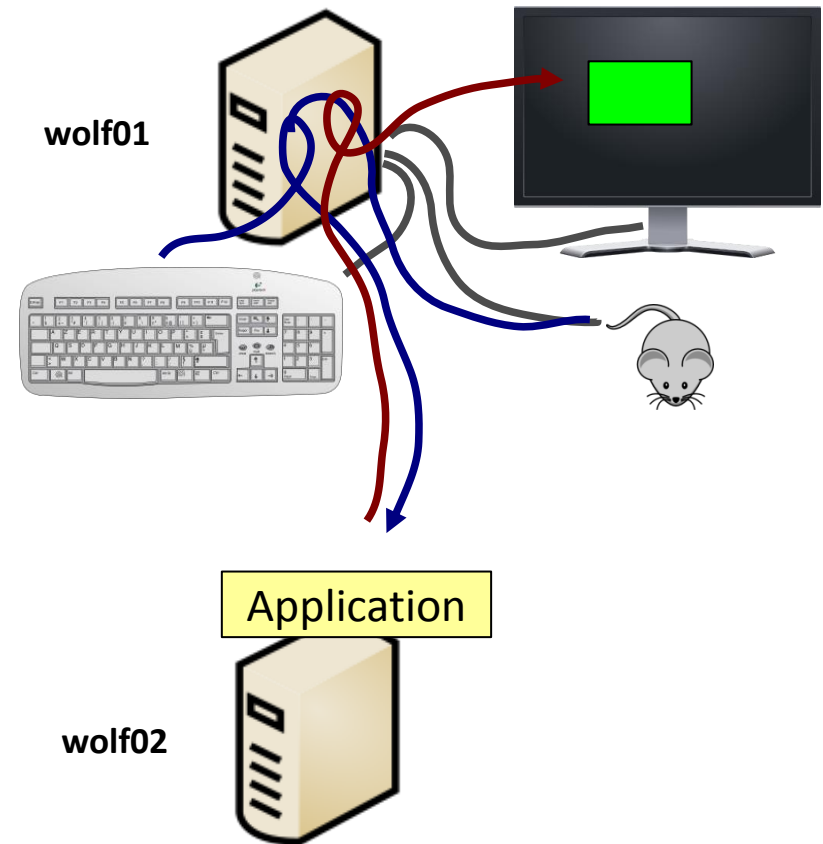
Running remote GUI application

Graphical applications can be run directly in X11 environment (graphical terminal) or with display export to remote desktop X11 environment.

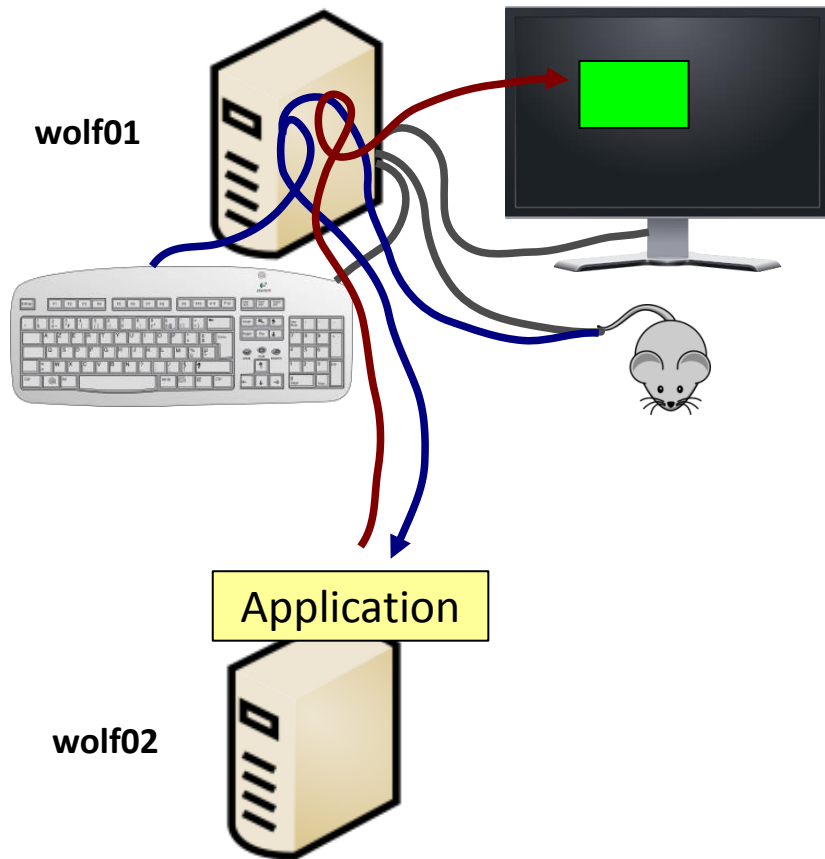
Direct run



Display export



Display export



Command `ssh` sets all necessities for display export automatically if option `-X` (uppercase X) is used.

```
[wolf01] $ ssh -X wolf02  
[wolf02] $ ./my_application
```

Option `-x` (lowercase x) disables export.

Display export can be done also manually, by setting variable `DISPLAY` and correct calls of commands `xhost` and `xauth`.

Exercise

1. Log to machine of your colleague using command **ssh**. Check your login mutually (command **w** or **who**).
2. Create subdirectory **pdb** in directory **/scratch/your_login**
3. Download structure **1SS9** from **PDB** database using command **wget** and save it as **test.pdb**.
4. Open structure in program **vmd**. Check, that your application runs on remote machine (**ps -e**). Check that application of your colleague runs on your machine (**ps -u his_login**).
5. Create subdirectory **structures** in directory **/scratch/your_login**
6. Copy file **1SS9.pdb** to your machine using command **scp** to directory **/scratch/your_login/structures**
7. Open structure in program **vmd** on your machine. Compare program qualitatively response (speed) for remote and local running.

Work in pairs.

Virtualization

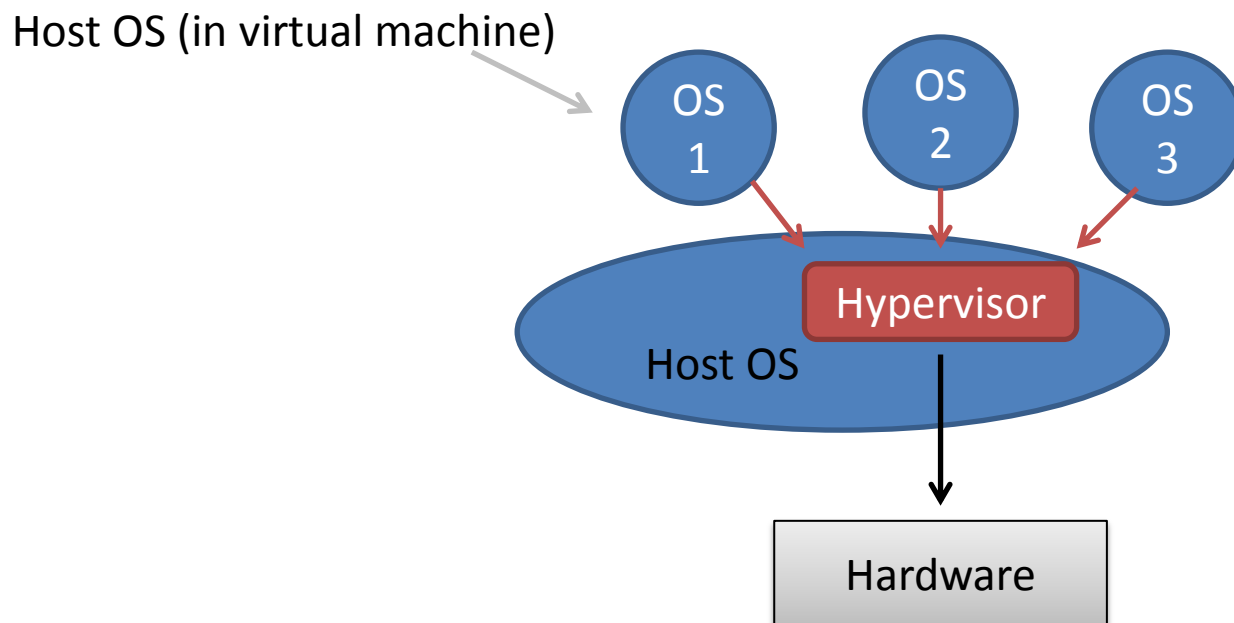
- **What is virtualization?**
- **Typical usage**
- **Hypervisor overview**
- **MS Windows in VirtualBox**
- **Ubuntu OS installation**

Virtualization – Hypervisor

Virtualization are procedures and techniques, that enables to approach computer hardware in different way, then they physically exist. Virtualization can be done **on different levels**, from whole computer (**virtual machine**), to particular hardware devices (virtual processors, memory etc.) or only software environment (virtualization of operating system).

source: www.wikipedia.org

Hypervisor – virtual machine manager



Virtualization advantages

- On one physical machine, there may run **multiple virtual machines** (each with different operating system).
- Physical hardware performance can be used more efficiently (lower costs).
- Easier backup. Virtual machine state maybe saved as **snapshots**, these can be used to **restore** original state.
- **Teleport**. Virtual machines can be transferred in between two physical machines with minimal stop time. Appropriate for hardware updates.
- **Easier testing** of OS.

Virtualization tools overview

VirtualBox

www.virtualbox.org

supported host OS: MS Windows, Mac OS X, Linux

Licence: freeware + proprietary extension for non-commerce usage

KVM

Linux kernel part

Supported host OS: Linux

Support programs: virt-manager, qemu

Licence: freeware

VMWare

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

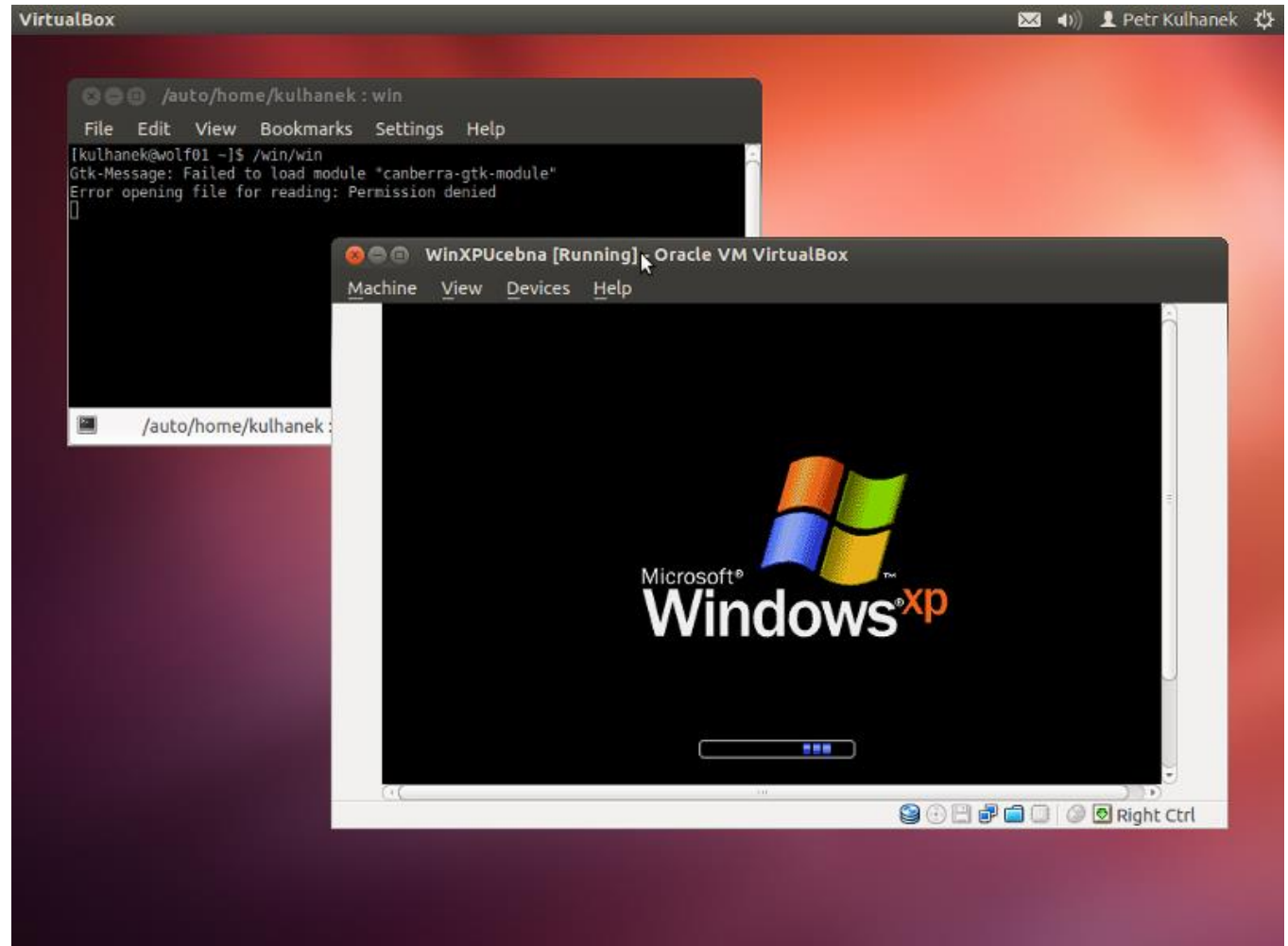
Supported host OS: MS Windows, Linux

Licence: commerce

MS Windows on WOLF cluster

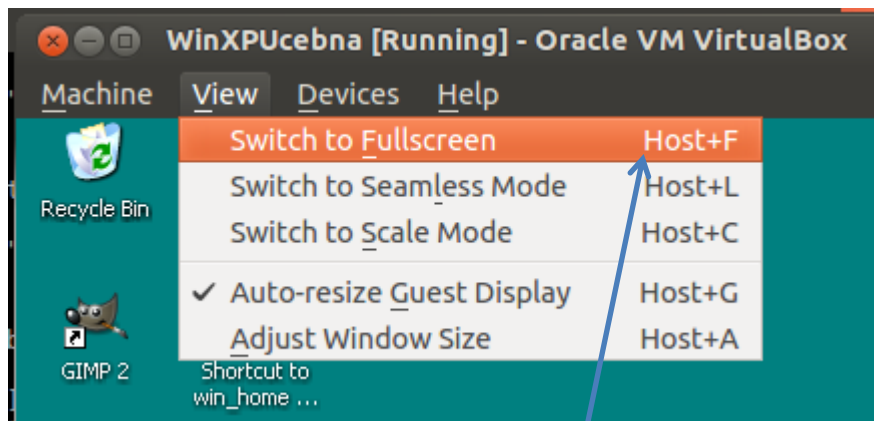
Running MS Windows XP in virtual machine (hypervisor VirtualBox)

```
$ /win/win
```



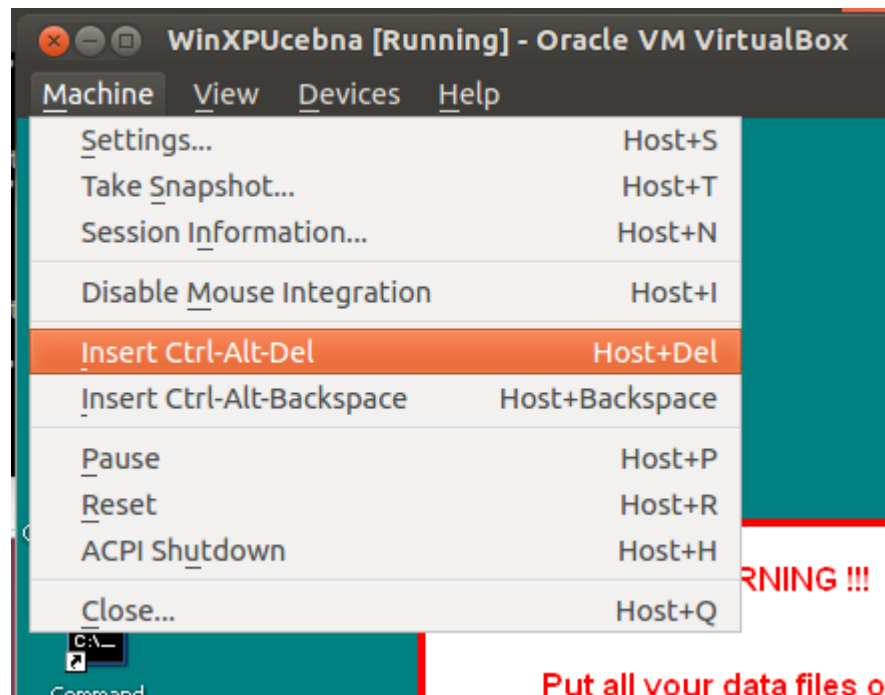
Virtual machine control

Full screen on / off switch



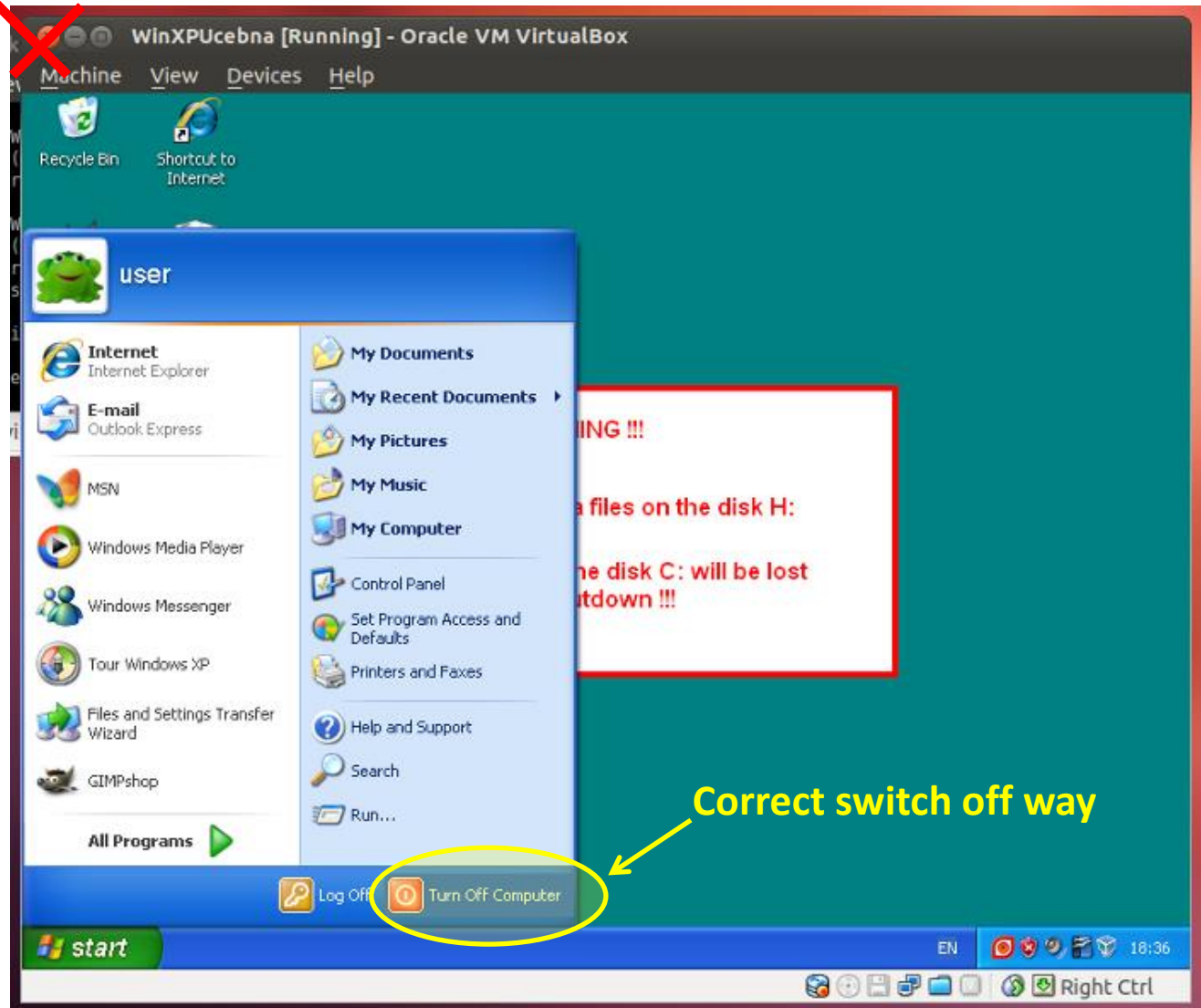
Host = (right Ctrl key)
(MS Windows and Linuxem)

How to input Ctrl+Alt+Del



Virtual machine switch off

Wrong switch off



Correct switch off way

Exercise

1. Run virtual machine with MS Windows XP (command **/win/win**).
2. Open **Internet Explorer** in virtual machine and find keyword Hypervisor in Wikipedia.
3. On host OS monitor hypervisor using command **top**.
4. Pause virtual machine.
5. Resume virtual machine.
6. Finish virtual machine.

Ubuntu 12.04 LTS installation

- Install program VirtualBox (<http://www.virtualbox.org>).
- Download installation image of OS Ubuntu as **iso** format:
<http://www.ubuntu.com/>
Ubuntu 12.04 LTS (Ubuntu Desktop)
- Create virtual machine in VirtualBoxu manager:
Choose OS **Linux** and **Ubuntu** version.
Other settings can be left on default values.
- First virtual machine run:
First run prompts for install media input. We attach **iso image** as installation media (icon on right and select downloaded iso image)
- System install
Then follow installation wizard hints.

Homework.

MS Windows as client

- Putty
- WinSCP
- Text file transfer

MS Windows as client – overview

Login to Linux from MS Windows (text terminal)

- **putty** www.chiark.greenend.org.uk/~sgtatham/putty
- **ssh** from Cygwin environment; www.cygwin.com

File transfer between Linux and MS Windows

- **WinSCP** www.winscp.com, twin-panel file manager
- **scp** from Cygwin environment;

Display export from Linux to MS Windows (X11 server)

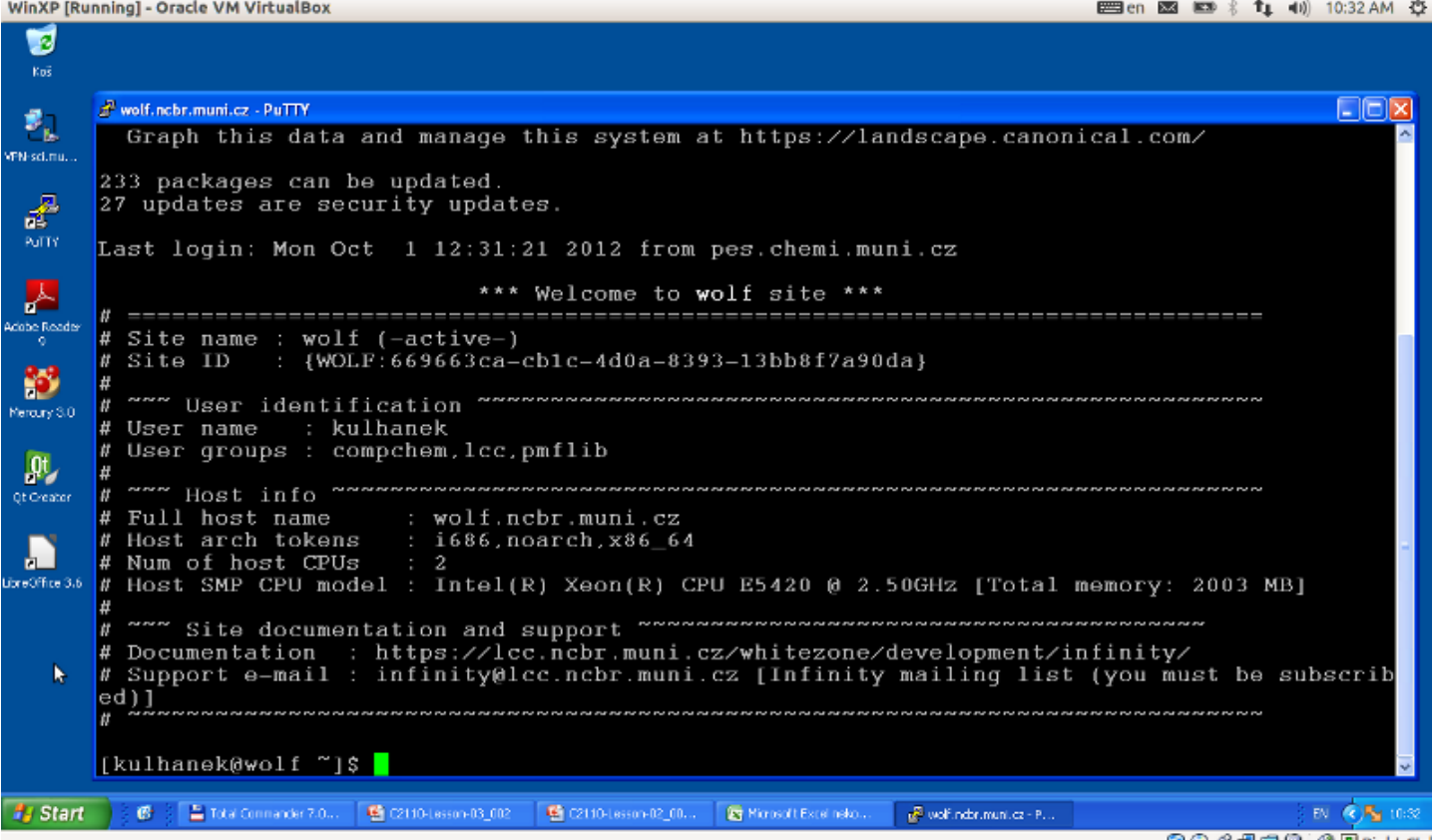
- **cygwin** www.cygwin.com
- **Xming** <http://sourceforge.net/projects/xming/>

Login from Linux to MS Windows (remote desktop)

- **rdesktop**

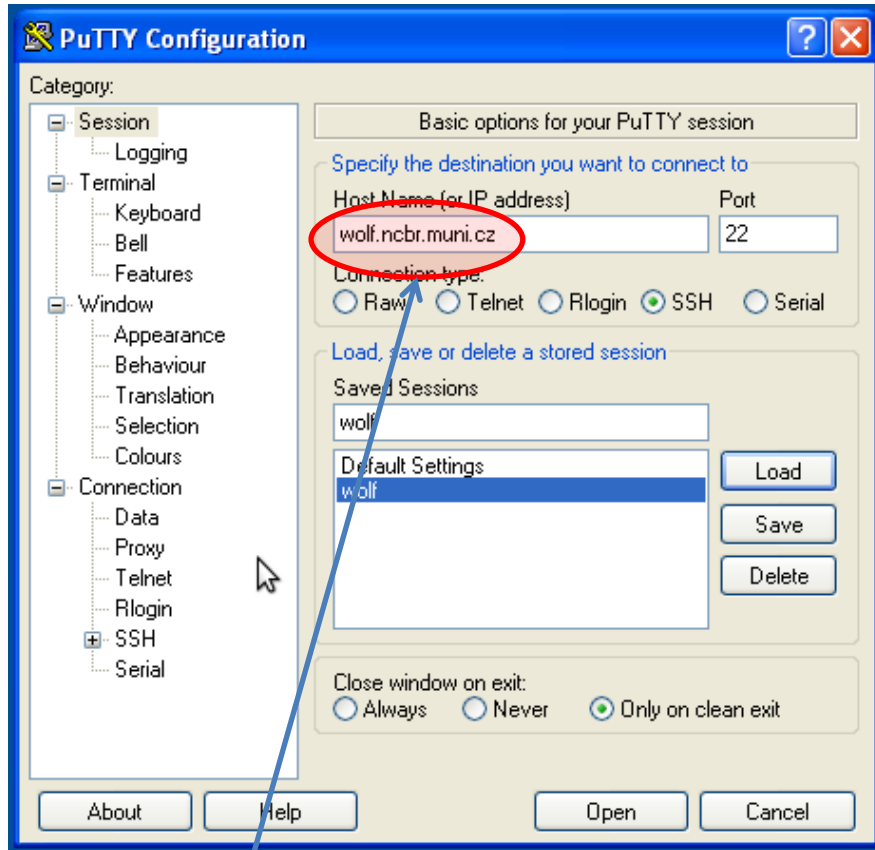
Putty

Putty <http://www.chiark.greenend.org.uk/~sgtatham/putty/>
Implementation of SSH (Secure Shell) for Windows, Putty enables remote connection to SSH servers (machines supporting ssh protocol and login – unix/linux type).



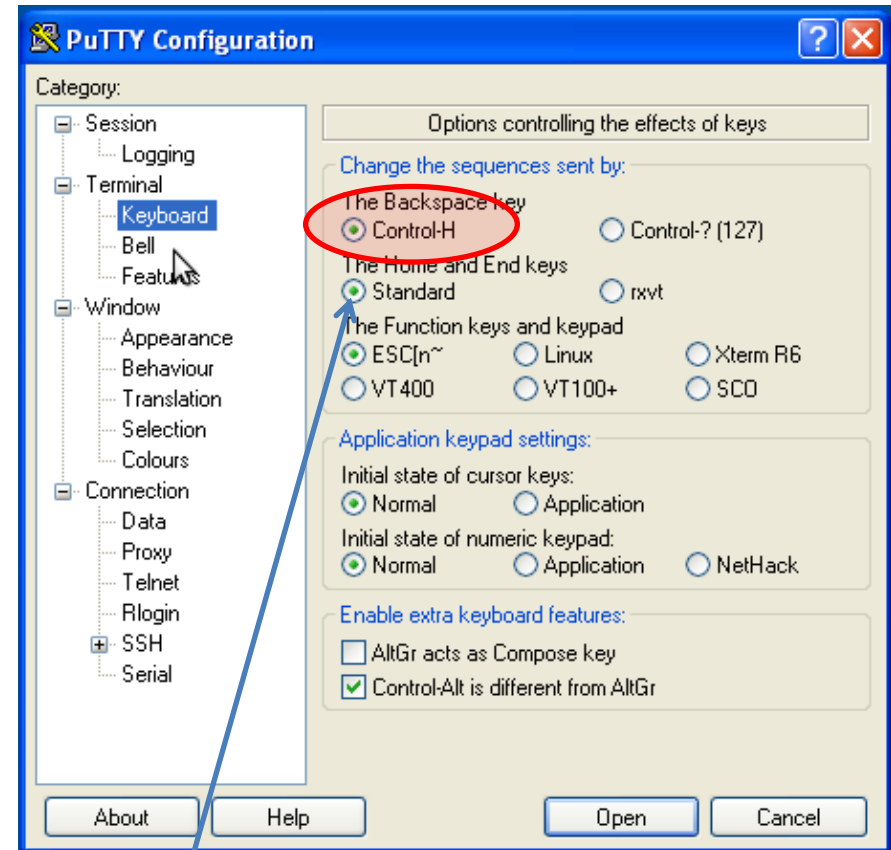
```
WinXP [Running] - Oracle VM VirtualBox
en 10:32 AM
wolf.ncbr.muni.cz - PuTTY
Graph this data and manage this system at https://landscape.canonical.com/
233 packages can be updated.
27 updates are security updates.
Last login: Mon Oct 1 12:31:21 2012 from pes.chemi.muni.cz
*** Welcome to wolf site ***
# =====
# Site name : wolf (-active-)
# Site ID : {WOLF:669663ca-cb1c-4d0a-8393-13bb8f7a90da}
#
# ~~~ User identification ~~~
# User name : kulhanek
# User groups : compchem,lcc,pmflib
#
# ~~~ Host info ~~~
# Full host name : wolf.ncbr.muni.cz
# Host arch tokens : i686,noarch,x86_64
# Num of host CPUs : 2
# Host SMP CPU model : Intel(R) Xeon(R) CPU E5420 @ 2.50GHz [Total memory: 2003 MB]
#
# ~~~ Site documentation and support ~~~
# Documentation : https://lcc.ncbr.muni.cz/whitezone/development/infinity/
# Support e-mail : infinity@lcc.ncbr.muni.cz [Infinity mailing list (you must be subscribed)]
#
[kulhanek@wolf ~]$
```


Putty – settings



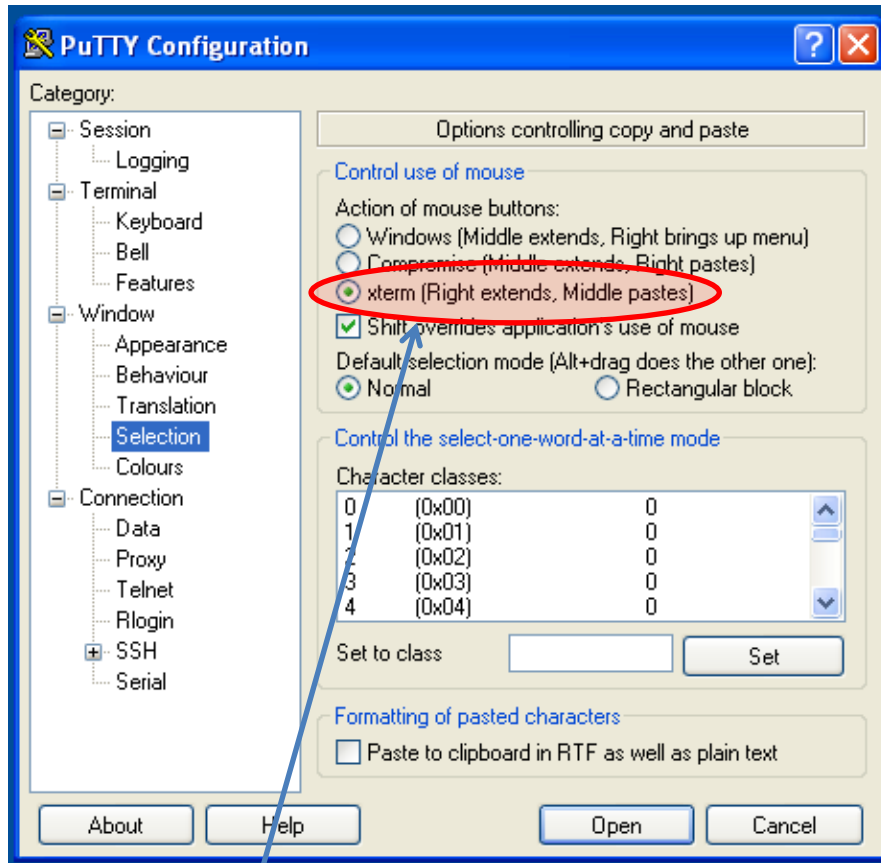
Remote machine address

wolf.ncbr.muni.cz

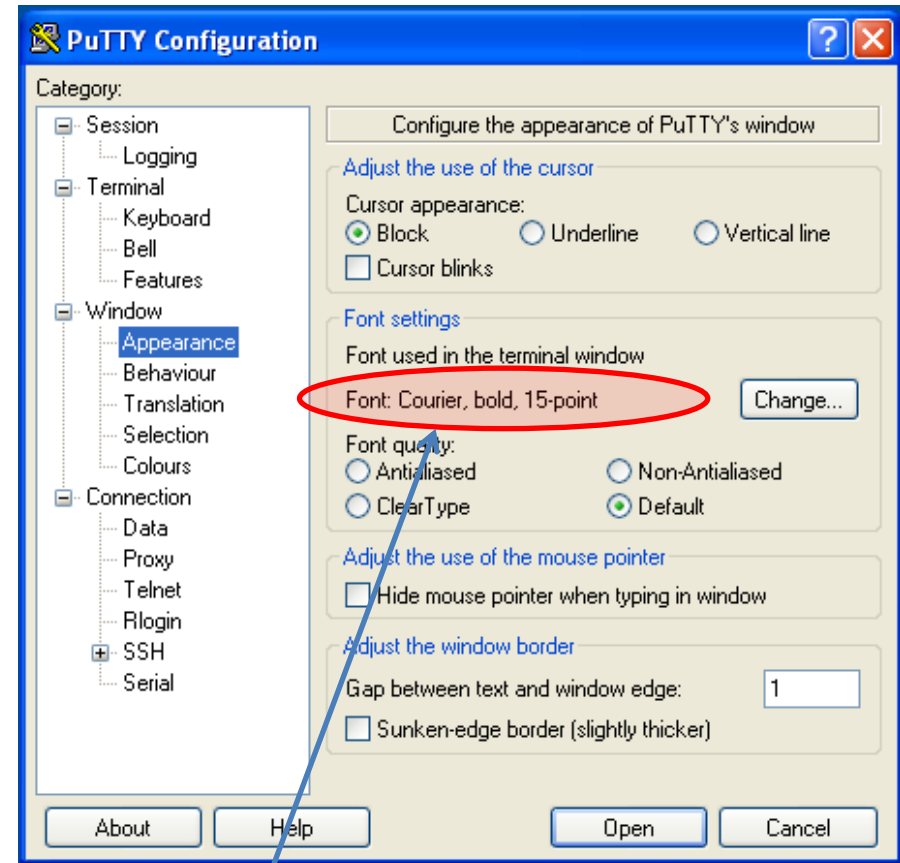


Backspace key interpretation.

Putty – settings II



Unix compatible mouse select / paste system.

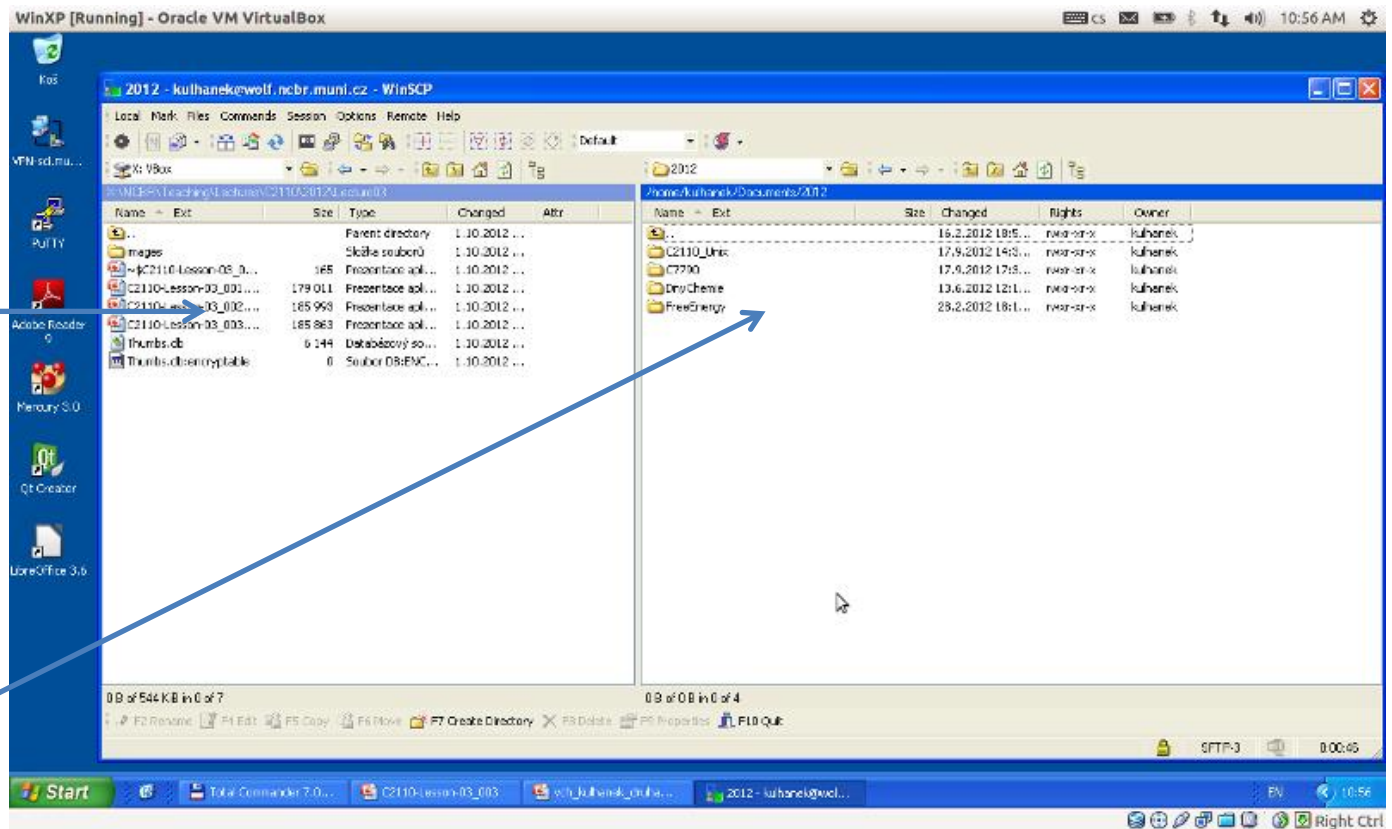


Non-proportional font
(all symbols have same width)

WinSCP

WinSCP <http://winscp.net/eng/docs/lang:cs>

Program for file transfer between MS Windows and computers supporting SFTP or SCP protocols (unix and linux type).



Local machine

Remote machine

Text files MS Win ↔ Linux

Text files created in MS Windows and Linuxem are **not** totally **compatible**, Each OS uses different coding of **line end**.

Linux: \n (line feed 0x0A)

MS Windows: \r+\n (carriage return 0x0D, line feed 0x0A)

For file conversion one can use programs **d2u** and **u2d** (on cluster WOLF).

1) Activation of cats module

```
$ module add cats
```

2) Conversion MS Windows => Linux

```
$ d2u file.com
```

3) Conversion Linux => MS Windows

```
$ u2d file.log
```

Exercise

1. Run virtual machine with MS Windows XP (**/win/win**).
2. Run application **Putty**.
3. Using terminal Putty log on machine **wolf.ncbr.muni.cz**.
4. Monitor who has logged on **wolf.ncbr.muni.cz**.
5. In terminal **Putty** try running application **vmd**. Why does it fail to run?
6. Run application **WinSCP**.
7. Download file **1SS9.pdb** to virtual machine. Open file in program **Notepad**. Is content shown correctly?
8. Correct line end coding in file **1SS9.pdb** and open file again in virtual machine program Notepad.