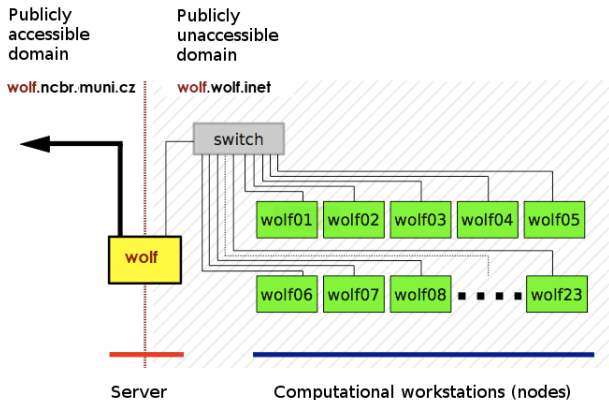


## Introduction to Unix

- Developed in 1970s in C language
- Open source code
- Multiuser system
- **Case-sensitive system**
- Many distributions developed since:
  - **Ubuntu**
  - Debian
  - BSD
  - Fedora
  - ...

# Cluster Wolf

- Head administrator: Mgr. Jakub Štěpán
- Scientific software administrator: RNDr. Petr Kulhánek, PhD.



- Unity
  - Native Ubuntu environment
- Gnome
- Xterm
  - Mac OS-like looking environment
- KDE
  - Windows-like looking environment
- Several text terminals
  - Accessed with CTRL+ALT+F1-F6

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

- 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

General advices aka “Good-To-Follow” rules:

- Case-sensitive system
- Do NOT use spaces in filenames (use underscore or dash)
- Good characters:
  - Alphanumerics
  - `_ . - +`
- Forbidden characters:
  - Any kind of diacritics
  - Quotation marks
  - Brackets
  - `# % ? ! , * ^ & @ / ~ ...`

- Found in Applications → Accessories → 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



# Terminal welcome output

- Useful information: Highly advisable to read
- Contains:
  - System statistics
  - Last login of user and IP address
  - Active site
  - User and Host info
  - **Site documentation and support**

# Useful commands I

Command	Action
<code>cd foo</code>	Change current working directory to “foo”
<code>ls</code>	List files in directory
<code>cp source target</code>	Copy source file to target file
<code>cp -r source target</code>	Copy source directory recursively into target
<code>mv source target</code>	Move source file to target file
<code>mkdir foo</code>	Create “foo” directory
<code>rmdir foo</code>	Remove <sup>a</sup> “foo” directory (only if empty)
<code>rm foo</code>	Remove <sup>a</sup> “foo” file
<code>rm -r foo</code>	Remove <sup>a</sup> “foo” directory recursively
<code>cat foo</code>	Print content of a “foo” file into terminal
<code>grep foo file</code>	Print only line containing “foo” keyword in “file”
<code>top</code>	See currently running processes

<sup>a</sup> Removing means deleting from the disc. **NOT** moving into trash.

## Useful commands II

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

- General way of use is:
  - `mnovak@wolf:~$ command [argument1, [argument2, ...]]`
- Switches
  - Alter output of commands
  - Short notation: `command -a -b -C`
  - Long notation: `command --alpha --beta --Gamma`
  - Use switch “-h” or “--help” for general help
- Manual pages
  - Help for basic commands
  - Accessed via command `man`
  - Close help with “q” key

- 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)

Will terminate current command!



# Example

- Run the following commands and compare results
  - `$ ls`
  - `$ ls -a`
  - `$ ls -l`
  - `$ ls -h`
  - `$ ls -lah`

# 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

# Running jobs in background

- Terminal is still usable for other tasks
- Two ways to achieve:
  - `$ command &`
  - Once job is running in terminal:
    - CTRL+z # Stops current task
    - `$ bg` # Puts all jobs into background



# 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 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  NI  VIRT  RES  SHR  S  %CPU  %MEM   TIME+  COMMAND
 5877 mnovak   20   0  133m 2228  840  S   0   0.1   0:00.08 sshd
 5878 mnovak   20   0 15976 5368 1656  S   0   0.3   0:00.55 bash
 7678 mnovak   20   0  9128 1136  852  R   0   0.1   0:00.07 top
```

# Password change

- `$ passwd`
- Insert current password
- Enter new password twice (check for typos)
- **No characters are printed in terminal during typing**

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.

- System of modules located on server
- Modules must be imported prior to running
- Some modules available only at selected nodes
- \$ **module avail** # Lists all available modules
- \$ **module add moduleName** # Adds selected module to path
- \$ **module remove moduleName** # Removes selected module
- Full description of imported module:
  - moduleName:version:arch:build
  - It is always a good practice to include version
- Full documentation at website:

<https://lcc.ncbr.muni.cz//whitezone/development/infinity/>

# Example

- Run following commands and see the results:

```
$ gabedit
```

```
$ module add gabedit:2.3.0
```

```
$ gabedit
```

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

- 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/html/doc/visual.html#Visual`

# 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

- 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

# Example

- 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](#)

# 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

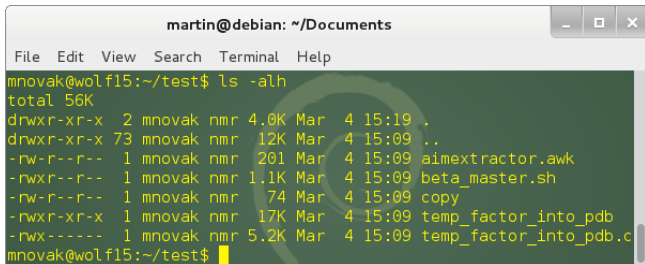
- \$ *scp* source target
  - Source and/or target can be on remote machine:
  - `mnovak@wolf12:~$ scp text.dat wolf13:/scratch/mnovak/`
  - `mnovak@wolf12:~$ scp -r wolf13:/scratch/mnovak/ directory/`
- \$ *mc*
  - Midnight commander - same as in Windows/Mac machines
  - “Graphical interface”
- \$ *gftp*
  - “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
File Edit View Search Terminal Help
mnovak@wolf15:~/test$ ls -alh
total 56K
drwxr-xr-x  2 mnovak nmr  4.0K Mar  4 15:19 .
drwxr-xr-x 73 mnovak nmr  12K Mar  4 15:09 ..
-rw-r--r--  1 mnovak nmr   201 Mar  4 15:09 aimextractor.awk
-rwxr--r--  1 mnovak nmr   1.1K Mar  4 15:09 beta_master.sh
-rw-r--r--  1 mnovak nmr    74 Mar  4 15:09 copy
-rwxr-xr-x  1 mnovak nmr   17K Mar  4 15:09 temp_factor_into_pdb
-rwx-----  1 mnovak nmr   5.2K Mar  4 15:09 temp_factor_into_pdb.c
mnovak@wolf15:~/test$
```

# Change permissions

- \$ *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

# Variables

- Variables are used for storing values
- Various languages/interpreters use different name schemes
  - bash/tcsh: CAPITAL\_LETTERS
  - awk: lowercase\_letters
  - c++: almostEveryFirstLetterCappitalized
  - ...
- Variable names follow in general the same rules as filenames
- Variables in bash/tcsh accessible via \$ sign, e.g. \$RANDOM, for example



# Scripts in bash

- Scripts are executable files which serve as storage of commands
- They are read line by line by interpreter and commands are run
- User does not have to type everything by hand
- Script must have executable permission
- Running scripts: `mnovak@wolf:~$ ./myscript.sh`
- Comments after hash “#” sign

```
mnovak@wolf:~
```

```
#!/bin/bash
```

```
# This is a script which makes a directory, enters it and, lists all files
```

```
mkdir test; # This commands makes the directory
```

```
cd test; # This command enters it
```

```
ls -alh; # This command lists all files inside
```

# Useful script in bash

```
mnovak@wolf:~
```

```
#!/bin/bash
```

```
# This script loads gaussian module and performs calculations
```

```
module add gaussian:09.A2; # Loads the module
```

```
g09 input.com;          # Performs the calculations
```

```
echo "All work done!";  # Prints info into terminal
```

```
return 0;                # Return code for the script can be accessed via '$?' variable
```