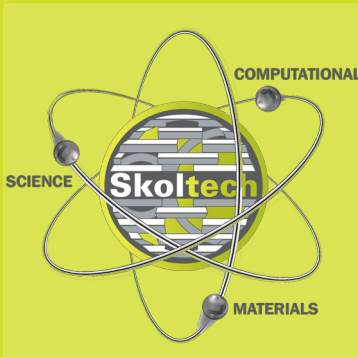




Tutorial 1: Introduction to linux command line interface and practice



Anton Boev, Dmitriy Aksyonov

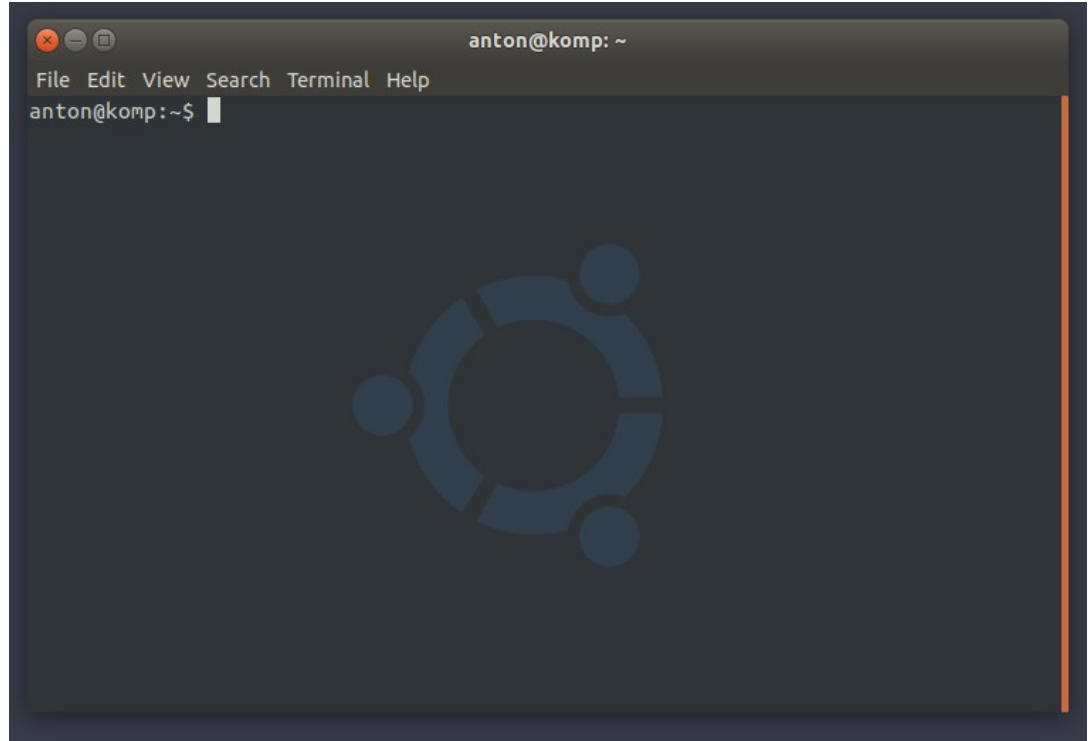
Theory

What is the Terminal in Linux?

The **terminal** is the GUI window that you see on the screen. It takes commands and shows output.

The **shell** is the software that interprets and executes the various commands that we type in the terminal.

Bash is a particular shell. It stands for **Bourne Again Shell**.



Basic bash commands

- ***ls*** - show the content of the current directory
- ***pwd*** - show the path to the current directory
- ***mkdir*** <name> - create a new directory
- ***touch*** <name.ext> - create a new file with extension *.ext*
- ***cat*** <file> - show a file

Midnight commander (MC) file manager

```
anton@komp:~$ mc
```

```
mc [anton@komp]:~
File Edit View Search Terminal Help
Left File Command Options Right
<- ~ -.[^]> <- ~ -.[^]>
.n Name Size Modify time .n Name Size Modify time
/.. UP--DIR мар 29 2020 /.. UP--DIR мар 29 2020
/Desktop 4096 ноя 1 12:18 /Desktop 4096 ноя 1 12:18
/Documents 4096 июл 3 11:53 /Documents 4096 июл 3 11:53
/Downloads 4096 окт 24 01:00 /Downloads 4096 окт 24 01:00
/Music 4096 апр 29 2020 /Music 4096 апр 29 2020
/Pictures 4096 июл 20 16:42 /Pictures 4096 июл 20 16:42
/Public 4096 мар 29 2020 /Public 4096 мар 29 2020
/Simulati~wrapper 4096 мая 18 22:43 /Simulati~wrapper 4096 мая 18 22:43
/Templates 4096 мар 29 2020 /Templates 4096 мар 29 2020
/hack 4096 апр 8 2020 /hack 4096 апр 8 2020
/mary 4096 мая 23 2020 /mary 4096 мая 23 2020
/media 4096 сен 8 12:12 /media 4096 сен 8 12:12
/newbtfix-4.15 4096 янв 18 2021 /newbtfix-4.15 4096 янв 18 2021
/screen_records 4096 мар 31 2021 /screen_records 4096 мар 31 2021
/sd 4096 мая 23 2020 /sd 4096 мая 23 2020

/Desktop 48G/109G (43%) UP--DIR 48G/109G (43%)
Hint: Use C-x t to copy tagged file names to the command line.
anton@komp:~$
1Help 2Menu 3View 4Edit 5Copy 6RenMov 7Mkdir 8Delete 9PullDn10Quit
```

<http://rus-linux.net/MyLDP/console/midnight-commander.html>

Hotkeys in MC

- **TAB** - switch active panel
- F<1-10>

1 Help	2 Menu	3 View	4 Edit	5 Copy
6 RenMov	7 Mkdir	8 Delete	9 PullDn	10 Quit

- Ctrl+O - switch between MC window and command line

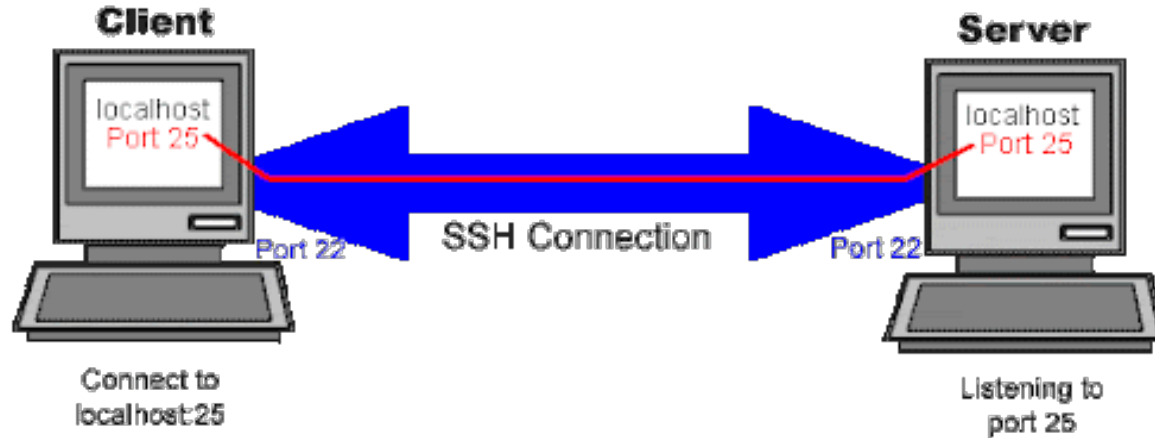
Open file using MC

- **F3/F4** - read only/edit mode

```
Left File Command Options Right
<- ~/vasp/surseg_tem/seg_paper/slab/LC.104.m05.7l.1ULC_g .[^]>
'n Name Size Modify time
/.. UP--DIR OKT 27 11:12
1.CHGCAR.gz 82407K OKT 2 09:07
1.CONTCAR 24954 OKT 2 09:05
1.OUTCAR 30373K OKT 2 09:06
1.POSCAR 14516 OKT 1 12:47
EIGENVAL 45032 OKT 2 09:06
IBZKPT 132 OKT 2 01:03
INCAR 1050 OKT 1 12:47
KPOINTS 37 OKT 1 12:47
LC.104.m05.7l.1ULC_g.1.log 29608 OKT 2 09:06
*LC.104.m05.7l.1ULC_g.run 843 OKT 1 12:47
POSCAR 14516 OKT 2 01:03
POTCAR 484219 OKT 1 12:47
sbatch.err 79 OKT 2 09:07
sbatch.out 0 OKT 2 01:03
```

```
1.POSCAR [----] 0 L:[ 1+ 0 1/233] *
i2a=[Co,Li,O] ; LC.104.22w.8.1.end
1.0000000000000000
11.348340 0.000000 -0.530610
-0.034760 11.478141 -0.743419
0.000000 0.000000 30.405135
Co Li O.
56 56 112.
Direct
0.0533931256896239 0.1889792849261411 0.969
0.5533931256896238 0.1889792849261411 0.969
0.0533931256896238 0.6889792849261411 0.969
0.5533931256896237 0.6889792849261411 0.969
0.3033931256896238 0.1889792849261411 0.969
0.8033931256896238 0.1889792849261411 0.969
0.3033931256896238 0.6889792849261411 0.969
```

How to connect to the remote machine?



Secure Shell (SSH) protocol for Linux-based machines

SSH for Linux

```
anton@komp:~$ ssh username@10.20.30.299
```

Write the following command into terminal, where

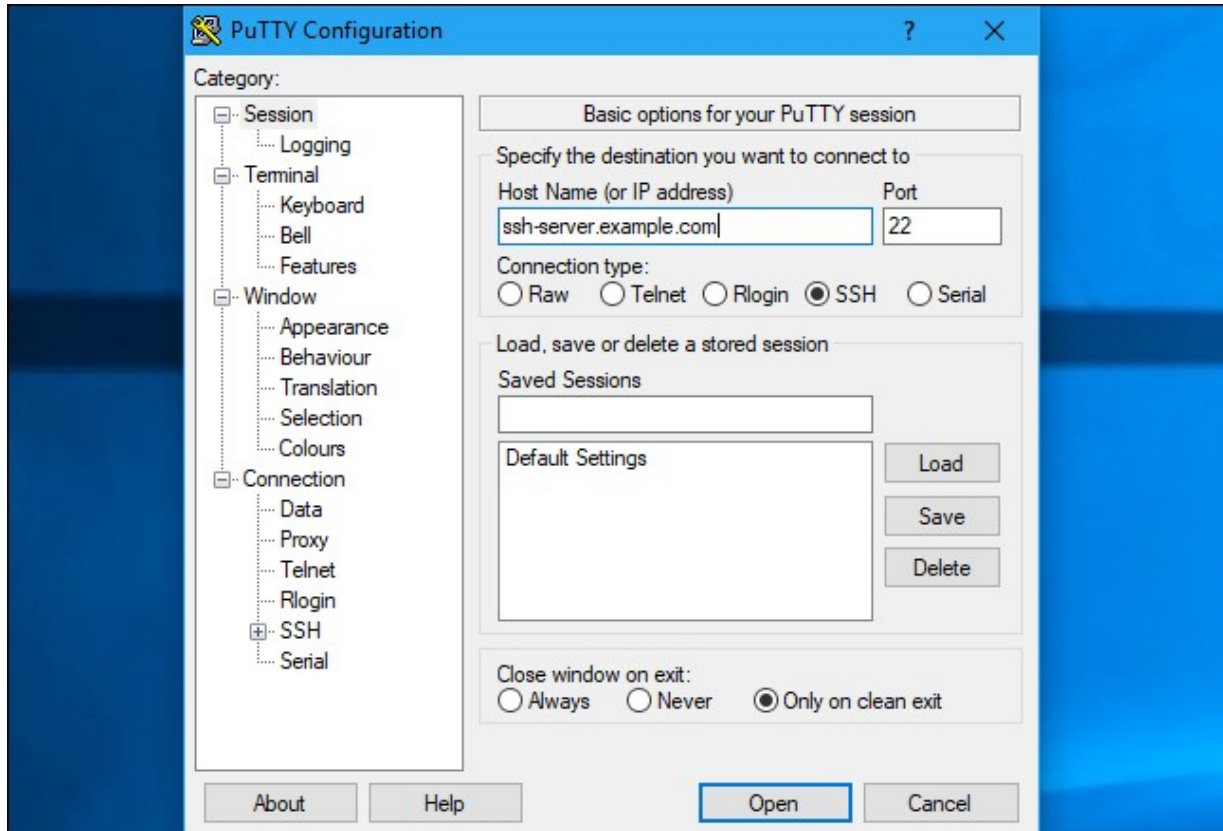
Username - your username on remote cluster

Numbers after @ - ip address of remote cluster

Then input your password



SSH for Windows - Putty client



Practice

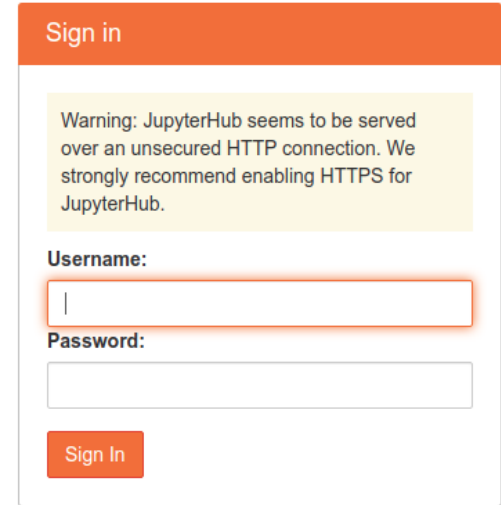
How can you connect to Jupyter server?

1. Visit a webpage: <http://10.30.99.214:8000/hub/login>
2. Input your credentials, which were sent to your email
3. Look around ;)



The screenshot shows the JupyterLab interface. At the top left is the Jupyter logo. On the right, there are buttons for 'Quit', 'Logout', and 'Control Panel'. Below the logo, there are tabs for 'Files', 'Running', and 'Clusters'. A message says 'Select items to perform actions on them.' followed by 'Upload', 'New', and a refresh icon. The main area is a file browser showing a directory structure with folders 'potcars', 'tutorial_5', 'tutorial_6', 'tutorial_7', and 'tutorial_8', and files 'pass_cys21' and 'simanrc.py'. The file browser has columns for 'Name', 'Last Modified', and 'File size'.

	Name	Last Modified	File size
<input type="checkbox"/>	potcars	20 часов назад	
<input type="checkbox"/>	tutorial_5	12 минут назад	
<input type="checkbox"/>	tutorial_6	10 минут назад	
<input type="checkbox"/>	tutorial_7	16 минут назад	
<input type="checkbox"/>	tutorial_8	10 минут назад	
<input type="checkbox"/>	pass_cys21	20 часов назад	133 Б
<input type="checkbox"/>	simanrc.py	6 минут назад	1.06 kB



The screenshot shows the JupyterLab login page. It has an orange header with the text 'Sign in'. Below the header, there is a warning message: 'Warning: JupyterHub seems to be served over an unsecured HTTP connection. We strongly recommend enabling HTTPS for JupyterHub.' Below the warning, there are two input fields: 'Username:' and 'Password:'. The 'Username:' field is highlighted with a red border. Below the input fields, there is an orange button labeled 'Sign In'.

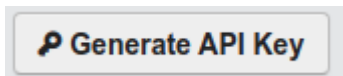
Manage simanrc.py file

input your username (the same as login)

generate own API key and input there

Just visit a web:

<https://materialsproject.org/dashboard>



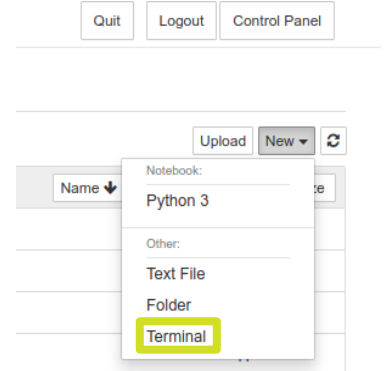
```
jupyter simanrc.py 9 минут назад
file Edit View Language Python

1 # -*- coding: utf-8 -*-
2 """
3 User-related parameters for siman, file is installed to home folder
4 """
5
6 from __future__ import division, unicode_literals, absolute_import
7 from siman.header import CLUSTERS
8
9 """Cluster constants"""
10 DEFAULT_CLUSTER = 'raz'
11 PATHZARCHIVE = '' # path to archive; if no files are found at home folder, siman will check here; relative paths should be same
12
13 user = 'a.boev'
14 CLUSTERS['raz'] = {'address':user+'@10.30.99.220',
15 'vasp_com':'mpirun vasp_std',
16 'homepath':'/home/'+user,
17 'schedule':'SLURM',
18 'walltime':'1:00:00',
19 'corenum':1,
20 'modules':'module load devtools/compiler/nvhpc/20.11; \
21 module load q-ch/vasp/5.4.4_OPT; \
22 \nulimit -s unlimited\n'
23 }
24
25
26 """Local constants"""
27 PATH2POTENTIALS = '/home/'+user+'/potcars/'
28 PATH2JMOL = 'java -jar /hdd/home/aksenov/installed/jmol-14.29.46/Jmol.jar'
29 PATH2PHONOPY = 'phonopy'
30 pmgkey = "AWqKPyV8EmTRlfl1" #API_KEY can be generated in the following webpage: https://materialsproject.org/dashboard
31 EXCLUDE_NODES = False
32
33 cluster_tools = 'tools'
34 show_head = None # show header for res_loop()
35
36
37
```

How to Setup Passwordless SSH Login

1. Open Terminal

```
Copyright (C) 2009-2016 Intel Corporation. All rights reserved.  
Intel(R) Inspector XE 2016 (build 460803)  
Copyright (C) 2009-2016 Intel Corporation. All rights reserved.  
Intel(R) VTune(TM) Amplifier XE 2016 (build 463186)  
Copyright (C) 2009-2016 Intel Corporation. All rights reserved.  
Intel(R) Advisor XE 2016 (build 463413)  
a.boev@Precision-T1700:~$
```

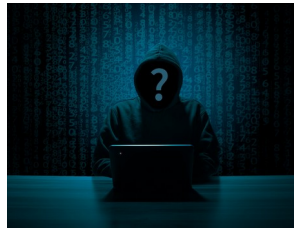


2. Generate personal keys (type command `ssh-keygen`)

3. Setup Passwordless ssh login (type command `ssh-copy-id username@10.30.99.220`)

4. If everything was ok you can access to cluster via command `ssh username@10.30.99.220`

5. Enjoy! You look like Russian hacker ;)



<https://linuxhint.com/use-ssh-copy-id-command/>

List of useful terminal commands

1. ***ssh username@10.30.99.220*** - access to the cluster
2. ***mc*** - run file manager
3. **Ctrl+O** - switch between MC and command line
4. **Tab** - switch between MC panels (left - right)
5. ***squeue*** - show job schedule on cluster
6. ***unzip name.zip*** - unzip archive
7. ***zip -r <name_of_new_archive>.zip <folder_name>*** - compress folder into zip archive

Thx

