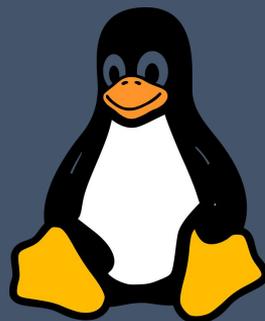


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Crystallography and Crystal Chemistry
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Young Scientists 2023

Tutorial 1-2: Introduction to linux command line and Jupyter notebook



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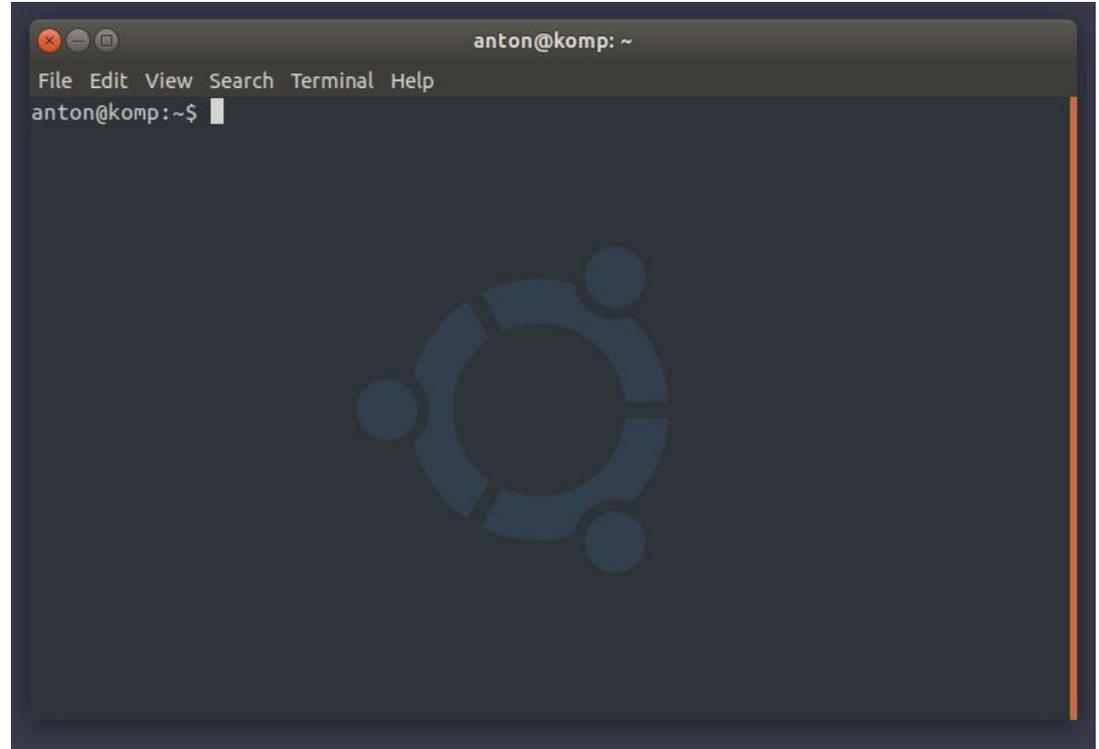
1. Terminal

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
```

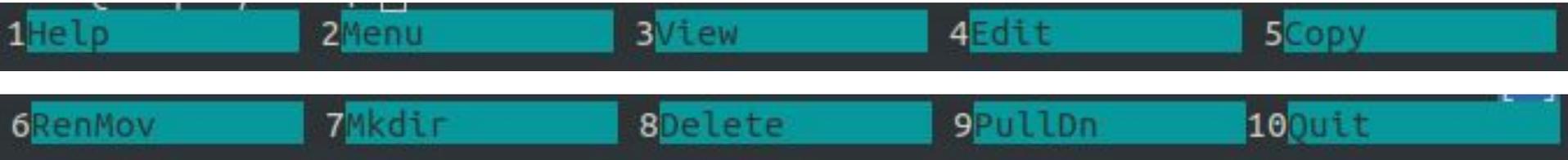
```
mc [anton@komp]:~
File Edit View Search Terminal Help
Left File Command Options Right
<- ~ .[^]> <- ~ .[^]>
.n Name Size Modify time .n Name Size Modify time
/.. UP--DIR мар 29 2020 /.. UP--DIR мар 29 2020
/Desktop 4096 ноя 1 12:18 /Desktop 4096 ноя 1 12:18
/Documents 4096 июл 3 11:53 /Documents 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 9PullDn 10Quit
```

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

Hotkeys in MC

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



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

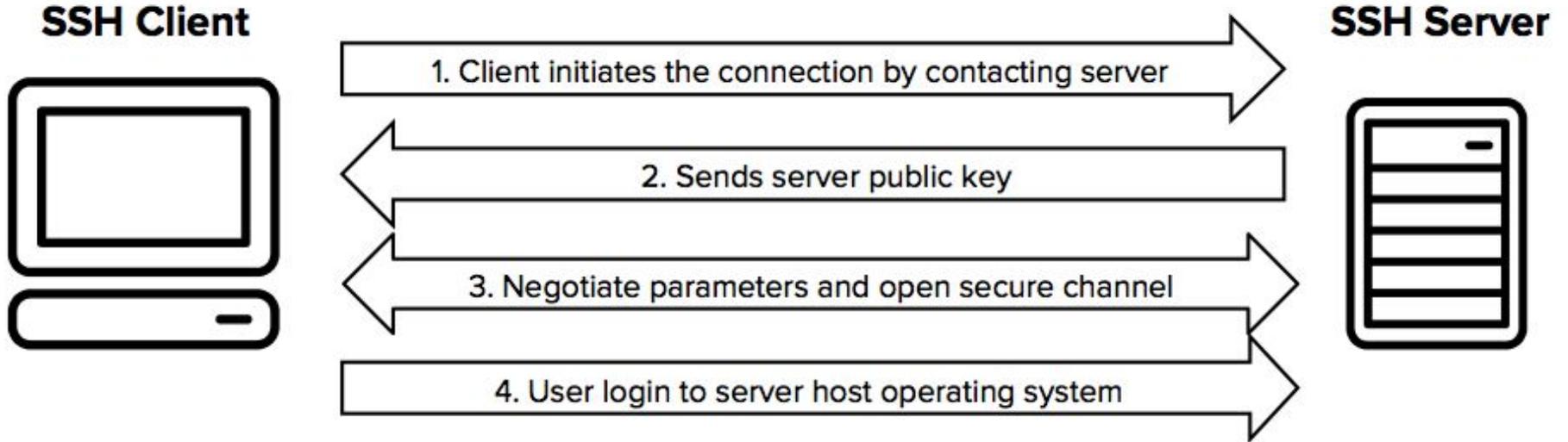
Open file using MC

- **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
/..            UP--DIR  OKT 27 11:12
1.CHGكار.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



```
ssh username@IP-address  
#for example ssh a.boev@10.16.77.19
```

Write the following command into terminal, where

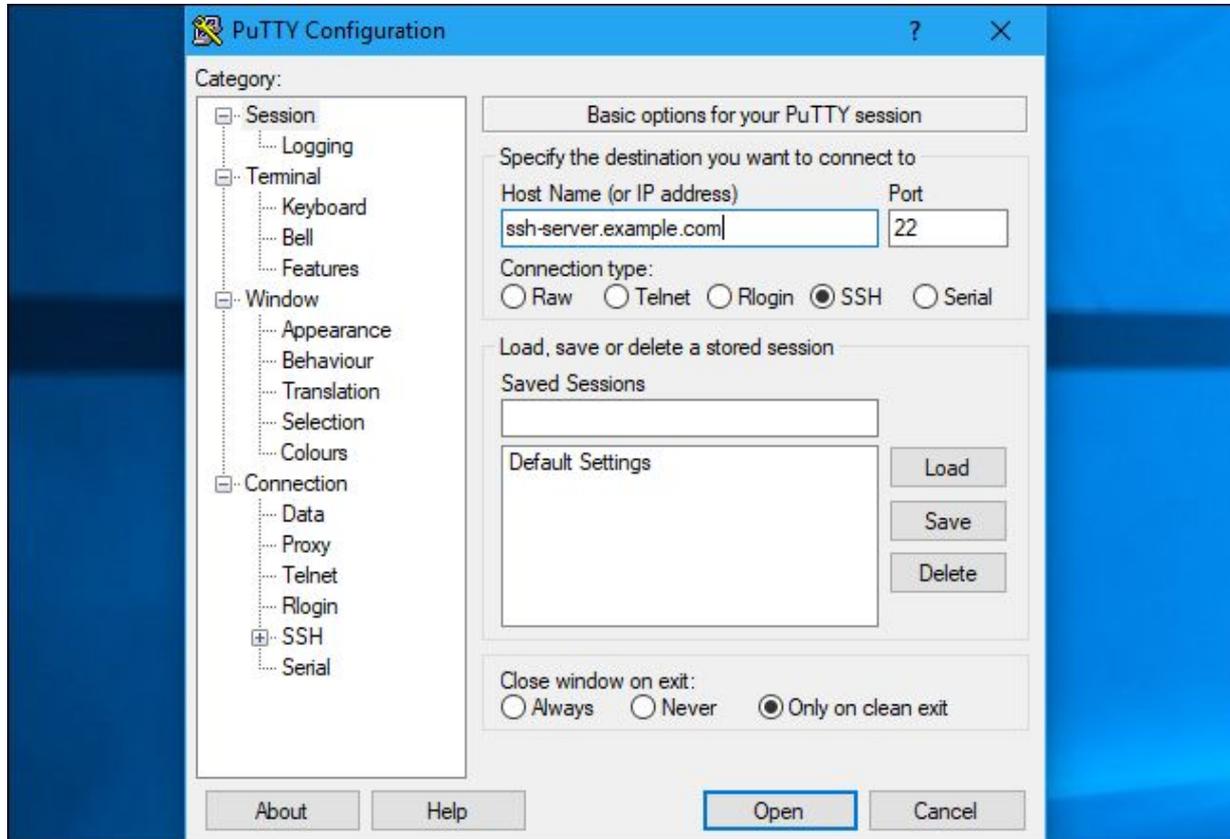
Username - your username on remote cluster

Numbers after @ - ip address of remote cluster

Then input your password



SSH for Windows - Putty client



2. Jupyter notebook

How can you connect to Jupyter server? (Skip it)

1. Visit a webpage: <http://10.16.77.5:8005/hub/login>
2. Input your credentials, which were sent to your email
3. Look around ;)



Quit Logout Control Panel

Files Running Clusters

Select items to perform actions on them. Upload New ↕

	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

Sign in

Warning: JupyterHub seems to be served over an unsecured HTTP connection. We strongly recommend enabling HTTPS for JupyterHub.

Username:

Password:

Sign In

How to set local Jupyter Notebook?

Linux

Install Python3 & PIP3 for Jupyter

```
1. sudo apt install python3-pip
```

Create a Python virtual environment for Jupyter

```
2. sudo pip3 install virtualenv
```

```
3. mkdir jupyter
```

```
4. cd jupyter
```

```
5. virtualenv notebookenv
```

```
6. source notebookenv/bin/activate
```

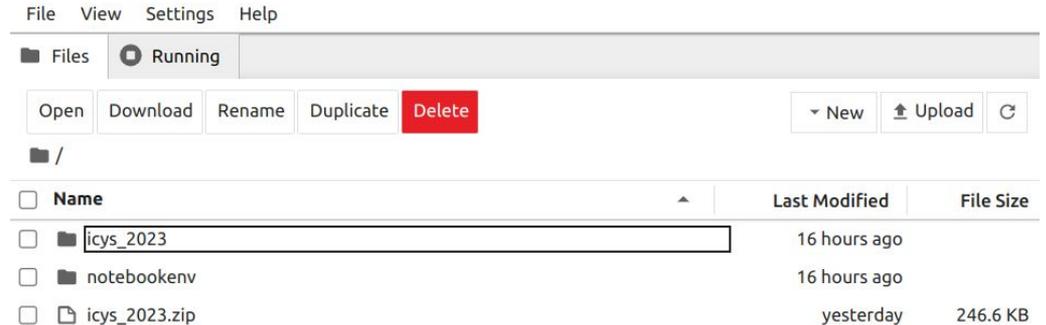
Install Jupyter Notebook

```
7. pip install jupyter
```

```
8. jupyter notebook
```

Windows

See [here](#) or elsewhere



Necessary setup

0. Open the terminal in your Jupyter Notebook panel

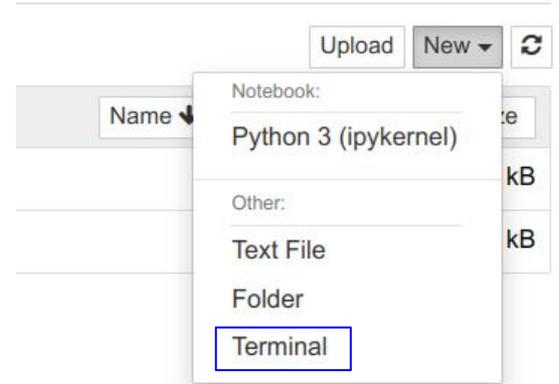
1. Install SIMAN python module - `pip install siman`

2. Check ssh connection to remote cluster - `ssh username@ip address`

3. Setup Passwordless ssh login - **see Slide 18**

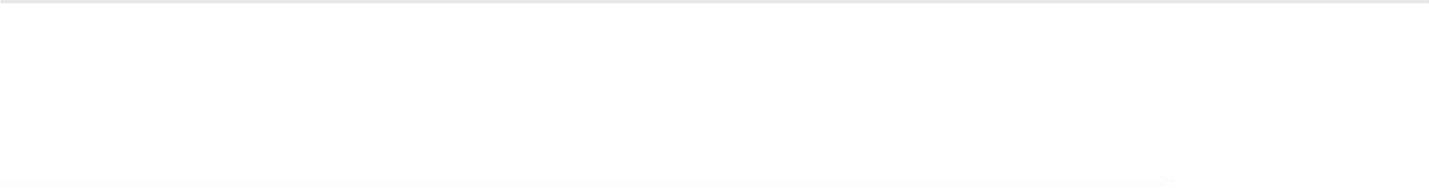
4. Download the archive with our tutorials and put it to your Jupyter Notebook panel -
see Slides 15-16

5. Install ipywidgets python module - `pip install ipywidgets`



Upload the archive into your directory

Quit Logout Control Panel

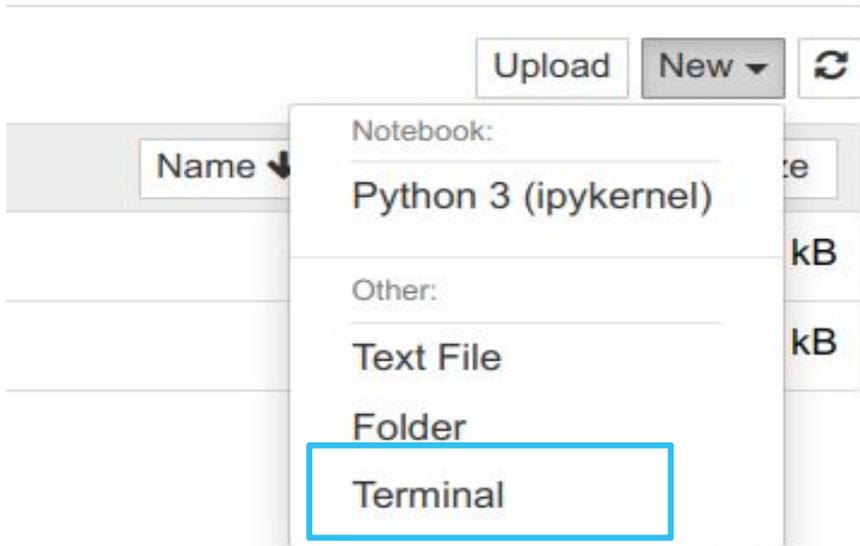


Upload New ▼ ↻

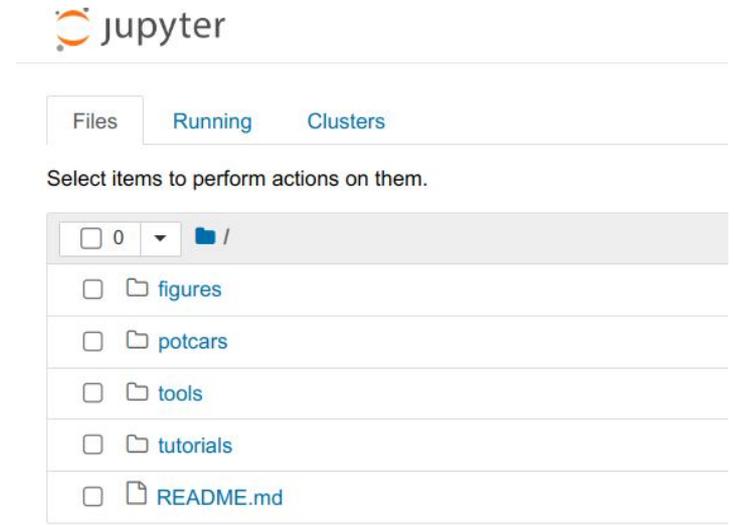
zip file with tutorials

Name ▼ Last Modified Click to browse for a file to upload.

Unzip it



```
$ unzip icys_2023
```



Manage tutorials/simanrc.py file

input local path to the unpacked archive
inside jupyter

generate own Materials Project API key
Just visit a web:
<https://materialsproject.org/dashboard>

A rectangular button with a grey background and rounded corners. On the left, there is a circular icon containing a key symbol. To the right of the icon, the text "Generate API Key" is written in a bold, black, sans-serif font.

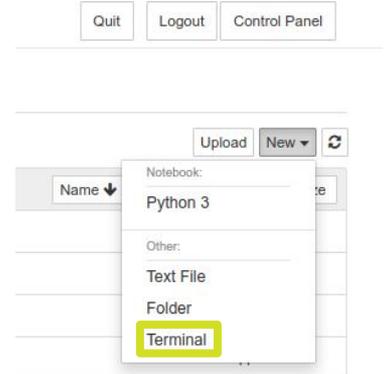
setup cluster parameters
(put your username, and
add a set for your cluster with VASP)
Don't forget to change DEFAULT_CLUSTER

```
1 """
2 User-related settings for siman
3 """
4
5 local_path = '/home/anton/jupyter/icys_2023/'
6 PATH2POTENTIALS = local_path+'potcars'
7 PATH2NEBMAKE = local_path+'tools/vts/nebmake.pl'
8 cluster_tools = local_path+'tools/'
9 PATH2JMOL = 'java -jar Jmol.jar'
10 AUTO_UPDATE_DB = True
11 pmgkey = "AWqKPyV8EmTRLfit" #API_KEY can be generated in the following webpage: https://materialspro;
12
13
14 """Cluster settings"""
15 DEFAULT_CLUSTER = 'geo' #short name of cluster
16 user = 'a.boev'
17
18 from siman.header import CLUSTERS
19
20 CLUSTERS['geo'] = {'address':user+'@95.71.121.195', #cluster address
21 'vasp_com':'mpirun /opt/vasp/bin/vasp_std', #command for VASP performing on cluster
22 'homepath': '/home/'+user, #path to home directory on cluster
23 'schedule':'SLURM', #type of schedule system using on cluster
24 'walltime':'2:00:00', #maximum time for job execution, hours:minutes:seconds, after this time since ;
25 system
26 'corenum':2, #number of cores for performing of one job on cluster
27 }
28
29 CLUSTERS['raz'] = {'address':user+'@10.16.77.19', #cluster address
30 'vasp_com':'mpirun vasp_std', #command for VASP performing on cluster
31 'homepath': '/home/'+user, #path to home directory on cluster
32 'schedule':'SLURM', #type of schedule system using on cluster
33 'walltime':'2:00:00', #maximum time for job execution, hours:minutes:seconds, after this time since ;
34 system
35 'corenum':2, #number of cores for performing of one job on cluster
36 'modules':'module load devtools/compiler/nvhpc/20.11; \
37 module load q-ch/vasp/5.4.4_OPT; \
38 \n\limit -s unlimited\n\
39 '
40
```

How to Setup Passwordless SSH Login

1. Open Terminal in Jupyter

```
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 ssh keys - `ssh-keygen`
3. Setup Passwordless ssh login - `ssh-copy-id username@ip address`
4. If everything was ok you can access to cluster via command `ssh username@ip address`
5. Enjoy! You look like a Russian hacker ;)



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

List of useful terminal commands

1. ***ssh username@ip_address*** - 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

