

How to use SSH

April 2021

1 Introduction

The practical classes require the use of Unix environment for some numerical simulations and analysis. Don't worry, you don't have to be very skillful at it. We would like you to complete the in-class practical exercise on the workstations prepared by the CIP-Pool of the physics faculty, so a connection to your workstation has to be set up beforehand. For this you need a computer account (send an email to sara.gabrielli@mpibpc.mpg.de as soon as possible if you don't have one!) and an SSH client (we advise you to use X2Go which proved to be stable enough in the previous semesters). **Please, make sure to be able to connect to the workstation before the beginning of the first tutorial**

2 How to use X2Go Client

1. Install X2Go Client from <https://wiki.x2go.org/doku.php/doc:installation:x2goclient>
2. Open X2Go Client and create a new session (Session → New session).
3. Edit the setting as shown in figure 1 and click on OK:

Session name: CIP-Pool

Host: *your computer ID, pick one randomly between c200 and c220, see Figure 1*

Login: your CIP-Pool account

SSH port: 22

Enable "Use Proxy server for SSH connection"

Proxy server host: login.physik.uni-goettingen.de

Port: 22

Enable "Same login as on X2Go Server" and "Same password as on X2Go Server" Session type: Choose "XFCE"

4. Launch the session "CIP-Pool" and enter your password.
5. You should see something like figure 2. Open "Terminal Emulator" and proceed to the next step.

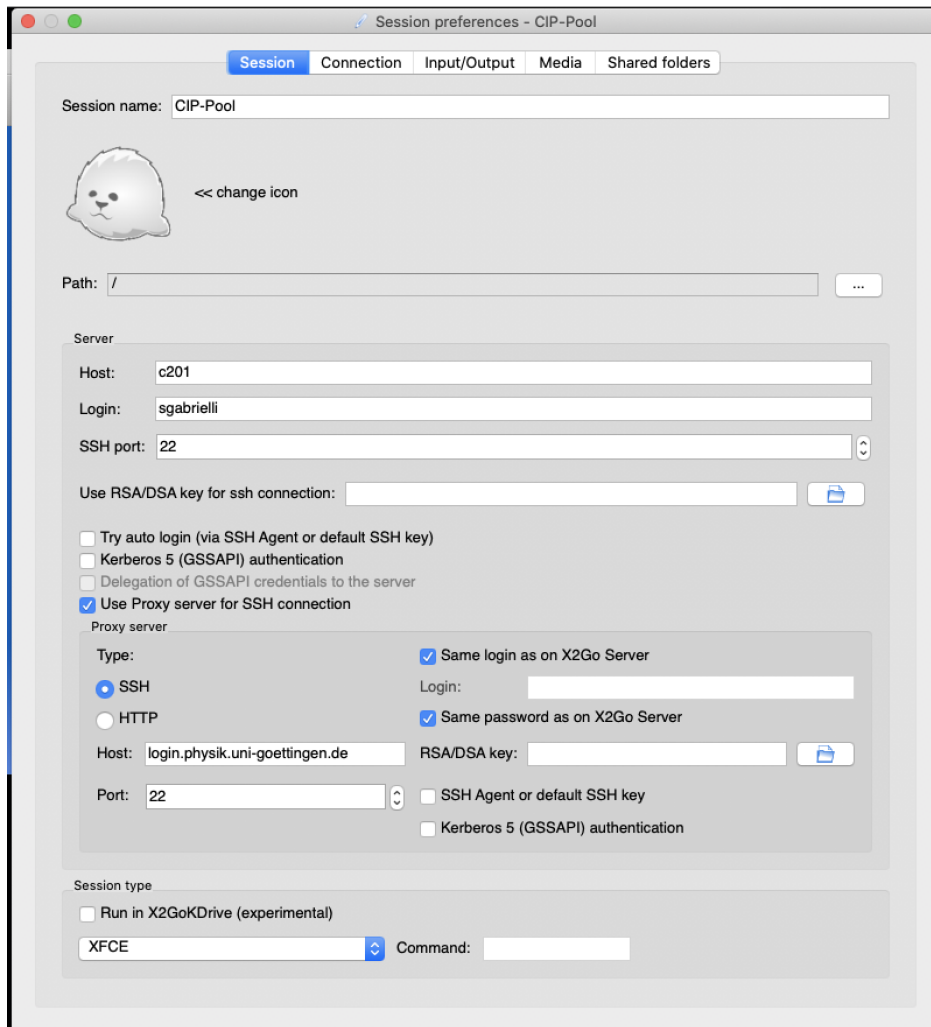


Figure 1: X2Go Client session setting

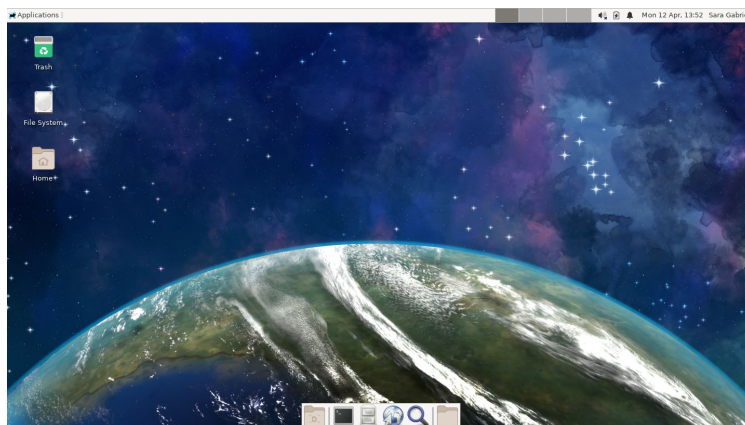


Figure 2: Workstation's desktop

3 Having fun with the Unix shell

Let's make a new directory called `practical1` and put the necessary files for the first practical into it:

```
mkdir practical1
```

Change the current directory to the newly created directory: `practical1`.

```
cd practical1
```

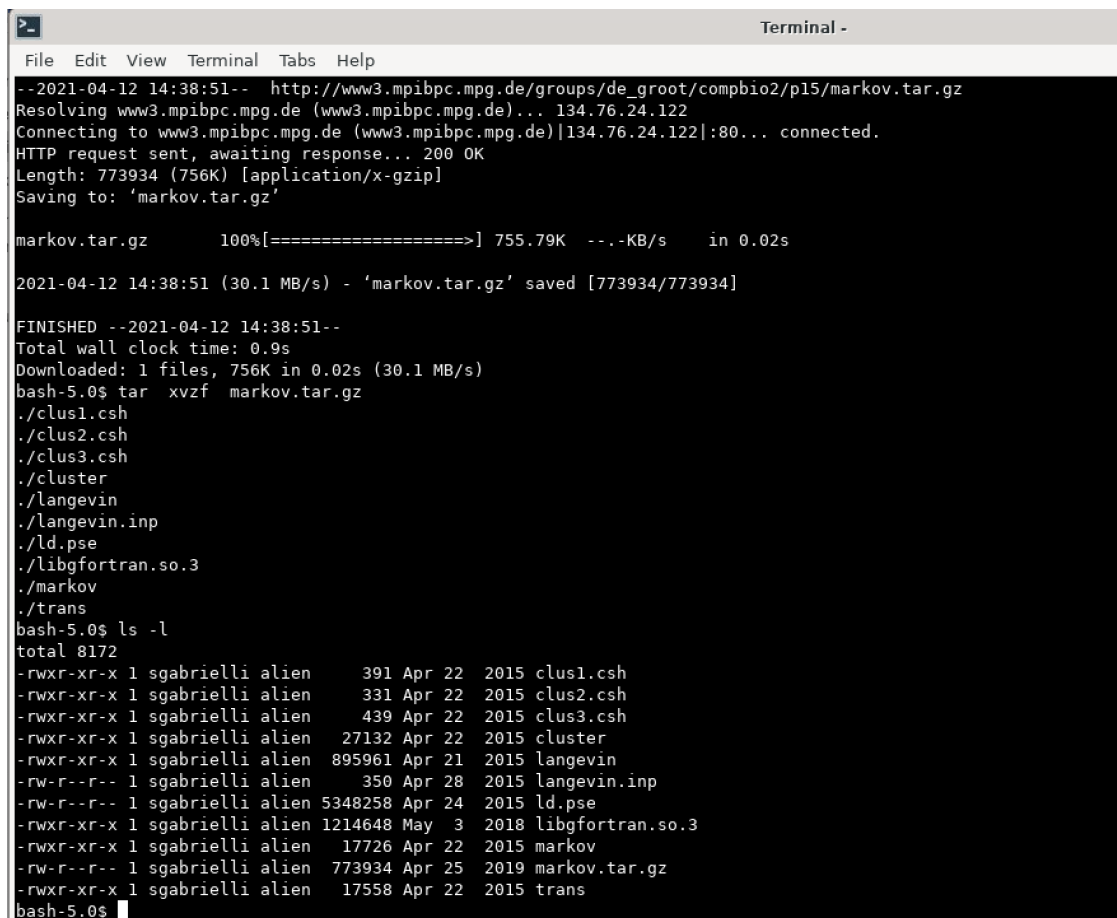
Download and unzip the material:

```
wget https://www3.mpibpc.mpg.de/groups/de_groot/compbio2/p15/markov.tar.gz
tar xvzf markov.tar.gz
```

Take a look at what files are extracted:

```
ls -l
```

You should get something as shown in figure 3.



```
Terminal -
File Edit View Terminal Tabs Help
--2021-04-12 14:38:51-- http://www3.mpibpc.mpg.de/groups/de_groot/compbio2/p15/markov.tar.gz
Resolving www3.mpibpc.mpg.de (www3.mpibpc.mpg.de)... 134.76.24.122
Connecting to www3.mpibpc.mpg.de (www3.mpibpc.mpg.de)|134.76.24.122|:80... connected.
HTTP request sent, awaiting response... 200 OK
Length: 773934 (756K) [application/x-gzip]
Saving to: 'markov.tar.gz'

markov.tar.gz      100%[=====] 755.79K  --.-KB/s   in 0.02s

2021-04-12 14:38:51 (30.1 MB/s) - 'markov.tar.gz' saved [773934/773934]

FINISHED --2021-04-12 14:38:51--
Total wall clock time: 0.9s
Downloaded: 1 files, 756K in 0.02s (30.1 MB/s)
bash-5.0$ tar xvzf markov.tar.gz
./clus1.csh
./clus2.csh
./clus3.csh
./cluster
./langevin
./langevin.inp
./ld.pse
./libgfortran.so.3
./markov
./trans
bash-5.0$ ls -l
total 8172
-rwxr-xr-x 1 sgabrielli alien    391 Apr 22  2015 clus1.csh
-rwxr-xr-x 1 sgabrielli alien    331 Apr 22  2015 clus2.csh
-rwxr-xr-x 1 sgabrielli alien    439 Apr 22  2015 clus3.csh
-rwxr-xr-x 1 sgabrielli alien  27132 Apr 22  2015 cluster
-rwxr-xr-x 1 sgabrielli alien  895961 Apr 21  2015 langevin
-rw-r--r-- 1 sgabrielli alien    350 Apr 28  2015 langevin.inp
-rw-r--r-- 1 sgabrielli alien 5348258 Apr 24  2015 ld.pse
-rwxr-xr-x 1 sgabrielli alien 1214648 May  3  2018 libgfortran.so.3
-rwxr-xr-x 1 sgabrielli alien   17726 Apr 22  2015 markov
-rw-r--r-- 1 sgabrielli alien  773934 Apr 25  2019 markov.tar.gz
-rwxr-xr-x 1 sgabrielli alien   17558 Apr 22  2015 trans
bash-5.0$
```

Figure 3: Basic operations

You can also test the stability of the connection when having a graphical interface remotely:

```
xmgrace
```

Xmgrace is a 2D plotting tool that will come in handy during the tutorials. You can also try to open PyMOL, which is one of the molecular visualization system that we are going to use:

```
pymol
```

If you completed the instructions successfully, congratulations! You are ready to start! You are also encouraged to try out the first practical (https://www3.mpibpc.mpg.de/groups/de_groot/compbio2/p15/index.html) and don't hesitate to get in touch with me sara.gabrielli@mpibpc.mpg.de if anything is unclear to you!