

Connecting from your own desktop/laptop

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Summary

This document is meant to help you for setting up your own desktop/laptop computer at the start of the semester, so that you can **connect remotely** to the PC's of our computer rooms. This will allow you to do part of the work, all of the work, or even extra work (for chemical or computational problems of your own interest!) from outside these rooms. It is still **strongly recommended** to attend the Informatik I exercise sessions with the assistants, as you will both learn more and save time when solving the exercises. In view of the particular **corona situation** this semester, a subset of students / groups will do on-line teaching. For this reason, please, **HAVE A LOOK AT THIS DOCUMENT TODAY (!)**, as we expect you **complete the present setup** already in the **first semester week** from 18 to 24.9.2023. If if you don't succeed on the sole basis of the present document, feel free to **contact our assistants** to get help.

Depending on the operating system of your personal desktop/laptop computer, go to the following section: for a PC running Windows, go to Sec. 0C.3; for a Mac, go to Sec. 0C.2; for a PC running linux, go to Sec. 0C.1. After that, you may read the remaining sections Secs. 0C.4 and 0C.5.

If you don't succeed on the sole basis of the present document, assistants will be available to help you. For this, send an e-mail to:

- If you use a PC running Windows: Carl Schiebrock, carl.schiebroek@phys.chem.ethz.ch
- If you use a Mac: Meghna Manae, meghna.manae@phys.chem.ethz.ch, please write **in English**
- If you use a PC running linux: Miguel Steiner, miguel.steiner@phys.chem.ethz.ch

0C.1 Connecting from a Linux PC

The description below refers to a system running Linux/Ubuntu, but things should be reasonably similar if you run other Linux variants.

Start a terminal window from the appropriate menu. Type `ssh -XY user@slabN.ethz.ch` where `user` is your ETHZ user (login) name, and `N` can be 1, 2, 3 or 4, press enter. If you have never connected to that specific machine before, some text about the "authenticity of the host" might pop up, and to confirm that you want to continue connecting to that machine, simply type `yes` and press enter. Then type in your ETHZ password (same as your email password) and press enter again. Note that when you are asked to enter your password, it is possible that no characters will appear in the terminal when you are typing (so that no one can spy over your shoulder and get your password!). Don't be confused by this, simply enter your password and finish by hitting enter. The `slab1` to `slab4` computers are the four login machines of the ETHZ Informatikdienste (they are not in the computer rooms).

```
Terminal File Edit View Search Terminal Help
luut@tran-trung-luu:~$ ssh -X luut@slab1.ethz.ch
luut@slab1.ethz.ch's password:
/usr/bin/xauth: file /tmp/.Xauthority.luut does not exist
[luut@slabivrt ~]$
```

Figure 0C.1: Linux installation, connecting to the ETHZ login machines

Only from these machines can you further connect to any machine in the computer rooms, by further typing `ssh -XY user@slabhcibNNN.ethz.ch`, where `user` is your ETHZ user (login) name and `NNN` runs from 002 to 041. Note that: (i) you don't need `vpn` (see Sec. 0C.5) to perform these operations; (ii) the first time you connect, you may have to confirm that you trust the computer you try to access (no worries, you can trust ETH); (iii) the machines in our computer rooms are sometimes switched off (inaccessible) when no one is working on them, so you might have to try different machines (*i.e.* different numbers between 002 and 041) until you can login to one that is switched on.

You can now work with your files and open programs by typing the appropriate command into the terminal, for example `xdg-open . &` for the file manager (don't forget the dot in this command), `gedit &` for the text editor, or `xmgrace &` for the graphics program). When you type one of these commands, the corresponding window should open on your screen, as would be the case if you were using a PC in one of our computer rooms. When you are done working, just type `exit` twice in the command line to log out (the first one to exit the machine of the computer room, and then the second one to exit the login machine of the ETHZ Informatikdienste).

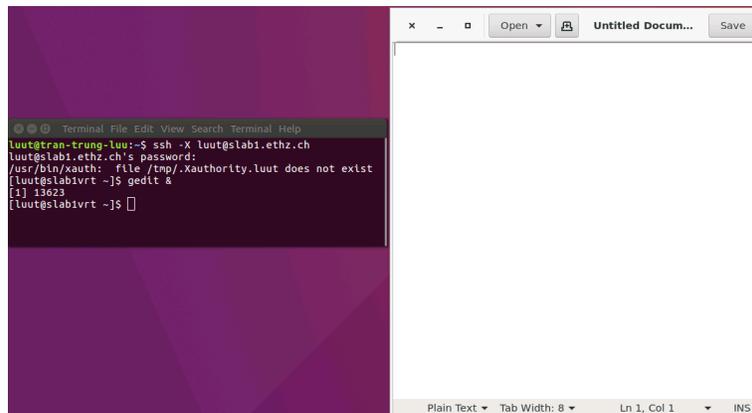


Figure 0C.2: Linux installation, opening a window for a particular application

In order to share files between the remote location (PC in the computer room) and your local workstation (your desktop/laptop at home):

- start a terminal
- if not yet installed, install `sshfs` (*e.g.* in ubuntu, use `sshfs --version` to check if installed, and use `sudo apt-get install sshfs` to install)
- if this is the first time you do this, create a directory (*e.g.* `mkdir john`, assuming your name is John)
- mount the remote filesystem by using `sshfs user@slab[1-4].ethz.ch: john`

- now, the remote filesystem will be accessible from your local workstation, like an external harddrive
- before logging out, use `fusermount -u john` to disconnect the remote filesystem

0C.2 Connecting from a Mac

Connecting from a Mac is only slightly more complicated compared to Linux (previous section), because the MacOS operating system, just like Linux, is in fact a variant of UNIX. However, there is generally no X11 server (the software responsible to display UNIX-type windows on your screen), and you will have to install one yourself. We suggest using **Xquartz**, which is a free software (this is one of many options; if you don't like **Xquartz**, just type *e.g.* "X11 server for Mac" in your favorite web search engine).

So, let's start by installing **Xquartz**. Go to the web page www.xquartz.org and install the **Xquartz** software on your computer.

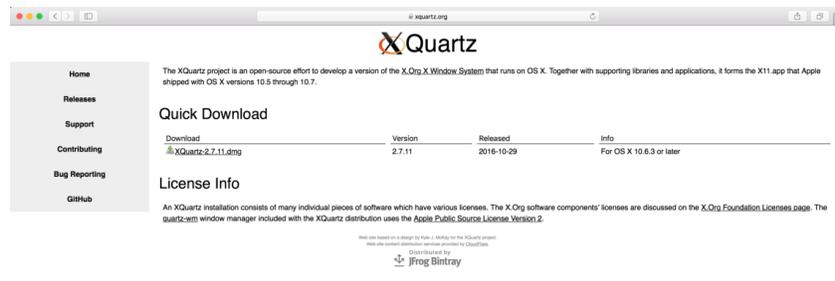


Figure 0C.3: Mac installation, installing Xquartz

Now, whenever you want to login remotely, first start a **Xquartz** window, either from **Finder** → **Go** → **Applications** → **Utilities** → **Xquartz**, or by typing "Xquartz" in the Launchpad. Then open a terminal window from **Finder** → **Go** → **Applications** → **Utilities** → **Terminal** or by typing "Terminal" in the Launchpad. Type `ssh -Y user@slabN.ethz.ch` where `user` is your ETHZ user (login) name, and `N` can be 1, 2, 3 or 4, press enter. If you have never connected to that specific machine before, some text about the "authenticity of the host" might pop up, and to confirm that you want to continue connecting to that machine, simply type `yes` and press enter. Then type in your ETHZ password (same as your email password) and press enter again. Note that when you are asked to enter your password, it is possible that no characters will appear in the terminal when you are typing (so that no one can spy over your shoulder and get your password!). Don't be confused by this, simply enter your password and finish by hitting enter. The `slab1` to `slab4` computers are the four login machines of the ETHZ Informatikdienste (they are not in the computer rooms).

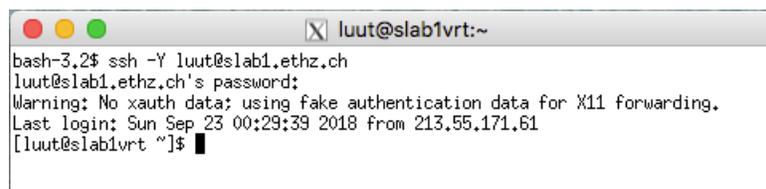


Figure 0C.4: Mac installation, connecting to the ETHZ login machines

Only from these machines can you further connect to any machine in the computer rooms, by further typing `ssh -XY user@slabhcibNNN.ethz.ch`, where `user` is your ETHZ user (login) name and `NNN` runs from 002 to 041. Note that: (i) you don't need `vpn` (see Sec. 0C.5) to perform these operations; (ii) the first time you connect, you may have to confirm that you trust the computer you try to access (no worries, you can trust ETH); (iii) the machines in our computer rooms are sometimes switched off (inaccessible) when no one is working on them, so you might have to try different machines (*i.e.* different numbers between 002 and 041) until you can login to one that is switched on.

You can now work with your files and open programs by typing the appropriate command into the terminal, for example `xdg-open . &` for the file manager (don't forget the dot in this command), `gedit &` for the text editor, or `xmgrace &` for the graphics program). When you type one of these commands, the corresponding window should open on your screen, as would be the case if you were using a PC in one of our computer rooms. When you are done working, just type `exit` twice in the command line to log out (the first one to exit the machine of the computer room, and then the second one to exit the login machine of the ETHZ Informatikdienste).

Important: Depending on your mac and its setup, you may get an error when typing `xdg-open . &`, `gedit &` or `xmgrace &`. In this case, try to follow the same login steps, but using the `XQuartz` terminal window (also called `xterm`). To reach it, click on the `XQuartz`. Now in the top left of the mac window, you can see `Applications`. Click on the `Applications`→`terminal` or use “command + N” to open the `xterm` window.

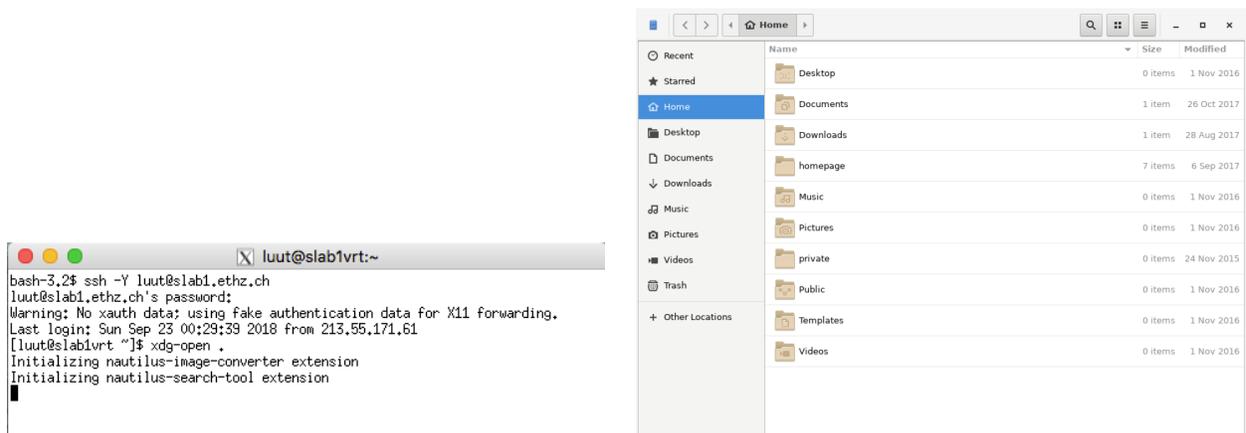


Figure 0C.5: Mac installation, opening a window for a particular application

The following step is optional, but will make your setup much more convenient for sharing files between the remote location (PC in the computer room at ETH) and your local workstation (your Mac desktop/laptop at home).

- start a terminal
- if not yet installed, install `sshfs` (download `OSXFuse` from <http://osxfuse.github.io/>, open the `OSXFuse` `dmg` and run the installer, download `SSHFS` from <https://osxfuse.github.io/> and run the `SSHFS` installer). If you're not sure whether `sshfs` is already installed, you can check with the command `sshfs --version`. If the output shows something

like “SSHFS version X.X.X”, it is already installed, and if the output shows something like “sshfs: command not found”, it is not yet installed.

- if this is the first time you do this, create a directory (e.g. `mkdir john`, assuming your name is John)
- mount the remote filesystem by using `sshfs user@slab[1-4].ethz.ch: john`
- now, the remote filesystem will be accessible from your local workstation, like an external harddrive
- (optional) before logging out, use `umount john` to disconnect the remote filesystem

This also allows you to easily use a locally installed text editor to work on your remote files.

0C.3 Connecting from a Windows PC

For the Microsoft Windows operating systems we recommend you to use MobaXterm. To get MobaXterm simply go to <https://mobaxterm.mobatek.net> and select “GET MOBAXTERM NOW!” followed by the free “Installer Edition”.

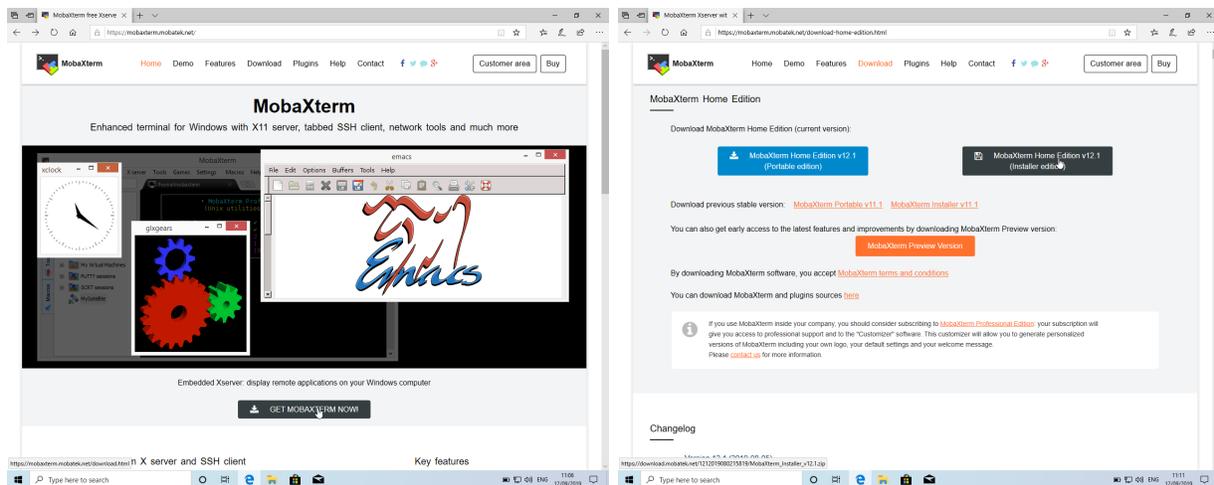


Figure 0C.6: Windows installation, installing MobaXterm (“Installer edition”)

After downloading the “Installer edition” you will end up with a `.zip` archive. This archive contains a bundle of files, which you have to extract by right-clicking on the `.zip` and selecting the extract option. You will then find yourself with a `.msi` Windows installer file. Run this installer and follow through the installation process. If at any point you get a popup window from Windows Defender Firewall asking you to grant permission to MobaXterm, do grant permissions for the type of network (public and/or private) you are going to be using.

You can now set up a `ssh` connection within MobaXterm. Once the program has finished its initial setup, open a local terminal by clicking on “Session” on the top left, selecting “Shell” and clicking “OK” (you don’t have to change any settings). This will open a new terminal window, where you have to type the following commands.

Type `ssh -XY user@slabN.ethz.ch` where `user` is your ETHZ user (login) name, and `N` can be 1, 2, 3 or 4, press enter. If you have never connected to that specific machine before, some text about the “authenticity of the host” might pop up, and to confirm that you want to continue

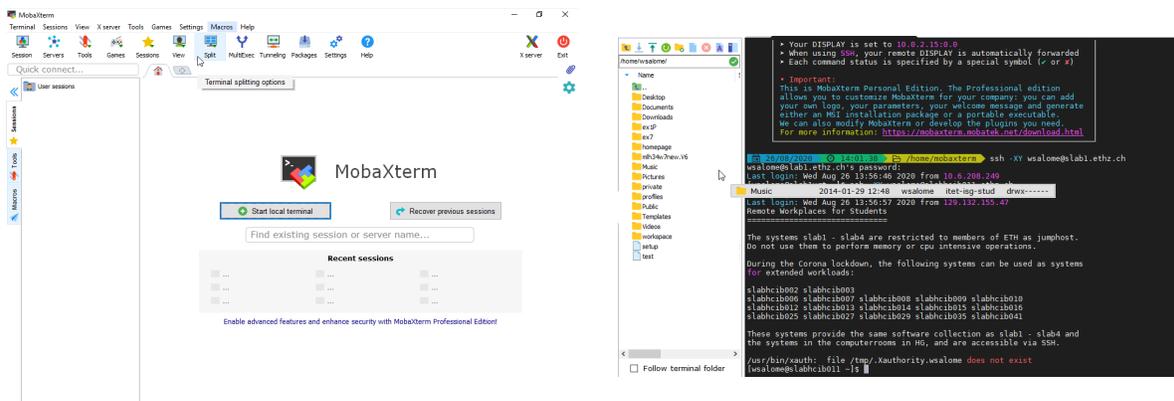


Figure 0C.7: Windows installation with MobaXterm. Left: Terminal-setup window in MobaXterm. Right: Terminal window and file browser once successfully logged in to one of the workstations in our computer rooms.

connecting to that machine, simply type `yes` and press enter. Then type in your ETHZ password (same as your email password) and press enter again. Note that when you are asked to enter your password, it is possible that no characters will appear in the terminal when you are typing (so that no one can spy over your shoulder and get your password!). Don't be confused by this, simply enter your password and finish by hitting enter. The `slab1` to `slab4` computers are the four login machines of the ETHZ Informatikdienste (they are not in the computer rooms).

Only from these machines can you further connect to any machine in the computer rooms, by further typing `ssh -XY user@slabhcibNNN.ethz.ch`, where `user` is your ETHZ user (login) name and `NNN` runs from 002 to 041. Note that: (i) you don't need `vpn` (see Sec. 0C.5) to perform these operations; (ii) the first time you connect, you may have to confirm that you trust the computer you try to access (no worries, you can trust ETH); (iii) the machines in our computer rooms are sometimes switched off (inaccessible) when no one is working on them, so you might have to try different machines (*i.e.* different numbers between 002 and 041) until you can login to one that is switched on.

The MobaXterm layout is fairly easy to understand. On the right you are presented with the same kind of UNIX terminal that you will be working on in the computer labs during the exercise classes. And on the left you will find file browser similar to a Windows Explorer, that shows the directory structure on the remote machine you are connected to. A nice feature of MobaXterm is that this file manager supports dragging and dropping (for copying & pasting, both internally as well as to and from the remote machine).

You can now work with your files and open programs by typing the appropriate command into the terminal, for example `xdg-open . &` for the file manager (don't forget the dot in this command), `gedit &` for the text editor, or `xmgrace &` for the graphics program). When you type one of these commands, the corresponding window should open on your screen, as would be the case if you were using a PC in one of our computer rooms. When you are done working, just type `exit` twice in the command line to log out (the first one to exit the machine of the computer room, and then the second one to exit the login machine of the ETHZ Informatikdienste).

Note that, sometimes, the window of a new program will not appear on top of the MobaXterm terminal window, but if you check your taskbar or cycle through open windows with `Alt + Tab`, you will find it.

0C.4 Useful Programs

Following the instructions of the previous sections, you should now be able to start and use remotely from your desktop/laptop all the programs available on the UNIX machines of our computer rooms (*e.g.* `gedit`, `firefox`, `xmgrace`, ...). However, this this can be quite slow. It is usually easier to install the programs you need directly on your desktop/laptop, and then use them to open the remote files you want to work on. In terms of text editor, you may try to install locally `gedit` (<https://wiki.gnome.org/Apps/Gedit>) or `SublimeText` (<https://www.sublimetext.com/3>). In terms of graphics program, you may try to install locally `xmgrace`, `gnuplot`, or the python `matplotlib` library. If you are familiar with `Excel`, which is available for free from the ETH Software Store, this is also an excellent alternative to `xmgrace` for making your graphs. Note, however, that the instructions in the exercise scripts assume that you use `xmgrace`. If you need help with your alternative plotting tools, just ask your assistant.

0C.4.1 VMD

For exercise 7 (last week of the semester), you will have to use VMD, which is a graphics software for molecular modelling. The easiest is to do this exercise from one of our computer rooms, where the program is installed and running. But if some corona-type virus decided one semester to prevent you from joining the in-presence sessions (who knows...), then only one option: follow the instructions below to install VMD on your own machine at home. It is recommended that you do this at least a week before the start of exercise 7, sso that you can ask for the help of your assistant if you have a problem.

In order to install VMD you first have to download the software. For this, go to <https://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=VMD>. We recommend that you choose version 1.9.3.¹

- If you are using a Linux PC, choose [LINUX_64 OpenGL, CUDA, OptiX, OSPRay](#).
- If you are using a Windows PC, choose [Windows OpenGL](#).
- If you are using a Mac with MacOS version 10.13.x² or lower, choose [MacOS X OpenGL \(32-bit Intel x86\)](#).
- If you are using a Mac with MacOS Catalina 10.14 or 10.15³ or higher, choose the VMD 1.9.4 version [MacOS X Catalina OpenGL \(64-bit Intel x86_64\)](#).

Once you click on the software version you want to install, you will be forwarded to a Registration/Login page. If this is the first time you install VMD, choose a username and password, otherwise, enter your existing username and password. Click on “Continue with registration or download”. Next, fill out the registration form (don’t worry, it is free for academic use) and click on “Register”. You will be prompted to confirm your identity and agree to the terms of the license⁴ by clicking on the corresponding button. This should prompt the download of the installation file. The next steps of the installation depend on the operating system you are using. You can find the instructions for the installation on a Linux, Windows or Mac PC in the following sections.

¹If you are adventurous you can of course also install the alpha version of VMD 1.9.4.

²To find out which OS version you have, click on the apple in the top left corner of your screen and choose “About This Mac”. In the Overview, you will find the name of your operating system and the version number.

³To find out which OS version you have, click on the apple in the top left corner of your screen and choose “About This Mac”. In the Overview, you will find the name of your operating system and the version number.

⁴If you have trouble falling asleep in the evening, this license agreement may actually be useful to you: save the text and read it three times before going to bed. It will help.

0C.4.1.1 Installing VMD on a Linux PC

If the download was successful, you should find a file beginning with `vmd-1.9.3` with the file extension `.tar.gz` in your download folder. Once you extract this archive, follow the instructions of `vmd-1.9.3/README` in the section **Quick Installation Instructions**. Once everything is completed, you can start VMD by typing `vmd` in your terminal.

0C.4.1.2 Installing VMD on a Mac

Once the download is finished, go to your Download directory and open the `dmg` file. You can now drag the VMD icon to your Applications folder. The first time you are opening the application, you will have to right click on the icon and choose “open” since Mac cannot verify the developer. After that, it should be possible to start the application by simply double clicking the icon.

0C.4.1.3 Installing VMD on a Windows PC

If the download was successful, you should find in your Download folder a Windows Installer Package file called `vmd193win32nocuda.msi`. Start the installation process by double-clicking on this file. This will start the InstallShield Wizard for VMD 1.9.3. Click “Next”. Choose the destination folder where you’d like to install VMD (if you are not sure, the default will be ok) and click “Next”. Click “Install”, which will start the installation process. Windows might ask you if you want to allow this app to make changes to your device, which you can answer by clicking “Yes”. Once the installation is finished you can click on “Finish”. If the installation was successful, you should now be able to start VMD by locating the VMD icon in the Windows start menu and clicking on it.

0C.5 Using the ETH virtual private network (VPN)

Irrespective whether you connect to ETH computers using a UNIX-type terminal or using your web browser, some ETH services will be refused to you by default because your computer is not recognized as belonging to ETH. Most prominently, you will not be able to access some documents (*e.g.* literature articles and databases) provided by the central ETHZ library or the D-CHAB Infozentrum. To enable these features, you will have to attach your PC to the so-called virtual private network of the ETH. You can find the instructions for setting up the ETH VPN at <https://www.isg.inf.ethz.ch/Main/ServicesNetworkVPN>