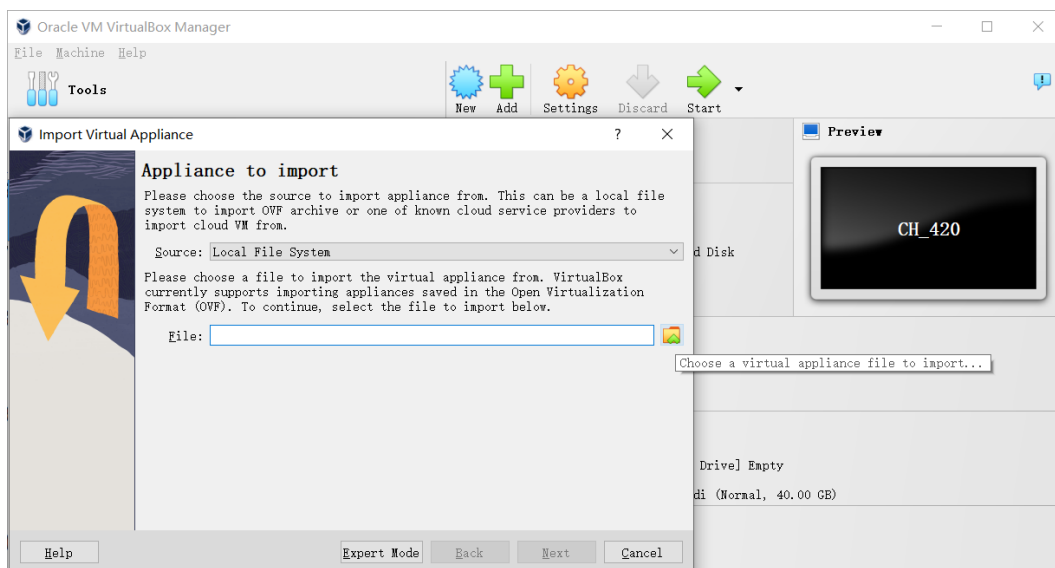



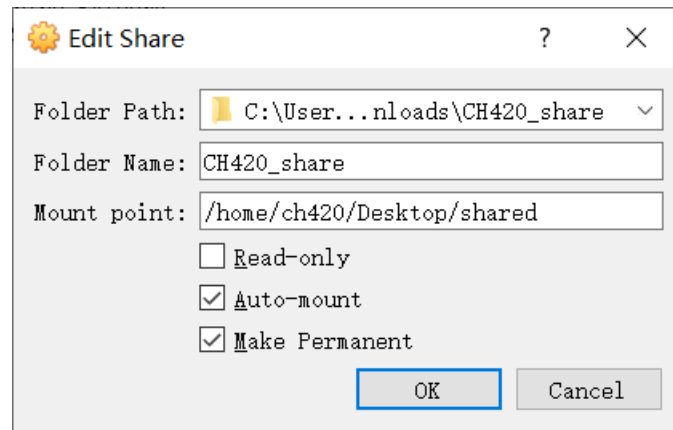
Virtual Machine (VirtualBox) Installation Guide

NOTE! DURING THIS PROCEDURE, YOU WILL NEED TO HAVE ABOUT 40GB OF FREE DISK SPACE. MAKE SURE THIS IS THE CASE BEFORE STARTING.

1. Install Oracle VirtualBox (if not installed).
Download and install the binary package corresponding to your operating system from: <https://www.virtualbox.org/wiki/Downloads> (There are Windows, Mac and Linux versions, choose the correct one). *We tested version 7.0.14.*
NOTE! Here we just provide Ubuntu image for windows system, if you are using Mac os and still have issues with package installation, please contact xin.jin@epfl.ch or yutao.li@epfl.ch.
2. (optional, but strongly suggested) From the same link <https://www.virtualbox.org/wiki/Downloads>, install also the “VirtualBox VM VirtualBox Extension Pack” (second section of the page). This will make the interaction with the VM much easier (the VM desktop will resize when you resize the window, you don't need to click in the VM to use it, you can use copy-paste from your computer into the VM and vice versa, you can drag-drop files between your computer and the VM, ...). You typically just need to download the file (with extension *.vbox-extpack*), double click on it and follow the instructions.
3. Download the file *CH_420.ova* to a folder of your local machine from this link: https://www.dropbox.com/scl/fi/ccfu4vh2bpcwlvej0i8k4/CH_420.ova?rlkey=iejx56p31fi80drl4ttiwmplx&st=jw3yj8ab&dl=0
4. Launch VirtualBox.
5. Choose from the menu the option “File > Import Appliance”.

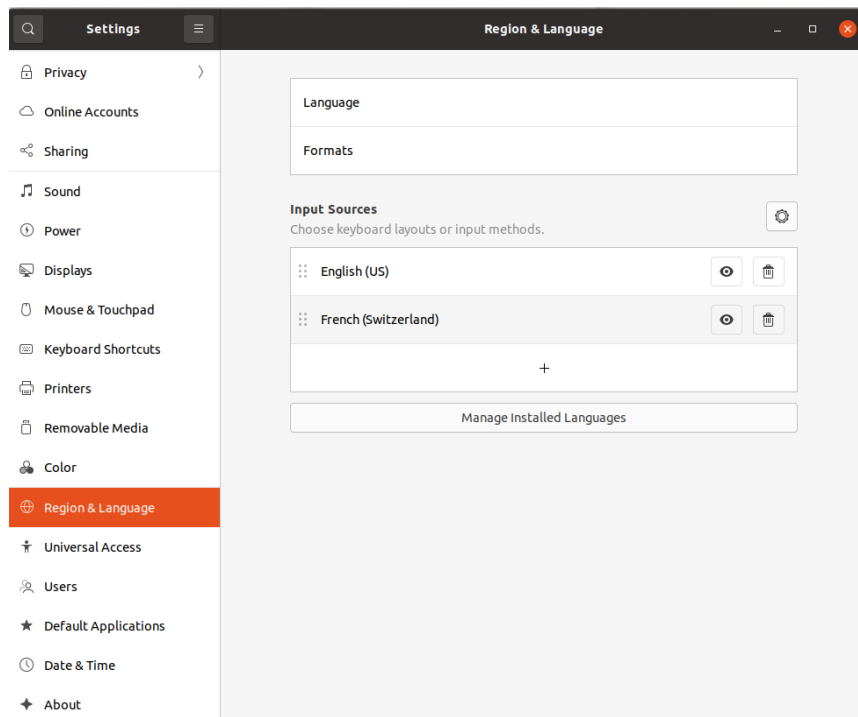


6. Click the button () next to the text box, reach the path where you downloaded *CH_420.ova*, and select it.
7. Click Next, then click Finish, and (if requested) agree on the license. The import will take up to a few minutes.
8. In the main window select the newly created entry “CH420” from the left pane, double click or click Start (green right arrow) from the upper toolbar. This will launch the virtual machine.
9. After a few minutes, the Ubuntu desktop is booted. The user is *ch420* and the password is *lsmo2025*. If it prompts a window for “Software Update”, click cancel! Do not update the virtual machine throughout the course, otherwise, it might break the necessary software for the course.
10. In the Ubuntu desktop, click the “Terminal” icon that appears in the sidebar on the left of the screen. In the terminal, you can test if everything works fine by typing `$ conda activate molsim`
Remember this is the environment that we always use in the following study.
11. To make the use of the VM smooth, you need to install the most recent version of the VirtualBox Guest Additions inside the VM. We pre-installed those for VirtualBox 6; if you are using VirtualBox 7, it's better to install those for version 7 (especially if you encounter problems such as slowness, etc.) following these instructions:
 - a. In the VirtualBox menu, select Devices -> Insert Guest Additions CD image...
 - b. Open the disk icon that appears in the sidebar on the left of the screen. In this folder, right click and choose 'open in terminal' to start a terminal.
 - c. Type in the terminal: `./VBoxLinuxAdditions.run`
 - d. If it needs password, it is *lsmo2025*. Wait a few minutes for installation.
 - e. Finally right click the disk icon that appears in the sidebar and choose Eject.
12. Set up a shared folder between the virtual machine and your host operating system. With the shared folder, you can easily exchange files and access your results from the host system.
 - a. Create a folder on the Desktop of your operating system (or in another place you prefer) called “CH420_share” (Or anything you like, but make sure it is consistent in the following steps).
 - b. In the VirtualBox toolbar, Click “Devices > Shared Folders > Shared Folders Settings...”.
 - c. If there is a shared folder, click the “Remove selected” button, and remove the folder/path already present.
 - d. Click the “Add new” button, fill in the entries as shown in the following screenshot, and click the OK button. Note that the folder path is the path to the shared folder in your host operating system i.e. “CH420_share” folder and mount point is the Desktop of the VM. Also, we suggest to tick “Auto-mount” and “Make Permanent”.
 - e. A folder with the name “shared” should automatically appear on the Ubuntu desktop. Take a try and create a file and verify it is effectively shared between the virtual machine and the host system (if you have issues, try to reboot the VM once). In the following study, we recommend not do simulation inside the shared folder but just transport files.



11. (Optional) Keyboard Switching

In the Virtual Machine, the keyboard is the US one. To change it go to “Settings” (the last icon on the left sidebar) and choose the same language as in the screenshot.



12. To test the molsim package, you can open the 'test' folder on the Desktop, first activate conda environment by typing:

```
$ conda activate molsim
```

```
$ code .
```

You can then open the test.ipynb file in VSCode and run each cell to test if it works. (you might be asked to choose the python environment, please choose molsim)