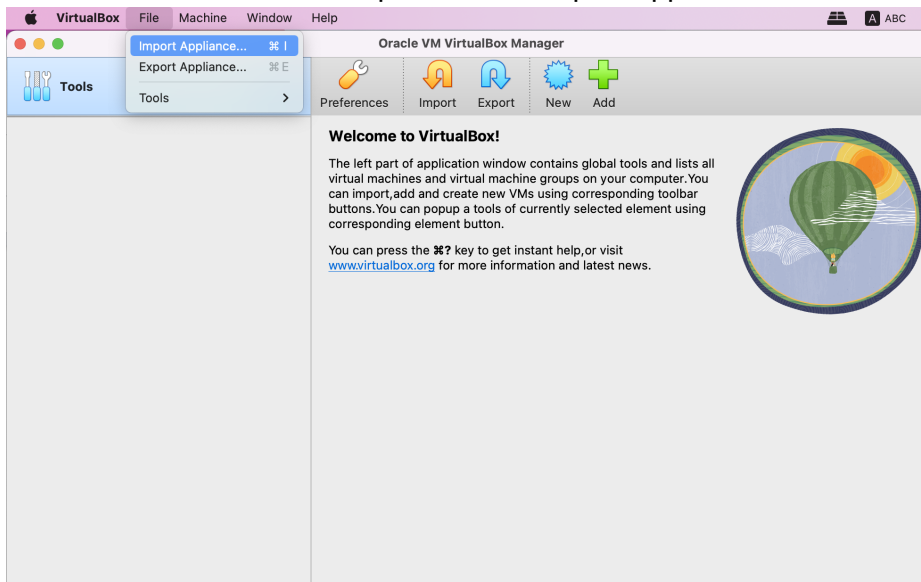



Virtual Machine (VirtualBox) Installation Guide

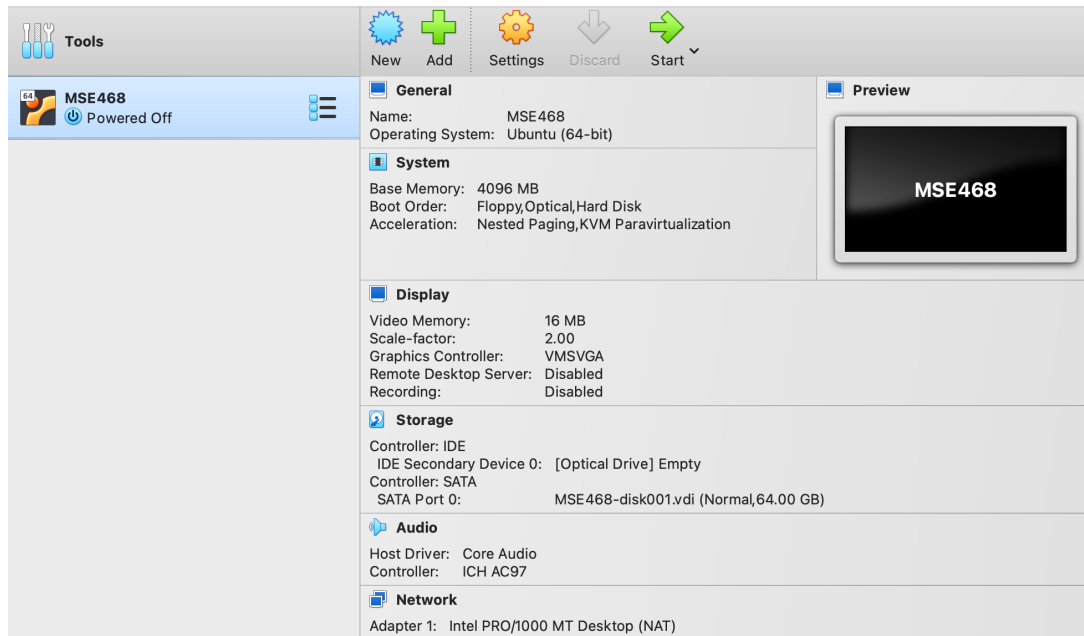
NOTE! DURING THIS PROCEDURE, YOU WILL NEED TO HAVE ABOUT 15GB OF FREE DISK SPACE. MAKE SURE THIS IS THE CASE BEFORE STARTING.

ALSO: PLEASE TEST THE INSTALLATION AND REPORT YOUR RESULTS (DEADLINE IS INDICATED ON MOODLE)

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! If you have a recent Apple Mac computer with an Apple M chip, you cannot use this version (VirtualBox) but you need to instead read the other instruction file, specific for MacBook M chips.
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 *MSE468Spring2025.ova* to a folder of your local machine using this link:
<https://drive.google.com/file/d/18ZzuZYLrFtZ2ZSaSNkuD-oo1xRbCcWS2/view?usp=sharing>
4. Launch VirtualBox.
5. Choose from the menu the option “File > Import Appliance”.



- Click the button () next to the text box, reach the path where you downloaded *MSE468Spring2025.ova*, and select it.
- Click Next, then click Finish, and (if requested) agree on the license. The import will take up to a few minutes.
- In the main window select the newly created entry “MSE468” from the left pane, double click or click Start (green right arrow) from the upper toolbar. This will launch the virtual machine.



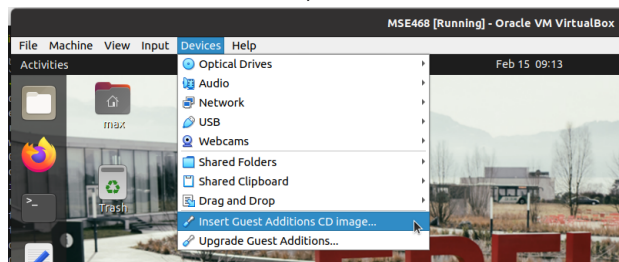
- After a few minutes, the Ubuntu desktop is booted. The user is **max** and the password is **aiida**. If it prompts a window for “Software Update”, click **cancel!** Do **not** update the virtual machine throughout the course, otherwise, it might break the necessary software for the course.



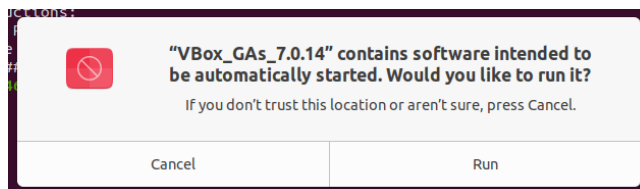
10. In the Ubuntu desktop, click the “Terminal” icon that appears in the sidebar on the left of the screen. In the terminal, you can launch LAMMPS, Quantum ESPRESSO, etc. for the calculations.



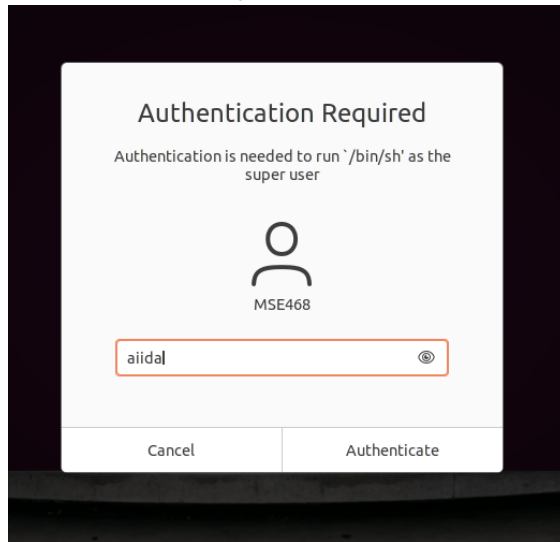
11. (Optional) To free up space, note that after importing the *MSE468Spring2025.ova* file in step 6, you can delete the file *MSE468Spring2025.ova* that you downloaded.
12. To make the use of the VM smooth, you need to install the most recent version of the VirtualBox Guest Additions inside the VM. 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...



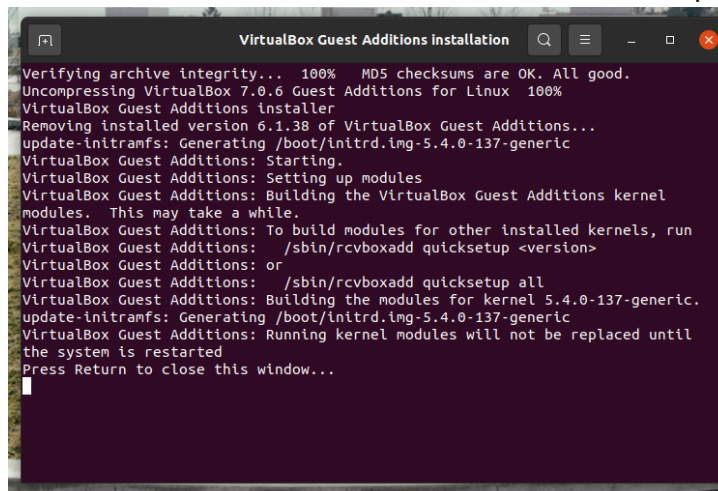
- b. A pop-up should appear asking confirmation that you want to automatically start some software: select “Run”



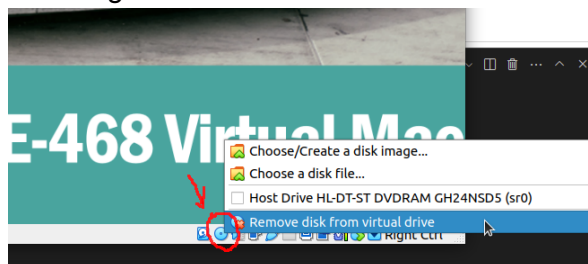
- c. Insert the password of the VM user (as a reminder: the user is **max**, the password is **aiida**)



- d. A terminal will open, and the process will take about 2-3 minutes. Wait for the final line “Press Return to close this window...”, then press return.



- e. Remove the Guest additions virtual disk by right-clicking on the “CD/DVD” icon at the bottom-right of the VirtualBox window (see next screenshot) and selecting “Remove disk from virtual drive”



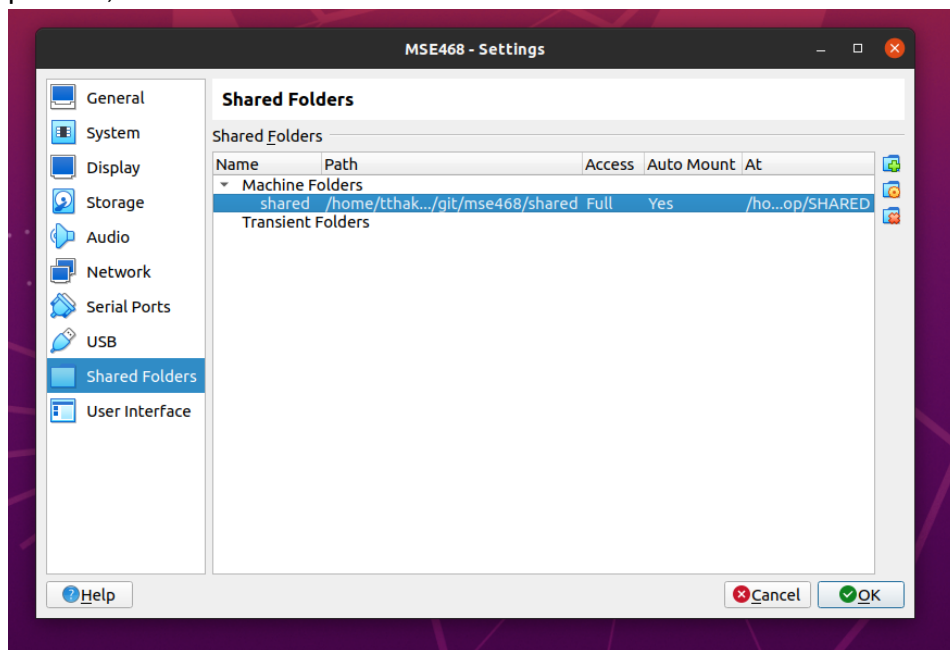
- f. Reboot the VM (not your computer, it's not needed) selecting the “shutdown icon” in the VM, then “Power Off/Log out”, and the “Power Off” (twice). You can then restart the VM.

13. 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.

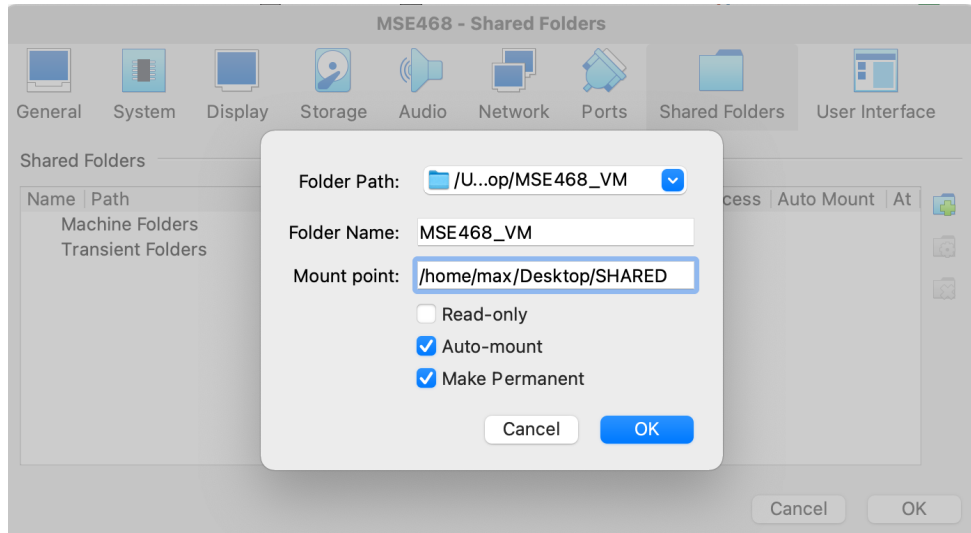
- a. Create a folder on the Desktop of your operating system (or in another place you prefer) called “MSE468_VM” (Or anything you like, but make sure it is consistent in the following steps).
- b. In the VirtualBox toolbar, Click “Devices > Shared Folders > Shared Folders Settings...”.



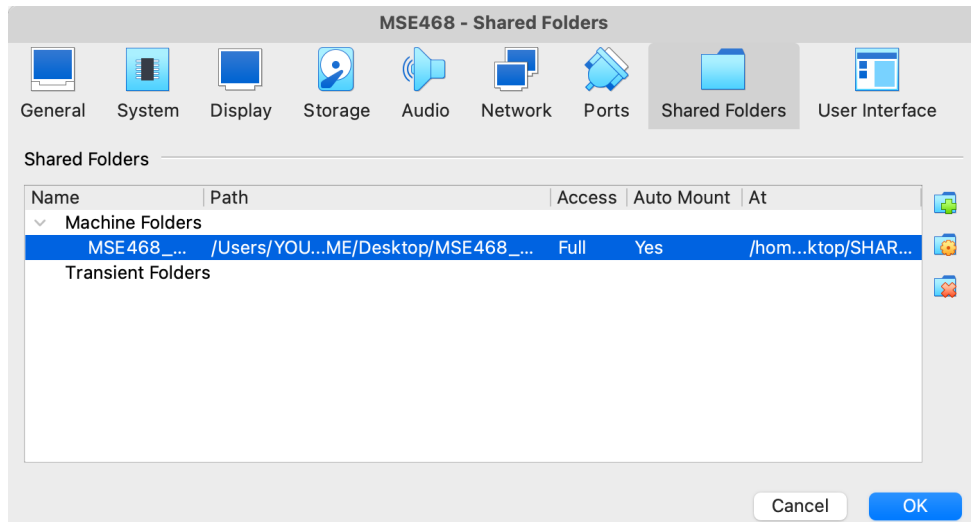
- c. Click the “Remove selected” button (🗑️), and remove the folder/path already present, as shown below.



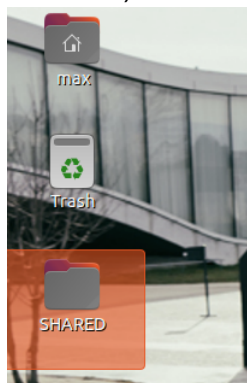
- d. Click the “Add new” button (➕), fill in the entries as shown in the following screenshot, and click the OK button. Note that the folder path is the path to the shared folder in your host operating system i.e. “MSE468_VM” folder and mount point is the Desktop of the VM. Also, we suggest to tick “Auto-mount” and “Make Permanent”.



Click OK and then the new shared folder is added to the list. Select OK.



- 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).

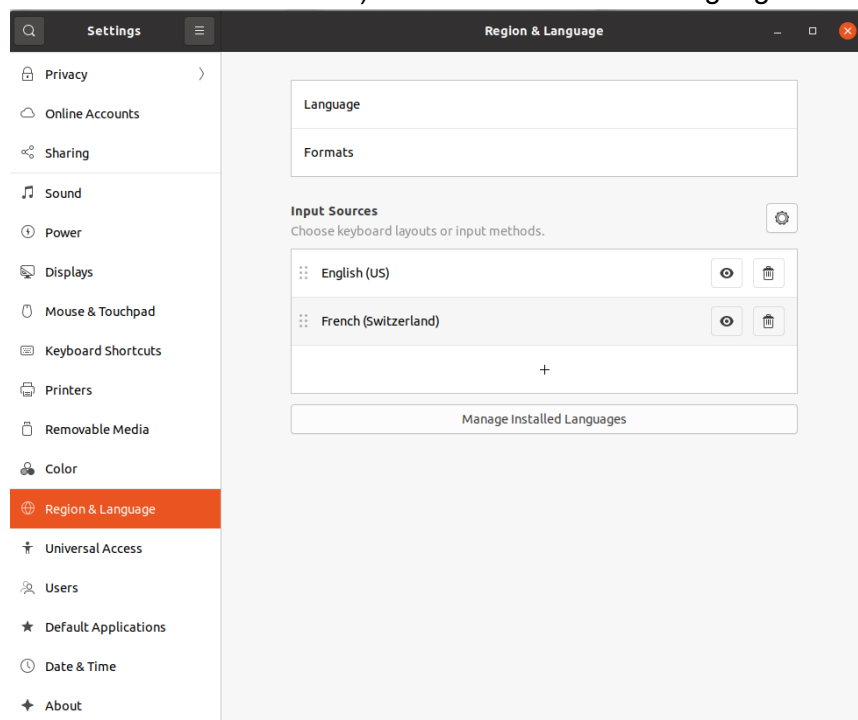


- f. We thus **recommend** that, inside the Linux Virtual Machine, you **save all your files always inside ~/Desktop/SHARED/**
- g. **IMPORTANT!** At the end of each class, we strongly encourage you to **save a copy of all the files you produced during the lab, in a USB stick or in any other**

safe backup location, to avoid data loss that can result into having to run again, and delays in providing your lab reports, with a consequent risk of losing points for your exercises.

14. (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.



15. Congratulations! You just managed to connect to a virtual machine preconfigured for the course!

NOTE: if needed, the user is **max** and the password is **aiida**.

Testing if everything works

To test that the virtual machine is properly configured, please complete the instructions contained in the document “*Testing the Virtual Machine (MSE-468).pdf*” (available on Moodle) **before the deadline that is indicated on Moodle** (so we have the time to help you solve any problem that you might have).

NOTE: In the document there is a link to a google form (very short) to fill by the date indicated above, to confirm that everything works well.

Final remarks

The virtual machine is generated based on *Quantum Mobile* (<https://quantum-mobile.readthedocs.io/en/latest/index.html>). If you encounter problems when using the virtual machine, here are some resources for FAQ and troubleshooting:

- <https://quantum-mobile.readthedocs.io/en/latest/users/faq.html>

- <https://quantum-mobile.readthedocs.io/en/latest/users/troubleshoot.html>

In case of doubts/problems, ask the instructors.