

Install Oracle VirtualBox

The computer image that you are going to use for the AiiDA tutorial has been made with VirtualBox 5.1.2, so we recommend to use such a version (or a higher one if existing).

Linux

Download the binary package corresponding to your linux distribution from <https://www.virtualbox.org/> and double click on it.

The installation should start automatically and finish without user intervention. For a better usage of VirtualBox, you might want to install also the extension from the same page where you downloaded the main binary package <https://www.virtualbox.org/>

MacOS

Download the **.dmg** package from <https://www.virtualbox.org/>, double click on it, and drag the virtualbox icon in your Application folder.

Windows

Download the installer from <https://www.virtualbox.org/> and run it.

Launch the virtual machine

1. Download **aiida_tutorial.ova** to a folder of your local machine.
2. Launch VirtualBox
3. Press CTRL+I to launch the appliance importer
4. Click the button next to the location bar, reach the path where you downloaded **aiida_tutorial.ova** and select it
5. Click **Next**, then click **Import**, and agree on the license. The import will take up to few minutes

6. In the main window select the newly created icon **aiida_tutorial** from the left menu, then click **Start** from the upper bar. This will launch the virtual machine
7. When the login prompt appear, type **aiida** as login and **tutorial** as password. The lightweight desktop manager xfce will start
8. In the desktop screen, find the **terminal icon** in the lower bar and click on it.
9. **(Optional)** In the terminal type **jupyter notebook**. The jupyter tree should appear in your browser. You will no longer use the first terminal, as it is being used by jupyter, so **open a new terminal** by clicking on the same icon as before

Connect to the virtual machine via SSH

If you are familiar with ssh connections you might not want to access the virtual machine directly, but via a ssh connection. This way, you will let aside the virtual machine and benefit from the advantages of a ssh connection (e.g. using **scp** to copy files from guest to host instead of using shared folders).

We assume that you executed successfully up to **step 6** of the previous list. Now:

1. Open in a text editor the file **~/.ssh/config** on your real machine and add the following lines at the bottom

```
Host aiida_tutorial
  HostName 127.0.0.1
  Port 2222
  User aiida
  LocalForward 8888 localhost:8888
```

Save and exit

2. Open a terminal on your real machine and type **ssh -Y -C aiida_tutorial** and type **tutorial** as password

From now on, you will access the virtual machine **only via the ssh terminal** that you just opened.

Congratulations! You just managed to connect to a virtual machine pre-configured for you. Now can go through the pdf of the tutorial and enjoy discovering AiiDA!

Optional: Run a jupyter notebook

In the ssh terminal enter the command

jupyter notebook --no-browser

Open a browser in your real machine and connect to the address

localhost:8888

The jupyter tree should appear in your browser.

You will no longer use the first ssh terminal, as it is being used by jupyter, so **open a new terminal and connect again to the virtual machine via SSH.**

If you do not manage to ssh into the virtual machine

This might be due to the fact that the IP assigned to your virtual machine might be a non-standard one (or you might have multiple virtual machines running).

1. Go into the window where the virtual machine is running, login with the following credentials:
2. Login: aiiida
3. Password: tutorial
4. Enter the **ifconfig** command. The output should look like
5. Copy the inet address of eth0. It should be the value of the first field of the second line.
6. In the virtualbox manager pane

7. In the virtualbox window click in the left menu on the **aiida_tutorial** virtual machine, type CTRL+F to shut it down, click OK to the warning. Then type **CTRL+s** to enter the settings. click on **Network** in the left menu, then click on **advanced**. In the new window there should be a row named **ssh**. Paste the inet address that you have just copied into the **Guest IP** field. Click OK twice to get back to the manager panel and start the virtual machine.
8. Try again to ssh into the virtual machine from the local terminal.