

Instructions to start the VirtualBox machine for the AiiDA tutorial

Step 1: Install Oracle VirtualBox (if not installed)

We recommend using VirtualBox 5.1.2 or a higher version.

Download the binary package corresponding to your operating system <https://www.virtualbox.org/>, and install it following the instructions. Linux, Mac OS X (called OS X on the download page) and Windows are all supported.

We suggest that you also download and install the “Virtual Box Extension pack” afterwards, downloadable from the same page, that makes the use of VirtualBox more performant, and allow to do copy-paste between your computer and the virtualbox image.

Step 2: Launch the virtual machine

1. Download **aiida_tutorial.ova** to a folder of your local machine.
2. Launch VirtualBox.
3. Choose from the menu the option “File > Import appliance”.
4. Click the button next to the text box, reach the path where you downloaded **aiida_tutorial.ova** and select it.
5. Click **Continue**, then click **Import**, and (if requested) 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, click on ‘Activities’ on the top left and click on the **terminal icon** that appears in the row of icons on the left of the screen.
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 choosing (in the terminal menu bar) the option “File > Open terminal”
10. To free up space, note that after importing the .ova file in step 5, you can delete the file .ova that you downloaded.

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!

Note: To access the jupyter, you must use a terminal started from within the virtualbox image (click on activities on the top bar, and search for ‘Firefox’). From there you can connect to the address

`http://localhost:8888`

(if you performed the optional step 9)

Some optional actions you might take, and some troubleshooting follows.

Optional: 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. In this way, you can reduce the VirtualBox window and work directly from your computer, keeping files there (e.g. using **scp** to copy files instead of 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. If the ssh connection does not work, see the troubleshooting section below.

Also, you will be able to access jupyter (if you started it before) directly from the browser on your computer rather than from a browser within the virtual machine, at the address

`http://localhost:8888`

Troubleshooting

You get errors when you try to start the virtualbox image

If you get error messages like “VT-x/AMD-V hardware acceleration is not available” or other similar errors, it is possible that you have to activate virtualization in the BIOS of your computer (note that you will need a 64-bit computer for the virtualbox image to work). Google for the error message, there are many posts that explain how to activate the correct setting.

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: aiida
3. Password: tutorial
4. Enter the **ifconfig** command. The output should look similar to this:

```
eth0      Link encap:Ethernet  HWaddr 08:00:27:49:08:fd
          inet addr 10.0.2.15  Bcast:10.0.2.255  Mask:255.255.255.0
          inet6 addr: fe80::a00:27ff:fe49:8fd/64 Scope:Link
          UP BROADCAST RUNNING MULTICAST  MTU:1500  Metric:1
          RX packets:4552 errors:0 dropped:0 overruns:0 frame:0
```

```
TX packets:2585 errors:0 dropped:0 overruns:0 carrier:0
collisions:0 txqueuelen:1000
RX bytes:5056186 (5.0 MB) TX bytes:206839 (206.8 KB)
Interrupt:19 Base address:0xd020
```

```
lo Link encap:Local Loopback
inet addr:127.0.0.1 Mask:255.0.0.0
inet6 addr: ::1/128 Scope:Host
UP LOOPBACK RUNNING MTU:65536 Metric:1
RX packets:376 errors:0 dropped:0 overruns:0 frame:0
TX packets:376 errors:0 dropped:0 overruns:0 carrier:0
collisions:0 txqueuelen:0
RX bytes:1516066 (1.5 MB) TX bytes:1516066 (1.5 MB)
```

5. Copy the IP address of eth0. It should be the value of the first field of the second line (near 'inet addr'), in the example above it is 10.0.2.15
6. Go to the virtualbox manager panel (that is the one from which you started the virtualbox image in the very first steps).
7. In the virtualbox window click in the left menu on the **Aiida Tutorial** virtual machine, choose **Settings**. Click on the **Network** section, then click on **advanced** (and, if present, click on **Port forwarding**). In the new window there should be a row named **ssh**. Type the inet address that you have obtained before into the **Guest IP** field. In the **host IP**, type 127.0.0.1.
8. Click **OK** twice to get back to the manager panel.
9. Try again to ssh into the virtual machine from the local terminal again (ssh aiida_tutorial). Also, in case there are still problems, you might change the port from 2222 to some other value (e.g. 2223, or 2224), both in the "Host port" section of the previous window, and in the line containing the string "Port" in the file `~/ssh/config` on your computer that you modified earlier.