



NMRProcFlow Installation Guide

This document describes how to install a virtual machine embedding the NMRProcFlow software on Oracle VM VirtualBox

© Copyright 2016-2021 Daniel J. Jacob

INRAE UMR 1332 BFP

Bordeaux Metabolome

France



NMRProcFlow Installation Guide

Content

1- Virtual Machine (VM)	4
2- System requirements	4
3- Disable the Hyper-V feature (Windows 10 Pro only)	5
4- Virtualization enabled	6
5- Installation procedures	7
6- Automated installation	7
7- Creation of the VM within Oracle VM VirtualBox.....	10
8- Using NMRProcFlow.....	14
9- Stop NMRProcFlow	16



License Agreement

NMRProcFlow is free software: you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version.

NMRProcFlow is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details.

You should have received a copy of the GNU General Public License along with this program. If not, see <<http://www.gnu.org/licenses/>>.



1- Virtual Machine (VM)

Characteristics of the NMRProcFlow Virtual Machine

- Distribution: CentOS 7.9 (Kernel 3.10)
- Memory: 4 Go (this parameter value can be modified in your virtualization software)
- 4 logical cores (this parameter value can be modified in your virtualization software)
- Thin provisioned system disk of 8 Go
- Network interface: NAT
- Docker CE 20.10.7
- **Warning:** Keyboard is AZERTY by default
 - After logging, the '**loadkeys us/loadkeys fr**' commands allow you respectively to switch to a QWERTY/AZERTY keyboard
- Default '**root**' password: **tomtom** (to;to; if you have a QWERTY keyboard)

2- System requirements

The installation and functionalities of the VM were successfully implemented based on the following items:

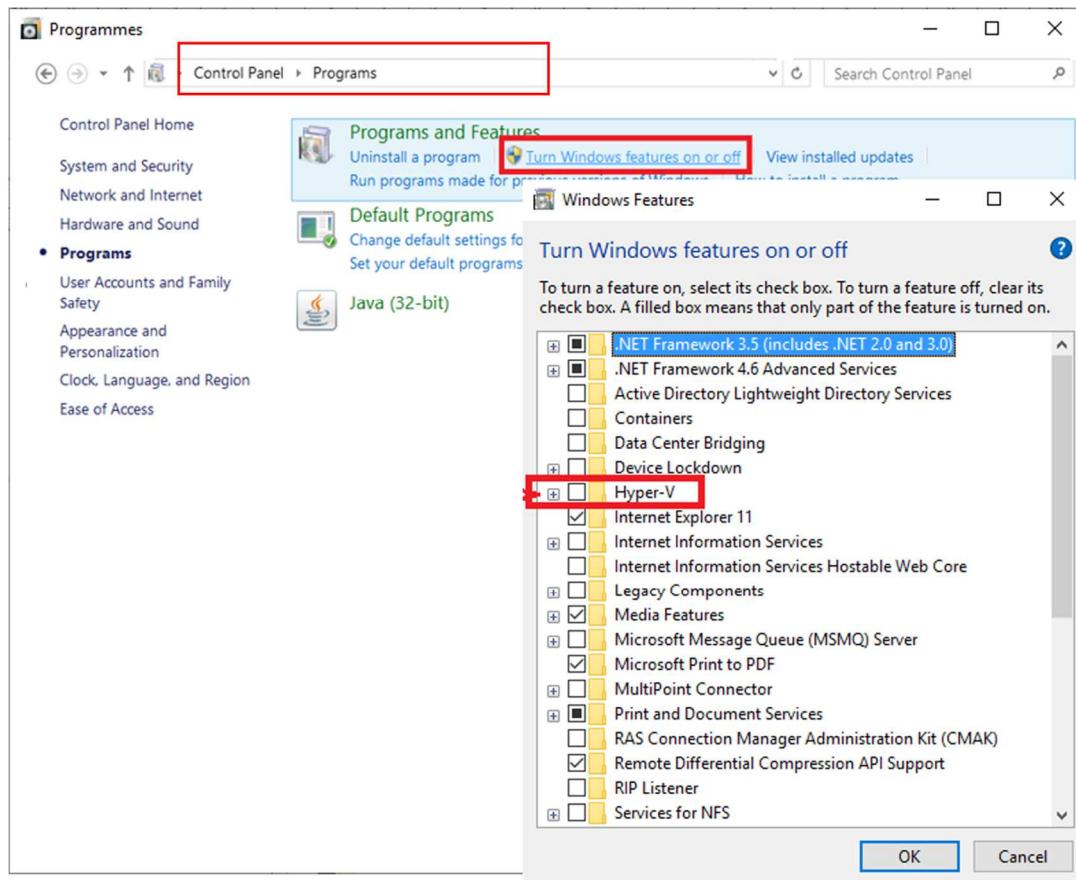
- Host machine under Windows 10 Pro (64bits)
- “Virtualization Technology” activated in the BIOS
- Host machine with a minimum of 4 Go RAM and 2 physical cores
- Host machine with a minimum of 20 Go disk free space
- You need to have Administrator privileges on the host machine
- Oracle VM VirtualBox 6.1.22

Other configurations may actually work well (i.e. with updated versions of the various elements or with Mac OS 10.11) but we cannot guarantee that the installation will run smoothly.



3- Disable the Hyper-V feature (Windows 10 Pro only)

On Windows 10 Pro, you have to disable the Hyper-V feature otherwise the virtual machine platforms do not work in 64-bit mode. Proceed as follow:



See

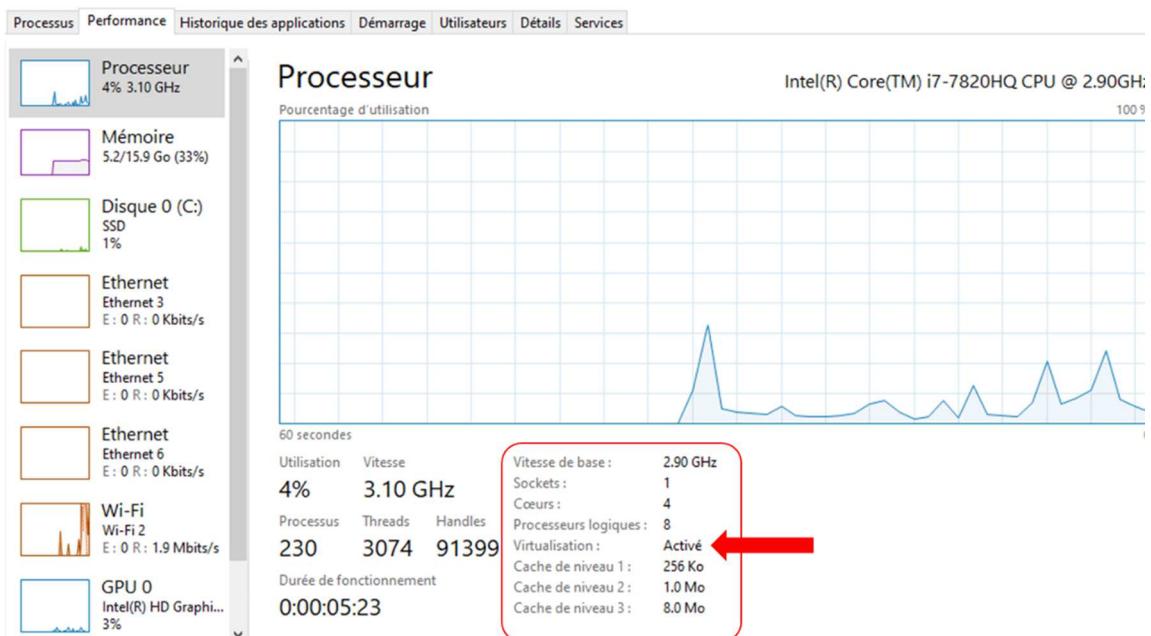
<https://ugetfix.com/ask/how-to-disable-hyper-v-in-windows-10/>

<https://www.poweronplatforms.com/enable-disable-hyper-v-windows-10-8/>



4- Virtualization enabled

You need to make sure that your PC supports virtualization. To do this, click on an area without an icon in the taskbar, and with the right mouse click, select "Task Manager".



You should normally see the information about the virtualization, and whether or not it is enabled. If this is not the case, then you should check with your hardware vendor for information on how to enable virtualization at the BIOS level. If not, go and take a look at <https://2nwiki.2n.cz/pages/viewpage.action?pageId=75202968>.



5- Installation procedures

There are two ways to proceed with the installation of the virtual machine containing NMRProcFlow software.

1. The first approach uses scripts, which further automates the installation.
2. The second approach is more manual, i.e. you have to perform the different steps yourself.

It is advisable to proceed according to the first approach. If something doesn't work properly, then you have to follow the second approach in order to see what went wrong with the first approach.

Before installation

Whichever approach you choose you must first download the latest version of the virtual machine which can be retrieved at:

https://nmrprocflow.org/themes/ova/npflow_vbox_vdi_x64.7z

Download the zipped virtual disk file (VDI - 7z) then unzip it in your workspace. To unzip, install first the 7zip tool (<https://www.7-zip.org/download.html>).

After unzipping the 7z file, you should have 4 files as shown below:



Warning: It is to be noted that these files should not be removed after the installation. So, you should take care to save it on a safe place on your disk.

Then proceed with the actual installation according to the chosen approach.

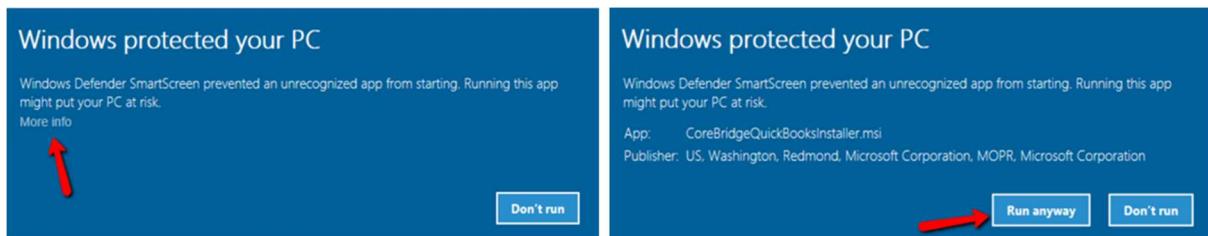
6- Automated installation

6.1- Creation of the Virtual Machine

To install the virtual machine, click on 'npflow_createVM.bat'.



If 'Windows Defender' is active, you should normally see a screen telling you that the script in question may be dangerous. To run it anyway (that's the goal), you have to click on 'More info', then 'Run anyway' as shown below:



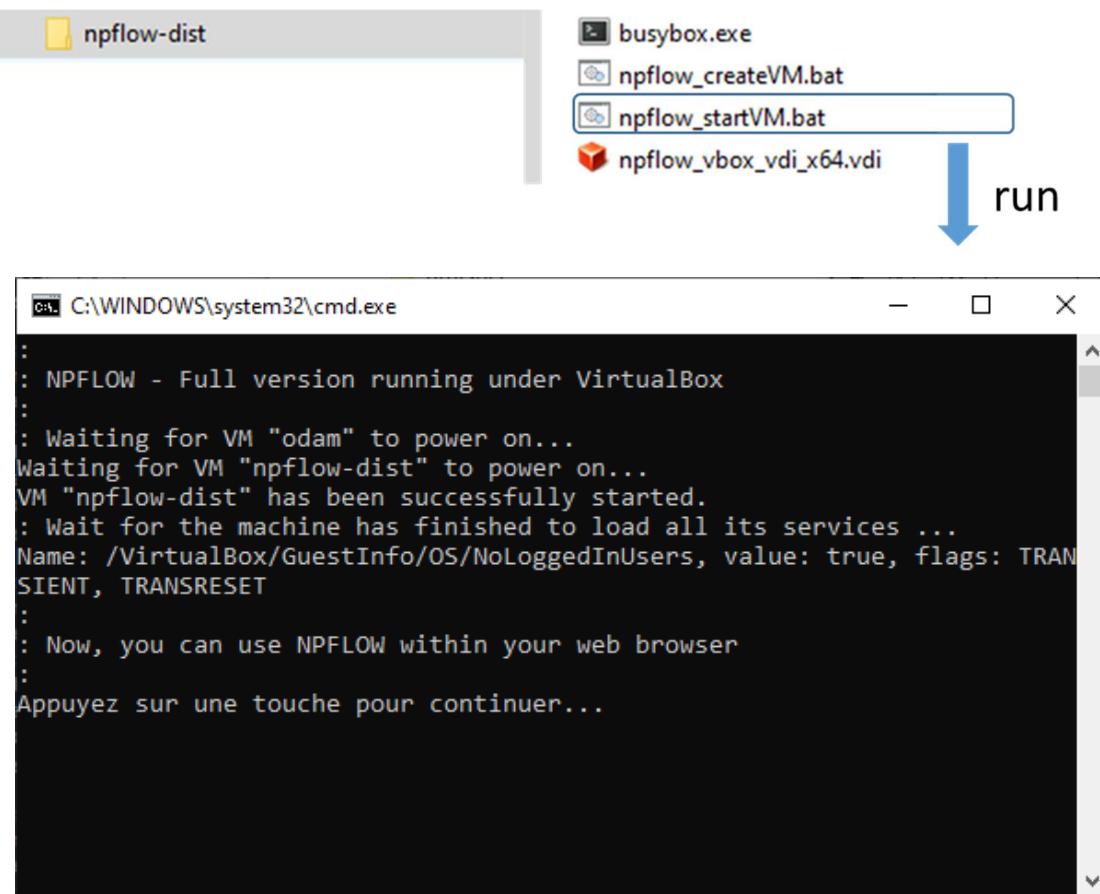
Then, a window will open.

```
C:\WINDOWS\system32\cmd.exe
:
: NPFLOW - Full version running under VirtualBox
:
Virtual machine 'npflow-dist' is created and registered.
UUID: 02acdf93-27d0-4772-9e74-00d08279ee20
Settings file: 'C:\Users\ djaco.GAIA\VirtualBox VMs\npflow-dist\npflow-dist.vbox'
: Ended
Appuyez sur une touche pour continuer...
```

Once the creation is finished, just press any key and the window will close.

6.2- Start of the Virtual Machine

To start the virtual machine, just click on 'npflow_startVM.bat'. Then a window opens asking you to wait until the virtual machine is fully started.



Once the virtual machine is started, just press any key and the window will close. Then Go to section “**Using NMRProcFlow**”.

Note1: If the virtual machine does not start correctly or fails due to an error, you may be forced to restart your PC (Welcome to the MS Windows world), then after restarting, try again. It is very likely that the problem will be solved.

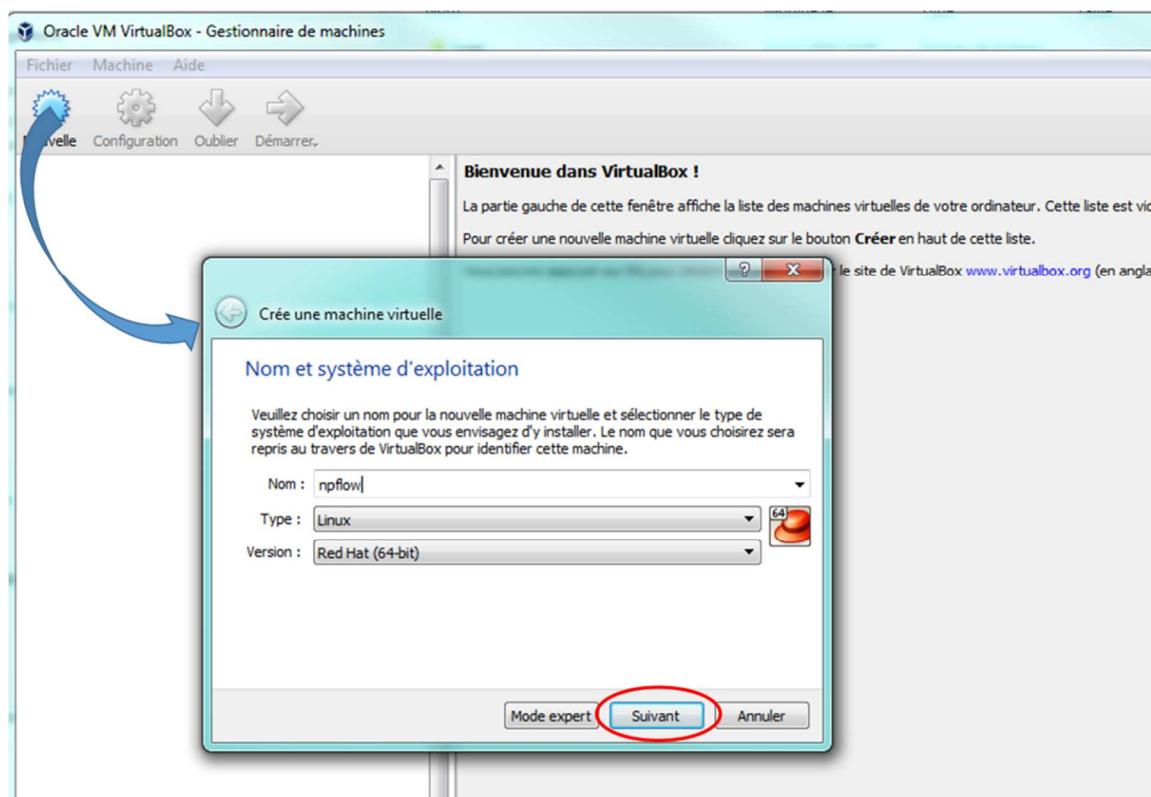
Note2: A good advice would be to create a shortcut of the 'npflow_startVM.bat' file and to move it to your desktop. In this way, you could easily start the application.



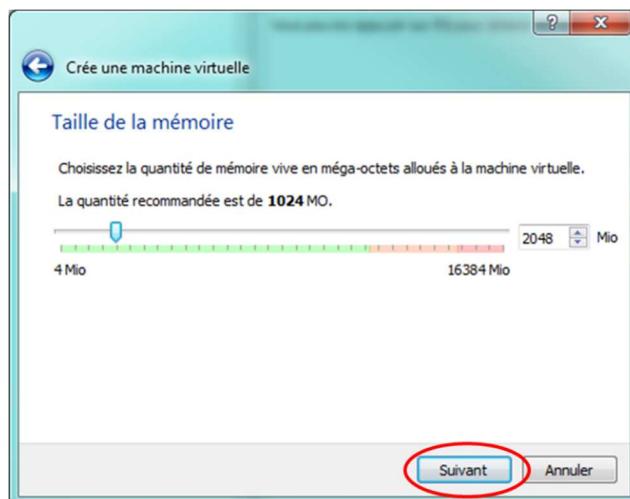
7- Creation of the VM within Oracle VM VirtualBox

You need to create a virtual machine directly in VirtualBox, except the virtual disk. The latter, already created (i.e. included in the compressed archive that obviously you should to unzip), will have to be connected to the virtual machine newly created. Some parameters will have to be adjusted and then normally, everything should work well.

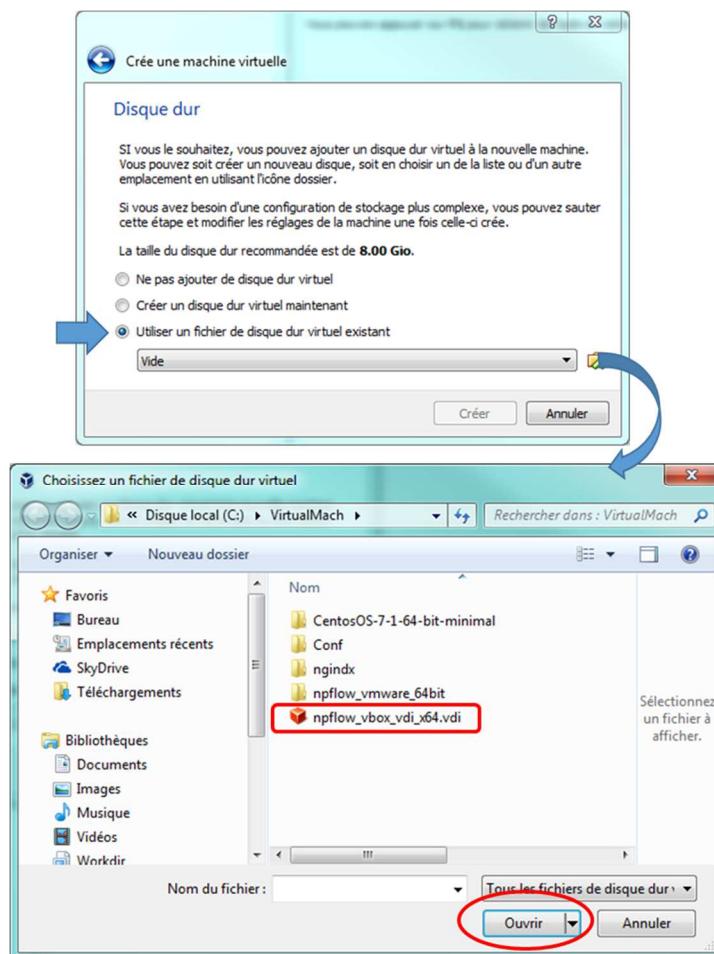
- **Creation of the new virtual machine:**



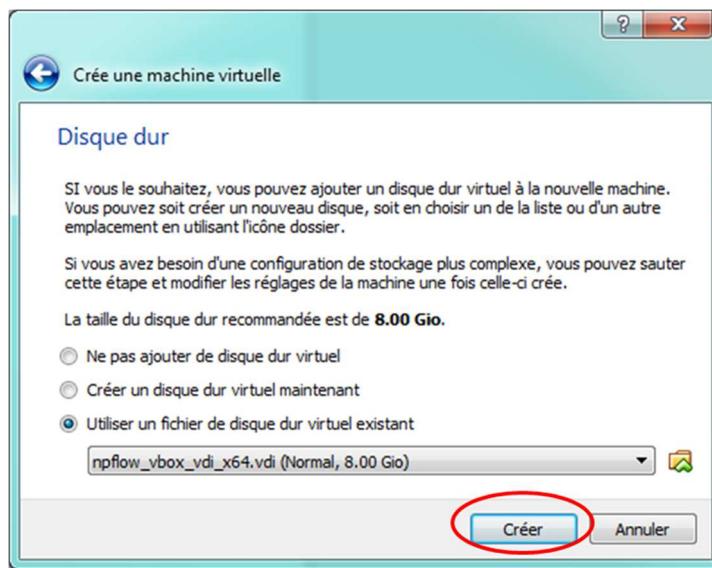
Choose '**Linux**' as Type, and '**Red Hat (64-bit)**' as Version. Of course, your computer has to be a 64-bit OS. Then, click to the '**Continue**' button.



Choose at least **1024Mo**; but **2048Mo** is better.



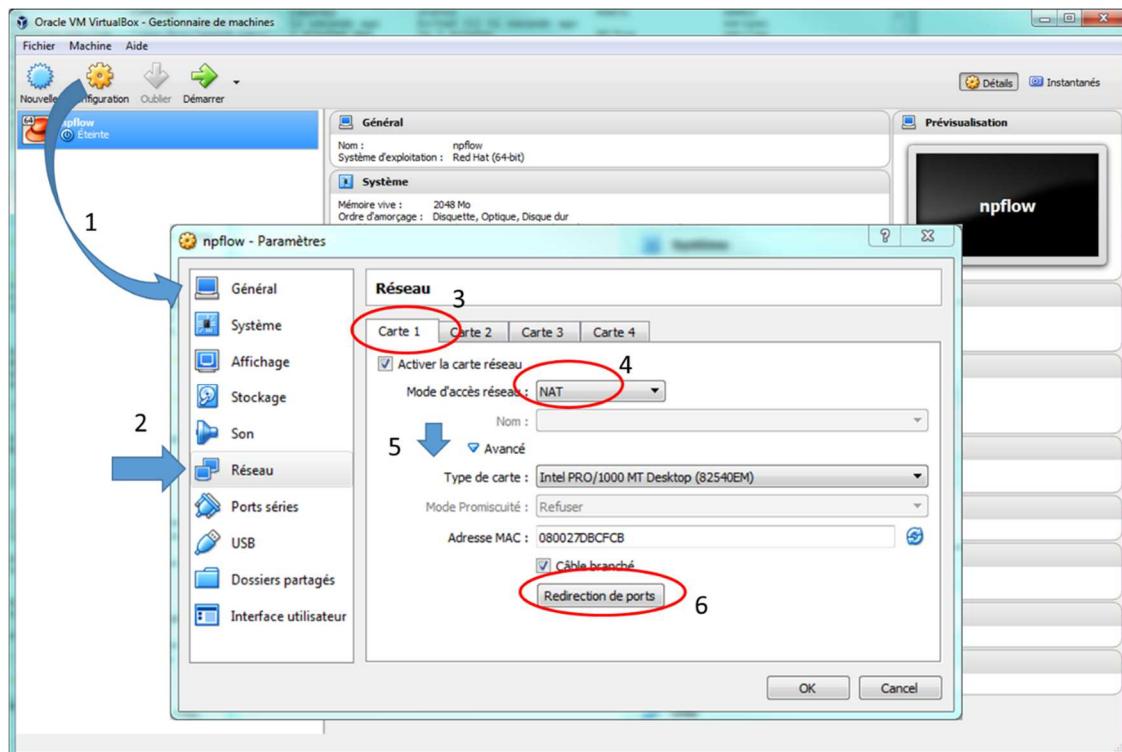
Instead of creating a new virtual disk, it is at this step that we have to connect the virtual disk embedded in the ZIP file (or 7z). Browse your file tree on your disk looking for where you've unpacked the virtual disk (i.e. the downloaded file).

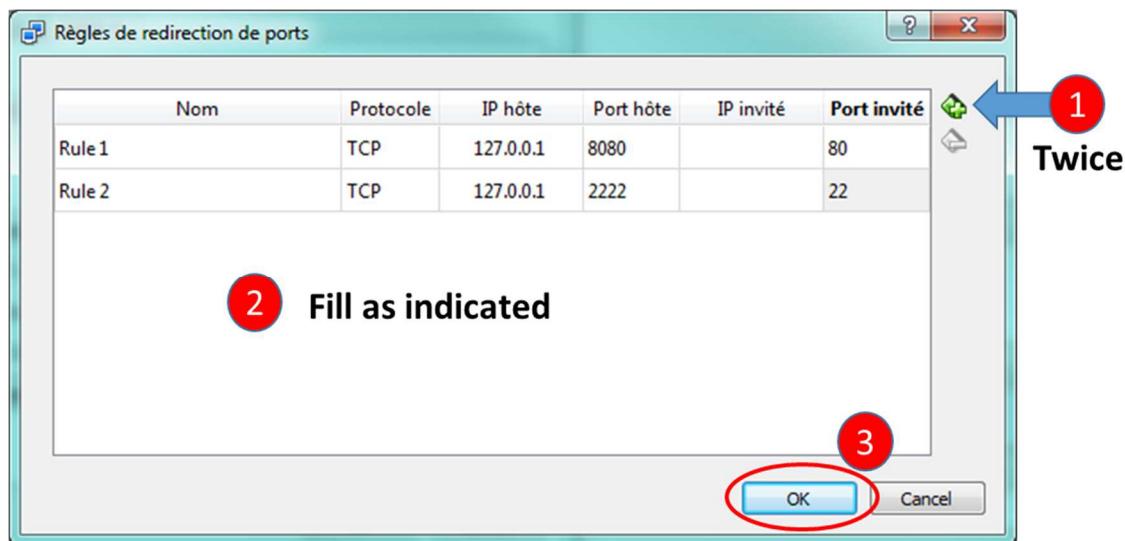


Then, click to the 'Create' button.

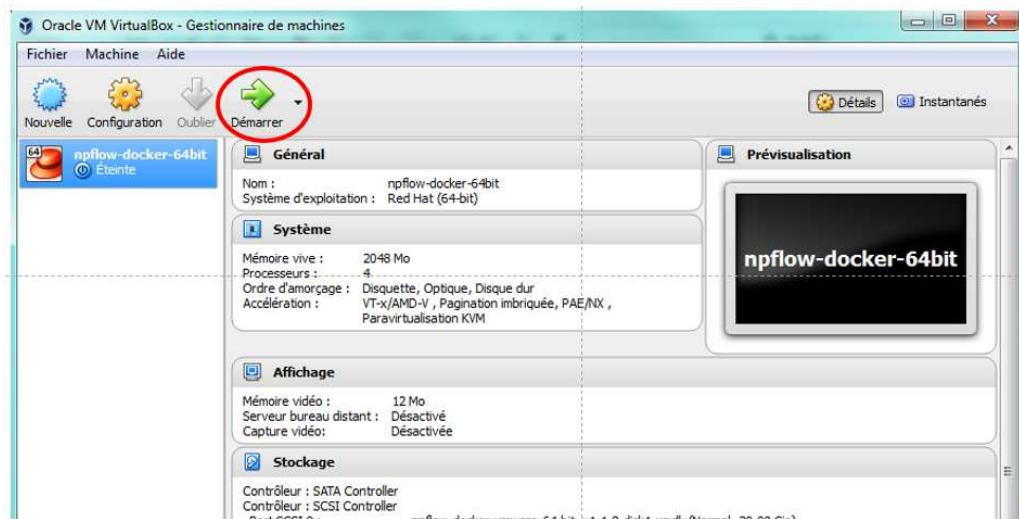
- **Adjusting some parameters:**

Now, the VM is created. We have to adjust some parameters concerning the network configuration. Proceed as shown below:





- Start your virtual machine





8- Using NMRProcFlow

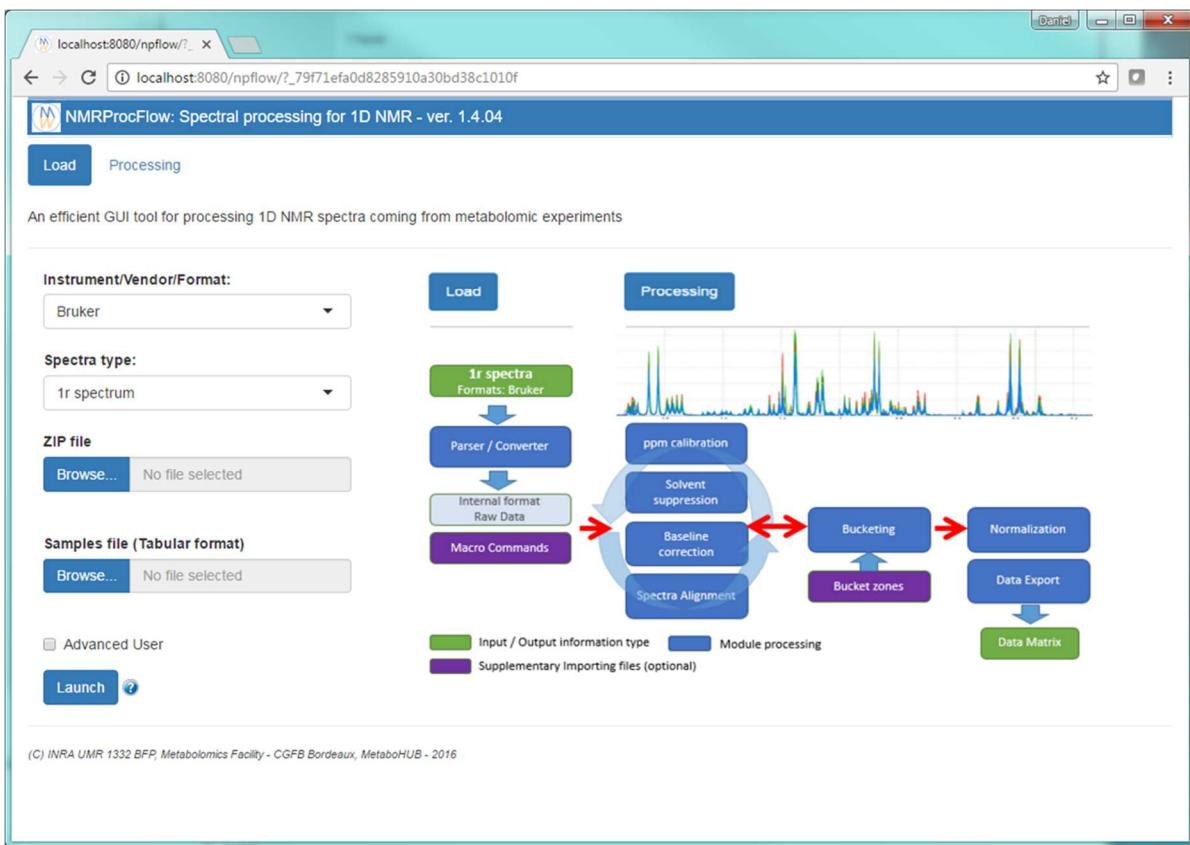
- Once the VM is started, the VM console will appear as shown below:

```
Fichier Machine Écran Entrée Périphériques Aide
waiting ...
NMRunview docker image: check and run ...
ba140780a2920d0ab1de06acedc37e19a931cddd91f85b5c1c4eaeae97296744
docker.io/nmrprocflow/nmrview    latest           2697b8953170      2 weeks
ago      562.9 MB
NMURspec docker image: check and run ...
08b384839360e0469e7cec7809c1356272b2667da?107b65420ac4e88a0f2833
docker.io/nmrprocflow/nmrspec   latest           f0d1af111e5c      4 days ago
go      1.227 GB
Purge sessions with no activities since 3 days ...Before: 0 ...OK
Starting shiny-server:OK
Starting apache2 server ...

=====
SSH Connection :
=====
ssh -p 2222 root@127.0.0.1

=====
URL Application (in your Internet Browser)
=====
http://localhost:8080/npflow/
```

- Note 1:** After starting, you should always wait for the URL application to appear in the console so that the various processes have time to start.
- Note 2:** To switch between the VirtualBox linux console and the Windows environment, press the right [Ctrl] key.
- Start your web browser to access the NMRProcFlow interface with the following URL (*JavaScript* functionalities must be enabled within your web browser).
 - <http://localhost:8080/npflow/>
- You will see the NMRProcFlow interface started:

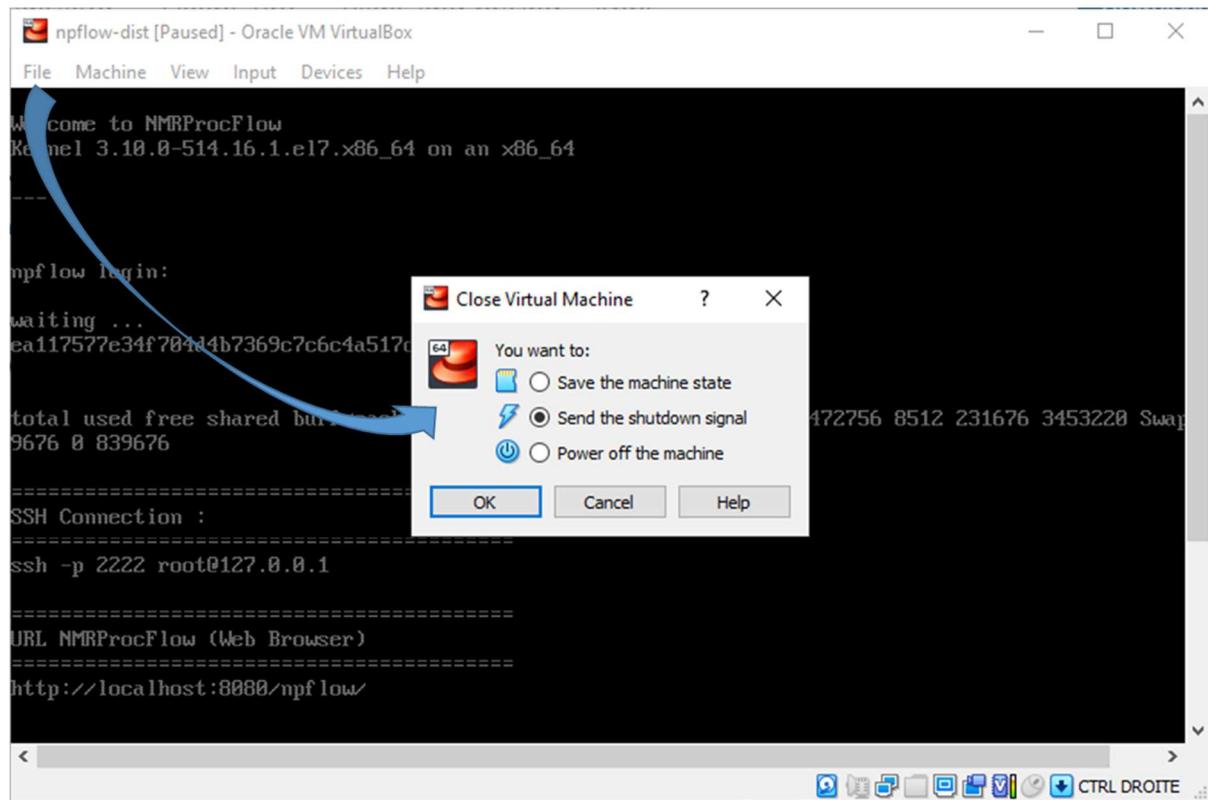


- **Note 1:** Sometimes you have to (re) try one minute after the launch, because the connection is not yet established. Just a problem of connection search a bit long (depending on your configuration).
- **Note 2:** When starting the interface, NMRProcFlow will create a new work session and its identifier will appear in the URL box of your web browser. You can bookmark the corresponding URL of your work session so that you could retrieve your session in the same state as you had left it, even if you had previously closed your web browser and/or restarted your VM or your PC.
- **Note 3:** The accumulation of work sessions can rapidly saturate the disk space of your VM. In order to avoid this, it is therefore necessary to clean periodically. **A cleaning process has been implemented to purge sessions without activities after 3 days.**



9- Stop NMRProcFlow

To stop properly the virtual machine, you have to click on ‘File’ in the menu on the top of the window application, as shown below:



Select “Close”, then “Send the shutdown signal” then click on the “OK” button. In this way, the virtual machine will properly close both services and applications and especially NMRProcFlow.