



DockM8 Installation Guide

Introduction

This is a guide to the installation and usage of the DockM8 package. It is meant for users testing the package before its release and is not a final production version.

Any queries/issues related to the installation process can be directed to Antoine Lacour at: alacournola@gmail.com. Please specify "DockM8 Installation Issue" in your email subject.

If any bugs within DockM8 are encountered, using the issue-reporting system on GitLab is preferred. (<https://gitlab.com/Tonylac77/DockM8/-/issues>). You can also contact Antoine.

1 Installation

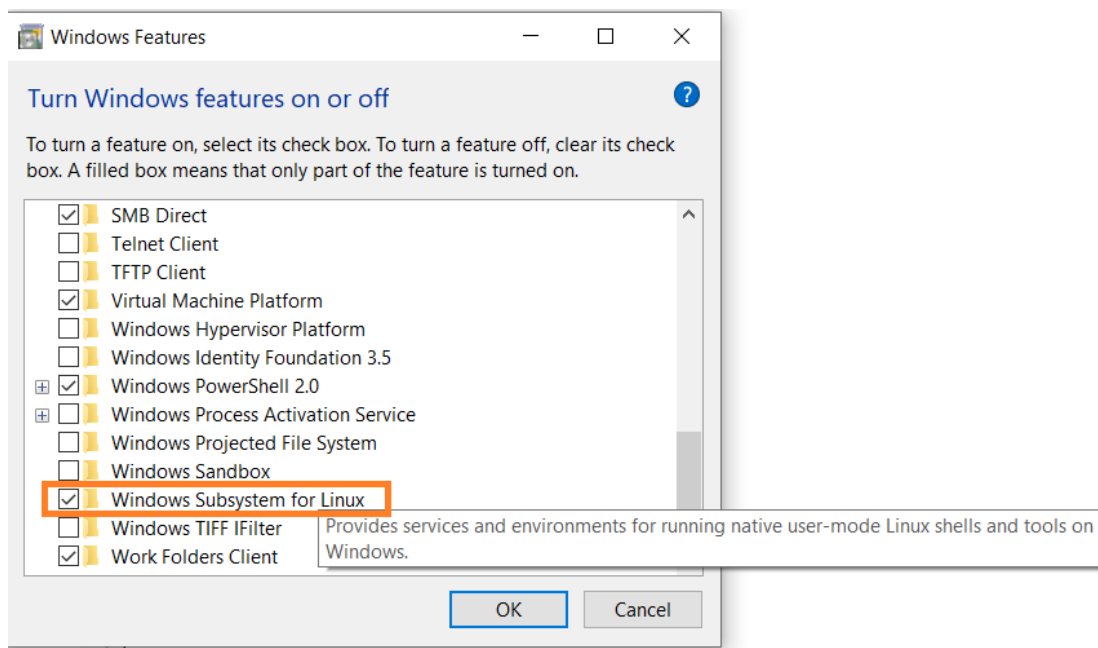
1.1 Windows

1.1.1 Using Windows Subsystem For Linux

In order to run DockM8 on Windows, you need to install the Windows Subsystem for Linux (WSL2), which is a way to run Linux inside of Windows. Once installed, you can follow the Ubuntu installation instructions in Section 1.2 as you will have an Ubuntu system running on your machine.

To install WSL2, follow these instructions (you may need administrator privileges for this) :

- Go to the start menu, and search for "Turn Windows features on and off".
- Check the "Windows Subsystem for Linux" and "Virtual Machine Platform" options.
- Ensure the "Windows Hypervisor Platform" and "Hyper-V" are turned off.

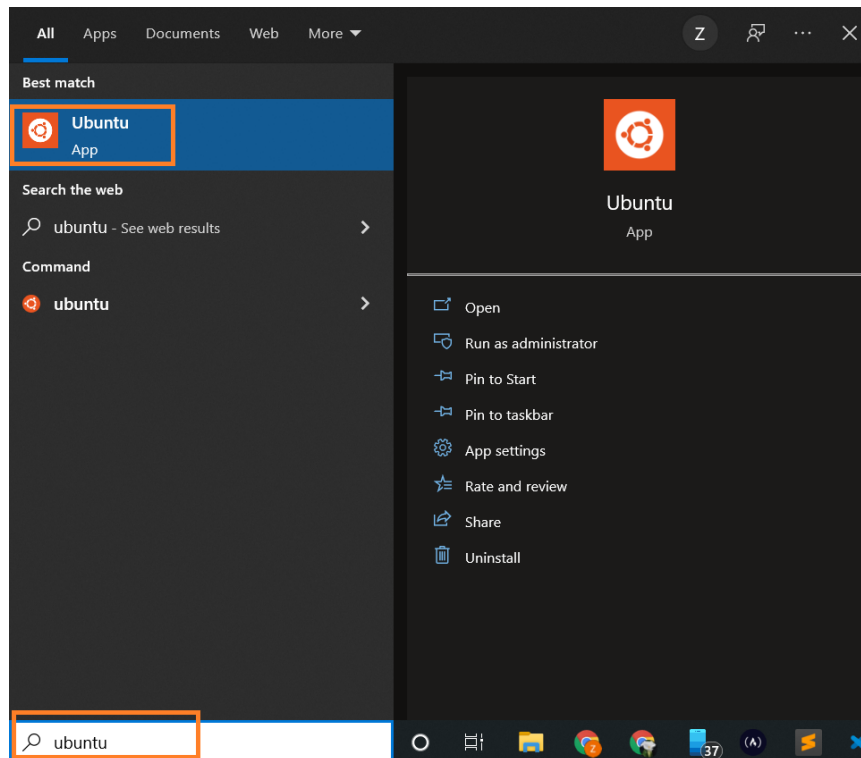


- Open the "Command Prompt" as an administrator (right-click, and choose "Run as administrator", you can search for it in the Start Menu).
- Run the following command (this will install Ubuntu by default):

```
wsl --install
```

- Restart your computer

You should now see Ubuntu when you search for it in the start menu. Launching the app will bring up a Ubuntu terminal, where you can type the commands listed in Section 1.2.



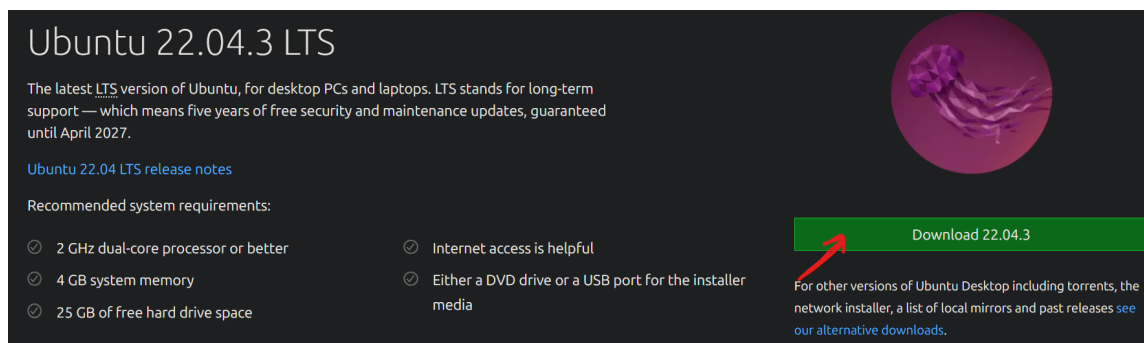
Should you encounter problems during the WSL2 installation, you can refer to the [Microsoft Documentation](#).

1.1.2 Using VirtualBox

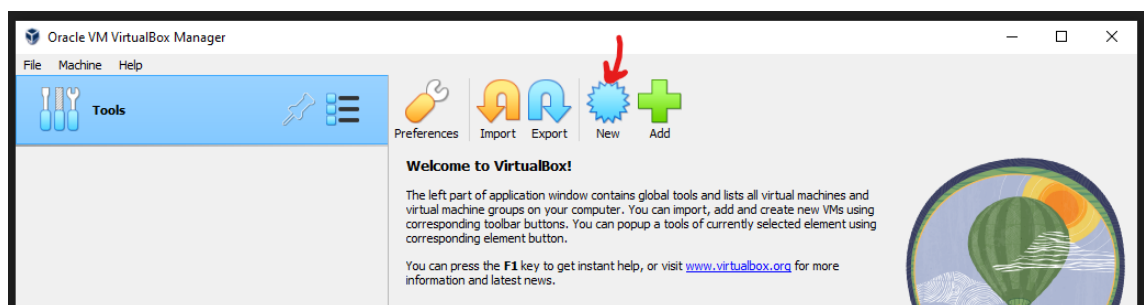
Download the VirtualBox installer [here](#).

Launch the installer (you will require administrator privileges) and click through the installation procedure, leaving all settings as default.

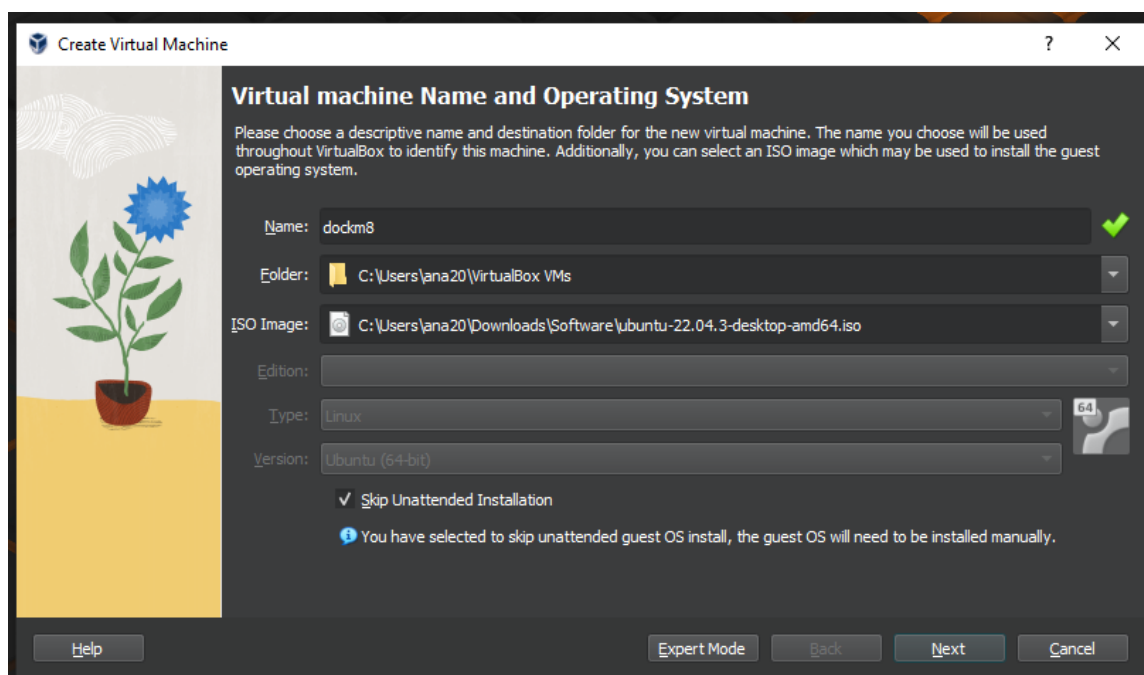
Download the Ubuntu 22.04 LTS .iso file [from the Ubuntu website](#). This will allow VirtualBox to create a new virtual machine running Ubuntu.



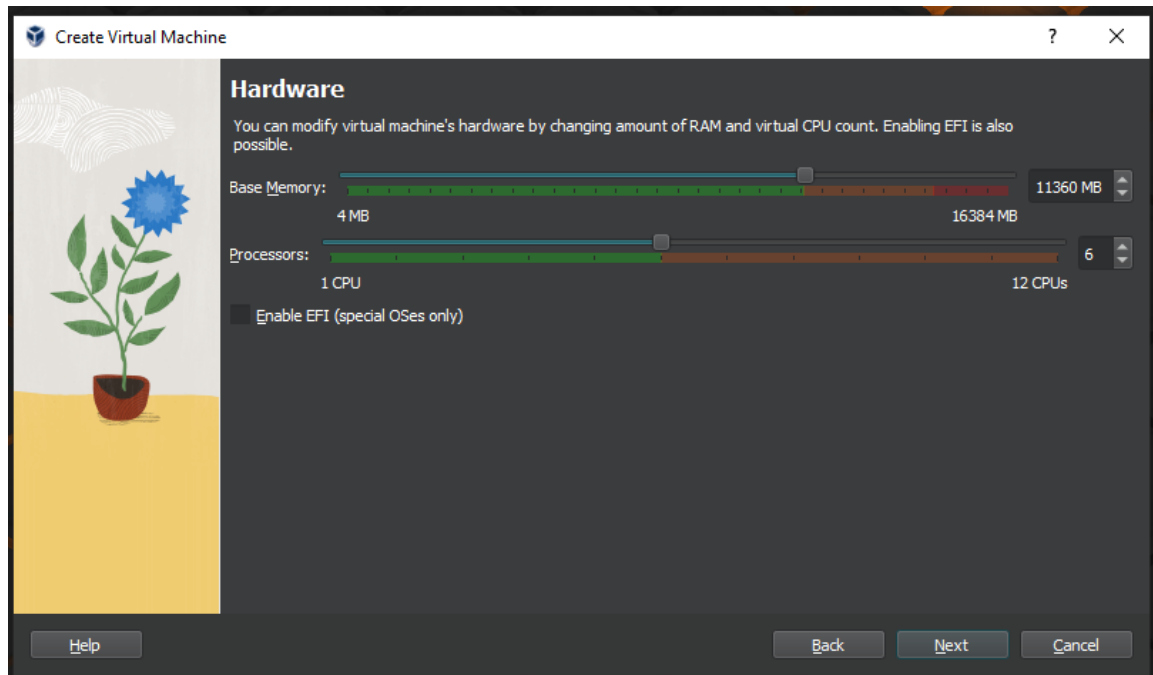
Save the .iso file to a convenient location, then launch the VirtualBox application from your Start Menu. Click the "New" button to create a new virtual machine.



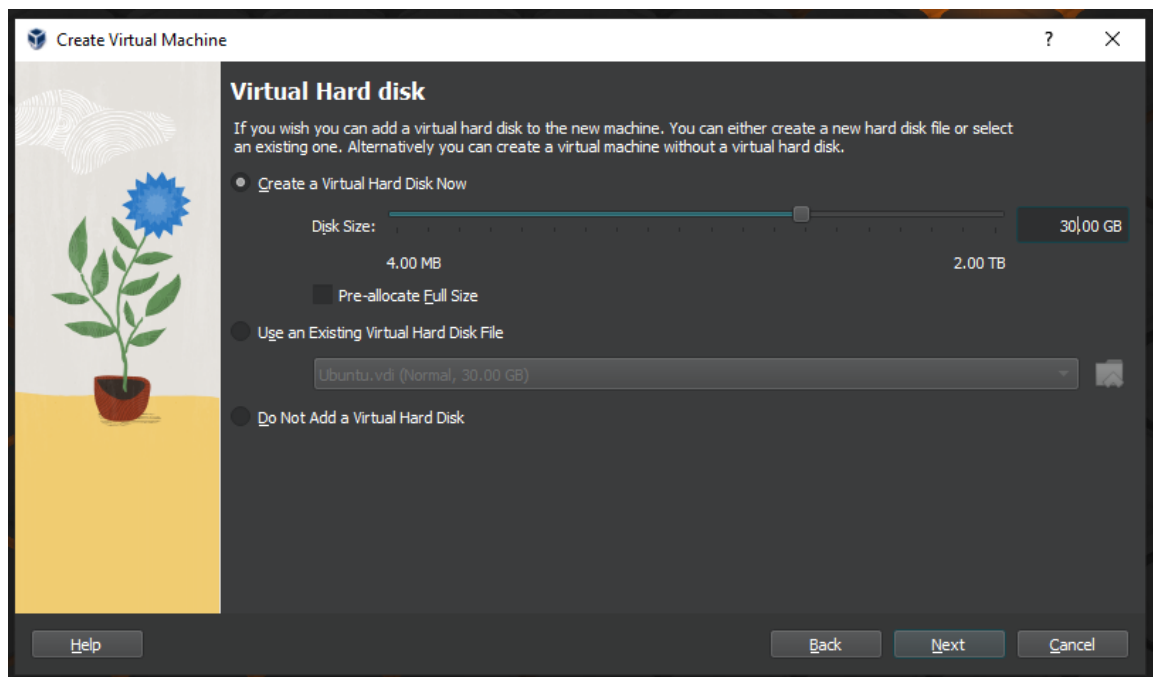
Select a name for your new virtual machine. Select the folder to which the machine should be saved. For the ISO Image, navigate to where you saved the .iso file you just downloaded. Be aware that VirtualBox may open the administrator user directory by default (wroot) but your downloaded file is likely in your user folder (ana20 in this example). Then click "Next". Make sure the "Skip Unattended Installation" checkbox is ticked.



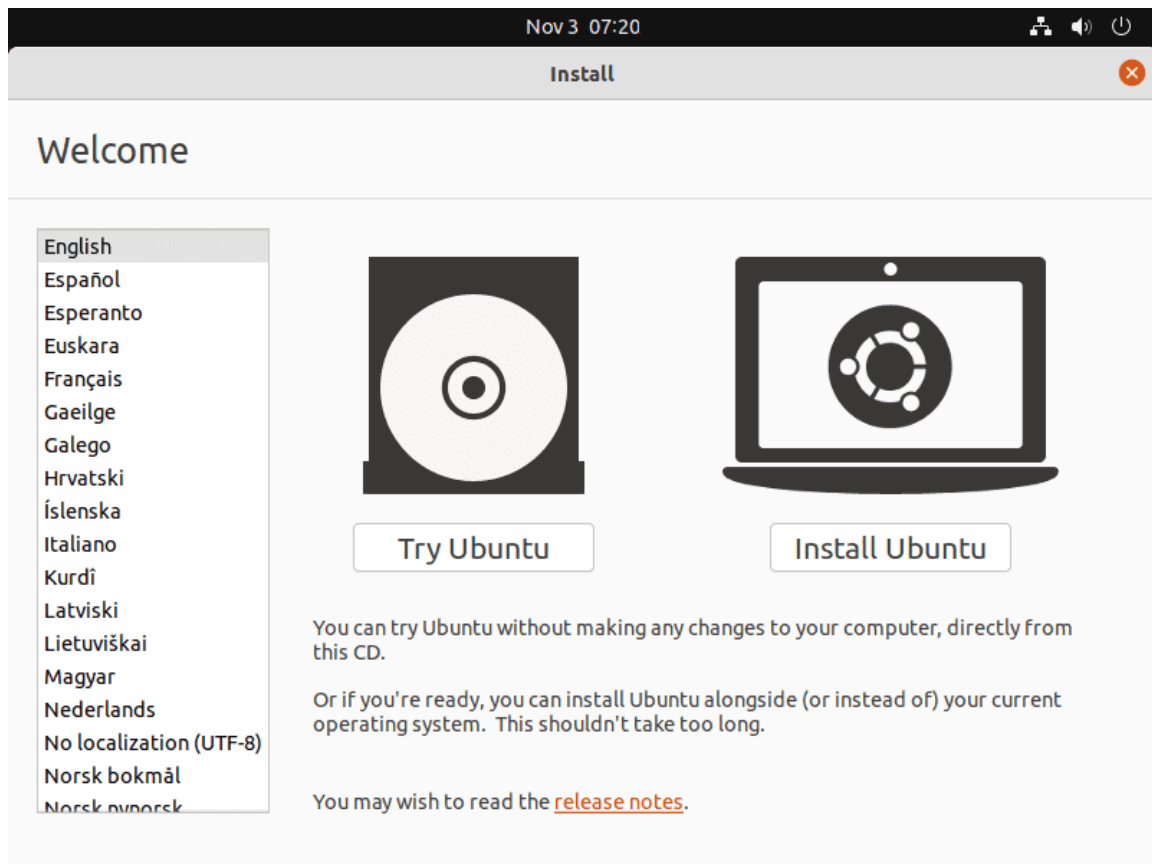
Next, you can set the number of CPUs and amount of RAM your virtual machine has access to. We recommend maxing out the number of CPUs (green bar) and ensuring that you leave some amount of memory free for Windows to run without issue.



We then need to create a virtual hard disk to store the virtual machine. Once you have selected the size you want, click "Next" and then "Finish" on the next screen.



Now, click "Start" in the VirtualBox interface, with the new virtual machine selected. A new window will appear, and the option to "Try or Install Ubuntu" will be available. Select that option. Wait a few seconds for the virtual machine to finish loading. A new screen will appear. Select "Install Ubuntu" and your preferred language and click "Continue".



Then select your keyboard layout and click "Continue".

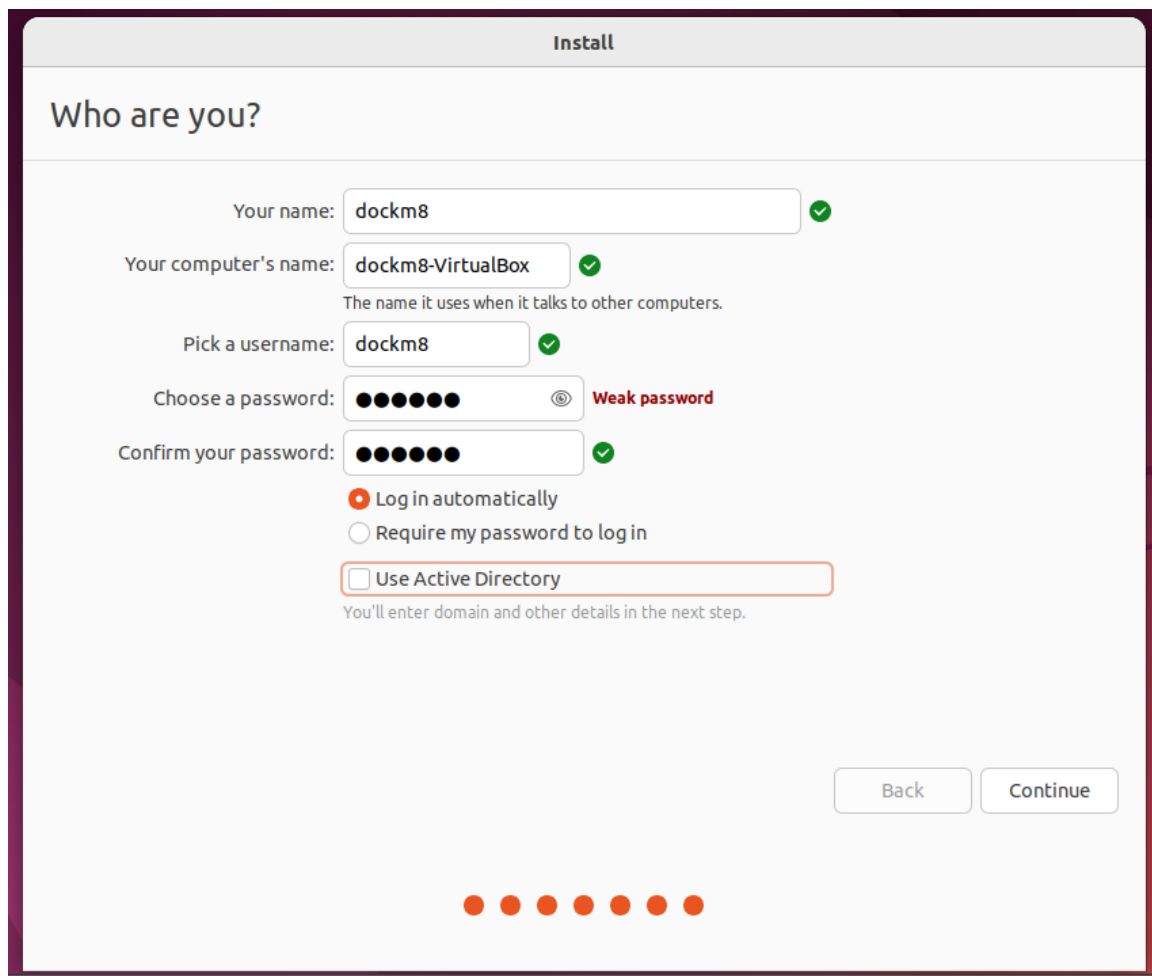
On the next screen, select "Minimal Installation" and "Download updates".

On the next screen, select "Erase disk and install Ubuntu" (this only applies to the virtual hard disk we created and will not delete any of your data).

Then click "Install Now" and confirm the disk changes.

Select your time zone.

On the "Who are you?" screen, you can set your username and password. Make sure to remember those as they will be required for the installation of further software.



The screenshot shows a window titled "Install" with a subtitle "Who are you?". It contains several input fields and checkboxes. The "Your name:" field is filled with "dockm8" and has a green checkmark. The "Your computer's name:" field is filled with "dockm8-VirtualBox" and has a green checkmark, with a note below it: "The name it uses when it talks to other computers." The "Pick a username:" field is filled with "dockm8" and has a green checkmark. The "Choose a password:" field is filled with dots and has a green checkmark, but a red "Weak password" warning is visible to its right. The "Confirm your password:" field is also filled with dots and has a green checkmark. Below these fields are two radio buttons: "Log in automatically" (selected) and "Require my password to log in". At the bottom, there is a checkbox for "Use Active Directory" which is unchecked, with a note below it: "You'll enter domain and other details in the next step." At the bottom right are "Back" and "Continue" buttons. At the very bottom center are seven orange dots, with the first one being slightly larger.

Once the installation is finished, close the window and shut down the machine.

You can now change some additional settings. We recommend setting the video memory to the maximum, and ensuring that the installation .iso file is unmounted. (right-click and "Remove Disk" if it is listed) You can now restart the virtual machine by clicking "Start" in the VirtualBox interface. Some configuration screens will appear where you can connect your Google account if needed and disable telemetry.

You can now proceed with the installation instructions in the 1.2 section.

1.2 Ubuntu Linux

1.2.1 Automatic Installation

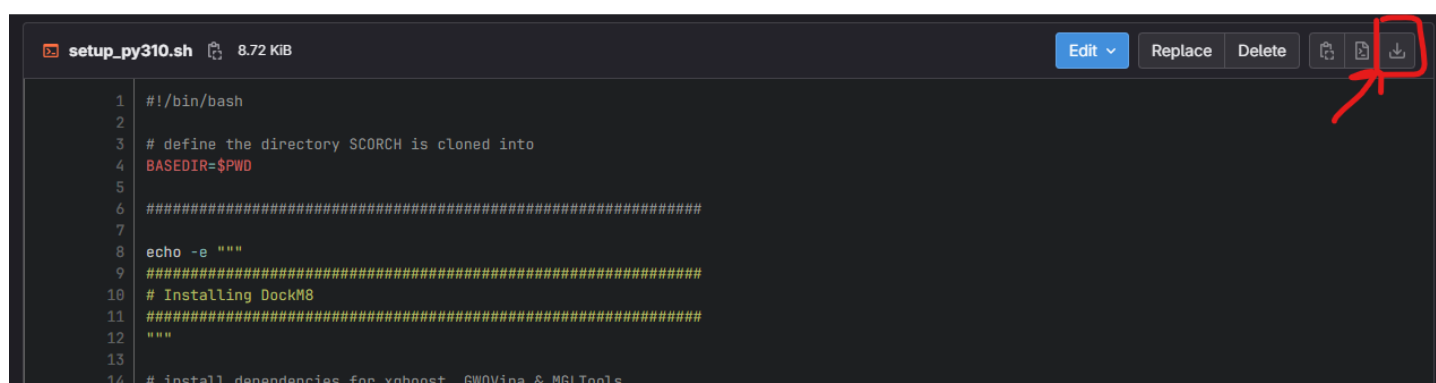
We provide an installation script to streamline the installation process. In order to use this option, please follow these steps :

We first need to make sure some essential programs are installed to build packages, decompress files etc. Please follow these instructions:

- Open Terminal (Ctrl + Alt + T on Ubuntu, or launch the Ubuntu app on Windows).
- Run the following commands (you will be prompted for your administrator (sudo) password):

```
sudo apt update
sudo apt install build-essential -y
sudo apt-get install wget -y
sudo apt-get install unzip -y
```

- Go the DockM8 setup script file in the repository : https://gitlab.com/Tonylac77/DockM8/-/blob/main/setup_py310.sh.
- Click the download button in the top right-hand corner :



- Save the file to where you want to install DockM8, we recommend installing in the /home/USERNAME directory.
- You will need to make the scripts executable in order to run it. You can do that in two different ways:

- Option 1: Right-click menu
 - * Right-click on the file.
 - * Select Properties.
 - * Go to the Permissions tab.
 - * Check the Allow executing file as program checkbox.

- Option 2 : Command line
 - * Open the terminal (Ctrl + Alt + T) and run :

```
chmod +x ~/setup_py310.sh
```

- You can now run the installation script in the command line.

- Open the terminal (Ctrl + Alt + T) and run :

```
bash ~/setup_py310.sh
```

The installation script will install Miniconda if there is no conda version installed. It will then create the environment and install all the required packages. All of the required executables and models will then be downloaded to the software folder. Please wait until the script is done running.

Note: Due to licensing restrictions, PLANTS is not installed automatically. If you would like to use it, please head to [the PLANTS website](#), sign up for a license, download the executable and put it in the ~/DockM8/software folder. Please also ensure the file is executable using `chmod +x PLANTS`.

Congratulations, you are now ready to run DockM8!

1.2.2 Manual Installation

This section assumes you are using Ubuntu 20.04 or Ubuntu 22.04 and that you have administrator privileges. Please note that orange arrow characters indicate that you should continue the command (the line with the arrow is not a new command).

We first need to make sure some essential programs are installed to build packages, decompress files etc. Please follow these instructions:

- Open Terminal (Ctrl + Alt + T on Ubuntu, or launch the Ubuntu app on Windows).
- Run the following commands (you will be prompted for your administrator (sudo) password):

```
sudo apt update
sudo apt install build-essential
sudo apt-get install wget
sudo apt-get install unzip
```

DockM8 runs in Python, in order to set up the Python environment easily, we recommend that you use Anaconda or Miniconda. To install Miniconda, follow these instructions.

- Open Terminal (Ctrl + Alt + T on Ubuntu, or launch the Ubuntu app on Windows).
- Run the following commands:

```
cd ~
mkdir miniconda3
cd ./miniconda3
wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh -O
→ miniconda.sh --no-check-certificate
chmod +x miniconda.sh
bash ~/miniconda3/miniconda.sh -b -u -p ~/miniconda3
rm -rf ~/miniconda3/miniconda.sh
~/miniconda3/bin/conda init bash
```

Miniconda is now installed. Next, we need to setup our Python environment and install the required packages. Please follow these instructions:

- Open Terminal (Ctrl + Alt + T on Ubuntu, or launch the Ubuntu app on Windows).
- Run the following commands:

```
conda create -n dockm8 python=3.10 -y
conda activate dockm8
conda config --add channels conda-forge
conda install rdkit ipykernel scipy spyrmsd kneed scikit-learn-extra molvs
→ seaborn xgboost openbabel docopt -q -y

pip install pymesh espsim oddt biopandas redo MDAnalysis==2.0.0 prody==2.1.0 dgl
→ Pebble tensorflow meeko chembl_structure_pipeline posebusters streamlit

pip3 install torch torchvision torchaudio --index-url
→ https://download.pytorch.org/whl/cpu

pip install torch_scatter torch_sparse torch_spline_conv torch_cluster
→ torch_geometric
```

The required dependencies for DockM8 are now installed. We now need to download DockM8 itself from GitLab:

- Open Terminal (Ctrl + Alt + T on Ubuntu, or launch the Ubuntu app on Windows).
- Run the following commands:

```
cd ~
wget https://github.com/Tonylac77/DockM8/main.zip -O DockM8.zip
unzip DockM8.zip
rm DockM8.zip
```

We now need to install the docking programs. If you plan to only use a selection of docking programs, you can only download the required ones. You may need to use sudo (administrator) to change the permissions of the executable files (the chmod commands). Unfortunately, due to license restrictions, we cannot redistribute the PLANTS docking software. If you would like to use it, please head to [the PLANTS website](#), sign up for a license, download the executable and put it in the ~/DockM8/software folder. Please also ensure the file is executable using chmod +x PLANTS.

- Open Terminal (Ctrl + Alt + T on Ubuntu, or launch the Ubuntu app on Windows).
- Navigate to the DockM8/software folder :

```
cd ~/DockM8/software
```

- Install GNINA:

```
wget https://github.com/gnina/gnina/releases/latest/download/gnina
→ --no-check-certificate
chmod +x gnina
```

- Install QVINA2:

```
wget https://github.com/QVina/qvina/raw/master/bin/qvina2.1
→ --no-check-certificate
chmod +x qvina2.1
```

- Install QVINAW:

```
wget https://github.com/QVina/qvina/raw/master/bin/qvina-w --no-check-certificate
chmod +x qvina-w
```

We now need to install the scoring functions. If you plan to only use a selection of scoring functions, you can only download the required ones. You may need to use sudo (administrator) to change the permissions of the executable files (the chmod commands).

- Install KORP-PL:

```
wget
→ https://files.inria.fr/NanoDFiles/Website/Software/KORP-PL/0.1.2/Linux/KORP-PL-LI
→ --no-check-certificate
tar -xvf KORP-PL-LINUX-v0.1.2.2.tar.gz
rm KORP-PL-LINUX-v0.1.2.2.tar.gz
chmod +x KORP-PL
```

- Install Convex-PLR:

```
wget
→ https://files.inria.fr/NanoDFiles/Website/Software/Convex-PL/Files/Convex-PL-Linu
→ --no-check-certificate
unzip Convex-PL-Linux-v0.5.tar.zip
tar -xvf Convex-PL-Linux-v0.5.tar
rm Convex-PL-Linux-v0.5.tar.zip
rm Convex-PL-Linux-v0.5.tar
rm -r __MACOSX
chmod +x Convex-PL
```

- Install SMINA:

```
wget https://github.com/cyangNYU/Lin_F9_test/raw/master/smina.static
→ --no-check-certificate
chmod +x smina.static
```

- Install AA-Score:

```
wget https://github.com/Xundrug/AA-Score-Tool/archive/refs/heads/main.zip
→ --no-check-certificate
unzip main.zip
rm main.zip
```

- Install GypsumDL:

```
wget https://github.com/durrantlab/gypsum_dl/archive/refs/tags/v1.2.1.tar.gz
→ --no-check-certificate
tar -xvf v1.2.1.tar.gz
rm v1.2.1.tar.gz
```

- Install SCORCH:

```
wget https://github.com/SMVDGroup/SCORCH/archive/refs/tags/v1.0.0.tar.gz
→ --no-check-certificate
tar -xvf v1.0.0.tar.gz
rm v1.0.0.tar.gz
```

- Install RF-Score-VS:

```
wget  
→ https://github.com/oddt/rf-scorevs_binary/releases/download/1.0/rf-score-vs_v1.0_1  
→ --no-check-certificate  
unzip rf-score-vs_v1.0_linux_2.7.zip  
rm rf-score-vs_v1.0_linux_2.7.zip  
rm -r ./test  
rm README.md  
chmod +x rf-score-vs
```

- Install RTMScore:

```
wget https://github.com/sc8668/RTMScore/archive/refs/heads/main.zip  
→ --no-check-certificate  
unzip main.zip  
rm main.zip
```

- Install DeepCoy models:

```
cd ./models  
wget https://opig.stats.ox.ac.uk/data/downloads/DeepCoy_pretrained_models.tar.gz  
tar -xvf DeepCoy_pretrained_models.tar.gz  
rm DeepCoy_pretrained_models.tar.gz
```

Congratulations, you are now ready to run DockM8! Please refer to the Usage Guide for more details about running DockM8