

The easiest and performance wise way to run QuantumEspresso on your machine

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QuantumEspresso is a suite of packages for the calculations of electronic structure and materials modeling. Today, many apps, and with them also QuantumEspresso can be run conveniently in a virtual environment, insulated from the machine and the software of the machine that hosts them.

Most of you are already aware of **virtual machines** and the way to use them. *Virtual machines* are supported by **Full Virtualization**: a program called **hypervisor** pretends to be a bare machine and so can load over itself any operating system.

There is a more lightweight sort of virtualization that reached maturity later on Linux and became popular in the last years : **os-level virtualization**.

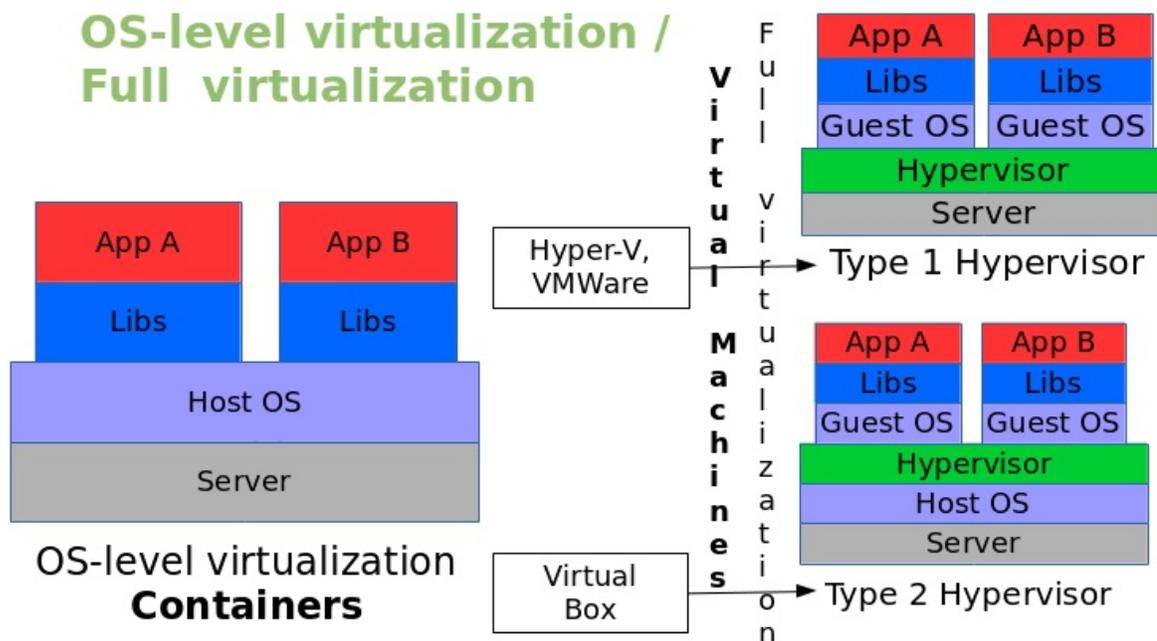
With this virtualization the Linux os keeps insulated the activities in **containers** (the equivalent of a VM in this context).

In this case the programs inside the container use the operating system services of the host and so they can't be apps for another os.

The good of this is that each process of the containers is a process of the host and so there is almost no penalty associated with this.

Furthermore for all the *containers* there is only one host os to take care of.

The most popular tool to provide **os-level virtualization** on Linux is **Docker**.



Docker runs containers formed according to **images**.

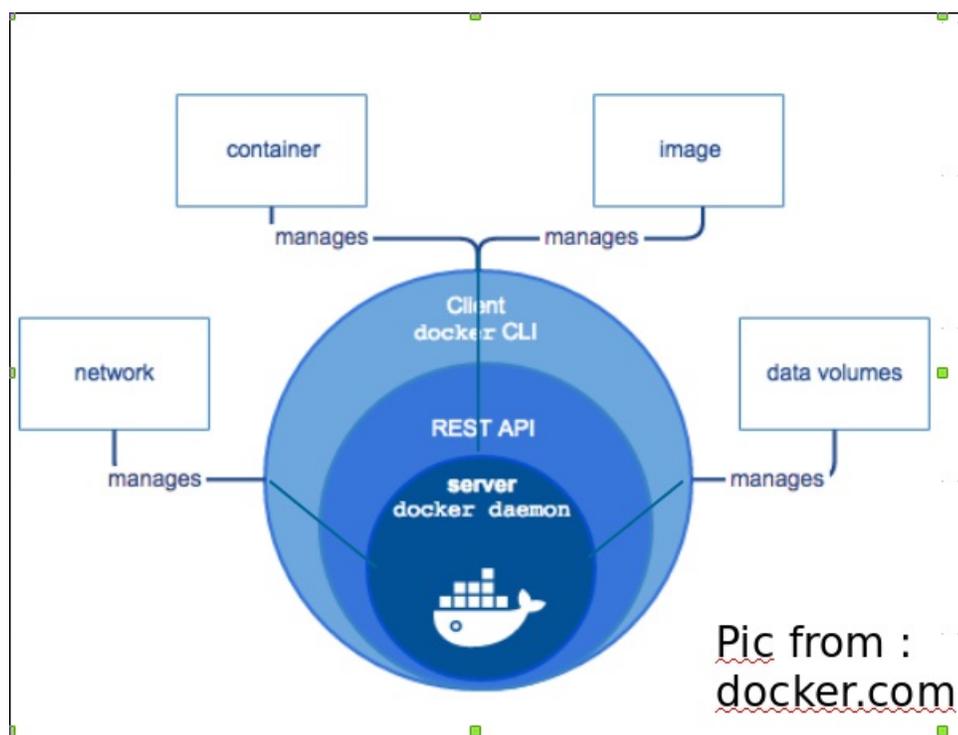
The *docker image* for QuantumEspresso is very large (up to 2 GB or more).

In any case prepare a sufficient space on disk, checking :

- On Linux :
 - docker images are stored under `/var/lib/docker`, if `df /var/lib` gives you not enough space you can create `$HOME/docker` and make a symbolic link from `/var/lib/docker` to your dir.
- On Windows :
 - docker images are stored under `c:\ProgramData\docker`
- On Mac : ?

Docker engine is the new way to call the client/server application once simply called **docker** and made of :

- a docker client (**docker CLI**)
- a docker server (**docker daemon**)



What to install on your machine

- If you have **Linux**: install **ssh**, **Docker Engine** and **docker-machine** :
 - **ssh** : if you don't have it, follow your distro instructions
 - **Docker Engine** , follow instructions for your distro on [*docker.com*](https://docs.docker.com/engine/installation/linux/ubuntulinux/) :
 - <https://docs.docker.com/engine/installation/linux/ubuntulinux/>
 - <https://docs.docker.com/engine/installation/linux/centos/>
 - <https://docs.docker.com/engine/installation/linux/fedora/>
 - <https://docs.docker.com/engine/installation/linux/debian/>
 - **docker-machine** :

```
$ curl -L https://github.com/docker/machine/releases/download/v0.9.0/docker-machine-`uname -s`-`uname -m` >/tmp/docker-machin
```

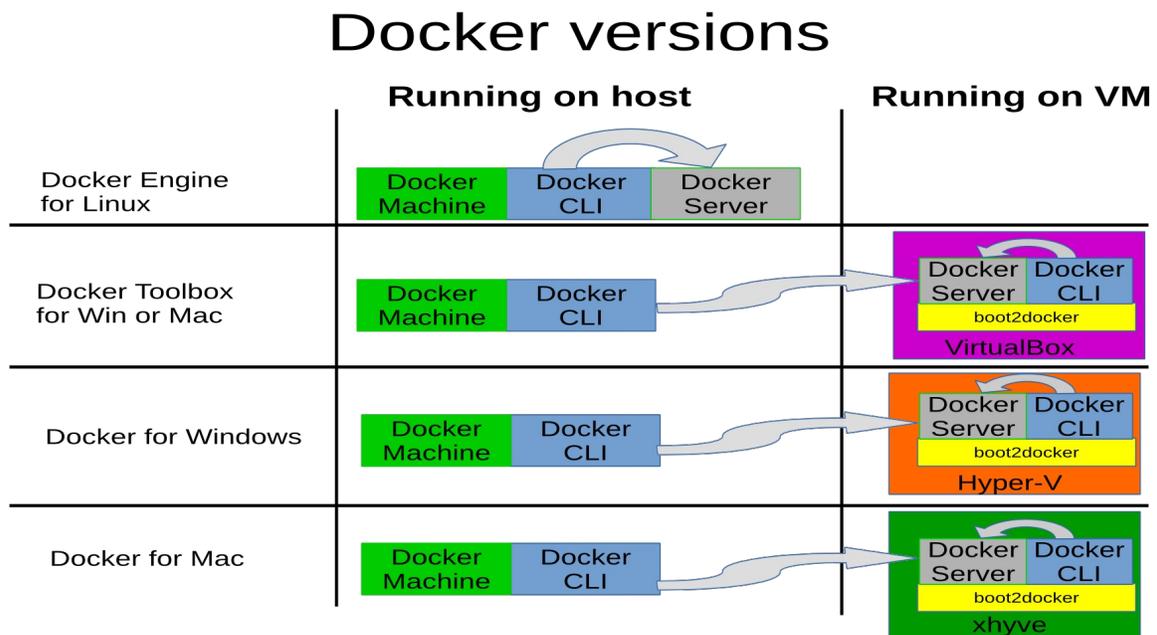
```
e &&
chmod +x /tmp/docker-machine &&
sudo cp /tmp/docker-machine /usr/local/bin/docker-machine
```

- If you have a Mac: install **ssh**, **Docker Toolbox** :
 - **ssh** : follow Apple instructions
 - **Docker Toolbox** , follow instructions on [*docker.com*](http://docker.com) :
 - https://docs.docker.com/toolbox/toolbox_install_mac/
- If you have **Windows** : install **putty**, **Docker Toolbox** :
 - **putty** : follow instructions on <http://www.putty.org/>
 - **Docker Toolbox** , follow instructions on :
 - https://docs.docker.com/toolbox/toolbox_install_windows/

docker-machine is installed along the **Docker Toolbox** on Win and Mac and so there is no need for a separate installation.

Different versions of Docker

Even if Docker is relatively recent, there is now a *plethora* of different **docker** versions.



Docker Engine

You should install it on Linux machines. For the other platforms is part of the Toolbox. Requires a Linux kernel at least 3.10. It uses the native Linux containers (cgroup/namespace) of the host.

On **Ubuntu 16.04** install it with :

```
sudo apt update
sudo apt-get install linux-image-extra-$(uname -r) linux-image-extra-virtual
sudo apt install -yq apt-transport-https ca-certificates
sudo echo "deb https://apt.dockerproject.org/repo ubuntu-xenial main" >>/etc/apt/sources.list
sudo apt-key add \
    --keyserver hkp://p80.pool.sks-keyservers.net:80 \
    --recv-keys 58118E89F3A912897C070ADB76221572C52609D
sudo apt update
sudo apt-cache policy docker-engine

sudo apt install -yq docker-engine
sudo service docker start

sudo groupadd docker
sudo usermod -aG docker *your_username*
```

On **Centos 7.X** :

```
sudo yum update
sudo yum update

sudo tee /etc/yum.repos.d/docker.repo <<-'EOF'
[dockerrepo]
name=Docker Repository
baseurl=https://yum.dockerproject.org/repo/main/centos/7/
enabled=1
gpgcheck=1
gpgkey=https://yum.dockerproject.org/gpg
EOF

sudo yum install docker-engine
sudo systemctl enable docker.service
sudo systemctl start docker
sudo groupadd docker
sudo usermod -aG docker **your_username**
```

Docker Toolbox

For other OS, Docker developed a Linux microkernel (**boot2docker**), that can run the docker daemon and containers and is installable over a **Virtual Machine** (in particular it will install **Oracle VirtualBox**).

This is the legacy solution that, for the time being, I suggest you to use if you don't run Linux. Here the instructions for Mac and Win :

- https://docs.docker.com/toolbox/toolbox_install_mac/
- https://docs.docker.com/toolbox/toolbox_install_windows/

Recently Docker released new versions of docker based on OS specific hypervisor (**xhyve** and **hyper-v**) for MacOS and Windows, it called them **Docker for Mac** and **Docker for Windows**.

I suggest you don't try first these two new solutions.

Docker for Mac

- <https://docs.docker.com/docker-for-mac/>

Requires a Mac produced after 2010 with processor supporting **ept** and **unrestricted mode**.

Requires at least 4 GB RAM.

Requires macOS at least Yosemite 10.10.3, but better ElCapitan 10.11 or newer .

This version uses a Mac specific Hypervisor : **HyperKit** (based on *xhyve*) .

Docker for Windows

- <https://docs.docker.com/docker-for-windows/>

Requires 64 bit Windows 10 Pro/Enterprise/Student Edition (November update 1511, build at least 10586).

Uses **Hyper-V** on Windows 10.

The last beta version can run both Linux and Windows containers.

QuantumEspresso images

Some **QuantumEspresso** images are available on the standard registry/repository <https://hub.docker.com/r/rinnocente>. You can list them with :

```
$ docker search rinnocente
```

In particular, for QE version 6.0, images available are :

- **rinnocente/qe-full-6.0** : all source/all binaries
- **rinnocente/qe-full-6.0-with-thermo-pw** : qe-full-6.0 + thermo_pw sources and binaries
- **rinnocente/qe-pb-6.0** : only all parallel binaries (good if your b/w is limited)

Only local access allowed :

You can use locally the container without logging in typing :

```
$ docker run -it -u qe rinnocente/qe-full-6.0 /bin/bash
```

in this way you will be inside the container as user `qe` .

Also remote access via ssh :

If you want to access directly the container from outside your machine or you want to share the container with collaborators, then you have to start it in background with a running **sshd** .

You can run the container in background with **sshd** typing :

```
$ CONT=`docker run -P -d -t rinnocente/qe-full-6.0`  
$ PORT=`docker port $CONT 22 |sed -e 's#.*:##`  
$ ssh -p $PORT qe@127.0.0.1
```

Change the password that initially is set to *mammamia* , with the **passwd** command.

More information available at dockerhub : <https://hub.docker.com/r/rinnocente/qe-full-6.0/> or at github <https://github.com/rinnocente/qe-full-6.0>

