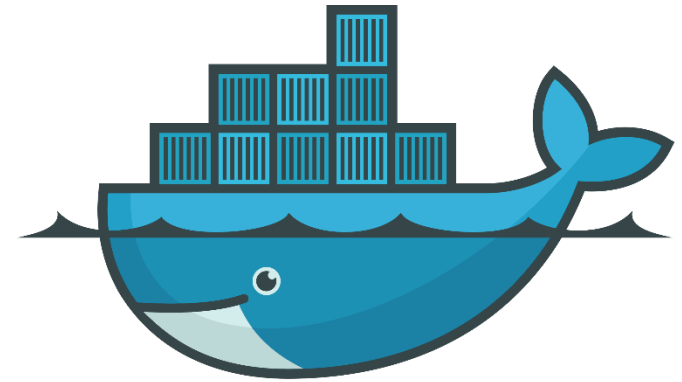
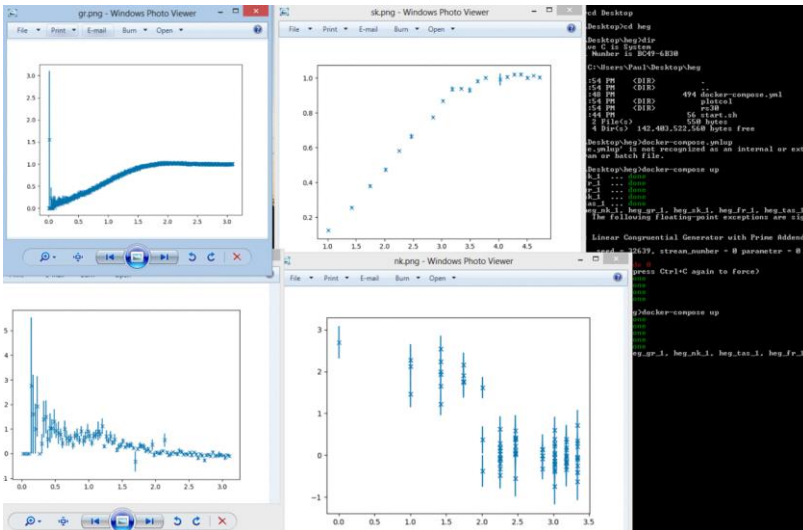


Docker Tutorial

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docker



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[paulyoung2018/harvest_qmcpack](#) ☆

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Dockerfile

```
FROM gcc:8.2.0
RUN apt-get update &&\
    apt-get install -y git &&\
    apt-get install -y libhdf5-dev &&\
    apt-get install -y python-pip
RUN git clone https://github.com/Paul-St-Young/harvest_qmcpack.git
WORKDIR /harvest_qmcpack
RUN pip install -r requirements.txt
ENV PYTHONPATH=/harvest_qmcpack:$PYTHONPATH
CMD pytest -v
```

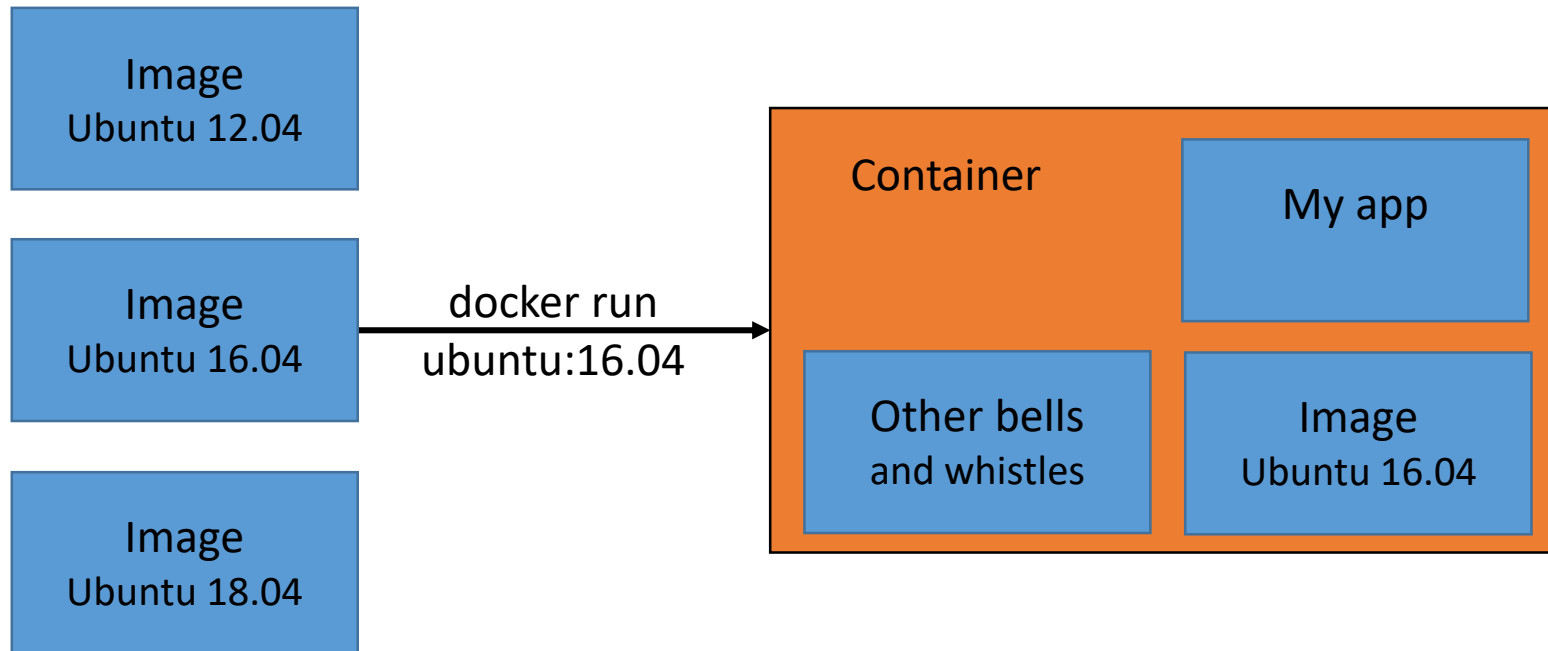
What is Docker?

Docker is *conceptually* a virtual machine **image** manager.

All dependencies are included in a single portable **container**.

Build in layers: modular and extendable.

(Like initial laptop setup. Only minimal, automated, and repeatable.)



Why use Docker?

Docker cleanses us of our **sins** and prepares us for the **heavens**

Photo by
Christopher Burns
on Unsplash

- Break out of dependency hell
- Easy deployment to the cloud



Photo by
Jeremy Perkins
on Unsplash

How to use Docker?

Level 0: Running one container – “docker -i -t -p -v”

Level 1: Building one image – “dockerfile”

Level 2: Modify container and image – “docker exec, commit”

Level 3: Using multiply containers – “docker-compose up”

Level 4: Run your application on the cloud – “docker swarm” & ECS on AWS

Great reference: [PyCon 2016 slides](https://us.pycon.org/2016/site_media/media/tutorial_handouts/DockerSlides.pdf)

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Reference bookmarks

Great reference: [PyCon 2016 slides](https://us.pycon.org/2016/site_media/media/tutorial_handouts/DockerSlides.pdf)

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Level 0: Run one container

Ubuntu base build: “-i” connect to standard-in; “-t” open pseudo terminal

```
docker run -it ubuntu  
# echo “hello from Ubuntu”
```

Web server: “-p” pass host port to container port i.e. [host port]:[container port]

```
docker run -p 200:80 nginx  
firefox localhost:200
```



rgbkrk commented on Mar 23, 2017 • edited ▼

Isolated Dev. Env.: “-v” mounts a local directory

```
docker run -v /soft/myapp/src:/src -it gcc  
# cd /src; make
```

Jo·vy·an

/ˈjōvēən/

noun – an inhabitant of Jupyter

Do Data Science Anywhere:

```
docker run -v /data:/data -p 8888:8888 --name mynb jupyter/datascience-notebook  
firefox localhost:8888/?token=[really long token for security]  
docker cp /data/mybigdata.json mynb:/home/jovyan/work
```

Level 1: Build one container

docker build and tag – [figlet example](#)

p125

Introducing: “dockerfile”

A list of commands to build your image.
(preferably from an official image as base)

```
FROM ubuntu
RUN apt-get update
RUN apt-get install -y figlet
```

Build the image: the natural way

```
docker build .
```

```
docker image ls
```

REPOSITORY	TAG	IMAGE ID	CREATED	SIZE
<none>	<none>	1b402d6bbb5e	About a minute ago	112MB

```
docker tag 1b402 figlet
```

Build the image: the right way

```
docker build -t figlet .
```



Level 1: Build one container

docker build and tag – [figlet example](#)

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Use interactively

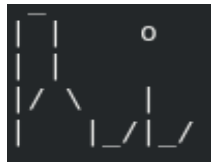
```
docker run -it figlet  
# figlet hello
```



```
FROM ubuntu  
RUN apt-get update  
RUN apt-get install -y figlet
```

Single-purpose application: CMD

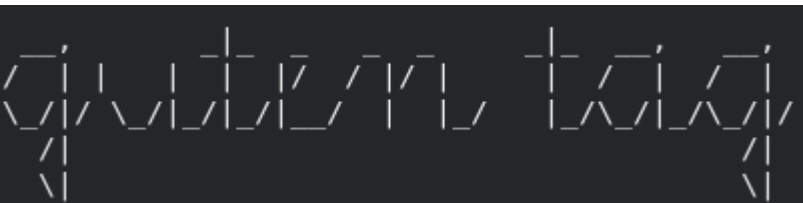
```
docker run figlet override  
docker run figlet figlet -f script hi
```



```
FROM ubuntu  
RUN apt-get update  
RUN apt-get install -y figlet  
CMD figlet hello
```

Multi-purpose application: ENTRYPOINT

```
docker run figlet guten tag
```



```
FROM ubuntu  
RUN apt-get update  
RUN apt-get install -y figlet  
ENTRYPOINT ["figlet", "-f", "script"]
```


Level 1: Build one container

docker build and tag – [figlet example](#)

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Publish container

```
docker tag figlet paulyoung2018/figlet:script
```

```
docker login --user paulyoung2018
```

```
docker push paulyoung2018/figlet:script
```

Tell your friends!

Run from anywhere

```
[not me]$ docker run paulyoung2018/figlet:script wuwuwuwuuut!
```

Pull to update

```
[not me]$ docker pull paulyoung2018/figlet:script
```

Level 2: Modify container and image

Log in to a container: the natural way

```
docker run -it --entrypoint=bash figlet
```

start a bash window in a new container

```
docker ps
```

list all running containers

CONTAINER ID	IMAGE	COMMAND	CREATED	STATUS	PORTS	NAMES
295aa35eaa82	figlet	"bash"	About a minute ago	Up About a minute		

```
docker rename 295aa myfig
```

rename container to something readable

```
docker exec -it myfig bash
```

start a new bash window

Log in to a container: the right way

```
docker run -it --name myfig --entrypoint=bash figlet
```

name container at start

Pop quiz: How to let figlet take a file's content as input?

Level 2: Modify container and image

Pop quiz solution: mount host file; then use bash

```
echo "make me a sandwich" > /tmp/figlet.in  
docker run -v /tmp/figlet.in:/home/figlet.in figlet /bin/bash -c "cat  
/home/figlet.in | sed 's/me/yourself/' | figlet"
```



Modify ENTRYPOINT (-c or --change)

```
docker commit -c 'ENTRYPOINT /bin/bash -c "cat /home/figlet.in | figlet"' myfig
```

sha256:773ec79ad35a17c25b38cabf968c61915d02c605793394aa0d76be38047bd167

```
docker tag 773ec figlet:file
```

Revert modification

```
docker history figlet:file
```

IMAGE	CREATED	CREATED BY	SIZE	COMMENT
773ec79ad35a	4 minutes ago		0B	
ffe572d63dcf	About an hour ago	/bin/sh -c #(nop) ENTRYPOINT ["figlet" "-f"...	0B	
a32c5b019c62	About an hour ago	/bin/sh -c apt-get update && apt-get install...	25.4MB	

```
docker tag ffe572d63dcf figlet:file
```

Level 2: Modify container and image

Publish new image

```
docker tag figlet:file paulyoung2018/figlet:file
```

```
docker push paulyoung2018/figlet:file
```

figlet:file is modified from figlet:script, so most **layers** are reused.

For more best practices regarding dockerfile. See official [docs](#) and

Great reference: [PyCon 2016 slides](#)

https://us.pycon.org/2016/site_media/media/tutorial_handouts/DockerSlides.pdf

write better dockerfile

p272-p296

Level 3: Using multiple containers

Introducing: “docker-compose.yml”

A list of containers and options to run.

Q/ How to do X with docker-compose?

A/ Use bash script and the docker API.

Basic usage 1: put docker API flags down in a file

```
echo “make me a sandwich” > /tmp/figlet.in
```

```
docker run -v /tmp/figlet.in:/home/figlet.in -- name myfig figlet
```



```
version: '3'
services:
  myfig:
    image: paulyoung2018/figlet:file
    volumes:
      - ./test/hello.txt:/home/figlet.in
```

Level 3: Using multiple containers

Basic usage 2: start multiple containers in order

```
version: '3'
services:
  myfig1:
    image: paulyoung2018/figlet:file
    volumes:
      - ./test/world.txt:/home/figlet.in
    depends_on:
      - myfig
  myfig:
    image: paulyoung2018/figlet:file
    volumes:
      - ./test/hello.txt:/home/figlet.in
```

More common useful examples compose:

Communicate between web front end interfaces and backend service

e.g. [website](#), [dockercoin](#), [voting app](#)

Level 4: Deploy applications to the cloud

Docker [swarm](#): takes a cluster of machines and make them look like one big machine.

[Kubernetes](#) (predates docker swarm) is Google's equivalent of docker swarm.

[Elastic Container Services](#) (ECS): scales the number of running containers & Amazon cloud servers based on load. "ecs-cli" is the command line tool.

Practical Example 1: Quantum Monte Carlo + Monitoring

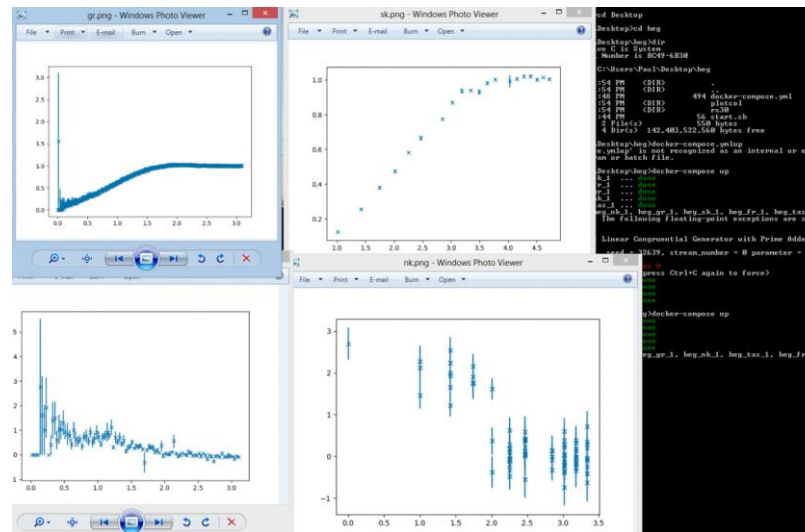
Step 1: compile code

Step 2: make image with reasonable entrypoint

Step 3: write analysis code

Step 4: write docker-compose.yml to orchestrate run and analysis

Step 5: go ham!

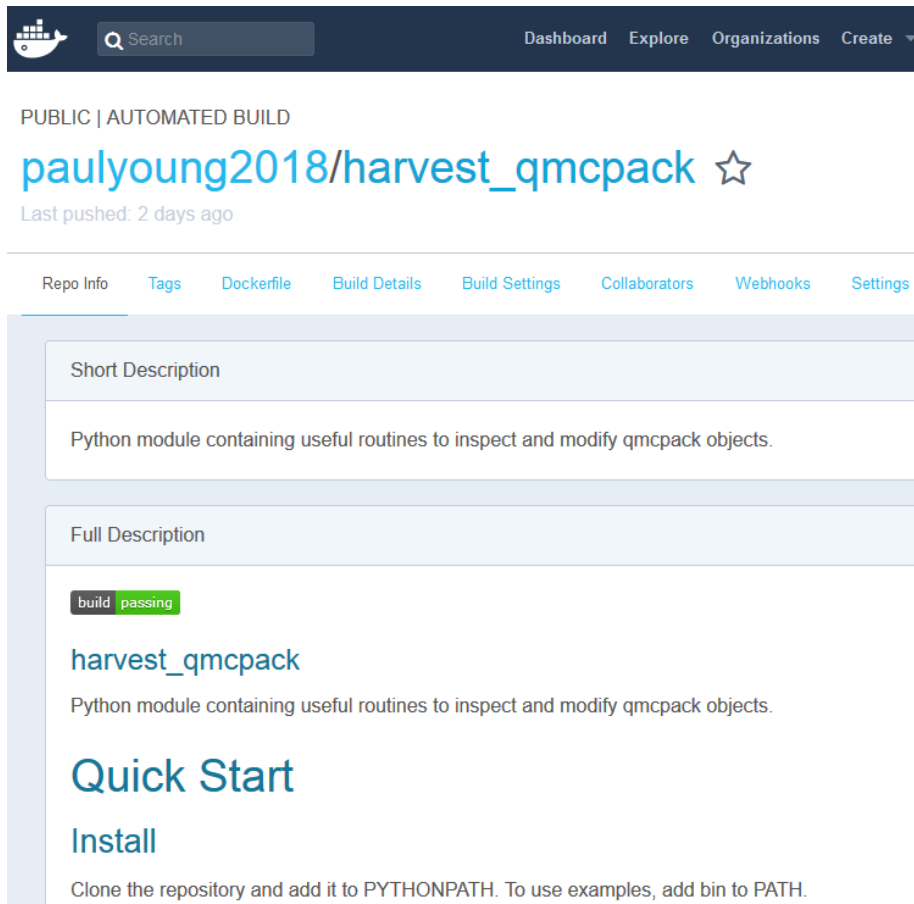


Practical Example 2: Make your GitHub repo. eternal

Step 1: add Dockerfile to your repo

Step 2: sell your soul to Docker Hub

Step 3: wait for your [automatically built image](#)!



The screenshot shows the Docker Hub interface for the repository `paulyoung2018/harvest_qmcpack`. The repository is public and has an automated build. The page includes a search bar, navigation links (Dashboard, Explore, Organizations, Create), and a tabbed interface. The 'Dockerfile' tab is selected, showing the Dockerfile content. Below the Dockerfile, there is a 'Short Description' section with the text 'Python module containing useful routines to inspect and modify qmcpack objects.' and a 'Full Description' section with a 'build passing' status. The 'Quick Start' section is also visible, with a sub-section 'Install' that says 'Clone the repository and add it to PYTHONPATH. To use examples, add bin to PATH.'

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WORKDIR /harvest_qmcpack
RUN pip install -r requirements.txt
ENV PYTHONPATH=/harvest_qmcpack:$PYTHONPATH
CMD pytest -v .
```

Short Description

Python module containing useful routines to inspect and modify qmcpack objects.

Full Description

build passing

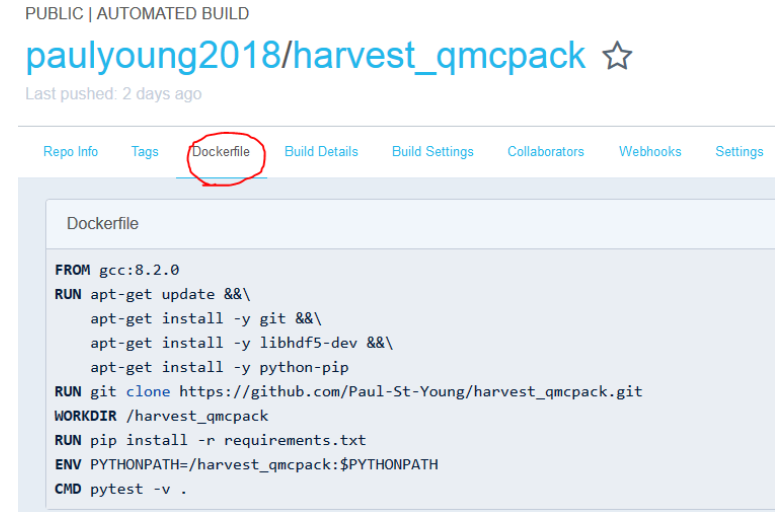
[harvest_qmcpack](#)

Python module containing useful routines to inspect and modify qmcpack objects.

Quick Start

Install

Clone the repository and add it to PYTHONPATH. To use examples, add bin to PATH.



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RUN pip install -r requirements.txt
ENV PYTHONPATH=/harvest_qmcpack:$PYTHONPATH
CMD pytest -v .
```

Last but not least: save your SSD

Docker keeps stopped containers and intermediate images on disk. In English, Moby Dock will gobble up your disk like krill.

Solution is simple:

`docker container prune`

`docker image prune`

All named containers and tagged images will be left alone.

You may wish to do [manual clean up](#) on a production server.

Conclusion:

Docker **container** = *future of* virtual machine instance

Docker **image** = *futher of* virtual machine snapshot

Containerized applications require no setup on any platform.

Growing support on:

- ✓ Amazon Web Service (AWS)
- ✓ Microsoft Azure Cloud
- ✓ Google Cloud (Kubernetes)

□ Run a single container using the docker API

```
docker run -it -p [host port]:[device port] --name me [owner/image:version]
```

□ Manage multiple containers using docker-compose.yml

```
docker-compose up
```

□ Write dockerfile to eternalize your GitHub repo.

□ Modify containers with exec and commit

□ Tag modified containers into images

□ Publish and be forever!