Containers

for

Scientific Computing and Data Science

Tommaso Buvoli

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Common Software Problems



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- No reproducibility across machines or across time.
- Packages end up littering your hard drive for years even after you've completed a project.
- Certain software can also be difficult to install.

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    - You can share containers across teams.

2. **Containers bundle your software dependencies.**

    - No clutter on your local machine.
    - Save your containers online and reuse them at a later date.

A Computer in a Computer

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- Similar in spirit to virtual machines.

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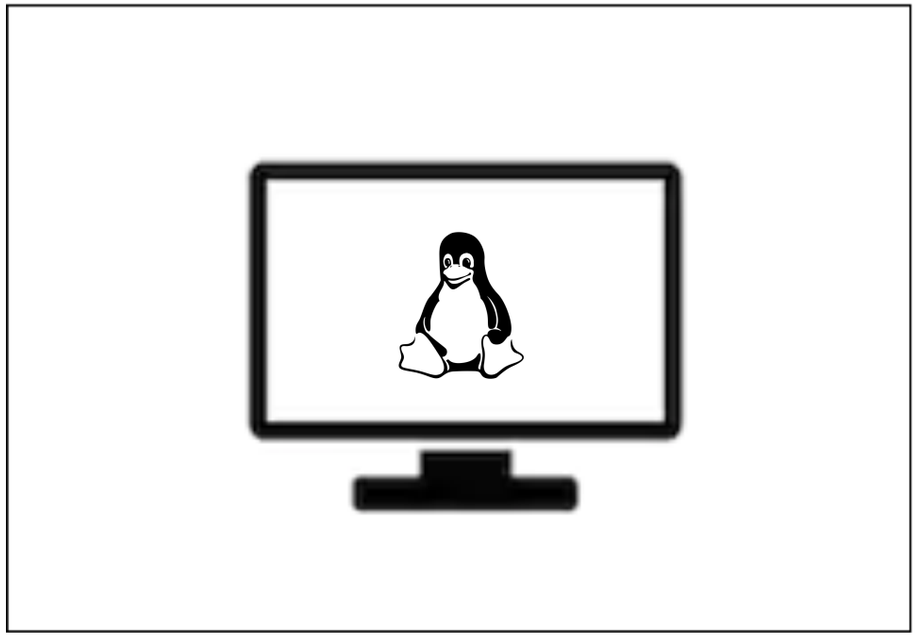
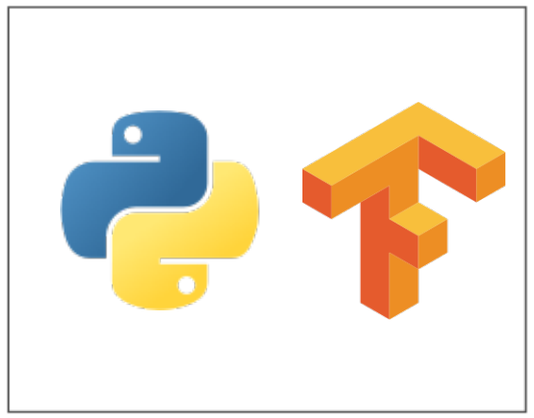
2. A **container** is a collection of processes that run from an image.

    - Multiple containers can be run from the same image.

Containers

Image





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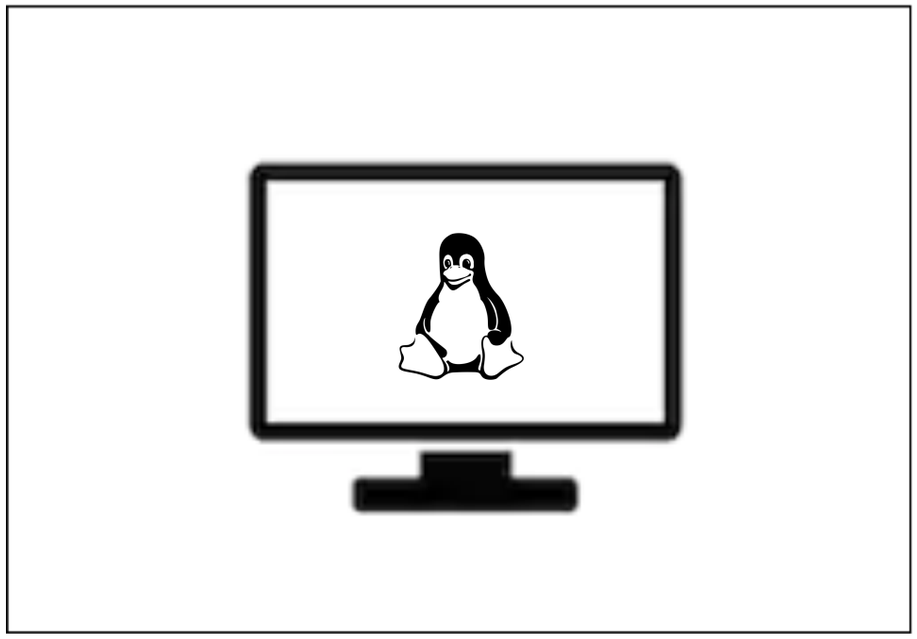

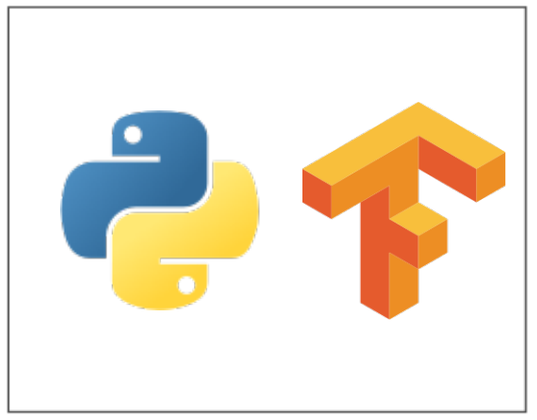

Remark: images are labeled as name:tag (e.g. myimage:v10)

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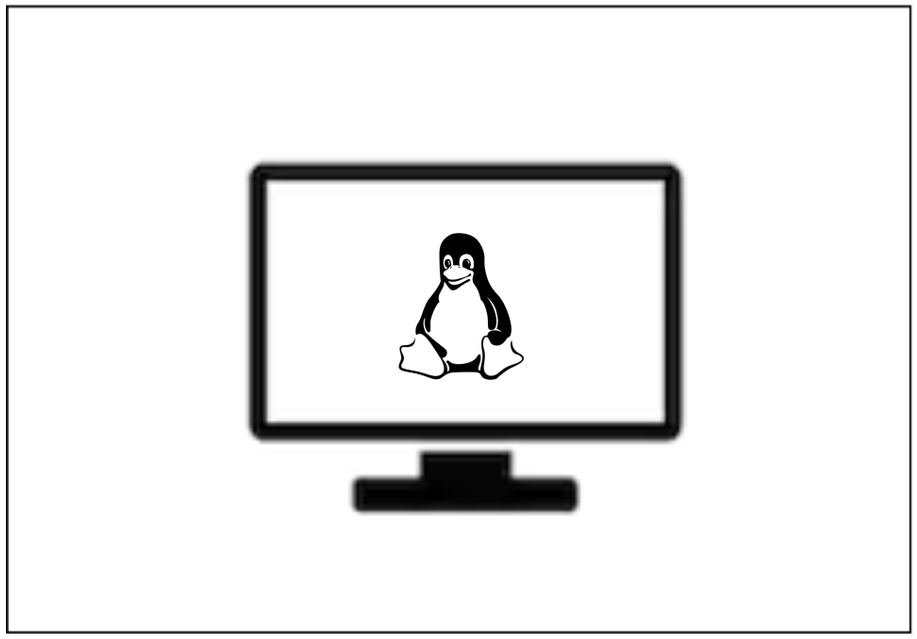

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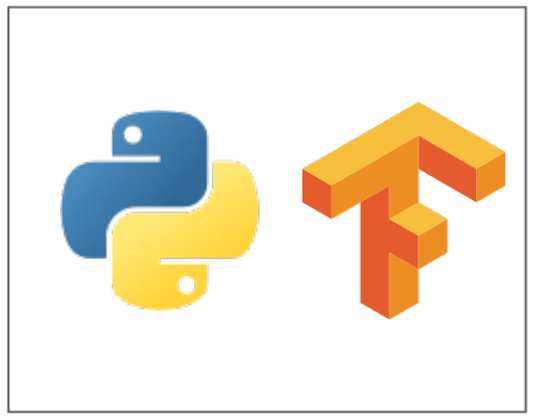
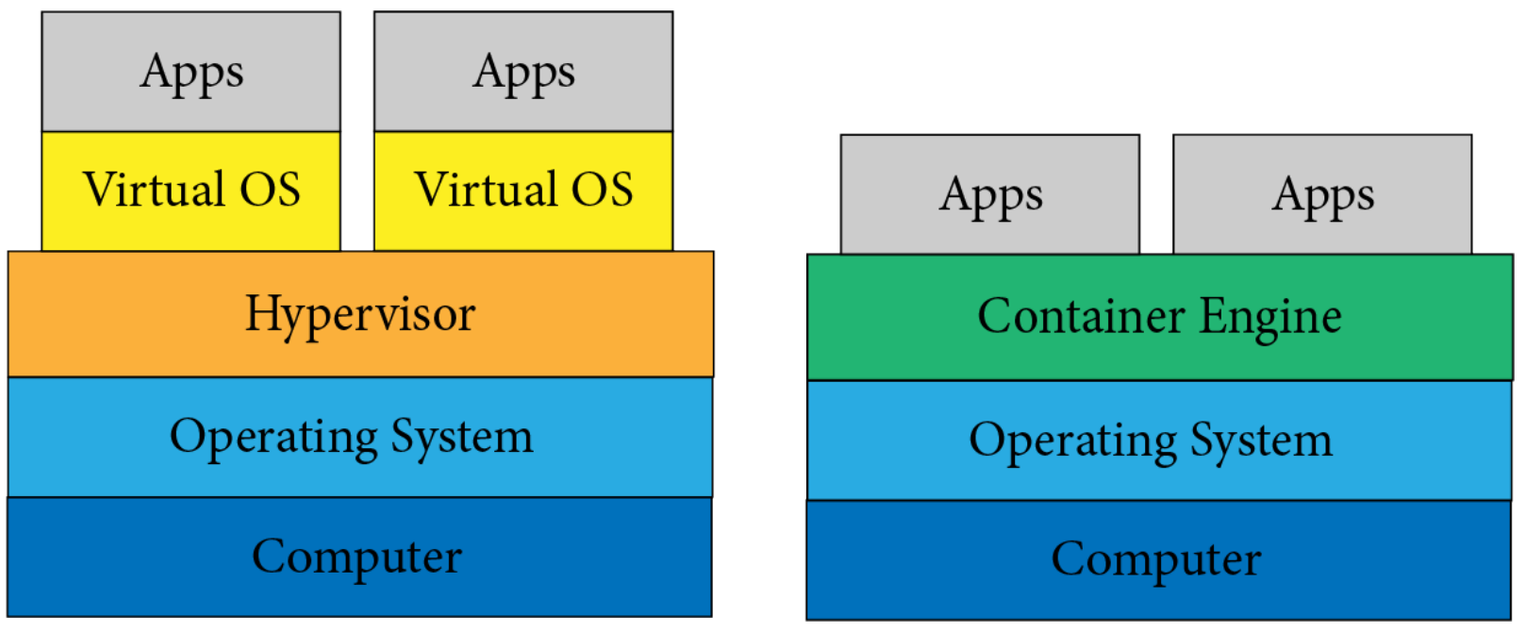


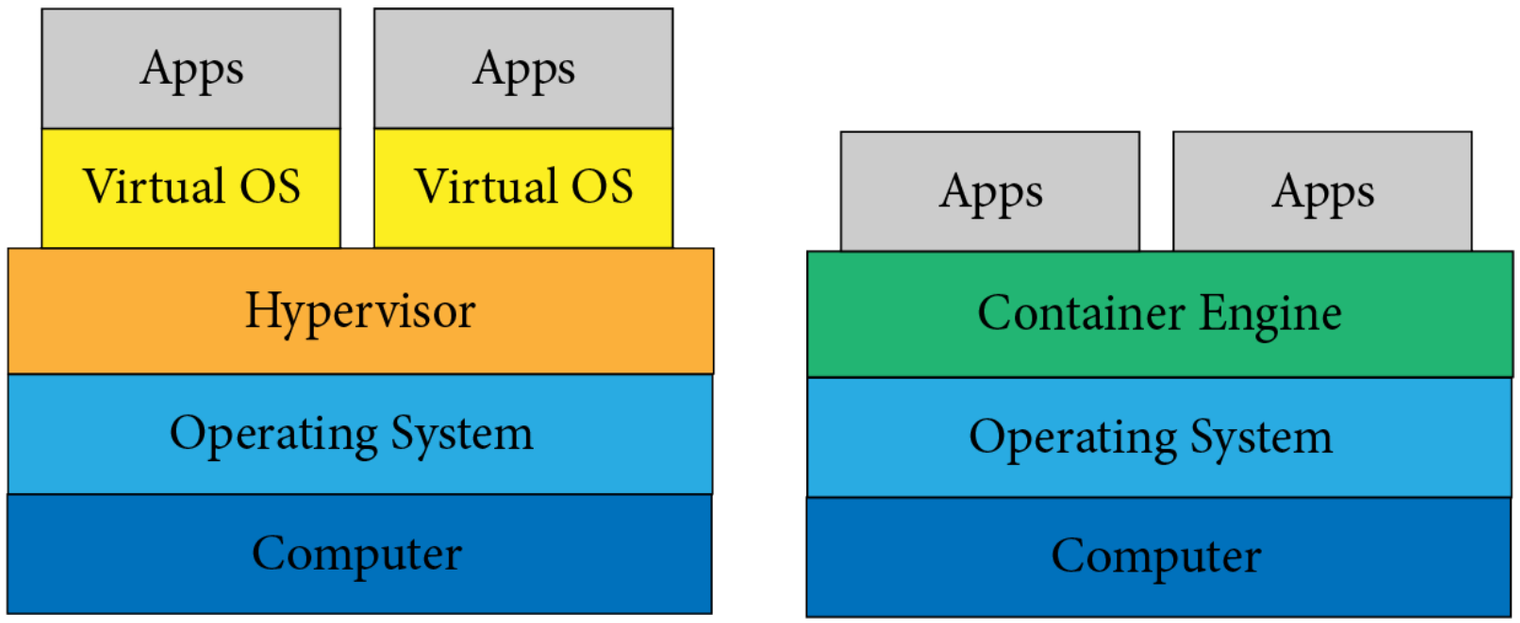
Remark: Containers are ephemeral.The image is never changed.

Containers vs Virtual Machines



Containers vs Virtual Machines

1. Containers are faster to start than virtual machines; no hypervisor, the kernel is shared with host the OS.



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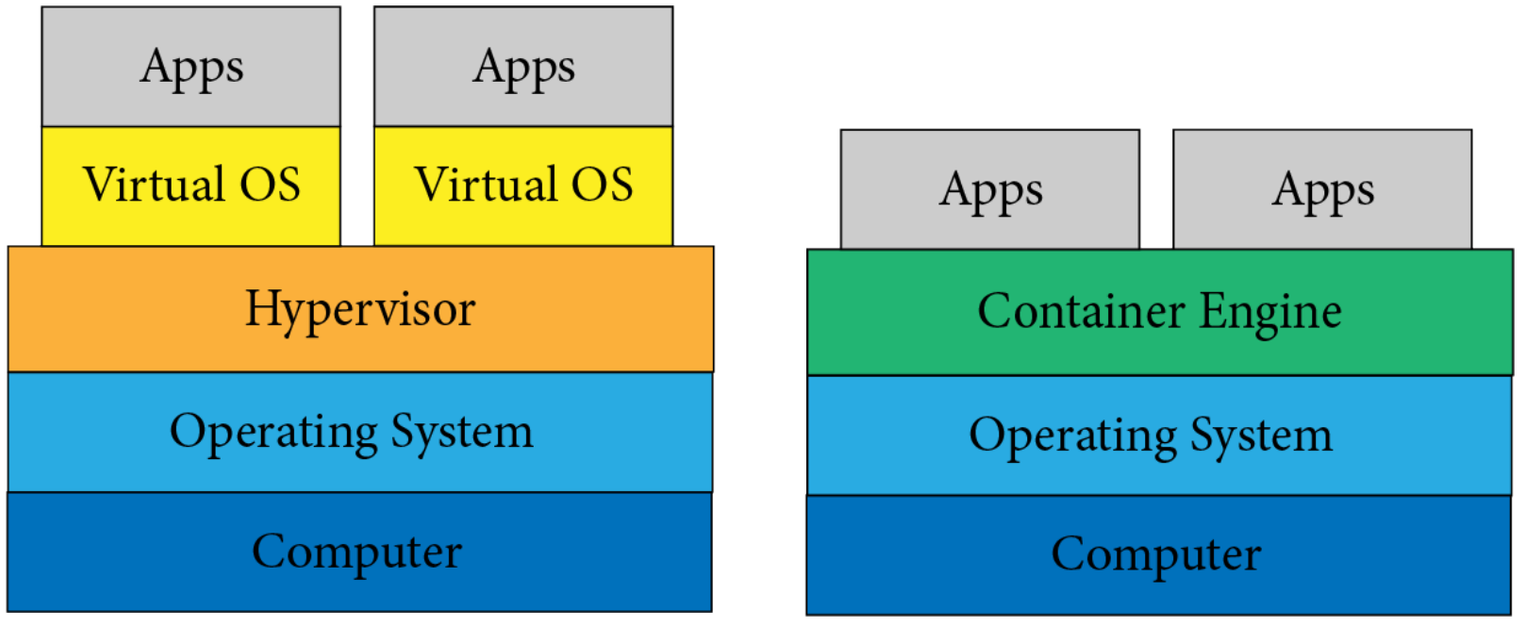
2. It is much simpler to share and distribute container images than VM images.



Three Container Engines

Docker is the most popular container engine and runs on Mac, Windows, and Linux.

Podman is a new, open-source container engine that runs on Linux.

Singularity is a container engine that was designed for HPC systems.

Container Orchestrators

Orchestrators manage multiple containers (advanced topic)

Compose is a simple orchestrator that ships with Docker.

Kubernetes is a much more sophisticated orchestrator aimed at deploying complex containerized apps.

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- Learn how to **build your own container images.**

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You can find a variety of images for:

- **Linux distributions** (e.g. Ubuntu, Fedora, Manjaro, Clear Linux)
- **Programming languages** (e.g. Python, Julia, c, C++, Fortran)
- **Software** (Jupyter Lab, Tensor Flow, Paraview)

```
$ docker pull fedora:latest
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pulls the image named fedora from docker hub onto your local computer

Starting a Container

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- The format for the command is:

```
$ docker run [FLAGS] image:tag command
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https://docs.docker.com/engine/reference/run/

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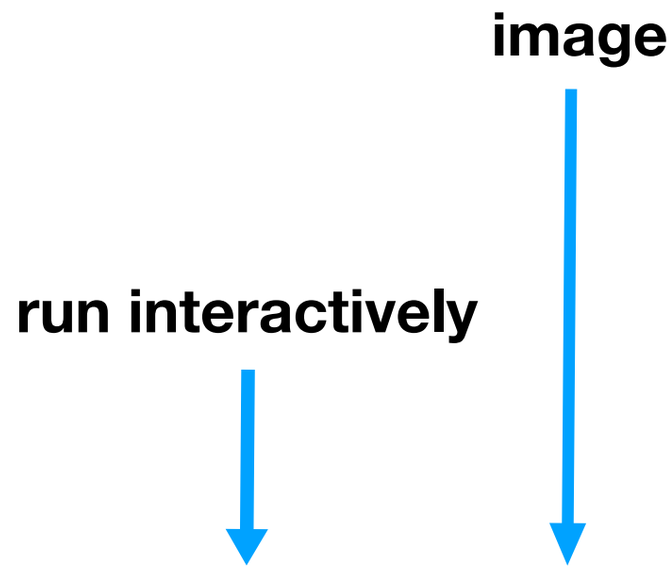


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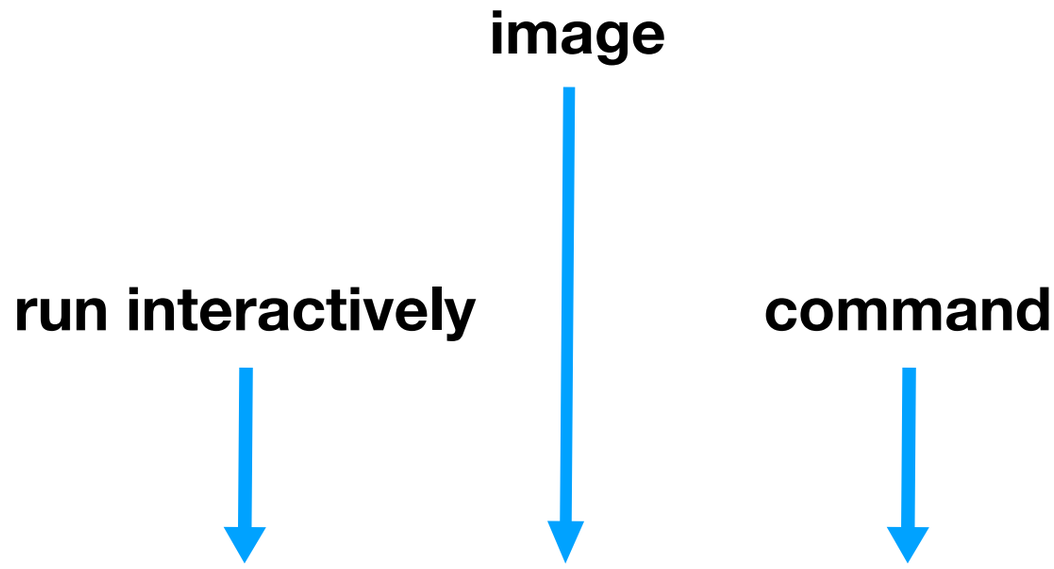
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run interactively
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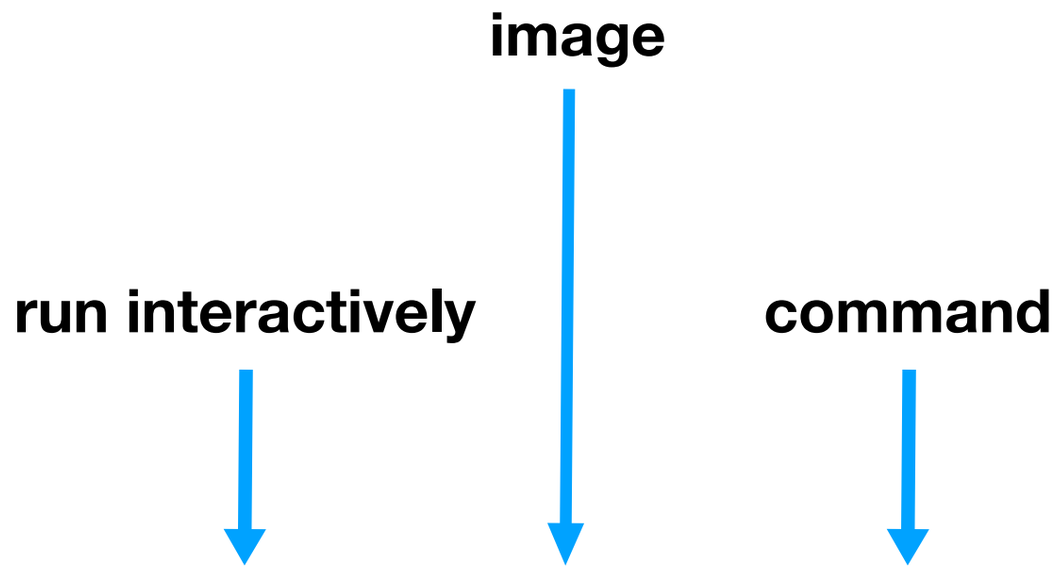


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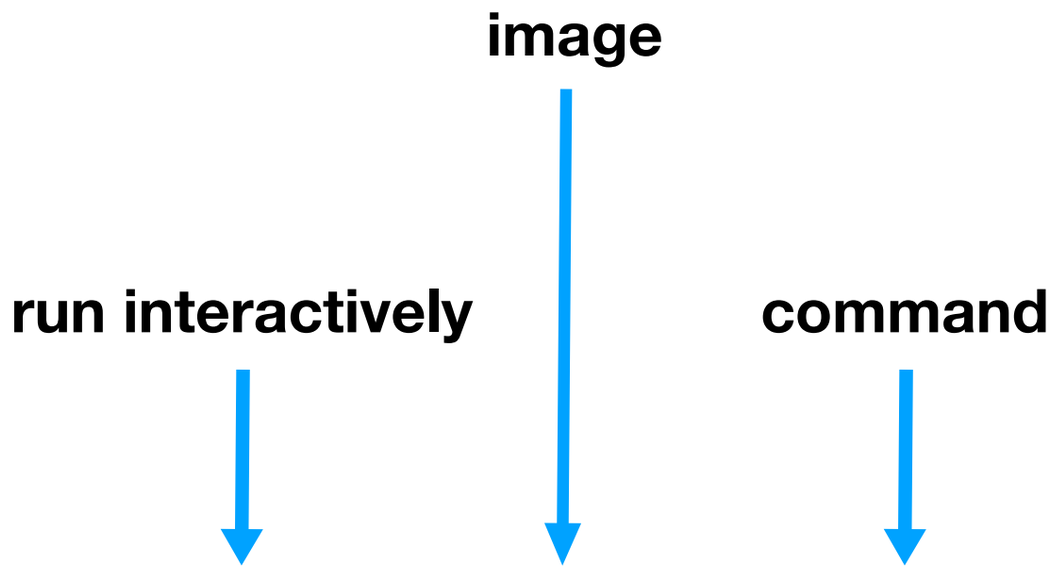
runs the command “bash” interactively using the image fedora:latest



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Let’s verify that containers are ephemeral.

```
$ docker run -ti ubuntu:latest bash
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It’s easy to try new Linux distributions.

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- This mounts the directory */path/on/host* on the **host**
  to */path/on/container* in the **container.**

```
$ docker run -v $(pwd):/files -ti fedora:latest bash
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Let’s try creating a file. It will also be on the host now.

Running Scripts

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We can run a script from inside the container interactively:

```
$ docker run -v "$(pwd)":/files -ti fedora:latest bash
[root@c092da88cd6c] $ python3 /files/hello-world.py
```

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Python does not need to be installed on the host!

Building Custom Images

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- The format for the command is:

```
$ docker build [FLAGS] -t=image:tag .
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https://docs.docker.com/engine/reference/build/

Two Build Commands

- `FROM image:tag`
  Allows you to start from an existing container image.

- `RUN command`
  Runs a command during the image build stage.

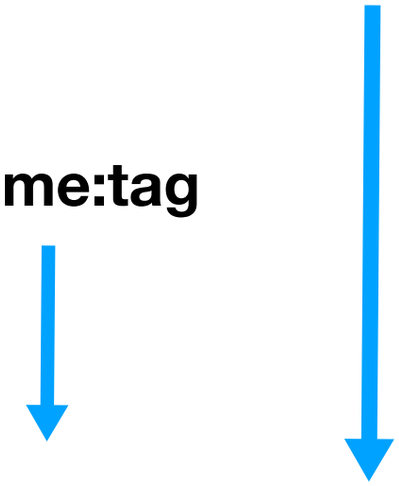
A Very Simple Dockerfile

```
FROM fedora:latest
RUN dnf -y install pip
```

```
# Starts from fedora image
# install pip
```

The build context; must contain the Dockerfile.

The image name:tag



```
$ docker build -t myfedora:pip .
```

this command will build the image specified by the Dockerfile in the cwd

Let’s discuss layers while our image builds.

Layers

Each line in a Dockerfile creates a new *layer*.

If you don't use the `--no-cache` flag when building, then previously computed layers will be reused.

```
FROM fedora:latest                  # starts from fedora image
RUN dnf -y install pip              # install pip
RUN pip install matplotlib          # install matplotlib
```

Let's try running an interactive bash session in our new image.

Additional Useful Docker Commands

Container Management

- Stop a container: `docker stop ID`
- Remove a container: `docker rm ID`
- List running a container: `docker ps`

Image Management

- Push an image to Dockerhub: `docker push image:tag`
- Remove an Image: `docker rmi image:tag`

Documentation

https://docs.docker.com/engine/reference/commandline/docker/

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- This is not a simple command.
- Using Docker Compose, we can encode this into a file.
- We can run the whole command with `docker-compose run`.

A Simple Compose File

docker-compose.yml

```
version: "3.8"
services:
  bash:
    image: myfedora:pip
    volumes:
       - .:/root/files
    command: bash
```

$ docker-compose run bash

If you find containers interesting…
Here is an even simpler tool

container job runner - a simple way to develop and run code in containers.

Local Development

```
$ cjr shell --here                    # start an interactive shell in local directory
$ cjr jupyter:start                   # start Jupyter Lab or notebook
```

Jobs

```
$ cjr job:start --resource=my-server  python myscript.py      # run remote job
$ cjr job:start --resource=localhost  python myscript.py      # run local job
```

website: https://container-job-runner.github.io/ **github:** https://github.com/container-job-runner/cjr

Thanks for your attention!