



Introduction to Containers for Data Science and Data Engineering



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<https://github.com/mafudge/odsc24>

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Part 1: Container Essentials

Important concepts for understanding containers and docker

Rationale

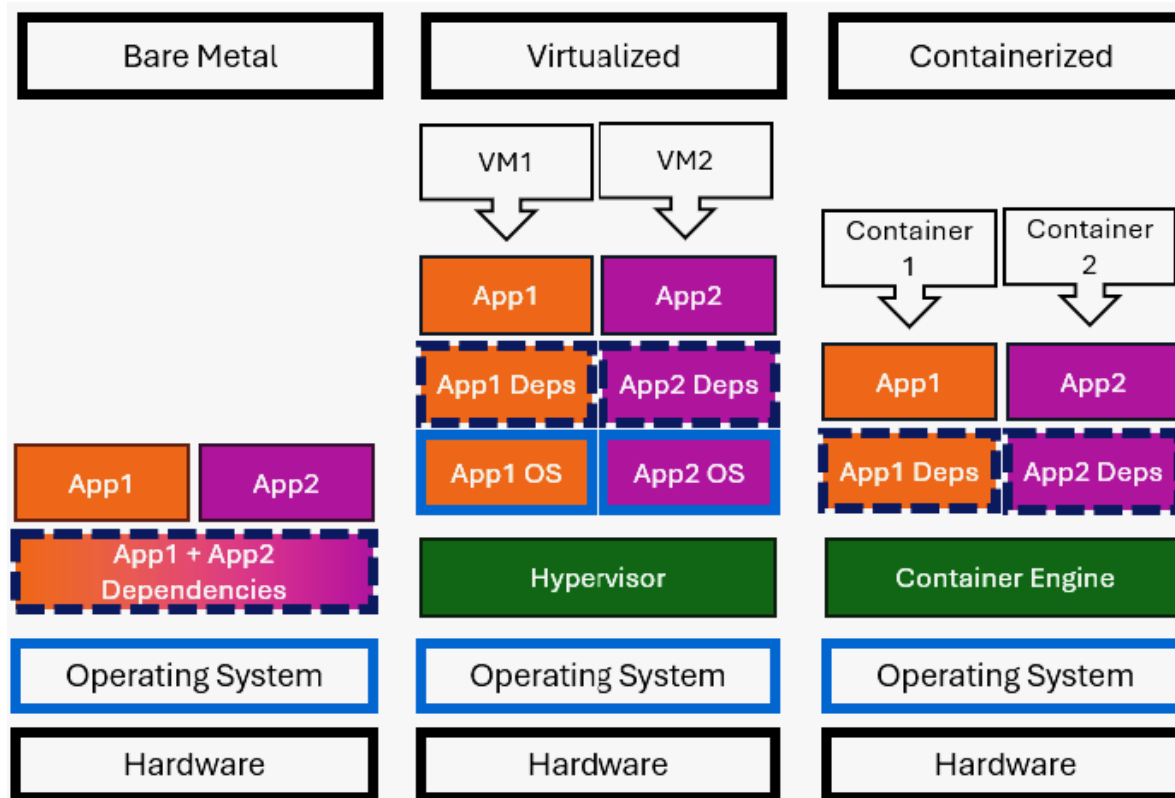
Have you ever:

- Worked on a project on more than one computer?
- Shared a project with a team?
- Said this: “but it works on my machine...”
- Spent hours trying to deploy your project live?
- If so, then containers are for YOU!

What is a container?

- A container is a form of virtualization.
- Containers virtualize the application and its dependencies.
- The virtualization occurs closer to the application than the hardware.

Containers, Virtualization, Bare Metal



Benefits of Containers

- **Reproducibility of work** - drastically minimizes “but it works on my machine”.
- Bundle the dependencies with your application.
- Can mimic complex environments with external systems.
- When combined with a git workflow, it can be team and cloud friendly.

Container Terminolog

- **Image** application + dependencies at rest, consumes disk
- **Tag** the version / release name of the image
- **Container** running image: consumes disk + RAM/CPU/Network
- **Port** expose a TCP/UDP Port outside the container
- **Volume** persistent storage for a container

Our first container

- It always starts with a need...
- Hmm. I'd like to use: <https://jupyter.org/install>
- Rather than install all those dependencies on your computer, run it in a container!
- Portability! Reproducibility!

Dockerhub: finding images

- Dockerhub is an example of a container registry.
<https://hub.docker.com>
- A catalog of container images in the cloud!
- <https://hub.docker.com/search?q=jupyter%2Fminimal-notebook>
- Red Hat's Quay.io is another:
<https://quay.io/repository/jupyter/minimal-notebook>

Demo 1: Pulling an image



- Pulling images
 - From Dockerhub
 - From Another public Image repository
- Viewing downloaded images

Demo 1: Summary of Commands

What	Command	Example
Download image from Docker registry	<code>docker pull <image>:<tag></code>	<code>docker pull jupyter/minimal-notebook:lab-4.1.6</code>
Download image from Another public registry	<code>docker pull <reg>/<image>:<tag></code>	<code>docker pull quay.io/jupyter/minimal-notebook:lab-4.1.6</code>
View downloaded images + tags	<code>docker images</code>	<code>docker images</code>
Delete an image	<code>docker image rm <image>:<tag></code>	

Running an image as a container

- To run the image:
`docker run --name <containername> -d <image>:<tag>`
- `--name` give the container a name.
- `-d` run in the background, return to the console.

Demo 2: Containers!



- Run the container
- See running containers
- View logs of running container
- Stop a running container
- See all containers (running and stopped)
- Delete container definition

Demo 2: Summary of Commands

What	Command	Example
Run a container	<code>docker run --name <container> -d <name>:<tag></code>	<code>docker run --name jupyter -d jupyter/minimal-notebook:lab-4.1.6</code>
List running containers	<code>docker ps</code>	<code>docker ps</code>
View output of running container	<code>docker logs <name></code>	<code>docker logs jupyter</code>
Stop a running container	<code>docker stop <name></code>	<code>docker stop jupyter</code>
List all containers (running and stopped)	<code>docker ps -a</code>	<code>docker ps -a</code>
Delete a container	<code>docker rm <name></code>	<code>docker rm jupyter</code>

Publishing TCP/UDP Ports

- What good is running an application in a container if you cannot access it?
- When the container is created, we must publish the exposed the port:
 - p published-port:exposed-port or
 - p OUTSIDE:INSIDE
- When you publish a port, you can connect to exposed application services on the published port.
- For example, if 8888 is published, then <http://localhost:8888>

Demo 3: Ports



- Run the container, exposing 8888
- See the port is exposed
- Visit <http://localhost:8888>
- Find the key in the container output!
- Login to the application!

Demo 3: Summary of Commands

What	Command	Example
Run a container and expose ports	<code>docker run --name <container> -p <pub>:<exp> -d <name>:<tag></code>	<code>docker run --name jupyter -p 8888:8888 -d quay.io/jupyter/minimal- notebook:lab-4.1.6</code>

Need for volumes

- Containers are ephemeral. Only what is in the image is retained between subsequent runs.
- When you `docker rm` the changes are gone!
- How does one save changes? Volumes!
 - v `host:image` or
 - v `OUTSIDE:INSIDE`

Demo 4: Volumes



- In the running container save a file.
- Stop and remove the container
- Re-run the container
- Check back into the App... file is gone. Ephemeral.
- Stop and remove the container... again
- Check out that local work folder
- Mount that folder as a container volume
- Stop and remove the container... last time

Demo 4: Summary of Commands

What	Command	Example
Run a container and expose ports and a volume	<code>docker run --name <container> -p <pub>:<exp> -d <name>:<tag></code>	<code>docker run --name jupyter -p 8888:8888 -v \$PWD/work:/home/jovyan/work -d quay.io/jupyter/minimal-notebook:lab-4.1.6</code>
List running containers	<code>docker stop jupyter && docker rm jupyter</code>	<code>docker stop jupyter && docker rm jupyter</code>

Orchestration with Docker Compose

- Docker compose allows you to manage containers through a configuration file, in `yaml` format.
- Makes Starting and Stopping containers easier.
- Infrastructure as code:
 - Clear separate of Configuration –vs- Commands

Docker vs Docker Compose

Command

```
$ docker run  
  --name jupyter  
  -p 8888:8888  
  -v $PWD/work:/home/jovyan/work  
  -e JUPYTER_TOKEN=osdc  
  quay.io/jupyter/minimal-  
  notebook:lab-4.1.6
```

Configuration file

```
version: "3"  
services:  
  jupyter:  
    ports:  
      - 8888:8888  
    volumes:  
      - ./work:/home/jovyan/work  
    environment:  
      - JUPYTER_TOKEN=osdc  
    image: quay.io/jupyter/minimal-  
    notebook:lab-4.1.6
```

Demo 5: Docker Compose

- Start with docker compose
- View running containers
- Stop with docker compose



Demo 5: Summary of Commands

What	Command	Example
Build the configuration and start the container(s)	<code>docker compose -f <file> up -d</code>	<code>docker compose -f jupyter.yaml up -d</code>
List running containers from the configuration	<code>docker compose -f <file> ps</code>	<code>docker compose -d jupyter.yaml ps</code>
Stop the running containers and remove them	<code>docker compose -f <file> down</code>	<code>docker compose -d jupyter.yaml down</code>



Part 2: Development with Containers

Containerizing your development pipeline

Simple Python ETL Pipeline

- Simple data Pipeline: read file, transform it, write another file
- Open part2 folder in Visual Studio Code.
- Open a terminal in the part2 folder



Dockerfile: Building your own image

- `Dockerfile` explains how to build an image
- `FROM` is the base image from a public image repository
- `COPY` copies files into the image
- `RUN` executes a command in the image
- `ENTRYPOINT` defines the default command from `docker run` or `docker compose up`

Demo 6: Building A Custom Image



- Look at the Dockerfile. No data... just code!
- Look at the docker-compose.yaml File.
Data in volumes.
- Build the Image with docker compose
 - Note we don't need -f here.
- What is the image name?
- Run the application with docker compose

Demo 6: Summary of Commands

What	Command	Example
Build an image using the docker-compose file	<code>docker compose -f <file> build</code>	<code>docker compose build</code>
View images created by docker compose file	<code>docker compose -f <file> images</code>	<code>docker compose images</code>
View images with docker	<code>docker images</code>	<code>docker images</code>
Run the application	<code>docker compose -f <file> up</code>	<code>docker compose up</code>
Remove the container definitions	<code>docker-compose -f <file> down</code>	<code>docker compose down</code>

Useful, but not Realistic: Enter Dev Containers

- This is a useful way to run your working programs
- It is impracticable to implement a dev-loop this way:
write → run → debug...
- Enter the Visual Studio Code dev containers!
- `devcontainer.json` points to an image with code + debugger
- You are coding inside a running container!
- Current folder is mounted as a volume!

Demo 7: VS Code Dev Containers



- Open `part2` in a dev container. It is building.
- Look at the `devcontainer.json`.
- Run code in container
- Set a breakpoint and debug!

Demo 7: Summary of Commands

What	Command
Open a Dev Container in VS Code	Open folder >< Remote window Reopen in container Dev Container builds
Run code in Dev Container	[F5]
Set a breakpoint	[F9]
Rebuild a dev container (if you add a new dependency, for example)	>< Remote Window Rebuild Container



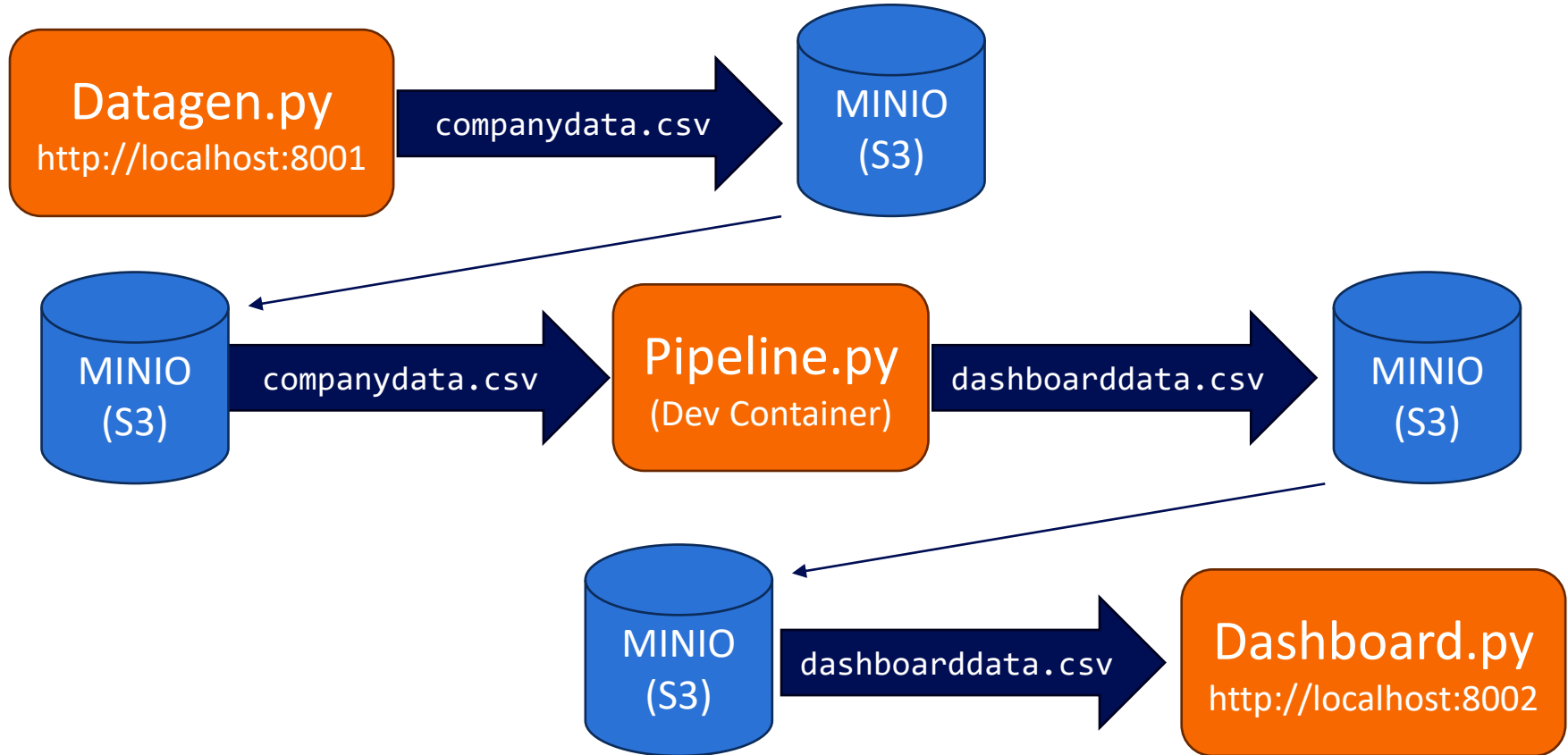
Part 3: Development with Containers and Other Container Dependencies

Use Docker Compose to orchestrate dependencies in your application

Overview of final pipeline

- Real world pipelines require many parts.
 - They read from/write to databases, for example.
 - Loosely coupled / No direct dependencies.
- Open `part3` folder in Visual Studio Code.
- This example uses `docker-compose.yml` with the dev container.
 - There are other containers used in this pipeline which demonstrate typical complexity.

Diagram of the pipeline



Demo 8: Complex Pipeline



- Open in Dev Container and build.
 - Look at all the running containers!
- Run `pipeline2.py`, Datagen <http://localhost:8001>, and Dashboard <http://localhost:8002>
- Watch the data update.
- Look at the `devcontainer.json`. Two docker-compose files.



Wrap-Up!

Summary

- Containers virtualize our applications,
 - bundling the dependencies with the app.
- Find images for your containers on repositories
 - docker hub and quay.io
- You can manage multiple containers with docker-compose and separate the configuration from the commands
- Write code inside containers with VS Code dev containers!
- Dev containers support docker compose for complex setups!

But Wait... There's more!

- How about a containerized Spark cluster With a Jupyter front-end and Minio storage?

<https://github.com/mafudge/docker-spark-cluster>

- Query your CSV/Excel files with SQL. Drop and go!

<https://github.com/mafudge/local-file-drill>

- Chat with your PDF file, 100% on device using llama2 (dev container example)

<https://github.com/mafudge/chat-pdf>

Cleaning up

- You might want to reclaim some disk space after the talk
- `docker system prune --all --volumes`

.....

Thank you For Attending!

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