Lecture 11:

Containerization

> Tomáš Báča

Containerization

BECM33MLE — Machine Learning Engineering

Dr. Tomáš Báča

Multi-Robot Systems group, Faculty of Electrical Engineering Czech Technical University in Prague









Why containers?

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Motivation

Docker

Manageme tools

Lazydock Portainer

Orchestrat

Apptaine

...

Reference

A solution to the dependency hell

When you need to run 2 apps with conflicting dependencies.

A solution to isolation

When you need to run two apps that might conflict on networking, file system or runtime level.

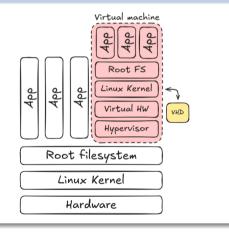
A solution to portability

Being able to share the whole system as well as a *prescription* for its installation.

Comparison to Virtual Machines (VMs)

The other extreme: complete isolation (almost hardware-like)

Virtual machines



Why containers?

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Motivation

A solution to the dependency hell

When you need to run 2 apps with conflicting dependencies.

A solution to isolation

When you need to run two apps that might conflict on networking, file system or runtime level.

A solution to portability

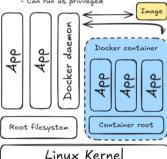
Being able to share the whole system as well as a prescription for its installation.

Comparison to Virtual Machines (VMs)

The other extreme: complete isolation (almost hardware-like)

Container system

- Complete namespace separation - Can run as privileged



Hardware

Core concepts

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Image

Layered file system with runtime, libraries, application code and configuration.

Container

A running instance of the software *spawned* from an image.

Networking

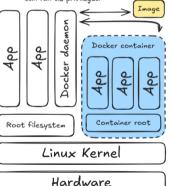
Containers connect by virtual network adapters.

Registries

Image are shared through registries where they are visioned and tagged.

Container system

- Complete namespace separation
- Can run as privileged



Docker — Architecture

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Docker

Docker client

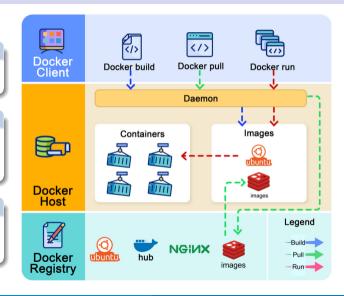
- user interaction
- control of the host

Docker daemon

- executes the image builds
- creates the runtime processes
- stores images locally

Docker registry

- analogue to git repository
- often hosted in cloud, can be local



Docker — Workflow

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References

1. Initial app development

- can happen natively (rare), or
- can already start with Docker in mind

2. Docker image build

- isolation of dependencies
- recipe for minimal image

3. Testing and development

- preparation of runtime instructions
- proparation of familiar modulation.
- recipe for minimal image

4. Orchestration

preparation of deployment

```
FROM alpine

ENV PYTHONUNBUFFERED=1

RUN apk add --update --no-cache python3 && ln -sf python3 /usr/bin/python

RUN ...

RUN ...

COPY my_script.py /

CMD ["python3", "-u", "/my_script.py"]
```

Figure 1: Illustration of a Dockerfile. See the lecture attachment for practical example.

Docker — Practical details

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Арреание

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Towards repeatability

• Containerizing your own work increases the chance that it will work not just on your own machine.

Minor points

- You can run linux-based docker containers on all major platfoms, but Windows and Mac virtualize the Kernel
- the current host's USER can be emulated but he needs to created during the image build phase
- GUI can piped from the containers xserver to the host's xserver
- you can connect to remote docker host by exporting DOCKER_HOST
- docker can be used completely offline:
 - images can be transport as '.tar'
 - images can be transport through self-hosted registry.
- images can be built as multi-platform (or for specific platform only)
 - the cross-platform build runs in QEMU

Docker compose

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Native Docker CLI interface

Not intended for normal daily use by people.

Docker compose

- well-organizable sessions
- yaml definition file
- containers aliased as services
- shared resources:
 - networks, volumes
- inter-service dependencies
- fine-grained control over
 - port forwarding
 - folder (volume) mounting
 - environment
 - container behavior

```
wolumee.
       db data:
     networks:
       frontend:
       backend:
     services:
9
10
11
         image: postgres:16-alpine
          volumes:
            - db data:/db/data
14
         restart: unless-stopped
          networks.
            - backend
18
       web.
10
20
            - "8000:8000"
         depends on:
         restart: unless-stopped
24
          networke.
25
            - frontend
26
            - hackend
```

Figure 2: Illustration of a compose file. See the lecture attachment for practical example.

Docker — devcontainers [1]

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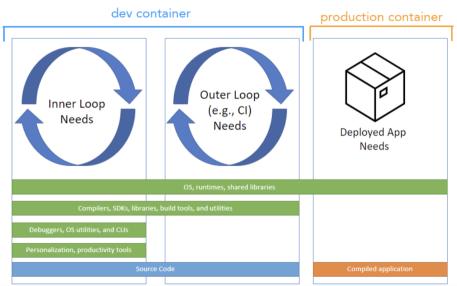
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References



Tomáš Báča (CTU in Prague) Lecture 11: Containerization December 9th, 2025

Lazydocker — container management in TUI

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Арреание

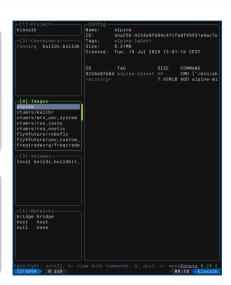
References

Lazydocker [2]

- TUI for local Docker management
 - (directly connecting to the Docker Host)
 - The brother of Lazygit
- image management
- container management
- volume management
- structured stdout visualization

Sidenote: use the right tool for the job

- Lazydocker, is not for everyone, but it can be the right tool for the job at a very specific time in your development, e.g., in the local testing phase.
- Aiming at the most ultimate tool for the job (unless you already know it) can be the wrong thing to do at the beginning of the project.



Portainer.io — "GUI for docker", [3]

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Universal UI for containers

- handles local, remote, Docker and Kubernetes
- Fine-grained access control

Portainer Community Edition

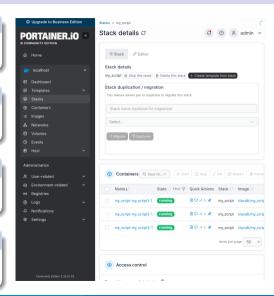
- Free, open source
- https://docs.portainer.io/start/install-ce

Portainer Agent (Docker API

- Connects to Docker host
- Thin, no UI, stateless

Portainer Server (UI)

- Connects to agents (or Docker host)
- Stores stacks per agent



Orchestration

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Orchestration

- health management of containers on a cluster
 - no program is 100% robust and reliable
 - downtime of containers is natural and it should be monitored and managed
- automatic load balancing using user-defined metric:
 - CPU load, memory usage, API request rate, etc.

Docker Swarm [4]

- orchestration built-in Docker
- automatic health monitoring
- automatic load-balancing
- automatic network management
 - Nodes get a dynamic hostname and ports
 - Nodes get the trafic routed automatically

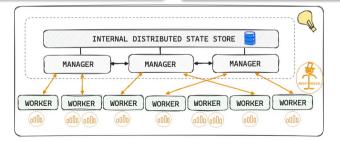


Figure 3: Source: [4]

Apptainer [5] — Motivation

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References

Docker's problems

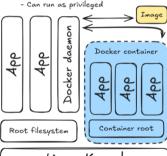
- Privileged execution
 - user can do "anything"
 - The existence of the daemon
 - centralized management of images
- sometimes the isolation is too good
 - the user inside is not the user outside

Apptainer's solution

- container as a user process
- images as single files
- integration over isolation
 - sits on top of the host's network stack, name resolution, /dev, \$HOME, user
 - GPU and hardware support
 - integrates well with HPC systems

Docker

- Complete namespace separation



Linux Kernel

Hardware

Apptainer [5] — Motivation

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Docker's problems

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 - user can do "anything"
- The existence of the daemon
 - centralized management of images
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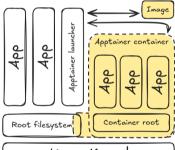
Apptainer's solution

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Apptainer







Linux Kernel

Hardware

Concepts

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Image recipe

- Can bootstrap from Docker image
- Can bootstrap from another Apptainer image

Image file

- *.sif Single Image File
- No local cash image cache
- Not layered images like Docker's
- Can be sandboxed
 - mutable by the user in runtime
 - can be packed back as an image
- Optional writable overlay

Runtime

 user spawns the process directly using an Apptainer's launcher system

Apptainer vs. Singularity

- Singularity used to be developed privately by Sylabs
 - SingularityCE (community Edition)
 - SingularityPro
- Apptainer developed by Linux Foundation
 - open source
 - backwards-compatible with the old Singularity

Practical comments

- similarly to Docker, the native CLI of Apptainer is not very pleasant
 - wrapping in custom scripts is usually beneficial

Apptainer — Workflow

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Usecase 1: sharing academic software

- preparing an image with a recipe or sandbox
- user is someone else than the creator

Usecase 2: "as a VM"

- long-term development of an obscure software
- starts by a recipe, ends with a sandbox

Usecase 3: as intended for HPC

- preparing an image with a recipe
- shipping the image to a cluster and computing

```
Bootstrap: docker
   From: ubuntu:20.04
   %post
        # location for the apptainer files
        touch /some file.txt
   %environment
        export CUSTOM ENV VAR=value
   %runscript
     CMD = "${@}"
14
     if [ -z "${CMD}" ]: then
        /bin/sh --login
     else
18
        /bin/sh --login -c "${CMD}"
20
     fi
     exit 0
```

Figure 4: An Illustration of an Apptainer recipe. See the lecture attachment for practical example.

Nix — (maybe) future solution to dependency hell

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Traditional dependency management (deb packaging system)

- you are expected to always update to the latest combination of stable versions
- versions are not encoded in dependencies
 - only version inequality constraints
 - only for a check.. the installer is not forced to install anything else than the latest version
- installing older versions is not supported
 - this leads to compilation from sources, but what if that needs older versions of dependencies?
 - To quote a famous Jedi: "Not updating is the path to the dark side, it leads to anger. Anger leads to hate. Hate leads to suffering".

Nix (https://nixos.org/)

- atomic and 100% replicable builds
 - the build should not rely on anything but static sources and Nix dependencies.
- build artifacts marked by hashes composed of:
 - source paths (and their hashes)
 - build dependencies (and their hashes)
 - svstem's hash
 - builder and build arguments
- two libyaml-1.0.0 can have different hash and can be installed simultaneously
- multiple instance of the library can be installed at once (even the same numeric version)
- dependencies can be encoded by hash
- [6] E. Dolstra, A. Löh, and N. Pierron, "Nixos: A purely functional linux distribution," *Journal of Functional Programming*, vol. 20, no. 5-6, pp. 577–615, 2010

Demos

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Kelerences

Prerequisities

- Install Docker
 - https://docs.docker.com/desktop/
- Install Apptainer
 - https://apptainer.org/docs/admin/main/installation.html

How to run

 ${\bf Example\ scripts\ are\ located\ in\ lecture\ attachment:\ {\tt scripts.zip}.}$

References I

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References

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- [3] Portainer, https://github.com/portainer/portainer, Accessed: 2025-12-09.
- [4] Docker swarm an indepth introduction, https://mesutoezdil.medium.com/docker-swarm-6efa43f7b68d, Accessed: 2025-12-09.
- [5] Apptainer, https://apptainer.org/, Accessed: 2025-12-09.
- [6] E. Dolstra, A. Löh, and N. Pierron, "Nixos: A purely functional linux distribution," Journal of Functional Programming, vol. 20, no. 5-6, pp. 577-615, 2010.