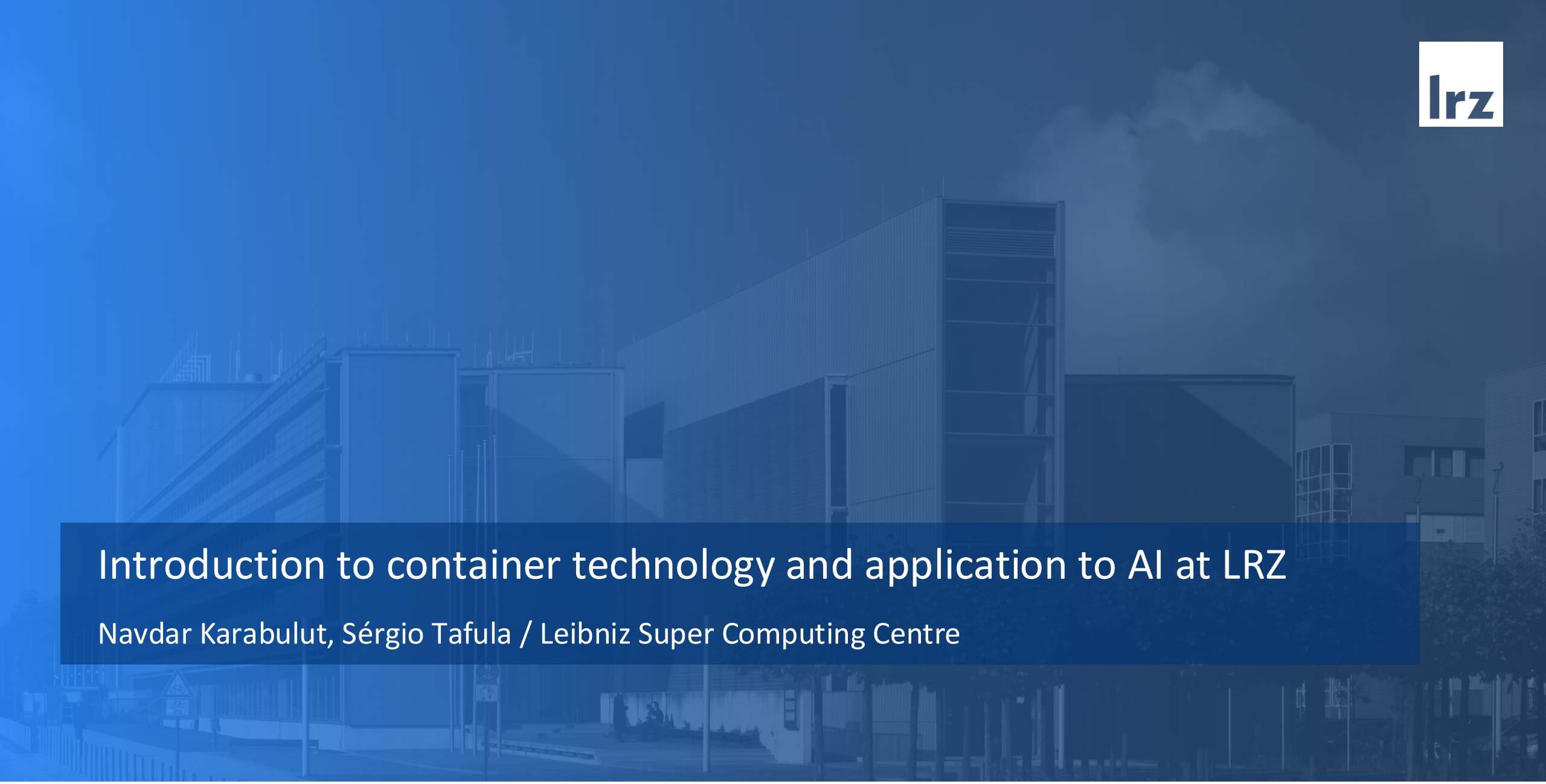
Leibniz Supercomputing Centre

of the Bavarian Academy of Sciences and Humanities



Introduction to container technology and application to AI at LRZ

Navdar Karabulut, Sérgio Tafula / Leibniz Super Computing Centre

Agenda

Course Structure and Learning Objectives

Part 1

- Motivation for Containerization
- Historical Evolution of Containerization
- Traditional Software Deployment
- Virtual Machines vs Containers
- Container Fundamentals
- Container Ecosystem

- Hands-on #1:Docker: Your First Steps With Containers

Part 2

- Container Runtime Architecture
- Container Image Construction
- Containers for AI Workloads
- HPC Container Runtime Systems

- Hands-on #2:Deep Learning: Make An ANN Dream in A Container

- Hands-on #3:HPC AI: Speech-to-Text With OpenAI Whisper.cpp in Enroot

Part 3

- Container Abstraction
- CI/CD with Containers
- Reproducible Scientific Workflows

- Hands-on #4: Reproducible RNA-seq Scientific Workflow With Nextflow and Docker:

Accessing Your Virtual Machine

The course resources: https://du4.link/containers

The exercises: https://github.com/LRZ-BADW/AITS-containers

An individual Virtual Machine (sandbox), look in your emails:

- Your IP address: 138.***.***.***
- Username: student**
- Password: ********

➢ Option 1 (easy): You can access the IDE

http://<138.***.***.***>:8080

➢ Option 2 (advanced): You can start SSH into the VM. Make yourself at home!

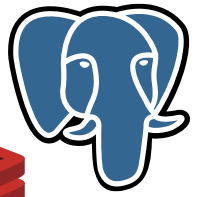
ssh <student**>@<138.***.***.***>

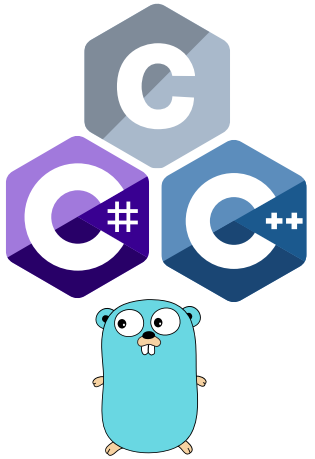
Part 1: Overview of Containerization

Motivation for Containerization

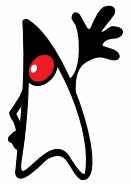
12, 14, 15

5, 8





7, 8, 10, 14



8, 11, 16

2.3, 2.4, 2.5

.gradle

.r

.cache

.conda

.jupyter

.m2

.node_modules

13, 12

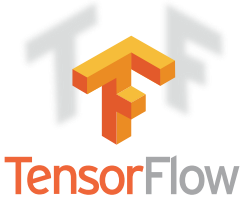
.npm

5, 7

2, 3, 4, 5

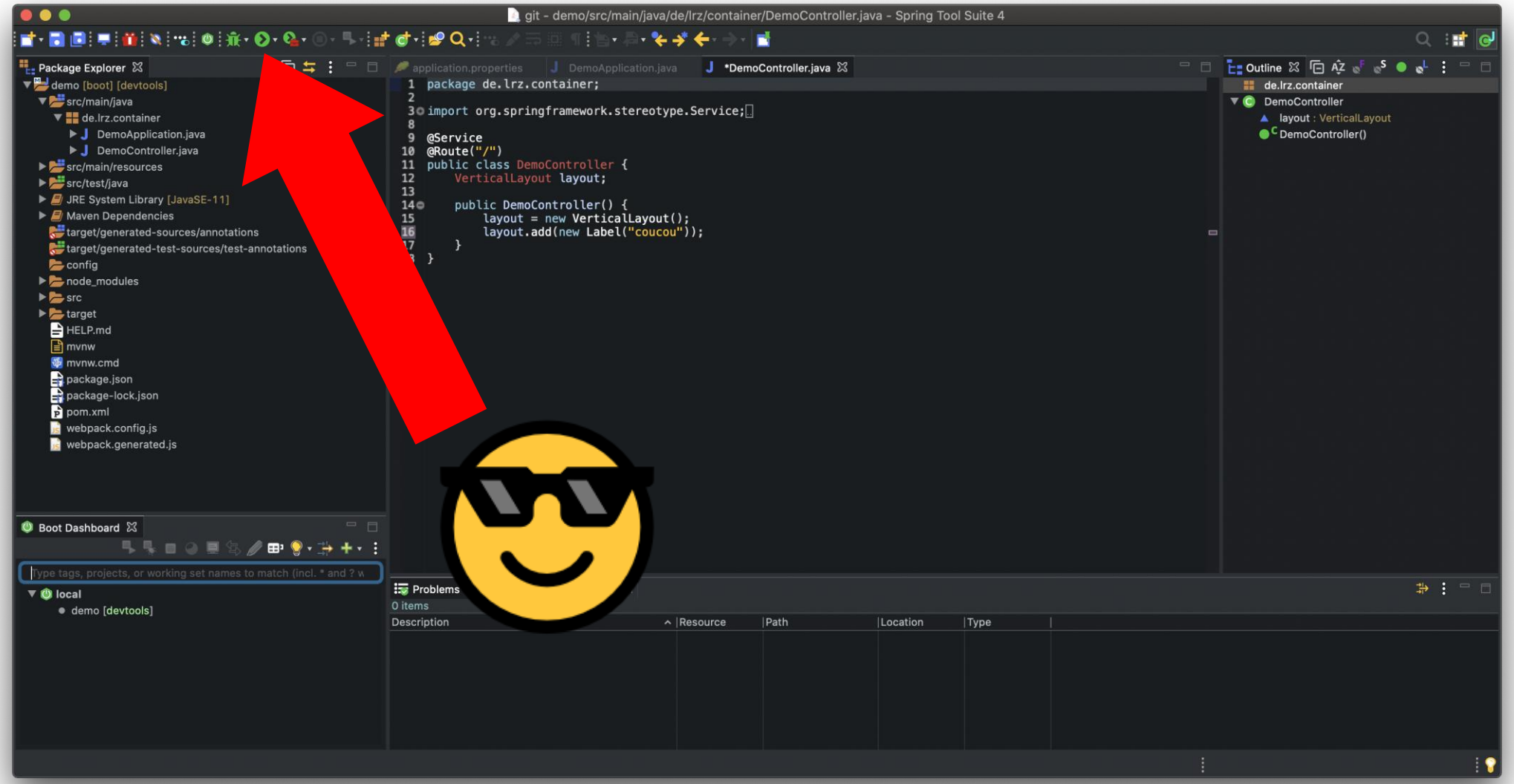
.config

/etc

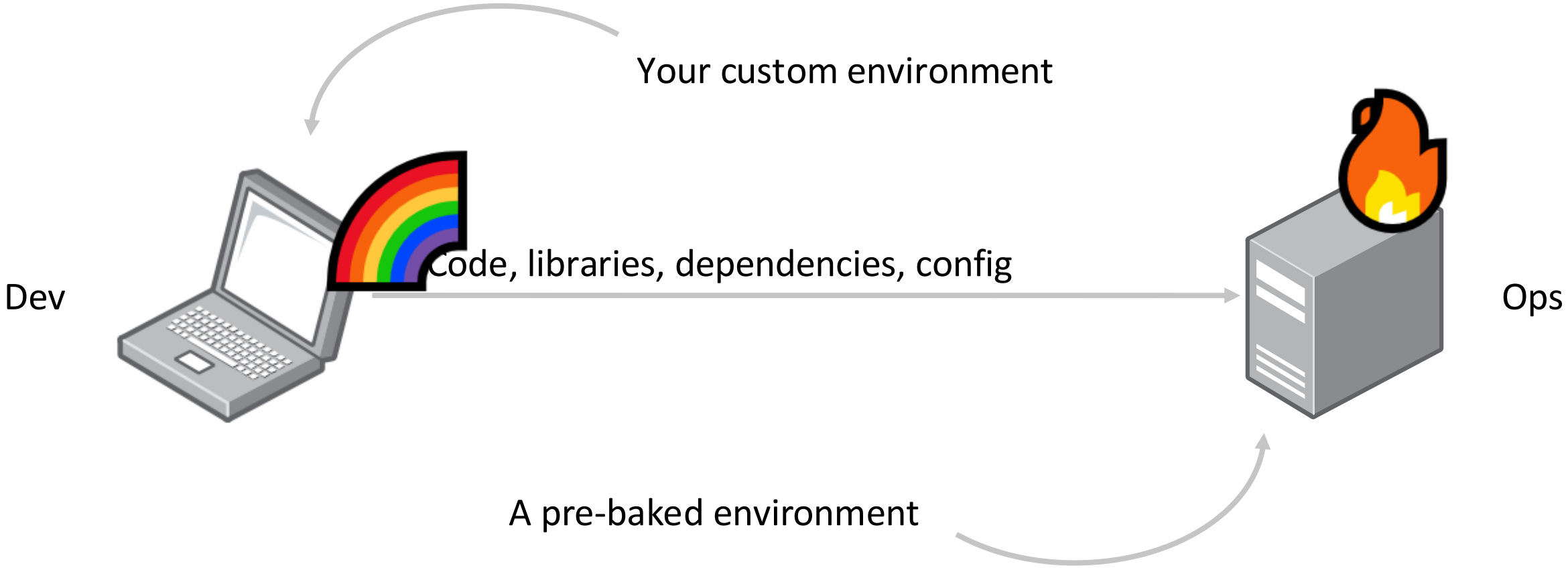


2.7, 3.6

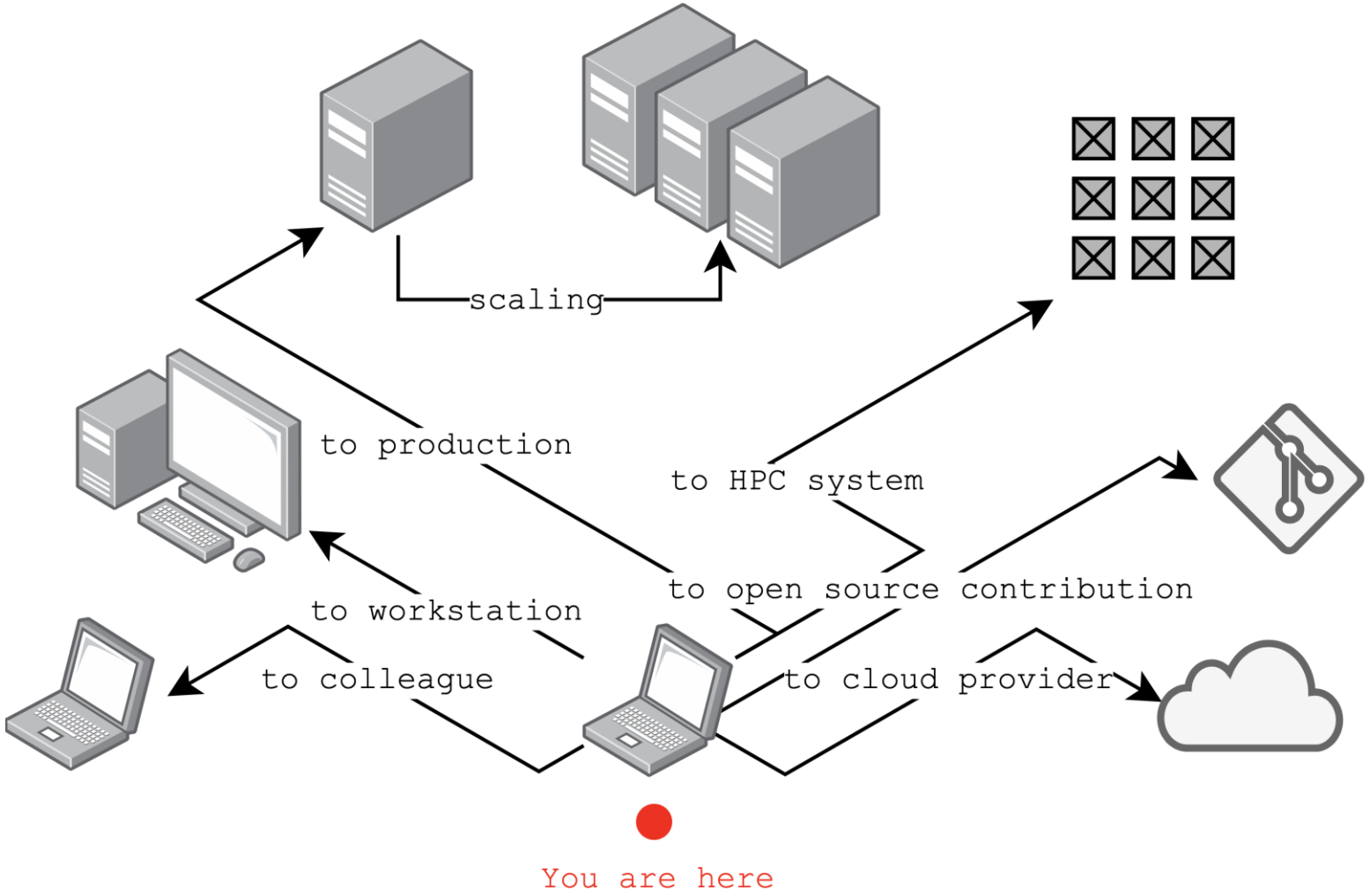
Motivation for Containerization



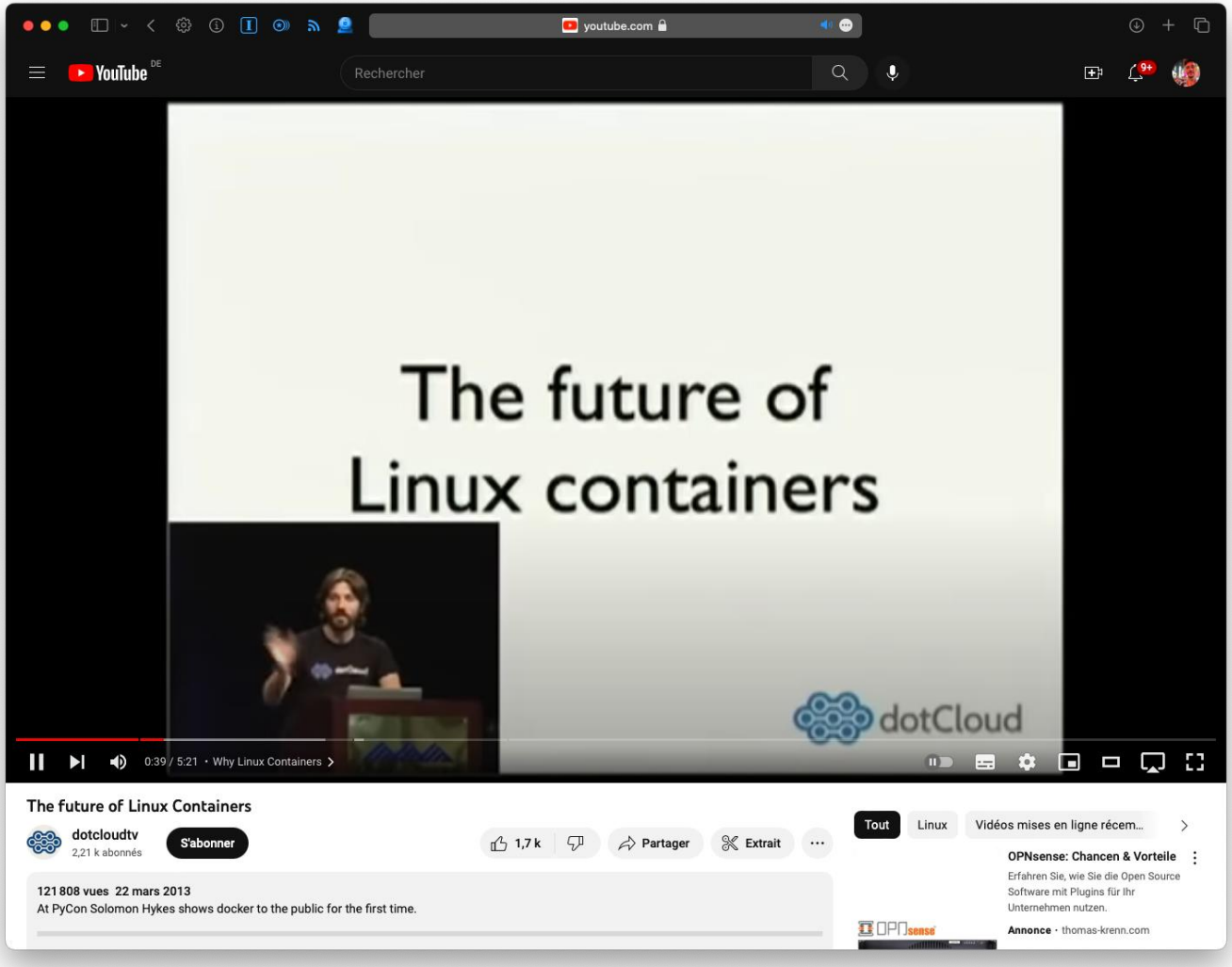
Motivation for Containerization



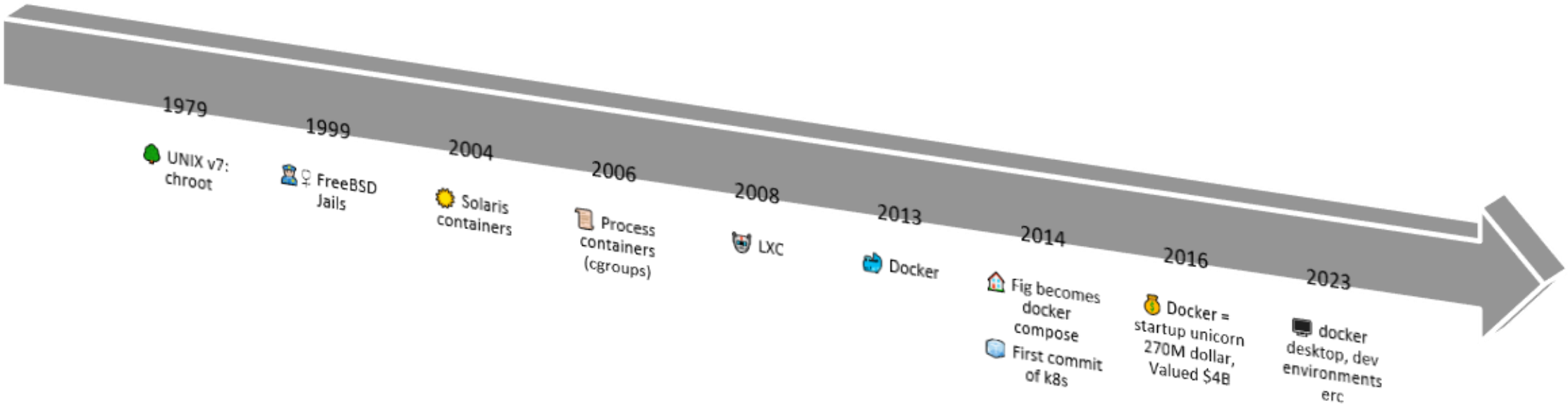
Motivation for Containerization



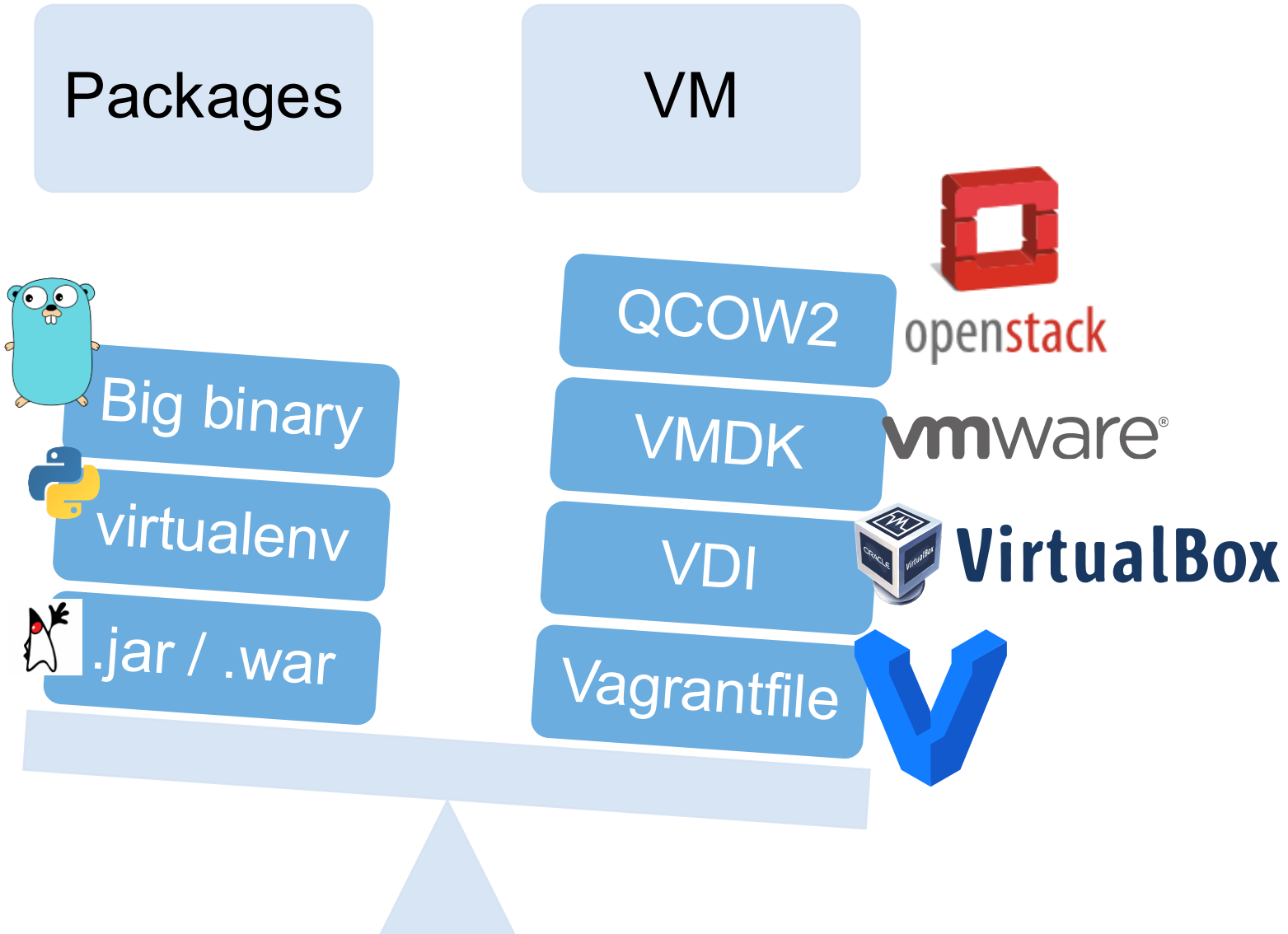
The future of Linux containers (15th March 2013)



Historical Evolution of Containerization



Traditional Software Deployment

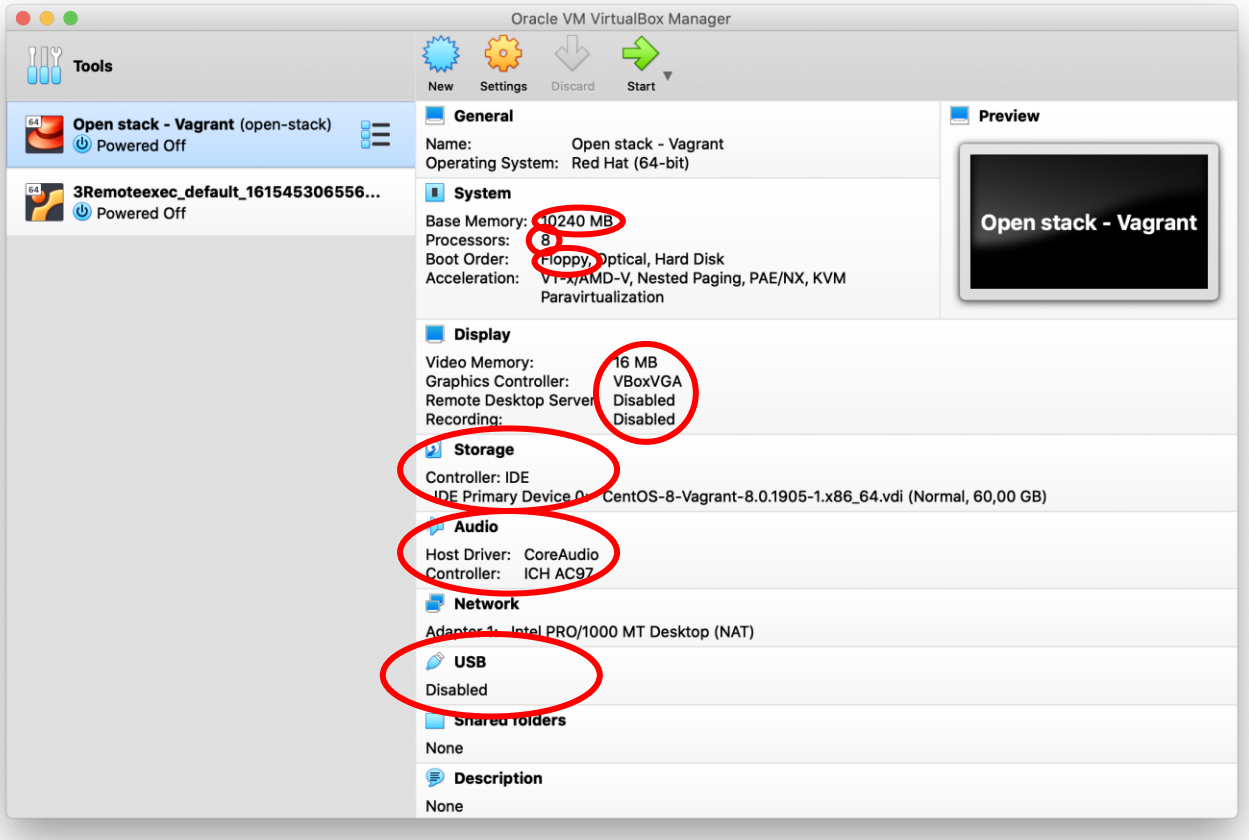


Virtual Machines vs. Containers

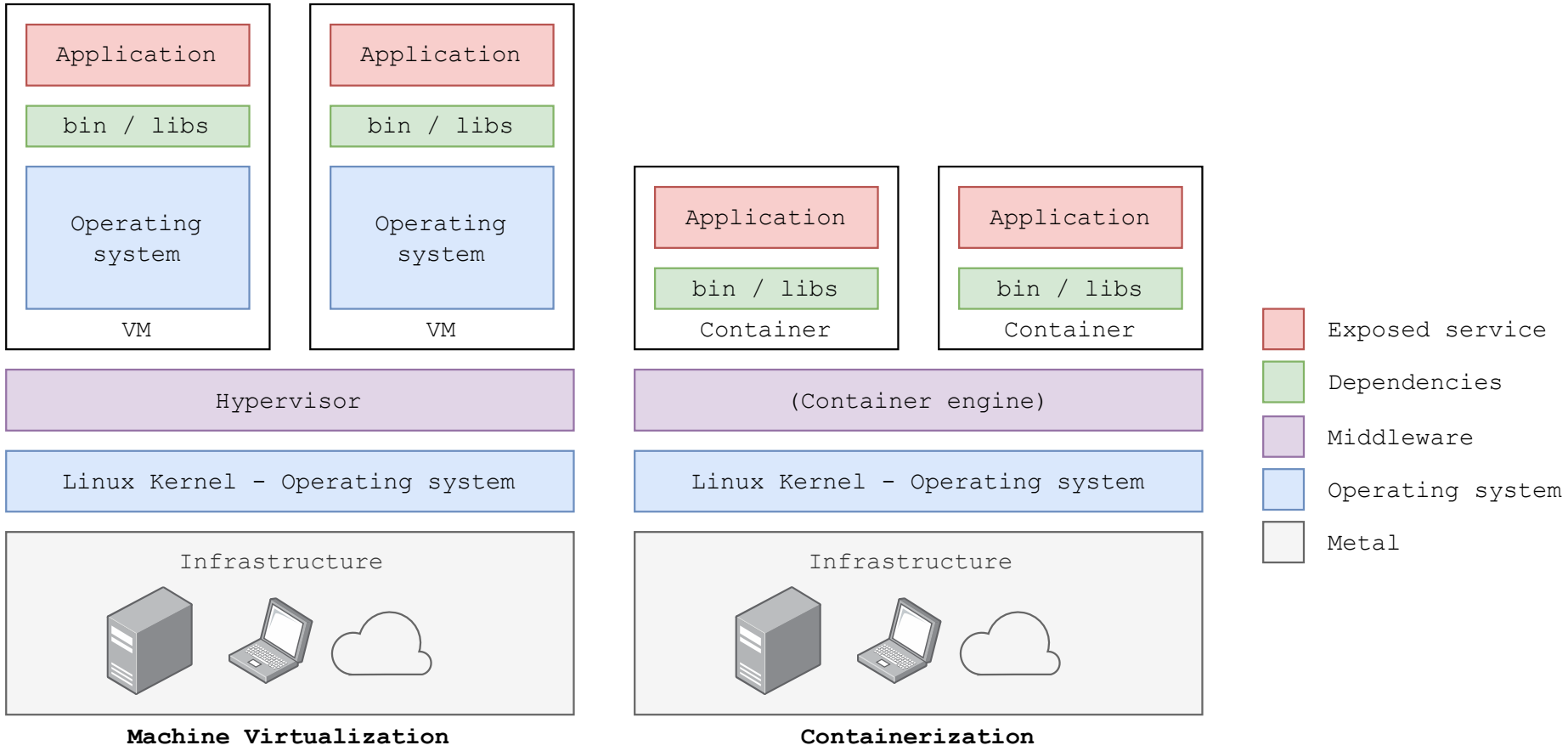
VMs Emulate Hardware

- RAM
- Processor
- Floppy drive?
- Graphics card
- Storage
- Audio card
- Networking
- Bunch of interfaces

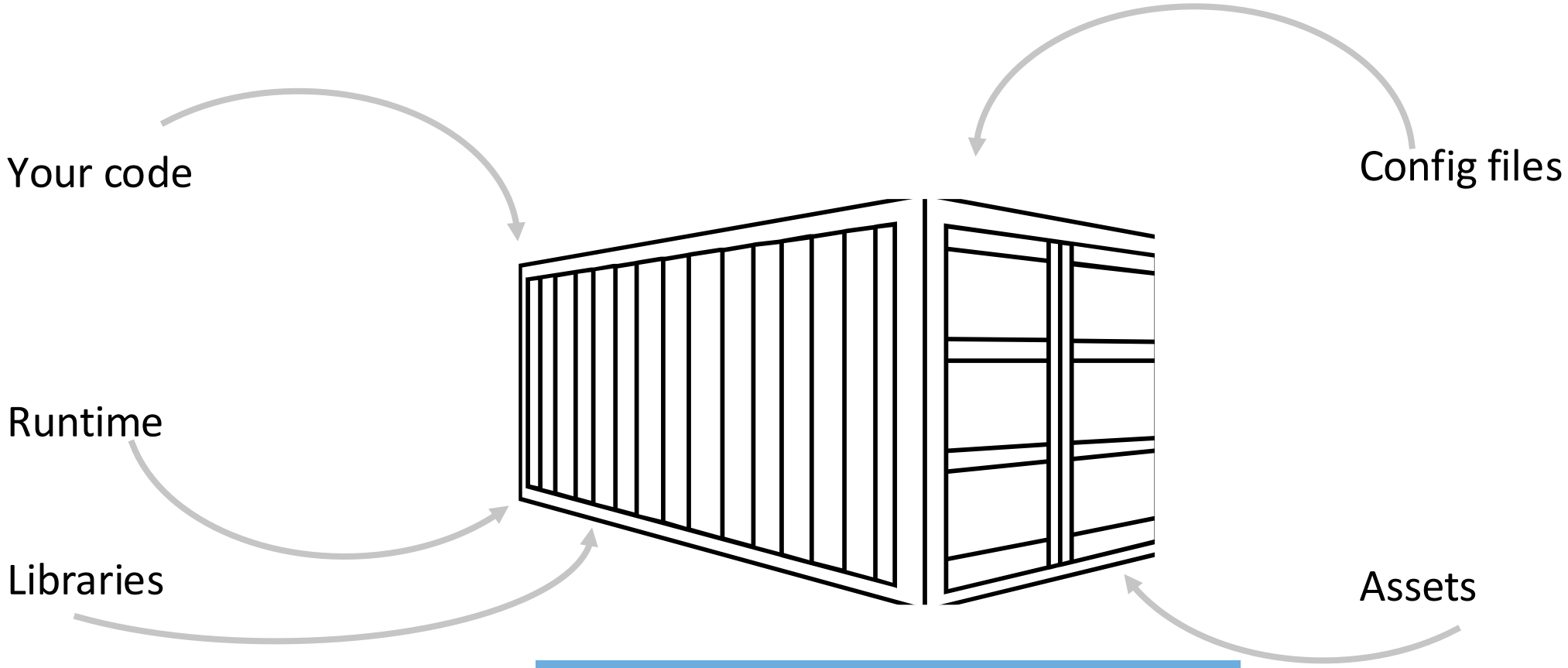
😱 WAIT! we don't want to worry about hardware!



Virtual Machines vs. Containers

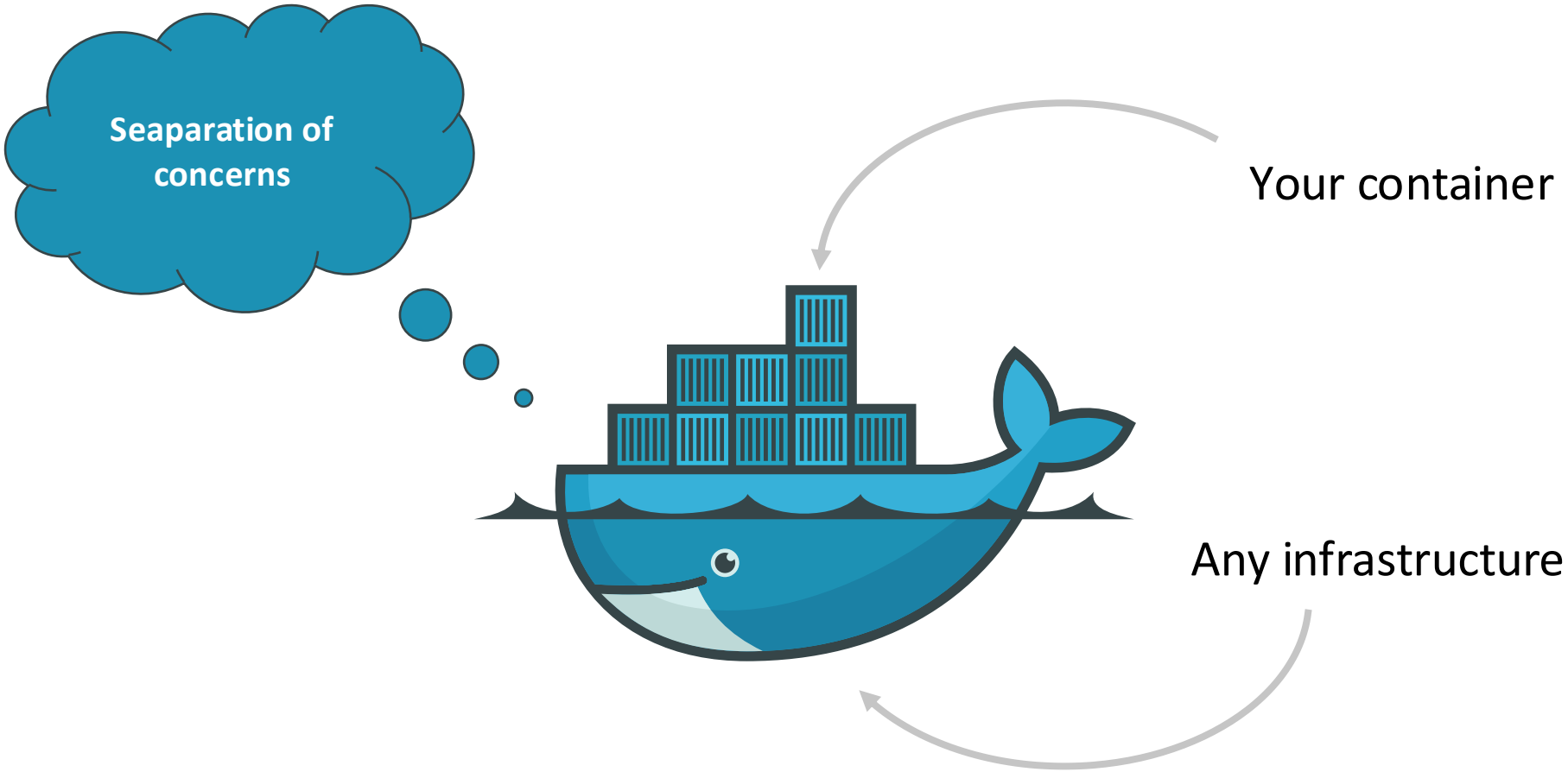


Container Fundamentals

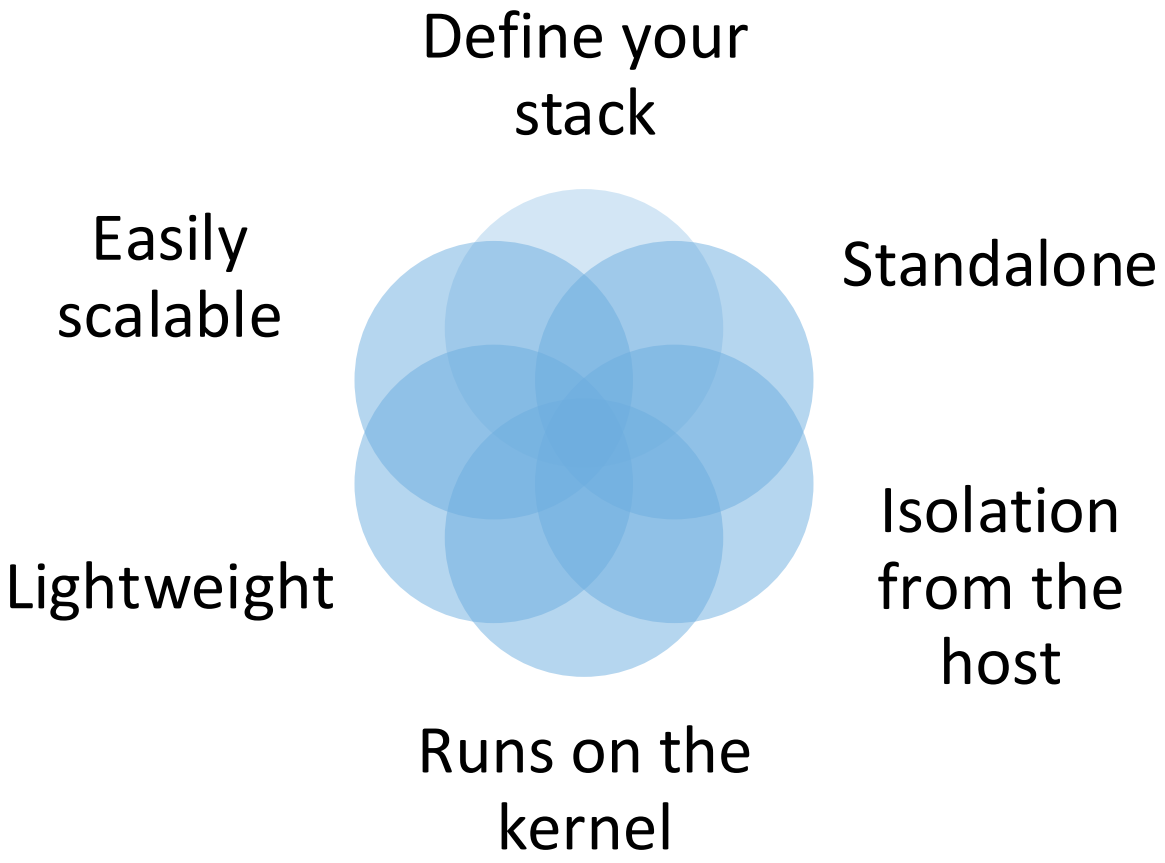


Containers allow: i) to sandbox the entire system ii) Without machine details iii) and without performance hit

Container Fundamentals



Containers allow UDSS



User Defined Software Stack

Container Ecosystem

Image

The way container software is shipped.

- Static, standardized, and portable **filesystem snapshot** with a **predefined executable** command or entry point.
- **Images are built** and can be stored and distributed.
- Images are a tool for **reproducibility** used to ship **fully built and packaged versions of application** components, assets etc.

~executable that bundles all the dependencies making it very portable.

Container

Isolated environment for running processes.

- **Running instance of an image**.
- Runs on a host machine and **shares the kernel** with OS.
- **The processes running in the container are isolated** from the rest of the system.
- Containers are **a tool for isolation** where components are segregated, providing better security and resiliency.

~ lightweight ephemeral virtual machines

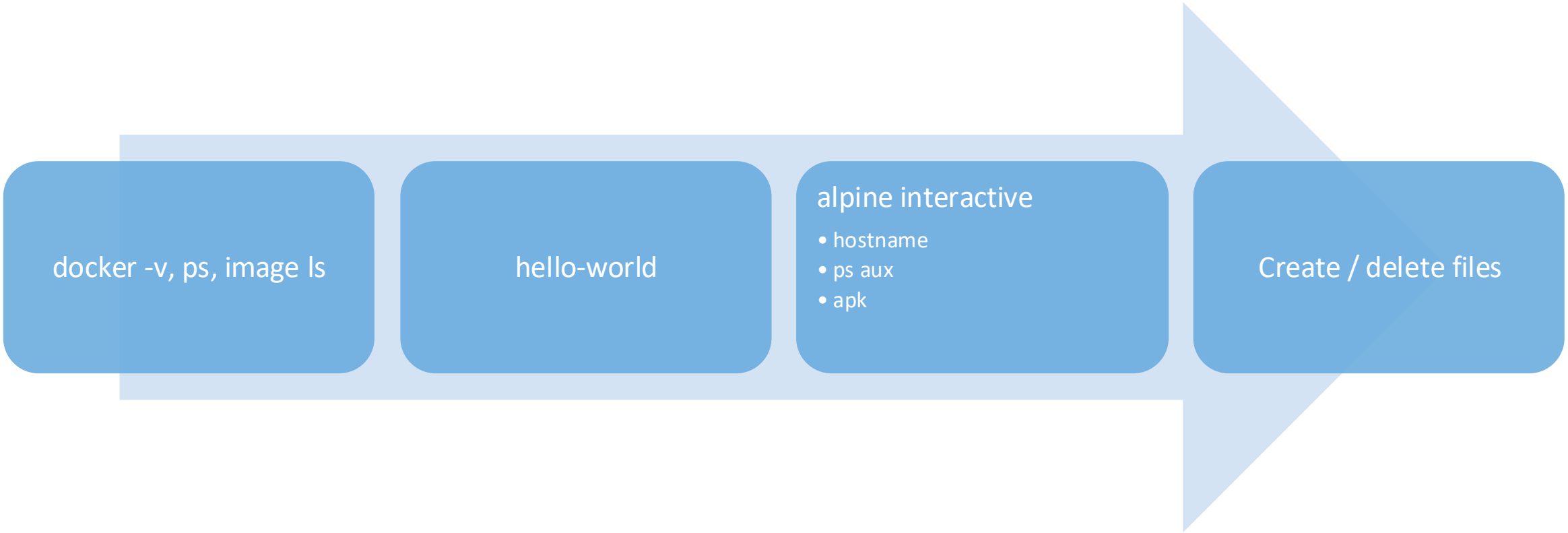
Orchestrator

Makes containers manageable.

- **Automates the lifecycle** of containers, networking, storage…
- Organizes containers into **abstract services** and handles dependencies. It allows to **declaratively describe how containers should behave.**
- An orchestrator is a tool for **managing complex applications** by providing load balancing, monitoring, automated restarts, version migration, and many other convenience capabilities.

Hands-on #1:Docker: Your First Steps With Containers

Exercise Guide



Exercise Guide

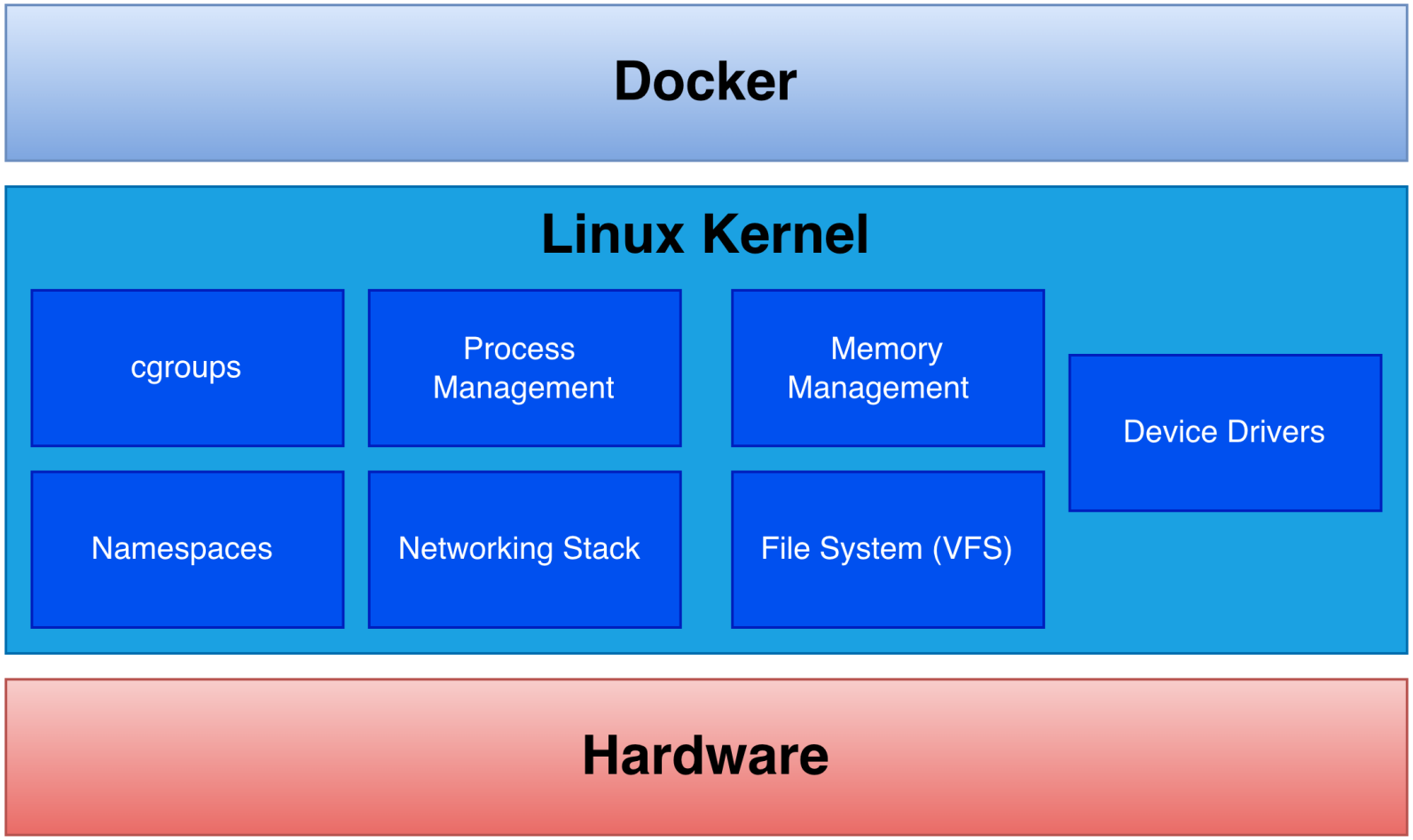
Let’s get into the workbench.

(easy) coder ide
(advanced) SSH

Part II: Container Technologies and Applications

Container Runtime Architecture

Linux Namespaces, cgroups, and Copy-on-Write (CoW) Storage



Linux Namespaces

Namespaces in Linux

- Isolation – a process sees only its own PID, network, filesystem,hostname
- Virtualization – Linux creates a virtual of the system for each process

Namespaces in Containers

- Isolation – own PID, network, filesystem, hostname per container
- Virtualization – root inside a container, unprivileged on the host system.
- Install & run software without affecting to the host system

Built into the kernel

Linux Control Groups (cgroups)

cgroups in Linux

- Organizes processes into hierarchical groups to control resource usage
- Limit – CPU, memory, disk I/O, process count per group
- Monitor – tracks usage per group, detects bottlenecks
- Freeze – suspends/resume processes (freezer controller v1, natively v2)

cgroups in Containers

- Limit – prevents one container from consuming all host resources
- Monitor – track resources usage per container, detects bottlenecks
- Freeze – suspends/resumes containers (freezer controller v1, natively v2)

Built into the kernel

Linux Copy-on-Write (CoW) Storage

CoW Storage in Linux

- Processes share data in RAM until write occurs
- Forking creates no immediate copy (only changed data is duplicated)
- Shared storage across copies saves disk space & speeds up operations

CoW Storage in Containers

- Layers stores only changes from the layer below
- Unchanged layers are shared across containers- no duplications
- Only modified layers stored or transferred
- Container add a thin witable layer over read-only image layers

Built into the kernel

Linux Namespaces, cgroups, and Copy-on-Write (CoW) Storage

- Containers are not a virtualization technology
- Linux uses namespaces, cgroups and Copy-on-Write(CoW) storage.
  - The system is a big container.
- Even when you're not in a container, you are in a container.

There is no performance hit.

I repeat, there is no performance hit.

Container Performance Considerations

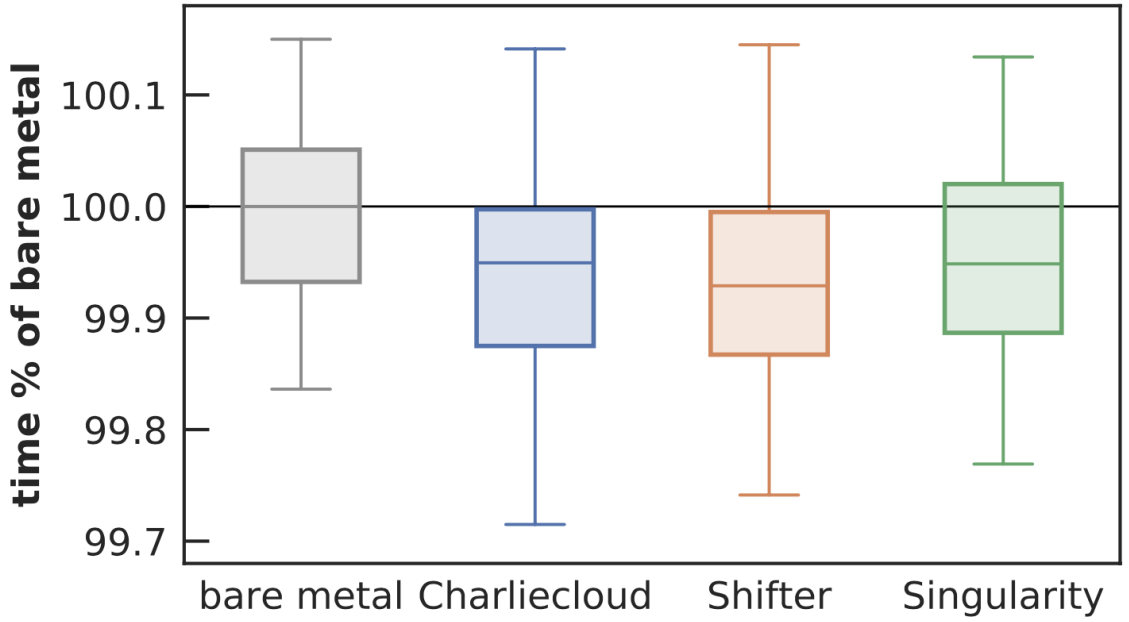


Fig. 1. SysBench prime number computation time relative to median bare metal performance of 129.36 seconds; lower is better. Boxes show the median and middle 50%, while whiskers show the maximum and minimum. The four environments showed essentially identical performance.

A. Torrez, T. Randles, and R. Priedhorsky, "HPC Container Runtimes have Minimal or No Performance Impact," in 2019 IEEE/ACM International Workshop on Containers and New Orchestration Paradigms for Isolated Environments in HPC (CANOPIE-HPC), Nov. 2019, pp. 37–42. doi: 10.1109/CANOPIE-HPC49598.2019.00010.

> Not to metion the time spared for humans (dev and ops)

Ephemerality, Statelessness, and Data Persistence

- Containers are ephemeral
- No data is persisted in a container
- Containers are meant to be stateless
  - No state
  - No information related to the state: amnesic
  - Just get the job done
  - Separation of data and process
- Containers can be replicated
  - No state = each container is the same
  - Allow for horizontal scaling

Volume Mapping

```
# ---------- #
# ON THE HOST #
# ---------- #

# Let's create a sample directory
# Its content will be mapped to the container
mkdir /tmp/data
# Let's create some files
echo "Monday, Tuesday, Wednesday"    > /tmp/data/week.txt
echo "Jeudi, Vendredi, Samedi"       > /tmp/data/semaine.txt
echo "Sonntag, Sonntag, Sonntag"     > /tmp/data/woche.txt

# -v let us map volumes with the syntax: <path_on_host>:<path_in_container>
docker run \
    -it \
    --rm \
    --name weeks \
    --hostname weeks \
    -v /tmp/data:/data \
    alpine

# --------------- #
# IN THE CONTAINER #
# --------------- #

ls -lah /data/
# total 20K
# drwxr-xr-x    2 root     root        4.0K Mar 26 10:07 .
# drwxr-xr-x    1 root     root        4.0K Mar 26 10:08 ..
# -rw-r--r--    1 root     root          24 Mar 26 10:07 semaine.txt
# -rw-r--r--    1 root     root          27 Mar 26 10:07 week.txt
# -rw-r--r--    1 root     root          26 Mar 26 10:07 woche.txt

# You can escape the container without killing it
# With ctrl-P ctrl-Q
```

host → `-v /tmp/data:/data` ← container

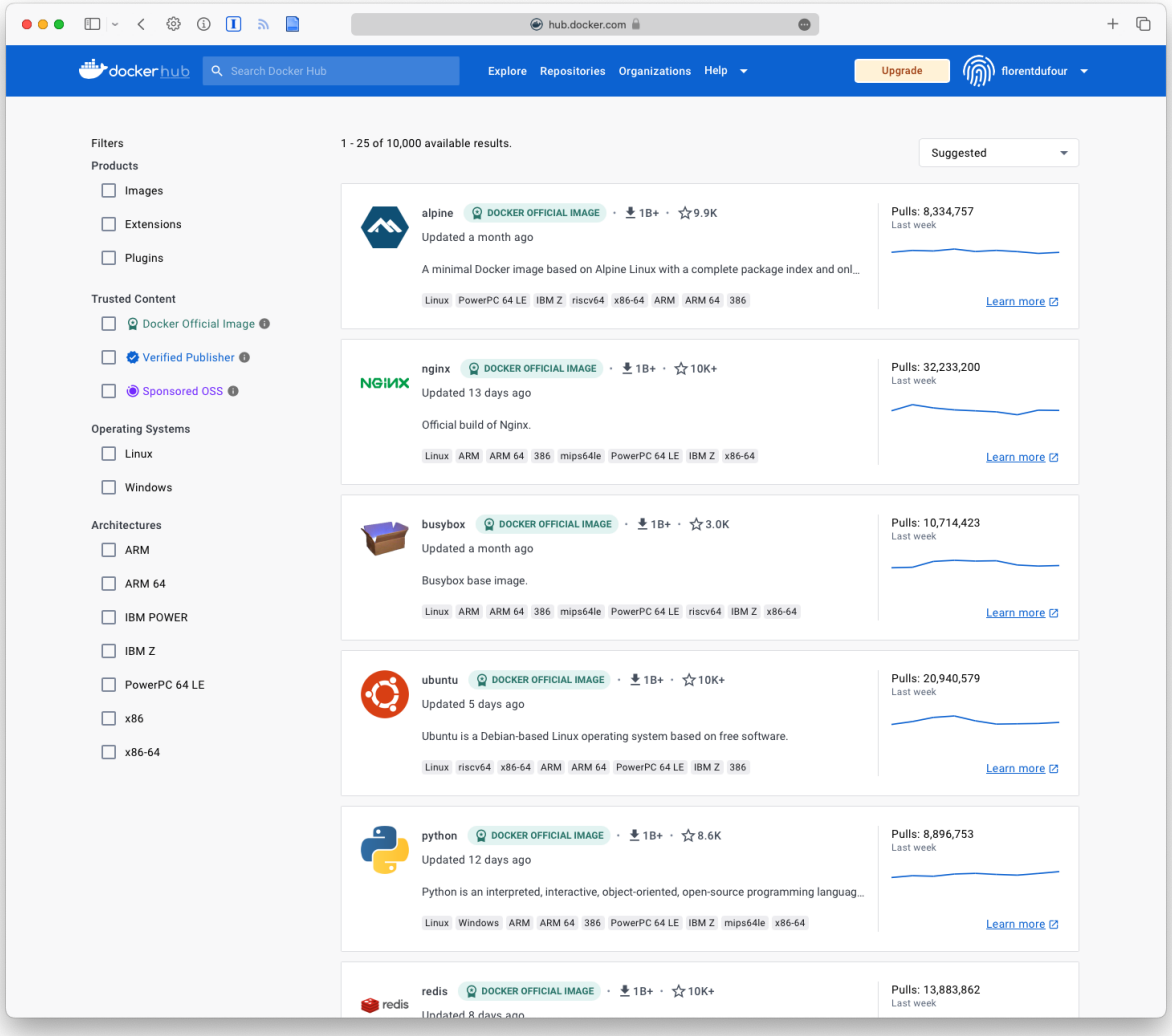
Port Mapping

```
# Let's expose a service, for example a website!

# Create your website
echo "<h1>Welcome...</h1><p>...to my awesome website running in a container ;-)</p
    >" > index.html

# -p lets us map ports with the syntax: <port_on_host>:<port_in_container>
# -v lets us mount the persitent file to the container
# -d Lets us run the container in detached mode (i.e. in the background)
# caddy is a web server. Kinda like nginx or apache, but shinier!
docker run \
    --name webserver \
    -d \
    -p 8888:80 \
    -v $PWD/index.html:/usr/share/caddy/index.html \
    caddy

# Visit http://<IP address>:8888 with your browser to see your website
```

host

container

Public Container Registries (Docker Hub)



https://hub.docker.com

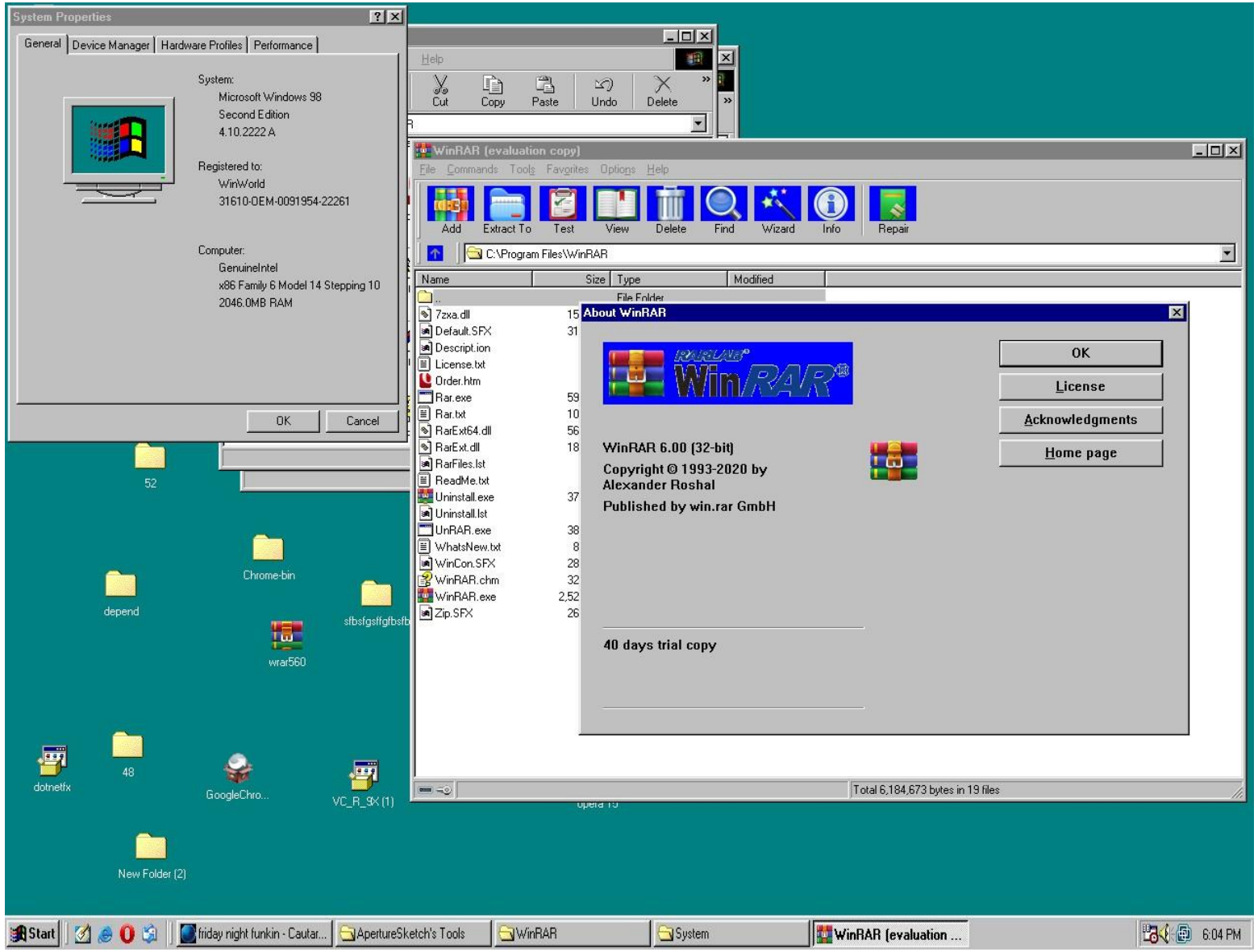
Container Image Construction

Commit-Based vs. Dockerfile-Based Approaches

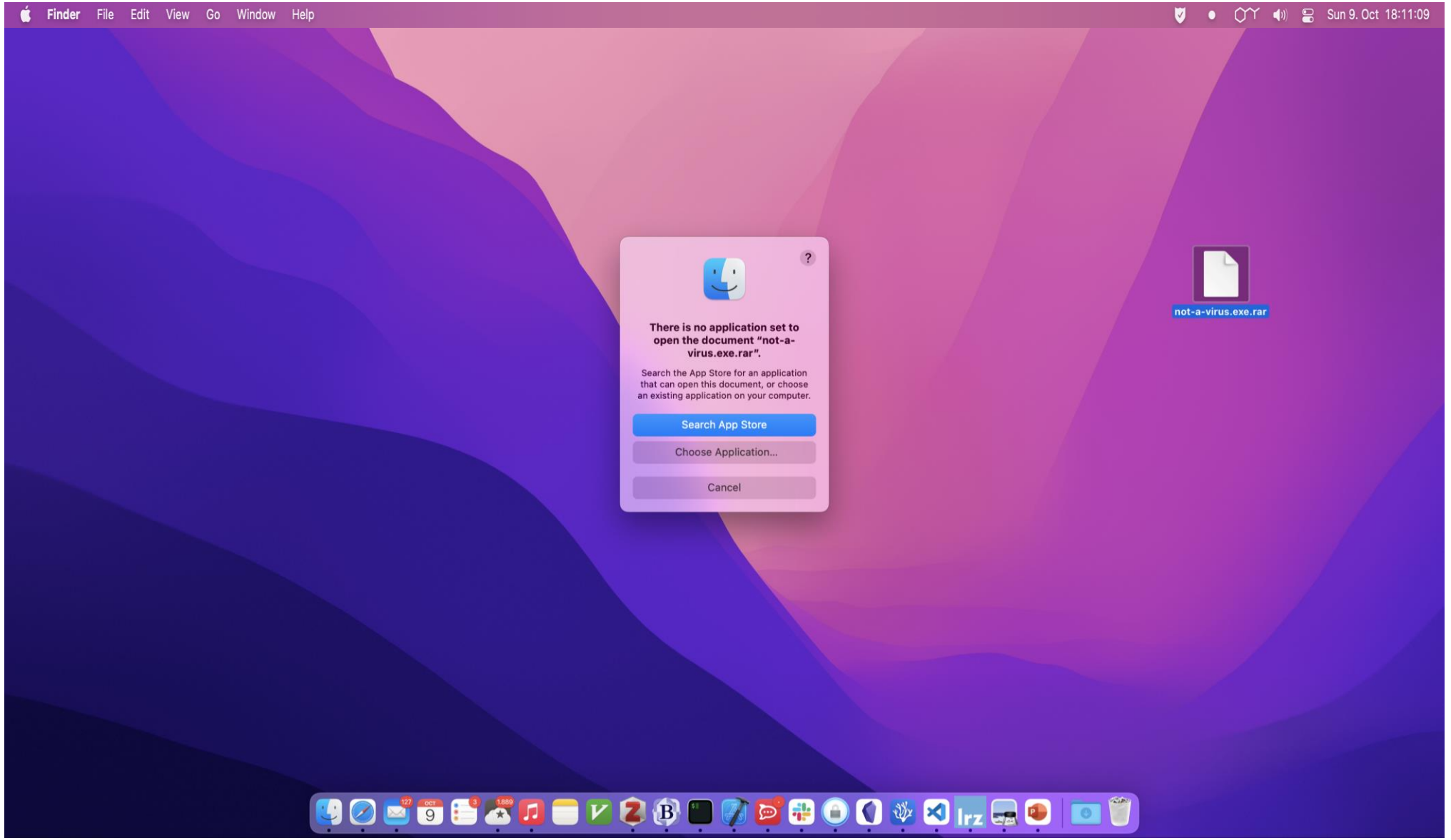
“Commit” a container

Create a “Dockerfile”

A Practical Example: Platform-Dependent Software Packaging



A Practical Example: Software Packing Challenges



Commit-Based Image Construction


```
# ---------- #
# On the host #
# ---------- #

docker image ls
# REPOSITORY          TAG                 IMAGE ID            CREATED
    SIZE
# alpine              latest              28f6e2705743        5 weeks ago
    5.61MB

# Only alpine is available as an ima
# Let's customize it in order to use                    xotic rar files
docker run -it alpine

# --------------- #
# In the container #
# --------------- #

# We add a package to the container
apk update && apk add unrar
# ctrl-P ctrl-Q

# ---------- #
# On the host #
# ---------- #

docker ps
# CONTAINER ID        IMAGE               COMMAND             CREATED
    STATUS              PORTS               NAMES
# 5a1c7e2f8491        alpine              "/bin/sh"           59 seconds ago
    Up 57 seconds                           musing_kilby

# We want to commit the container 5a1c7e2f8491
docker commit -m "unrar capability added to the container" 5a1c7e2f8491 unrar-
    apine
# sha256:e5e572c22a2c84ebcb07c963203c07f89a4b47f848aceb4d80be8afbb884fa3e

docker image ls
# REPOSITORY          TAG                 IMAGE ID            CREATED
    SIZE
# unrar-apine         latest              e5e572c22a2c        55 seconds ago
    9.67MB
# alpine              latest              28f6e2705743        5 weeks ago
    5.61MB

# A new image is created, we can now run alpine container with unrar installed
    already!
```

Dockerfile-Based Image Construction

Create an empty directory

The file must be named Dockerfile

The format is *very* simple:

```
# comment
INSTRUCTION arguments
```

Ignored

Uppercase by convention

https://docs.docker.com/engine/reference/builder/#format

Dockerfile-Based Image Construction

Command to execute when starting container

Volume

Command to execute

Parent image

```
FROM alpine:latest

RUN apk update && apk add unrar
VOLUME data_to_unrar

ENTRYPOINT /usr/bin/unrar
```

```
# Then build the image with:
# docker build . -t "alpine_unrar"
```

Tag of the image „name:version“

Directory containing the Dockerfile

Dockerfile-Based Image Construction

```
~$ ls -lah
 232 -rw-r--r--@  1 di67pif  wheel   115K Apr 14 17:23 Module-3_220420.pptx
2056 -rw-r--r--@  1 di67pif  wheel   977K Apr 19 11:40 not-a-virus.exe.rar

~$ docker run –v $PWD:/data_to_unrar alpine_unrar not-a-virus.exe.rar

~$ ls –lah
 232 -rw-r--r--@  1 di67pif  wheel   115K Apr 14 17:23 Module-3_220420.pptx
2056 -rw-r--r--@  1 di67pif  wheel   977K Apr 19 11:40 not-a-virus.exe.rar
2056 -rw-r--r--@  1 di67pif  wheel   2.1M Apr 19 11:43 not-a-virus.exe
```

Example: Dockerfile-Based Image Construction

```
.
├── Dockerfile
├── app
│   ├── assets
│   │   ├── static.lst
│   │   ├── image1.tiff
│   │   └── image2.tiff
│   ├── extractor.py
│   ├── main.py
│   ├── user.py
│   └── utils.py
└── requirements.txt

2 directories, 9 files
```

```
FROM ubuntu:bionic

RUN apt-get update
RUN apt-get –y upgrade
RUN apt-get –y install python3 python3-pip

COPY ./requirements.txt /tmp/requirements.txt
COPY ./app /app

RUN pip install –r /tmp/requirements.txt

ENV DEBUG=true

WORKDIR /app
ENTRYPOINT ./main.py
```

```
~$ docker build . –t “my-image:1.0”
~$ docker run my-image:1.0
```

Dockerfile-Based Image Construction

Instruction	Description
FROM	Set the parent image for the subsequent instructions (must be the first line) e.g., FROM alpine:latest
LABEL	Adds metadata to an image e.g., LABEL maintainer="Florent Dufour <florent@lrz.de>"
ARG	Defines a variables for build time or runtime
RUN	execute any commands in a new layer on top of the current image and commit the results. The resulting committed image will be used for the next step e.g., (shell form), RUN apt-get update e.g. (exec form) RUN ["apt", "update"]
WORKDIR	sets the working directory for any command to follow
ENV	Set environment variables that must be persistent after image build e.g., ENV DB_PASSWORD="Chang3me!"
USER	Sets the user name (or UID) and optionally the user group (or GID) to use when running the image and for later commands to run
ADD	Add files, directories or remote file URLs from to the filesystem of the image. It supports wildcards. Automatically expand archives ⚠ Can be unpredictable. e.g., ADD /source/file/path /destination/path e.g., ADD http://example.com/file.txt /destination
COPY	Newer than ADD but with limited functionalities. Much safer and predictable, prefer using COPY over ADD e.g., COPY /host/source/file/path /container/destination/path
VOLUME	creates a mount point with the specified name and marks it as holding externally mounted volumes from native host or other containers
EXPOSE	Make the container listen to a specific port at runtime. Can specify UDP/TCP. Must be used with –p when runing container e.g., EXPOSE 8090
ENTRYPOINT	Configure a container that will run as an executable. Either a command in $PATH or an executable

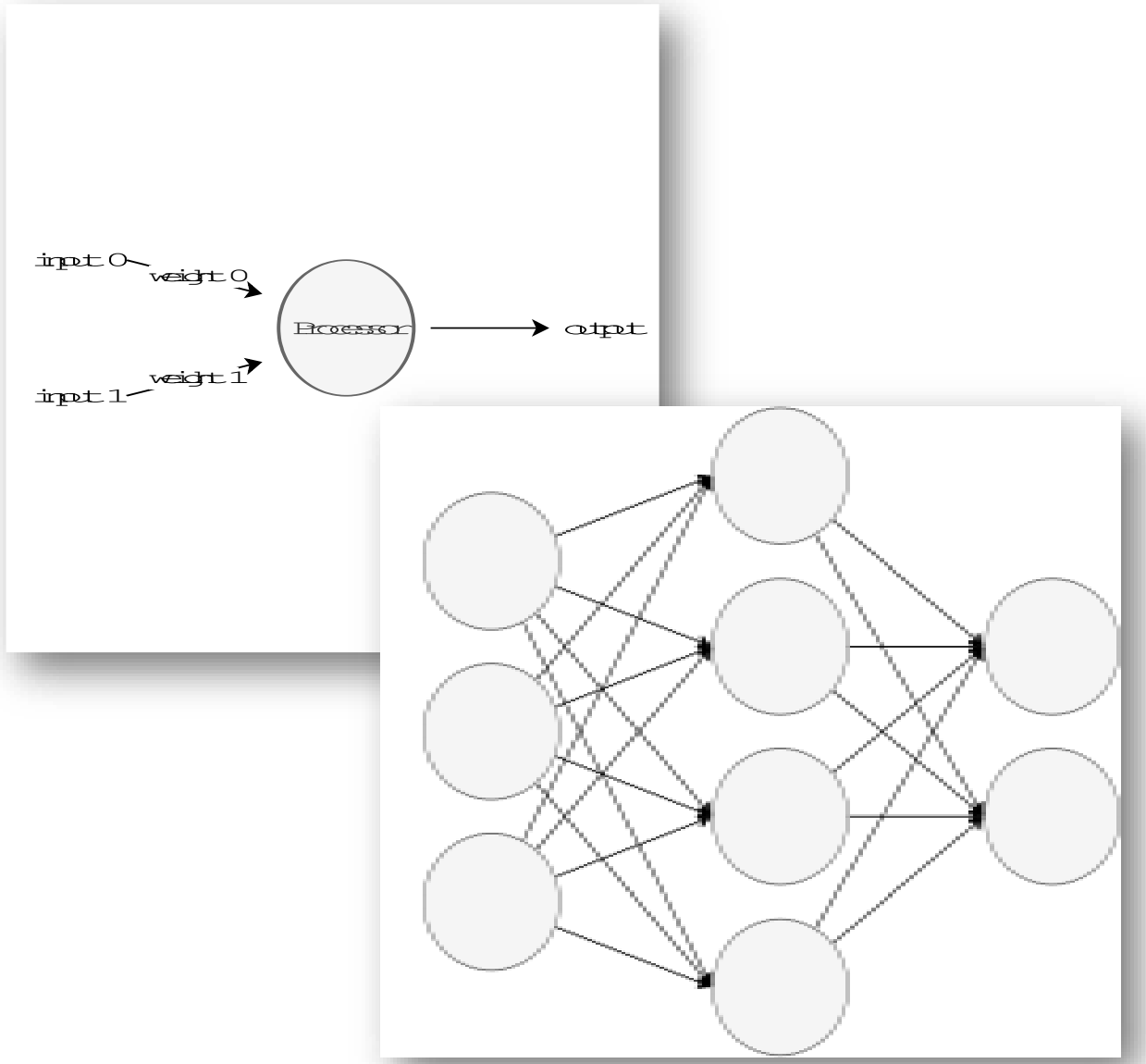
Hands-on #2:Deep Learning: Make An Artificial Neural Dream in A Container

History of Artificial Neural Networks

"DeepDream is a computer vision program created by Google engineer Alexander Mordvintsev that uses a convolutional neural network to find and enhance patterns in images via algorithmic pareidolia, thus creating a dream-like hallucinogenic appearance in the deliberately over-processed images"

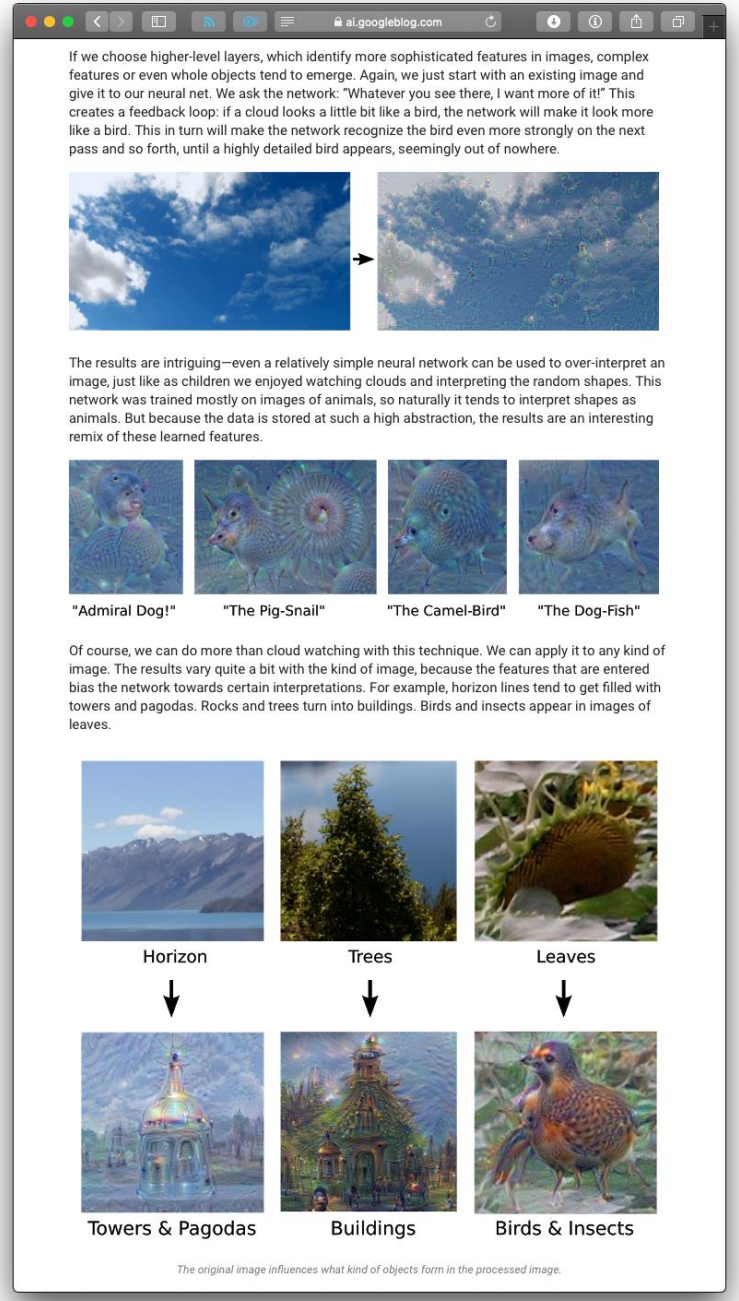
What is an Artificial Neural Network?

- Like in the brain: a “neuron” lives in a network, receives inputs, processes them, and generates an output.
- An ANN is a “connectionist” computational system that processes information collectively, in parallel throughout a network of neurons organized in layers.
- An ANN is adaptive and has the ability to learn by changing its internal structure based on the information flowing through it.
- This is achieved by tuning weights, the number that controls the signal between two neurons.
- Today, ANN are used to perform “easy-for-a-human, difficult-for-a-machine” tasks like optical character recognition, image classification, and speech and facial recognition for example.



History of Artificial Neural Networks

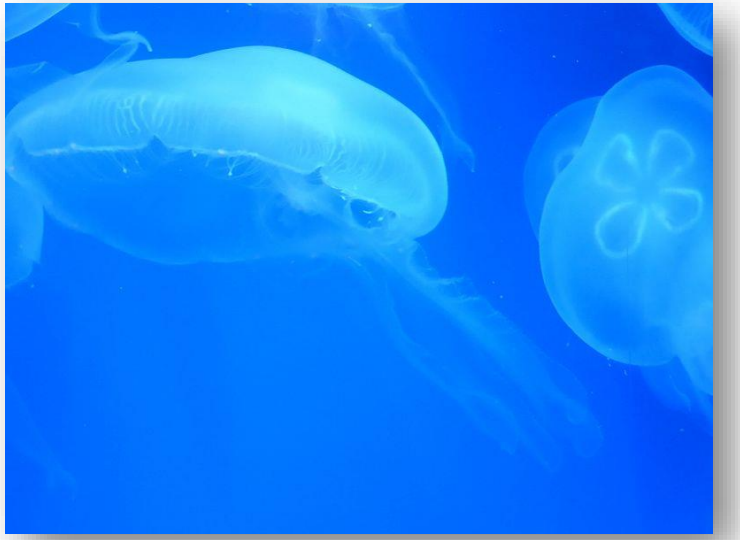
- Originally designed to detect patterns in images for classification (what ANN are good at!)
  - Ex: Find features of a dog: Fur, Dog snout then it's a 🐶
  - Ex: Find features of a fork: a handle and 2-4 tines and ignore what doesn't matter (size, color, number of teeth, orientation) : it's a 🍴
- Arised the question: Why do some models perform well and others don't?
- Idea: Reverse the process! And peek into the network
  - What is happening in each layer?
  - Pick a layer and enhance whatever is detected
  - Elicit a particular interpretation: What layer is responsible for what feature?

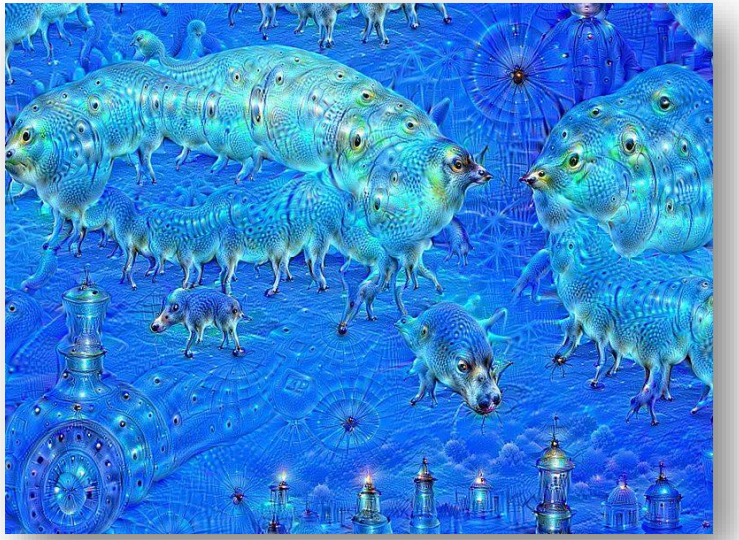


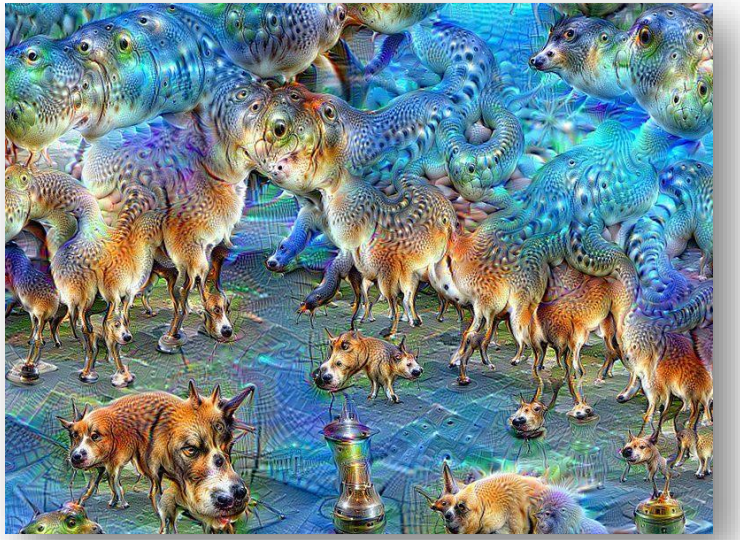
https://ai.googleblog.com/2015/06/inceptionism-going-deeper-into-neural.html

Iterative DeepDream: From Jellyfish to Dog Features

With an ANN trained to recognize dogs







x10

x5

https://ai.googleblog.com/2015/06/inceptionism-going-deeper-into-neural.html

Exercise Guide

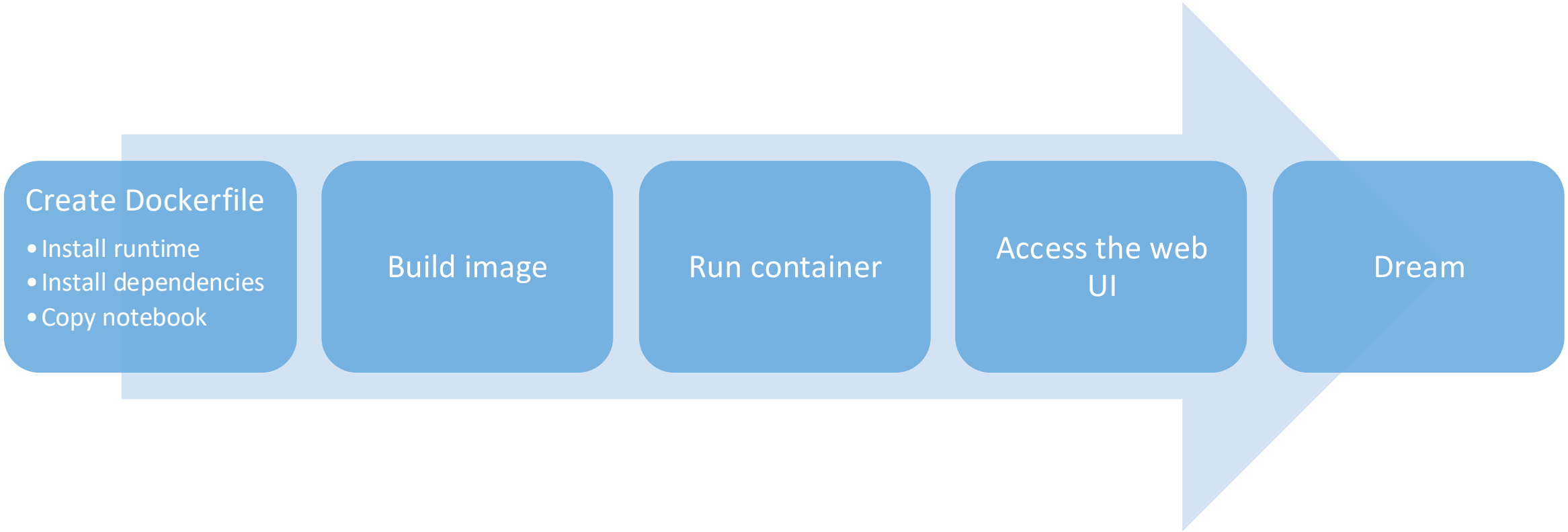
- We already have a Jupyter Notebook
- We have to build an image in which the notebook can run
  - Install the dependencies python3-dev and python3-pip with apt
  - Install the dependencies tensorflow matplotlib and jupyterlab with pip
  - Copy the notebook with the container
- We will run a container out of this image and map the port 8888:8888 to access the interface to execute the code from the Jupyter notebook

Exercise Guide

git clone https://github.com/LRZ-BADW/AITS-containers.git

- 2-Deep-Learning > question

Exercise Guide



Exercise Solution

- You can look into the solution subfolder
- You can run the full solution with make solution
- You can individually perform build and run tasks
  - make build
  - make run

Containers for AI Workloads

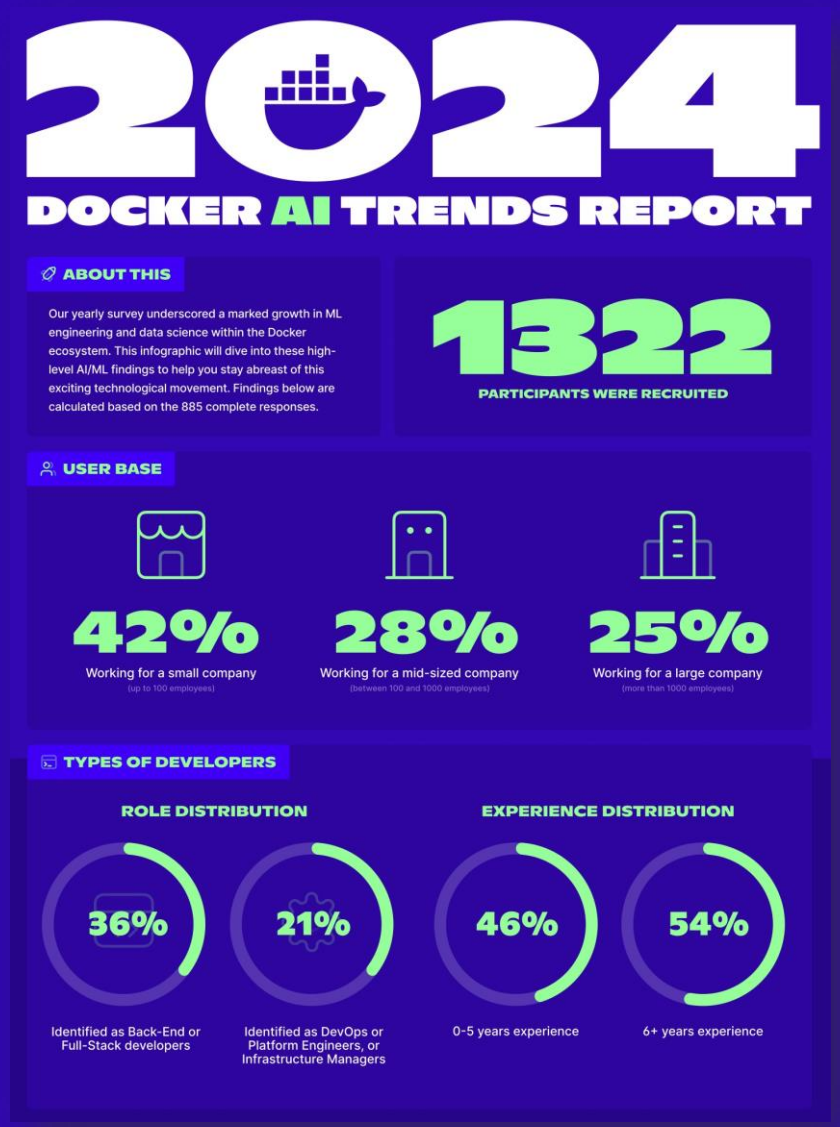
Rationale: Container Adoption in AI

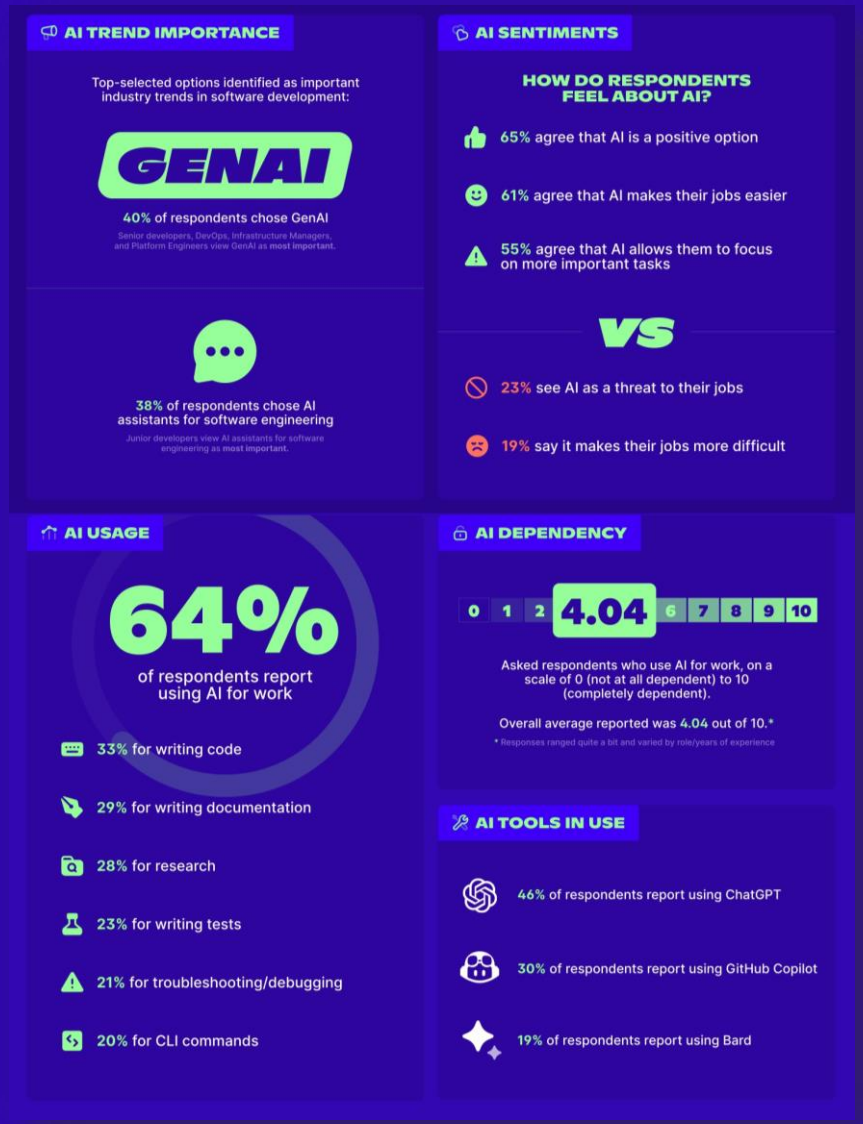
1. **AI workloads are inherently very heterogeneous**
   - Software: Python 3.x, PyTorch, RAG, Front-end etc.
   - Example AUTOMATIC1111/stable-diffusion-webui (what a mess…)

2. **AI workloads need to be portable (MLOps)**
   - Local development (laptop / workstation)
   - Remote training (AI GPU Cluster)
   - Cloud inference

3. **AI community tend to be younger**
   - early adopters of new technology like containers
   - More open to “new” paradigms like containers
   - Often prefers ease of use

Trends and Recent Developments in AI and Containers





Adoption of Container Technologies in HPC

HPC Capabilities and Constraints

What you get:

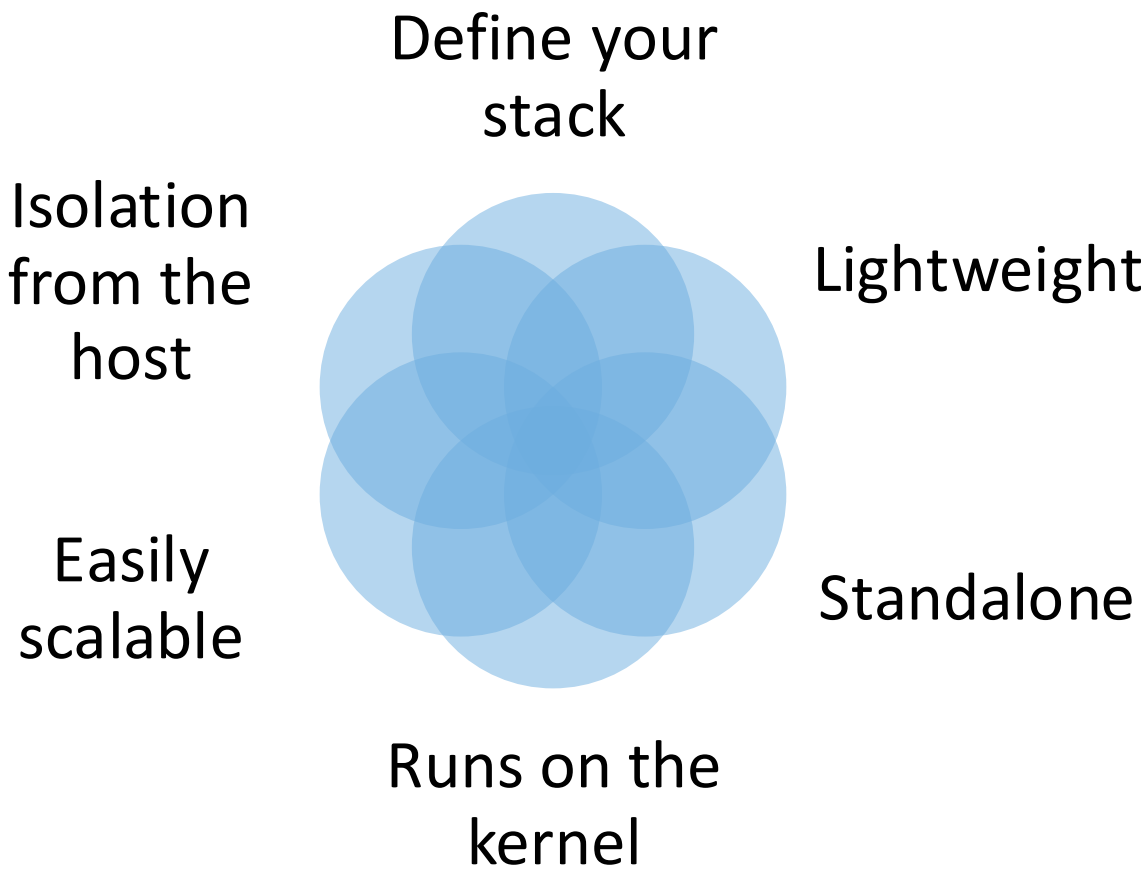
- High Performance
- Massive parallelism

What you don’t get:

- Root access
- Internet access
- Choice of OS
- `apt install exotic-library`

> Need for UDSS !

Containers as User-Defined Software Stack (UDSS)



User Defined Software Stack

Advantages of Containers in HPC

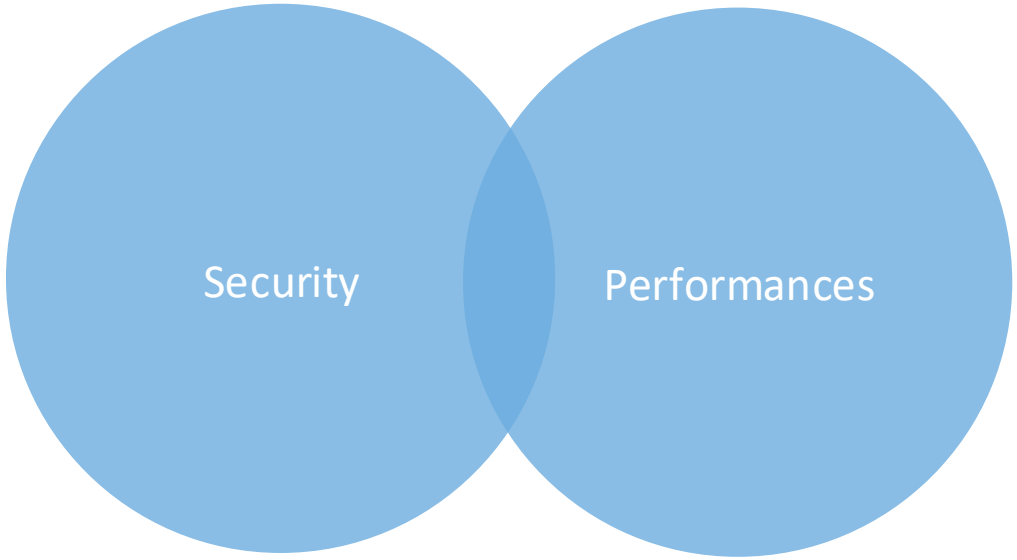
Containers are appealing for HPC

- UDSS
  - Circumvent root access
  - Use exotic libraries and framework
  - A researcher must research
- Bare metal performances
- Security
- Less burden on HPC staff = better Support

Docker Security Limitations in HPC Environments

Namespace

Docker socket



Filesystem

Integrity

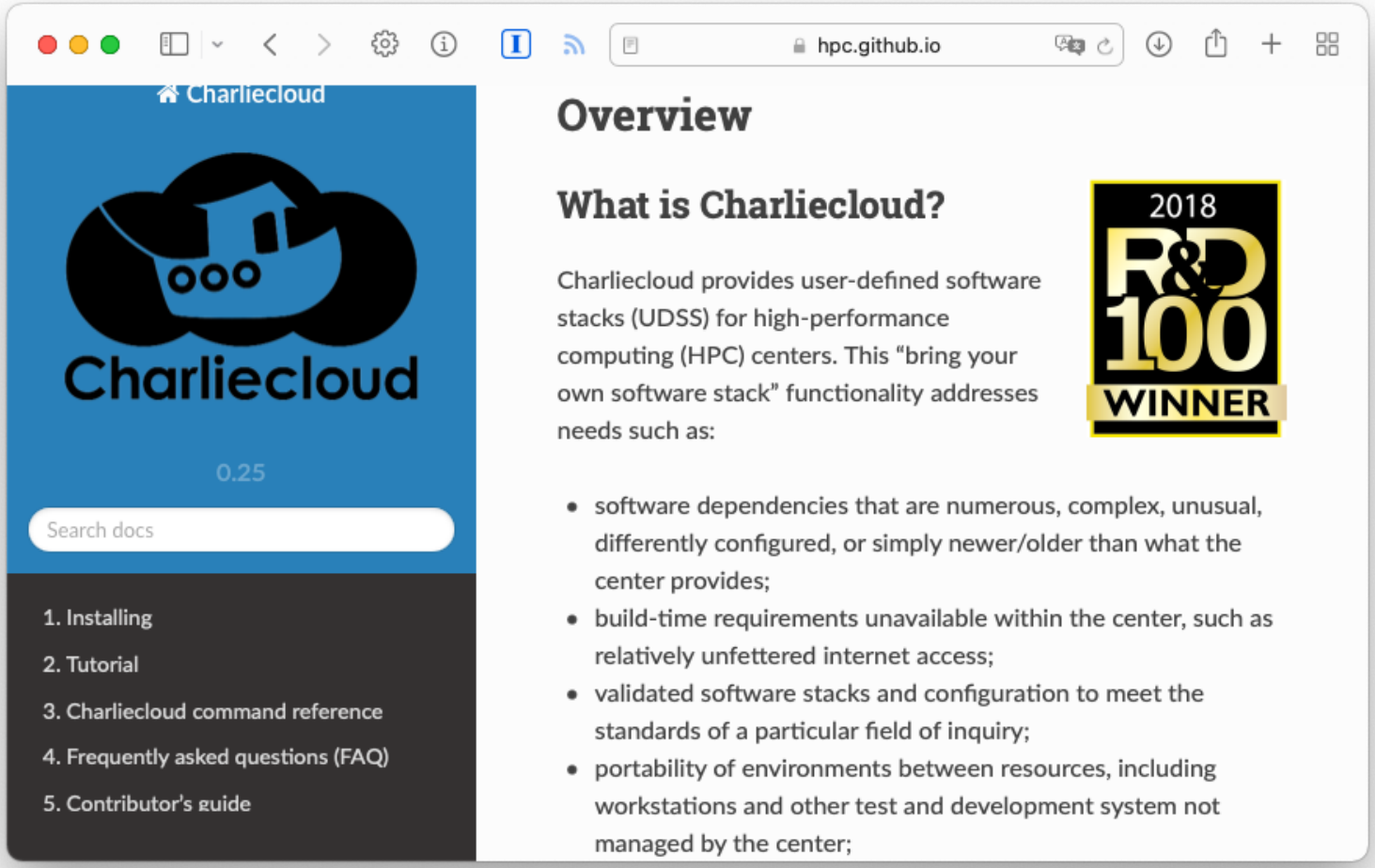
Docker is not HPC friendly

HPC Container Runtime Systems

Charliecloud

- Still relies on Docker images and Dockerfile as they are widespread BUT do not require any privileged operation
- Makes use of the unprivileged user namespace

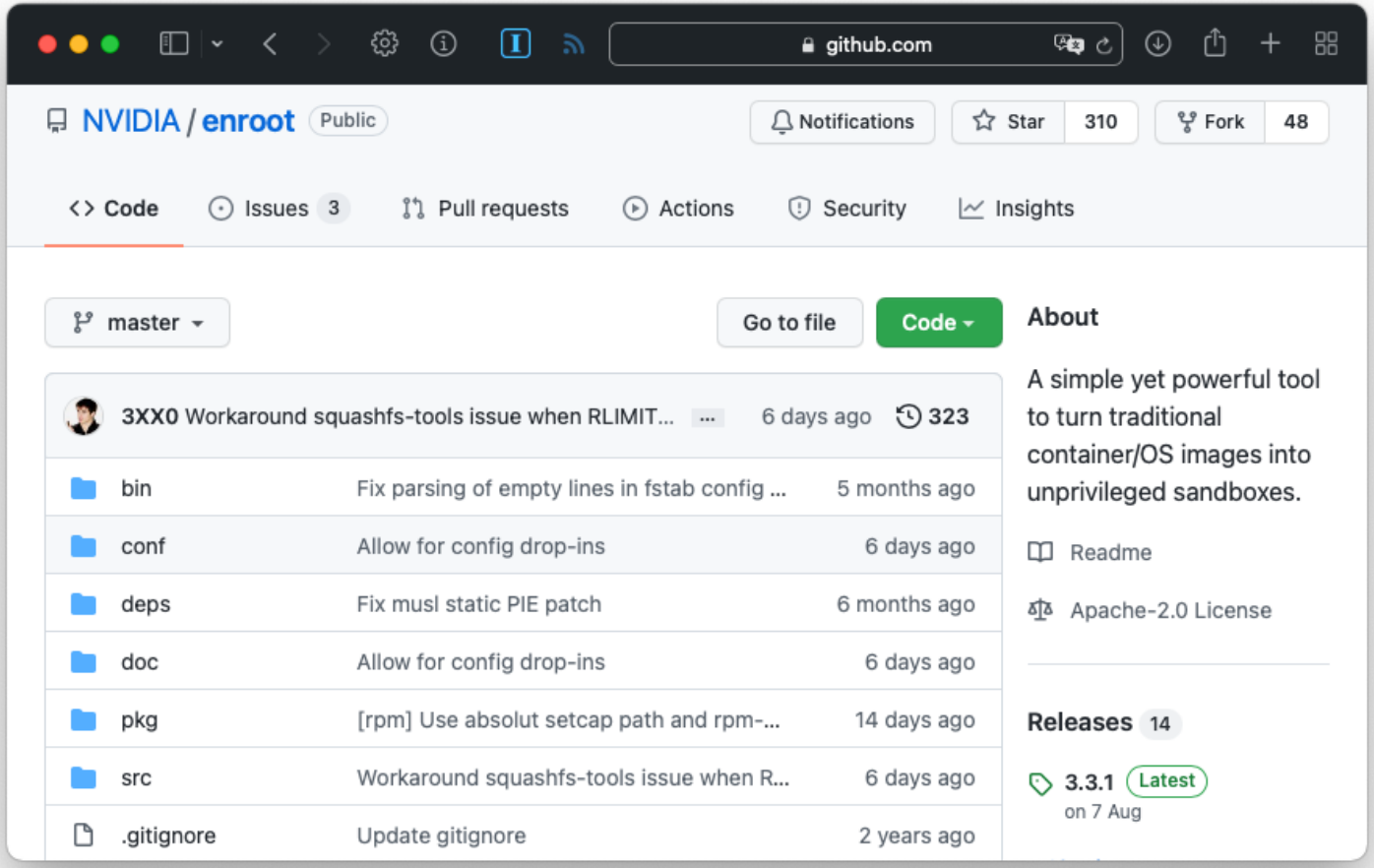
1. Create your Docker image
2. Convert and flatten the image
3. Upload it to the HPC system
4. Submit your job with a Slurm script



Enroot

- Developed by NVIDIA for AI / HPC workloads and Supports Docker images (Docker Hub /NGC) WITHOUT root privileges
- Lightweight and near-native performance

1. Create or import a Docker image
2. Convert to a .sqsh format
3. Upload it to the HPC system
4. Submit your job with a Slurm script



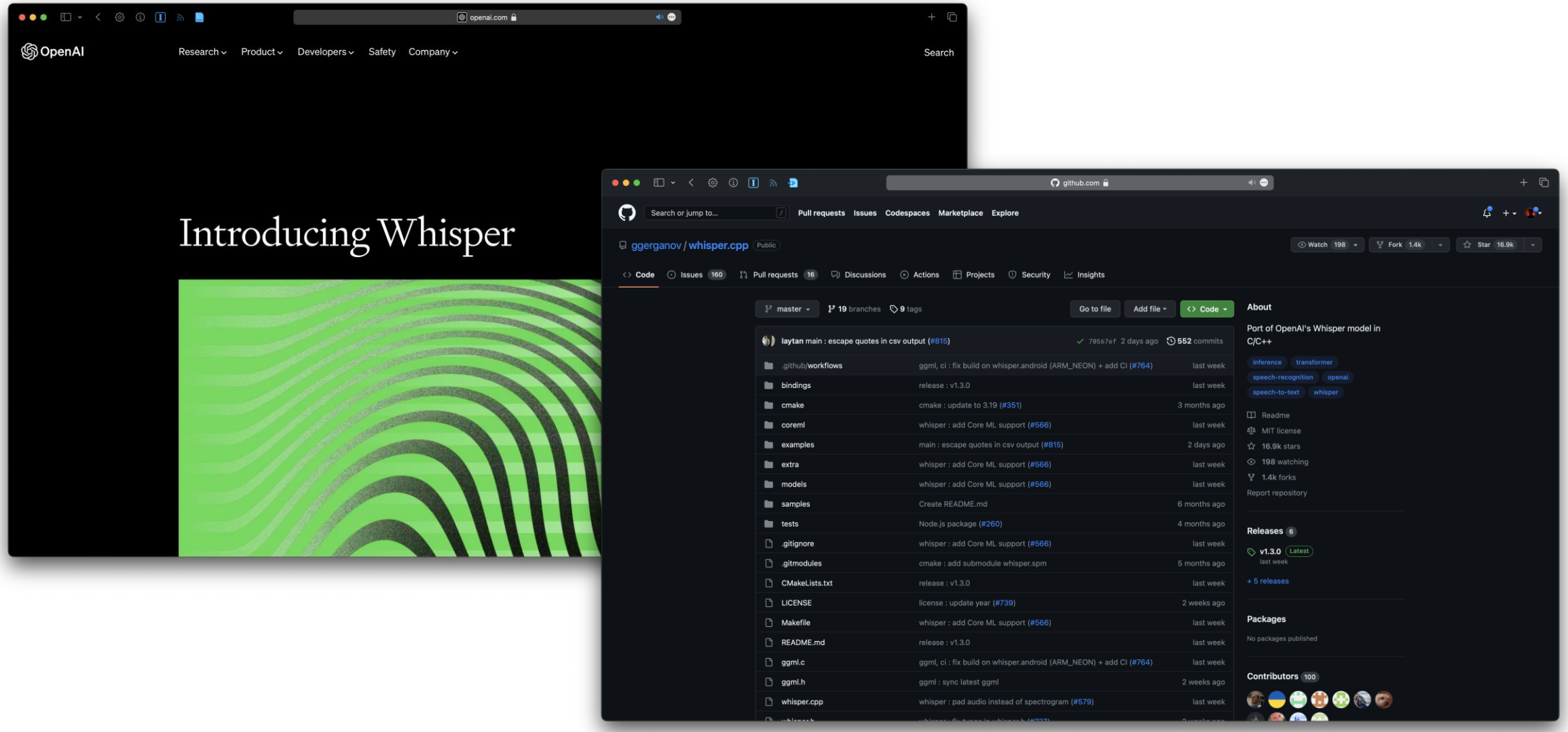
Charliecloud vs. Enroot

Charliecloud	Enroot
HPC systems - Use docker image - Create a tar file - chroot into it - Run isolate from the system - Fake root inside the container	**AI systems** - Use docker images (from Docker Hub or NGC catalog) - Run in user space - Flow: import, create, start - .sqsh images - Associated with a scheduler - More adapted to AI

Hands-on #3:HPC AI: Speech-to-Text With OpenAI Whicper.cpp in Enroot

OpenAI Whisper.cpp

https://openai.com/research/whisper



https://github.com/ggerganov/whisper.cpp

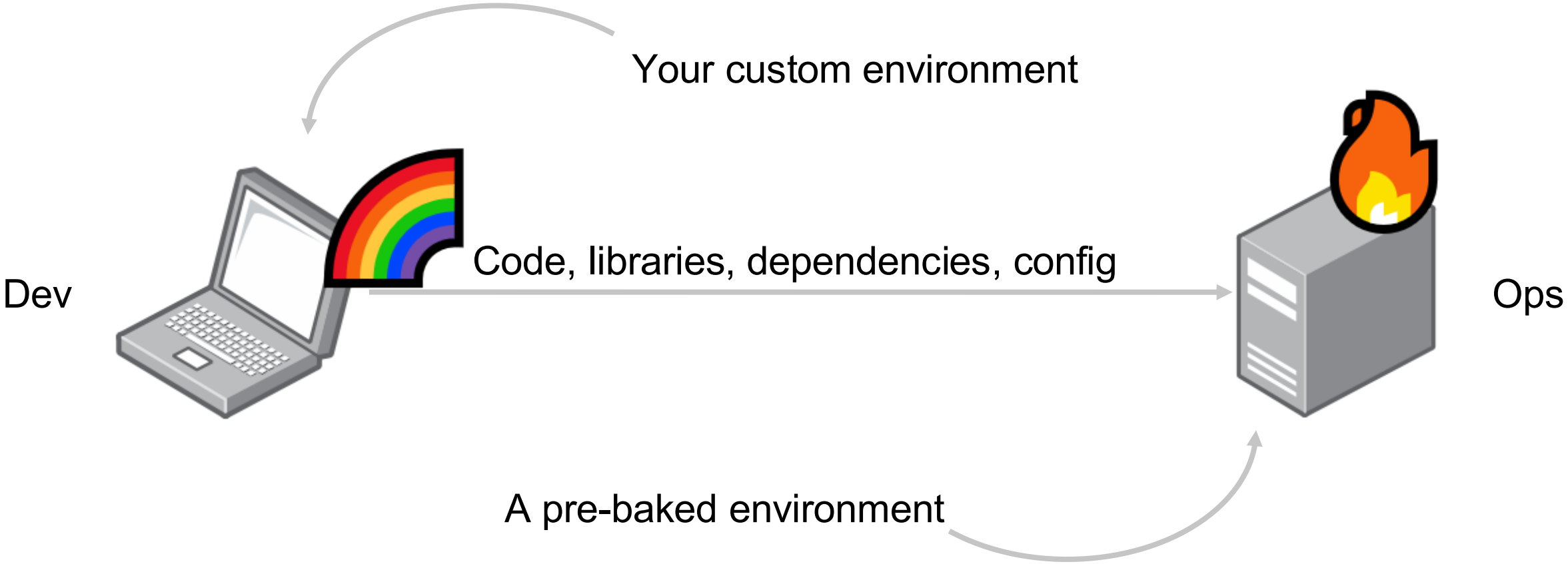
Exercise Guide and Solution

- In the question, we provide Dockerfile. You need to
  - Build the image
  - Convert to enroot
  - Create an enroot container
  - Start it while mounting /data to get audio files and a model
- You can convert speech to text!

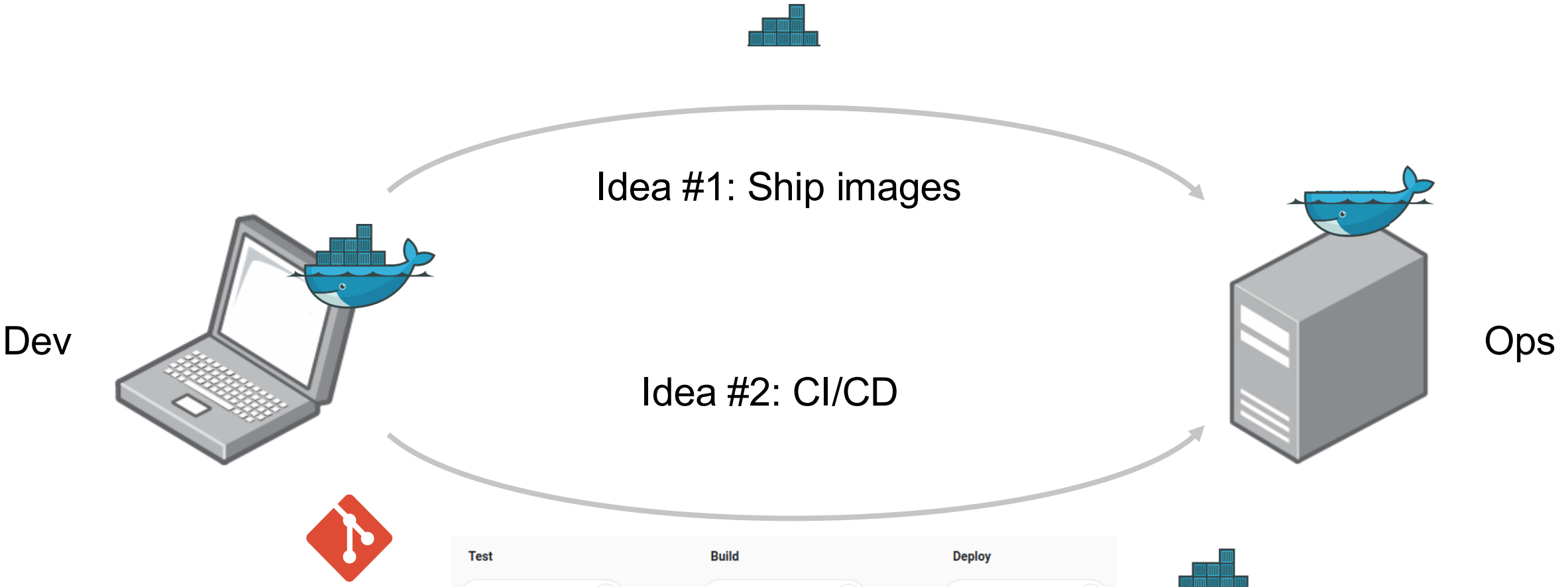
- You can also go into the solution and use make solution

Part III: Container Abstraction and Scientific Workflows

Container Abstraction



CI/CD with Containers



Reproducible Scientific Workflows

www.nature.com/scientificdata

SCIENTIFIC DATA

Amended: Addendum

OPEN

SUBJECT CATEGORIES
» Research data
» Publication characteristics

Comment: The FAIR Guiding Principles for scientific data management and stewardship

Mark D. Wilkinson *et al.*#

Received: 10 December 2015
Accepted: 12 February 2016
Published: 15 March 2016

There is an urgent need to improve the infrastructure supporting the reuse of scholarly data. A diverse set of stakeholders—representing academia, industry, funding agencies, and scholarly publishers—have come together to design and jointly endorse a concise and measureable set of principles that we refer to as the FAIR Data Principles. The intent is that these may act as a guideline for those wishing to enhance the reusability of their data holdings. Distinct from peer initiatives that focus on the human scholar, the FAIR Principles put specific emphasis on enhancing the ability of machines to automatically find and use the data, in addition to supporting its reuse by individuals. This Comment is the first formal publication of the FAIR Principles, and includes the rationale behind them, and some exemplar implementations in the community.

Supporting discovery through good data management

Good data management is not a goal in itself, but rather is the key conduit leading to knowledge discovery and innovation, and to subsequent data and knowledge integration and reuse by the community after the data publication process. Unfortunately, the existing digital ecosystem surrounding scholarly data publication prevents us from extracting maximum benefit from our research investments (e.g., ref. 1). Partially in response to this, science funders, publishers and governmental agencies are beginning to require data management and stewardship plans for data generated in publicly funded experiments. Beyond proper collection, annotation, and archival, data stewardship includes the notion of 'long-term care' of valuable digital assets, with the goal that they should be discovered and re-used for downstream investigations, either alone, or in combination with newly generated data. The outcomes from good data management and stewardship, therefore, are high quality digital publications that facilitate and simplify this ongoing process of discovery, evaluation, and reuse in downstream studies. What constitutes 'good data management' is, however, largely undefined, and is generally left as a decision for the data or repository owner. Therefore, bringing some clarity around the goals and desiderata of good data management and stewardship, and defining simple guideposts to inform those who publish and/or preserve scholarly data, would be of great utility.

This article describes four foundational principles—Findability, Accessibility, Interoperability, and Reusability—that serve to guide data producers and publishers as they navigate around these obstacles, thereby helping to maximize the added-value gained by contemporary, formal scholarly digital publishing. Importantly, it is our intent that the principles apply not only to 'data' in the conventional sense, but also to the algorithms, tools, and workflows that led to that data. All scholarly digital research objects[2]—from data to analytical pipelines—benefit from application of these principles, since all components of the research process must be available to ensure transparency, reproducibility, and reusability.

There are numerous and diverse stakeholders who stand to benefit from overcoming these obstacles: researchers wanting to share, get credit, and reuse each other's data and interpretations; professional data publishers offering their services; software and tool-builders providing data analysis and processing services such as reusable workflows; funding agencies (private and public) increasingly

Correspondence and requests for materials should be addressed to B.M. (email: barend.mons@dtls.nl).
#A full list of authors and their affiliations appears at the end of the paper.

COMPUTER SCIENCE

Accessible Reproducible Research

As use of computation in research grows, new tools are needed to expand recording, reporting, and reproduction of methods and data.

Jill P. Mesirov

Scientific publications have at least two goals: (i) to announce a result and (ii) to convince readers that the result is correct. Mathematics papers are expected to contain a proof complete enough to allow knowledgeable readers to fill in any details. Papers in experimental science should describe the results and provide a clear enough protocol to allow successful repetition and extension.

Over the past ~35 years, computational science has posed challenges to this traditional paradigm—from the publication of the four-color theorem in mathematics (*1*), in which the proof was partially performed by a computer program, to results depending on computer simulation in chemistry, materials science, astrophysics, geophysics, and climate modeling. In these settings, the scientists are often sophisticated, skilled, and innovative programmers who develop large, robust software packages.

More recently, scientists who are not themselves computational experts are conducting data analysis with a wide range of modular software tools and packages. Users may often combine these tools in unusual or novel ways. In biology, scientists are now routinely able to acquire and explore data sets far beyond the scope of manual analysis, including billions of DNA bases, millions of genotypes, and hundreds of thousands of RNA measurements. Similar issues may arise in other fields, such as astronomy, seismology, and meteorology. While propelling enormous progress, this increasing and sometimes "indirect" use of computation poses new challenges for scientific publication and replication. Large data sets are often analyzed many times, with modifications to the methods and parameters, and sometimes even updates of the data, until the final results are produced. The resulting publication often gives only scant attention to the computational details. Some have suggested these papers are "merely the advertisement of scholarship whereas the computer programs, input data, parameter values, etc. embody the scholarship itself" (*2*). However, the actual code or software "mashup" that gave rise to the final analysis may be lost or unrecoverable.

For example, colleagues and I published a computational method for distinguishing between two types of acute leukemia, based on large-scale gene expression profiles obtained from DNA microarrays (*3*). This paper generated hundreds of requests from scientists interested in replicating and extending the results. The method involved a complex pipeline of steps, including (i) preprocessing of the data, to eliminate likely artifacts; (ii) selection of genes to be used in the model; (iii) building the actual model and setting the appropriate parameters for it from the training data; (iv) preprocessing independent test data; and finally (v) applying the model to test its efficacy. The result was robust and replicable, and the original data were available online, but there was no standardized form in which to make available the various software components and the precise details of their use.

Reproducible Research

This experience motivated the creation of a way to encapsulate all aspects of our in silico analyses (*3*) in a manner that would facilitate independent replication by another scientist (*4*). Computer and computational scientists refer to this goal as "reproducible research" (*5*), a coinage attributed to the geophysicist Jon Claerbout in 1990, who imposed the standard of makefiles for construction of all the figures and computational results in papers published by the Stanford Exploration Project (*6*). Since that time, other approaches have been proposed (*7*–*14*), including the ability to insert active scripts within a text document (*15*) and the use of a markup language that can produce all of the text, figures, code, algorithms, and settings used for the computational research (*16*). Although these approaches may accomplish the goal, they are not practical for many nonprogramming experimental scientists using other groups' or commercial software tools today.

A similar challenge was encountered more than 20 years ago when scientists wanting to access data from remote computers had to write their own retrieval programs. The solution was the invention of the World Wide Web (*17*), together with the concept of "Web browsers" such as MOSAIC (*18*) and its successors. The approach was so effective that we now take it for granted.

In the same spirit, we need a paradigm that makes it simple, even for scientists who do not themselves program, to perform and publish reproducible computational research. Toward this end, we propose a Reproducible Research System (RRS), consisting of two components. The first element is a Reproducible Research Environment (RRE) for doing the computational work. An RRE provides computational tools together with the ability to automatically track the provenance of data, analyses, and results and to package them (or pointers to persistent versions of them) for redistribution. The second element is a Reproducible Research Publisher (RRP), which is a document-preparation system, such as standard word-processing software, that provides an easy link to the RRE. The RRS thus makes it easy to perform analyses and then to embed them directly into a

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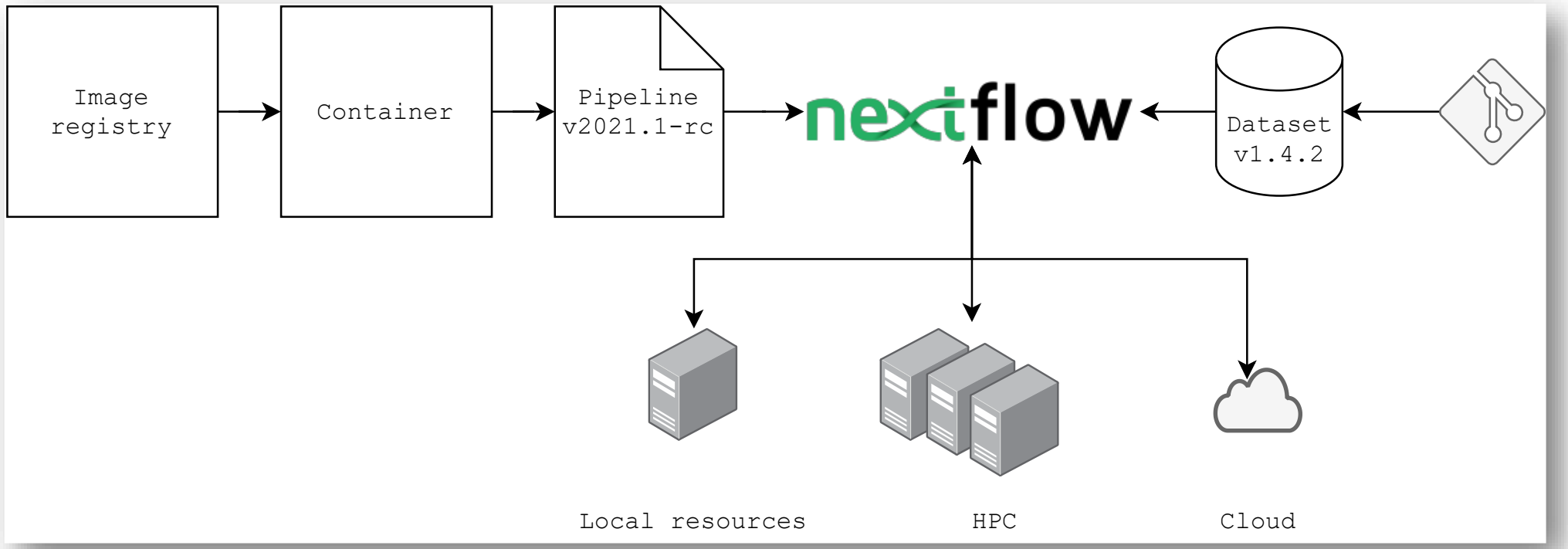
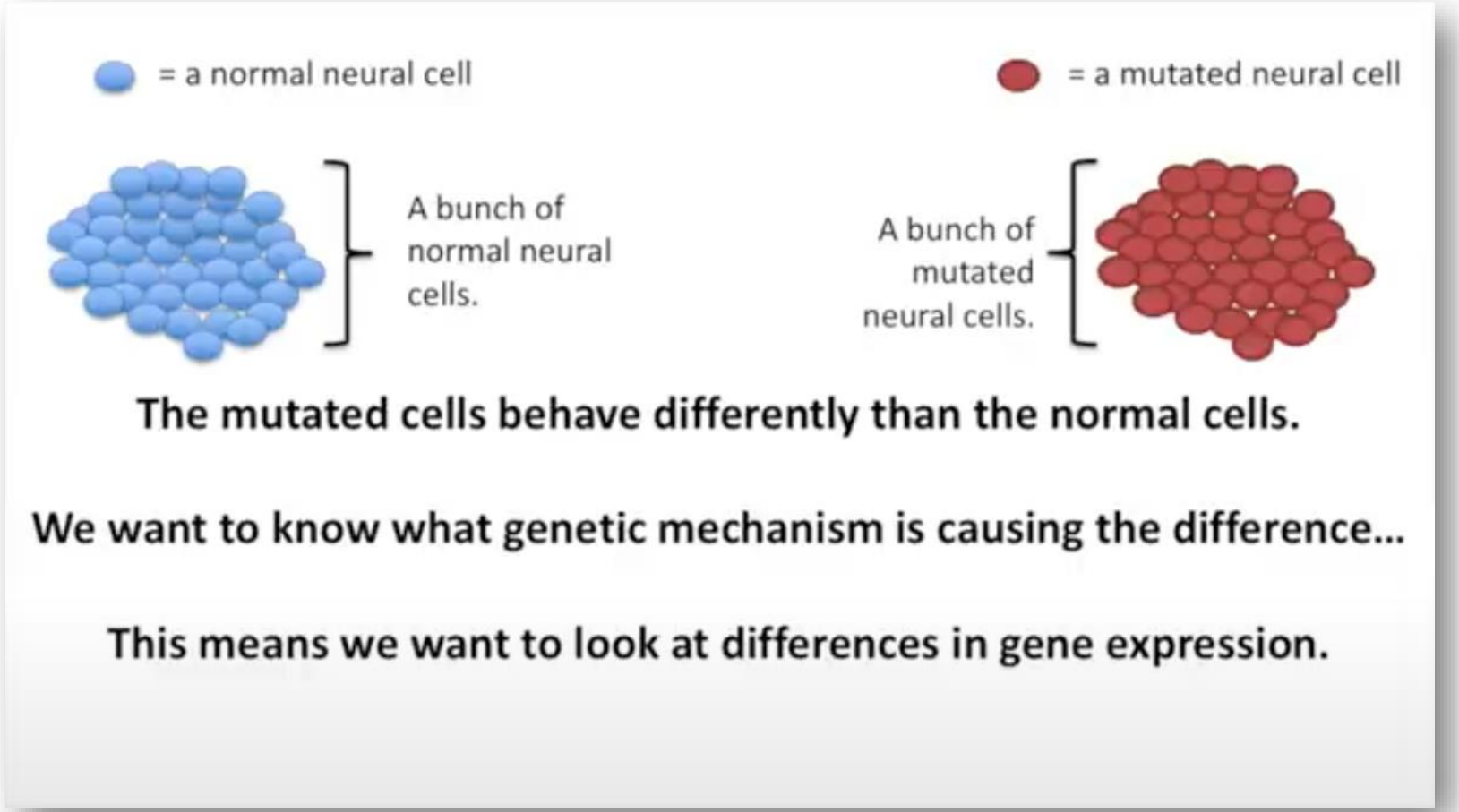
CREDIT: JOE BUTLER/WWW.CSMD.COM.AU/DE

Reproducible Scientific Workflows

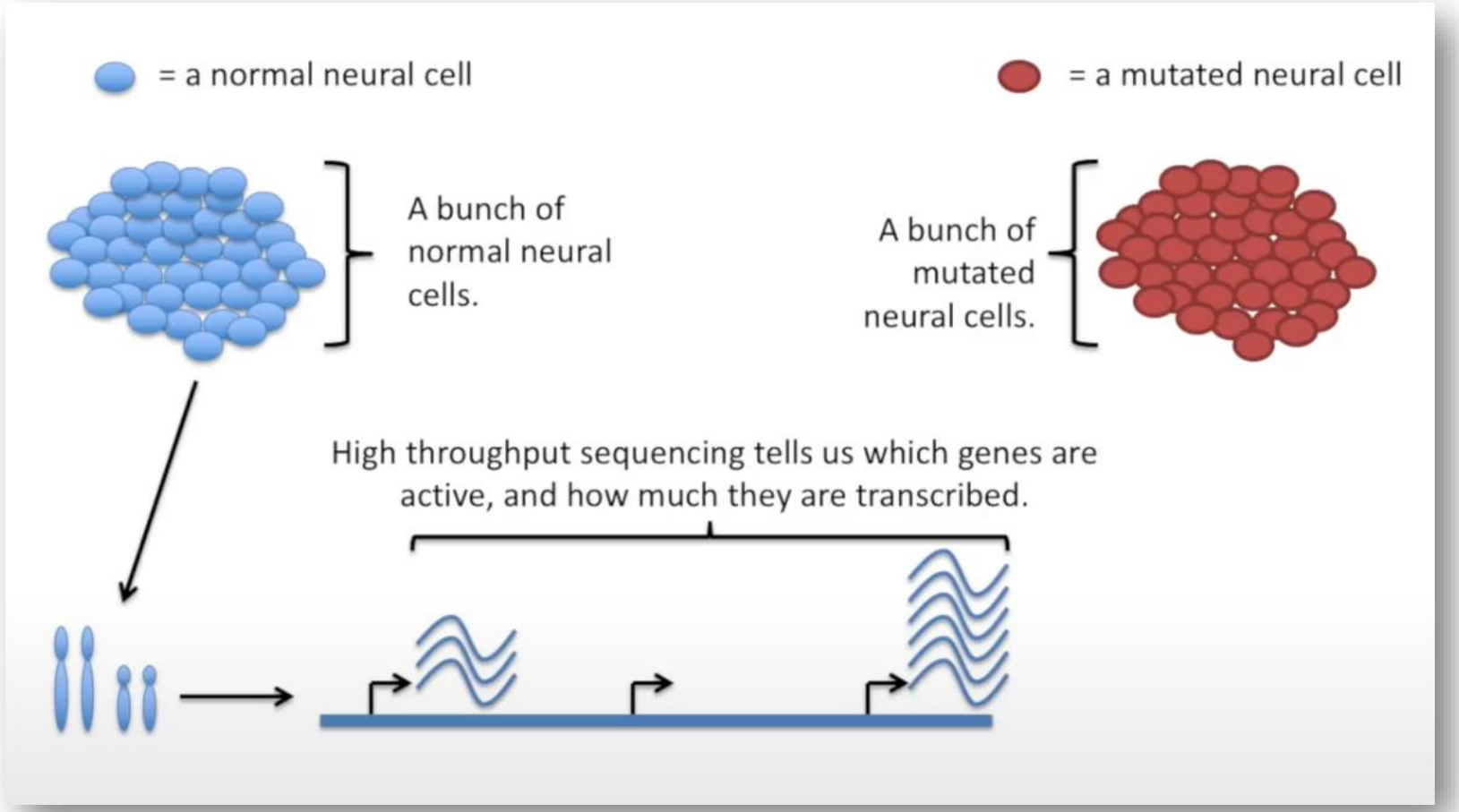


Hands-on #4: Reproducible RNA-seq Scientific Workflow With Nextflow and Docker

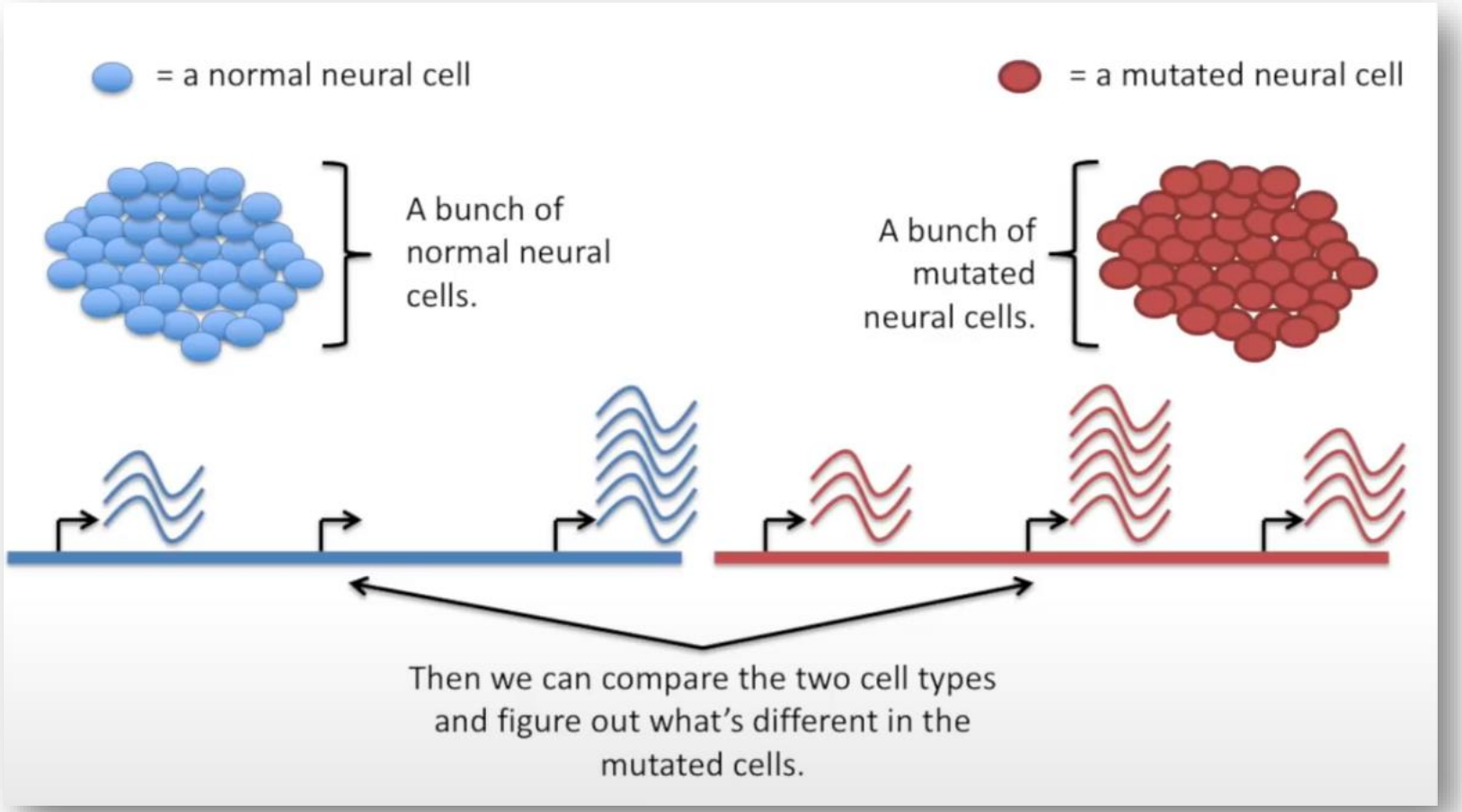
RNA Sequencing: Principles and Motivation



Measuring Gene Expression With High-Throughput Sequencing



Differential Gene Expression Analysis



RNA-seq Experiment Workflow

We measure the gene expression in both cell populations and compare the results to see what's happening in the mutated cells.

A RNA-Seq experiment usually occurs in 3 main steps:

i) Biological sample preparation (preparation of the library)
ii) Sequencing
iii) Data analysis

An illumina sequencer

RNA-seq Data Analysis Pipeline: FastQC, MultiQC, and Salmon

Data analysis:

- FastQC: To quality check the sequencing. Sequences with poor quality must be trimmed or filtered.
- MultiQC: Also to quality check, with additional information.
- Salmon: That must be run after the quality check and reads filtering. Salmon allows the mapping of high quality reads on a genome and a genes set in order to establish the differential gene expression.

Exercise Guide and Solution

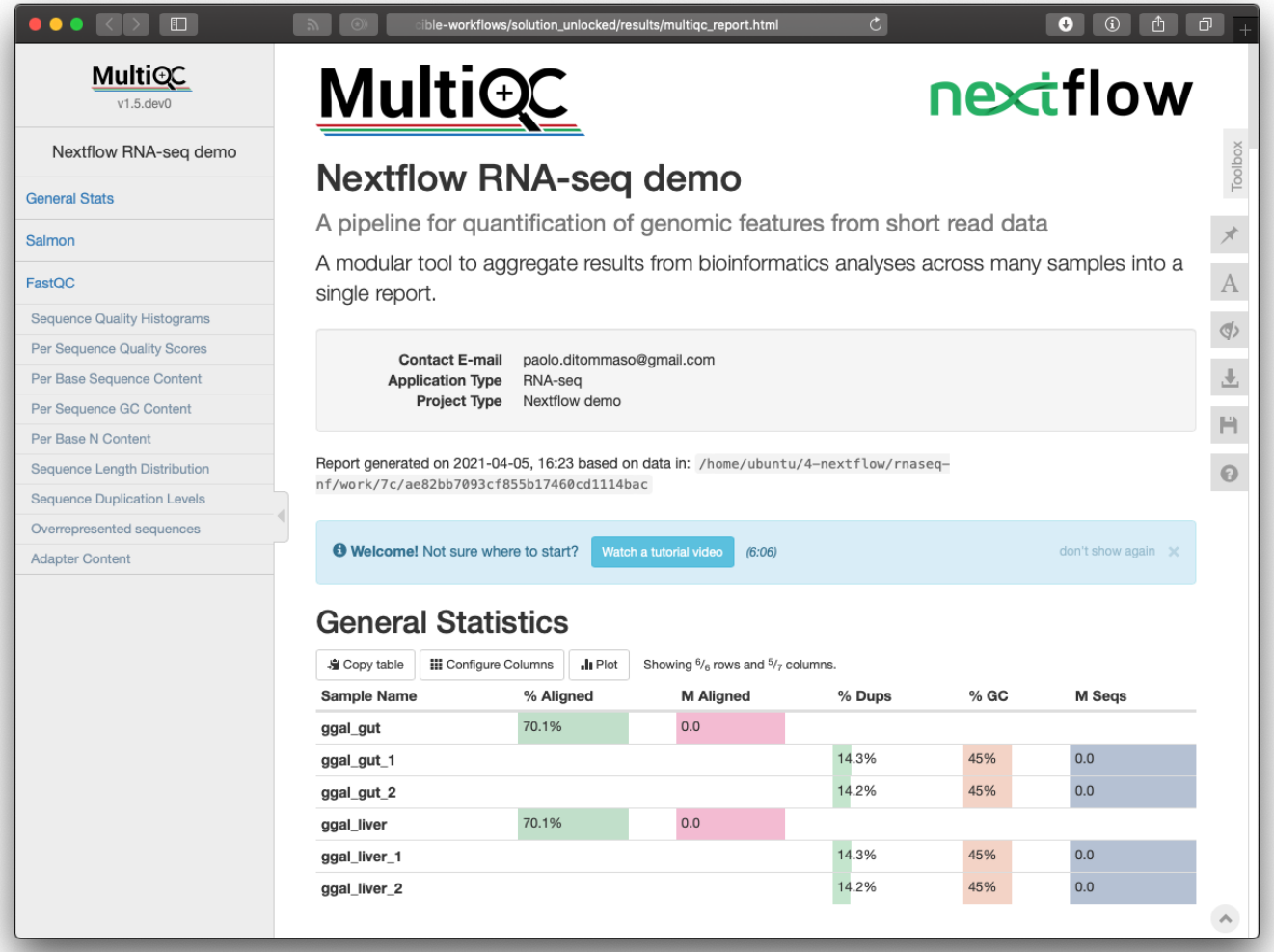
```
# Let's get the Nextflow code along with the dataset
git clone "https://github.com/nextflow-io/rnaseq-nf.git"
#Cloning into 'rnaseq-nf'...

# And run the pipeline locally in a docker container
cd rnaseq-nf
nextflow run nextflow-io/rnaseq-nf -with-docker
# R N A S E Q - N F   P I P E L I N E
#  ===================================
#  transcriptome: /home/ubuntu/.nextflow/assets/nextflow-io/rnaseq-nf/data/ggal/
    ggal_1_48850000_49020000.Ggal71.500bpflank.fa
#  reads        : /home/ubuntu/.nextflow/assets/nextflow-io/rnaseq-nf/data/ggal/*_
    {1,2}.fq
#  outdir       : results
# executor >  local (6)
# [06/dd0ce9] process > RNASEQ:INDEX (ggal_1_48850000_49020000) [100%] 1 of 1 /
# [a5/514067] process > RNASEQ:FASTQC (FASTQC on ggal_liver)    [100%] 2 of 2 /
# [9c/af0a9d] process > RNASEQ:QUANT (ggal_liver)               [100%] 2 of 2 /
# [70/d1650e] process > MULTIQC                                 [100%] 1 of 1 /
# Done! Open the following report in your browser --> results/multiqc_report.html

# That's it ! The rport is published in the results folder!
# Use scp to get visualize it on your local machine
```

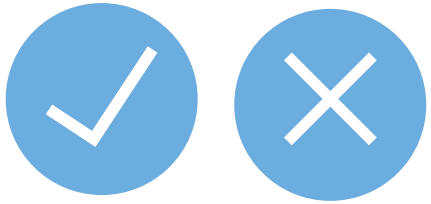
Can you use the caddy web server (as illustrated on code snippet 6) to expose the result of the pipeline as a web page accessible on port 8888?

Exercise Guide and Solution

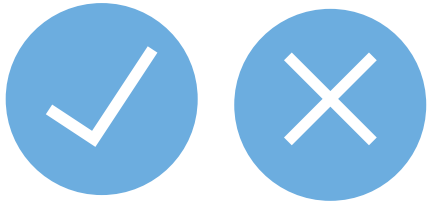


Take home message

Containers are the ephemeral running instance of an environment: an application, its runtime, dependencies, libraries, settings etc.

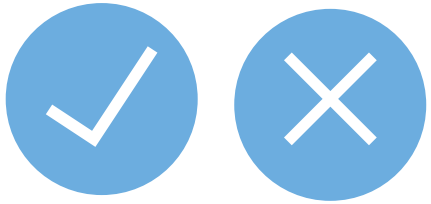


Virtual Machine (VM)s and containers are different technologies, each with its own advantages depending on the use case



Take-home message

Containers can not mount volumes from the host and expose ports.

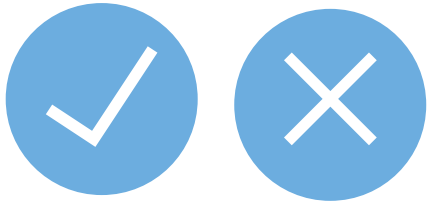


Containers can be committed to images, manually or thanks to a Domain-Specific Language (DSL) like the Dockerfile.

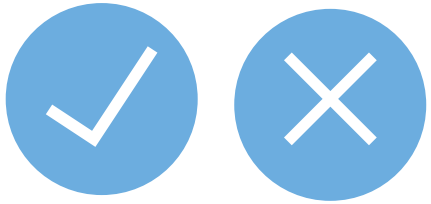
The syntax of the Dockerfile is expressive.

The Dockerfile is the cornerstone of all container platforms.

They are easy to write, share, and build.



One can convert a Docker image to other format like enroot and Charliecloud which are suited to HPC applications



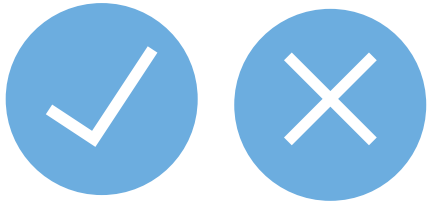
Take-home message

Containers allow

Containers allow consistency and reproducibility:

software build, scientific pipelines etc.

You to spend more time on your research that managing software



Upcoming courses

Look for the AI Training Series (free)

AI Training Series - Orientation Session	08.04.2026 – 09.04.2026	ONLINE
Intel Developer Workshop	20.04.2026 – 21.04.2026	Leibniz Rech
AI Training Series - Introduction to Container Technology & Application to AI at LRZ	27.04.2026 – 27.04.2026	ONLINE
AI Training Series - Introduction to the LRZ AI Systems	04.05.2026 – 04.05.2026	ONLINE
Introduction to C++	11.05.2026 – 13.05.2026	ONLINE
POSTPONED AI Training Series - Scaling Deep Learning - From Single GPU to Clusters	18.05.2026 – 20.05.2026	Leibniz Rech
Introduction to CoolMUC-4 with Focus on CFD and FEM Workflows	21.05.2026 – 21.05.2026	ONLINE

https://app1.edoobox.com/en/LRZ