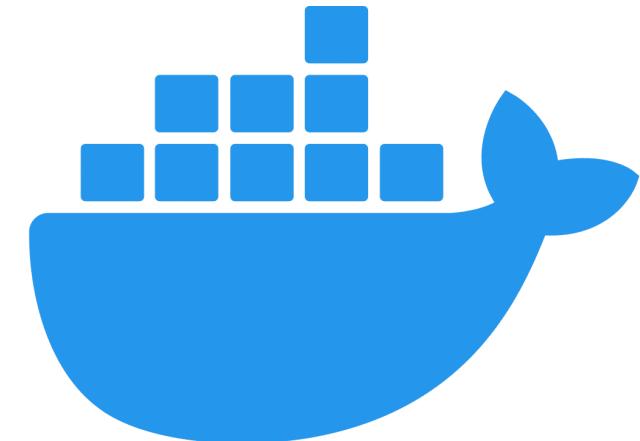




jimmyliu1326/cidgoh\_docker\_2023

# Software Containerization with Docker

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Feb 14th 2023

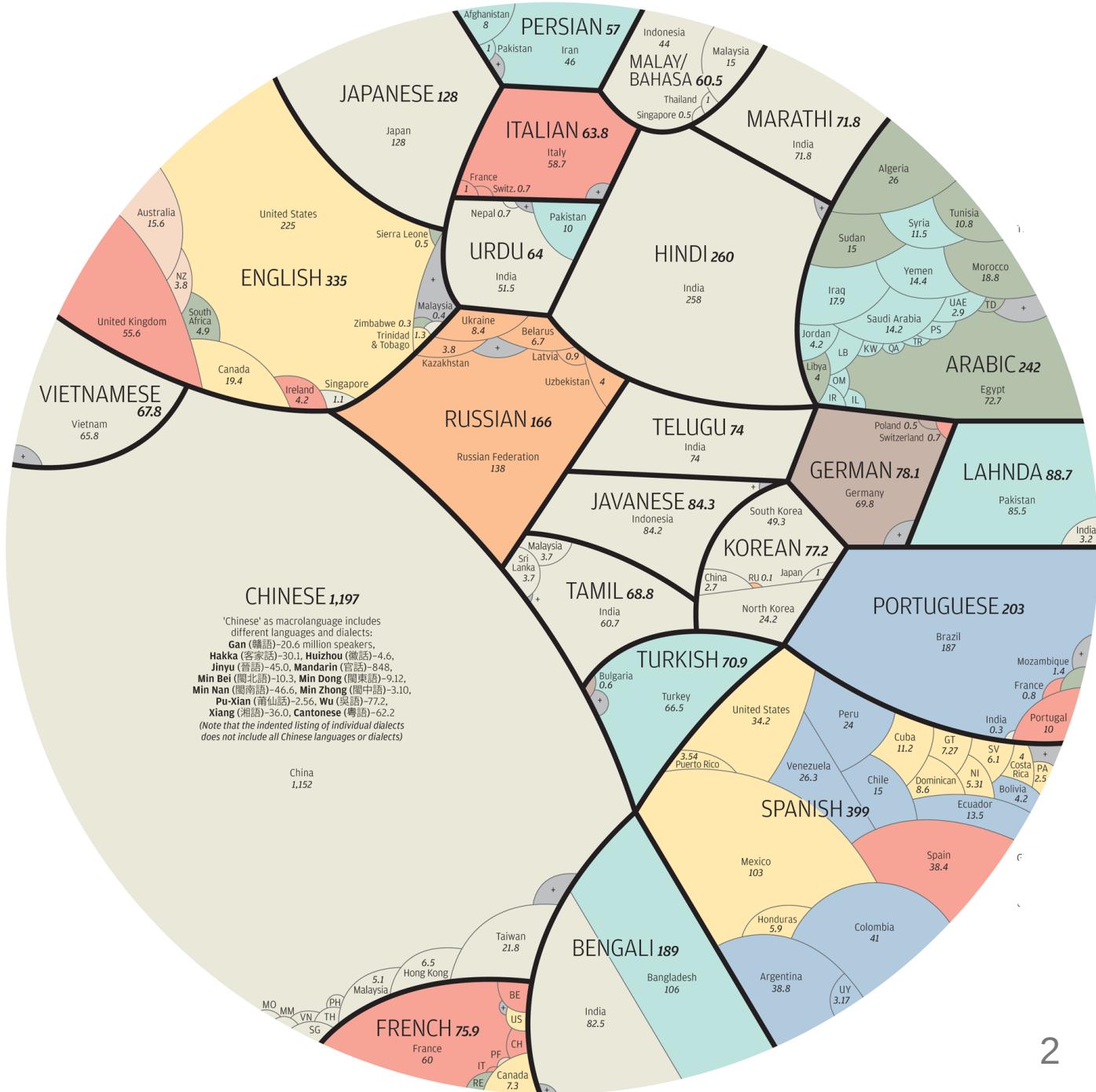


docker®



CENTRE FOR  
INFECTIOUS DISEASE  
GENOMICS AND  
ONE HEALTH

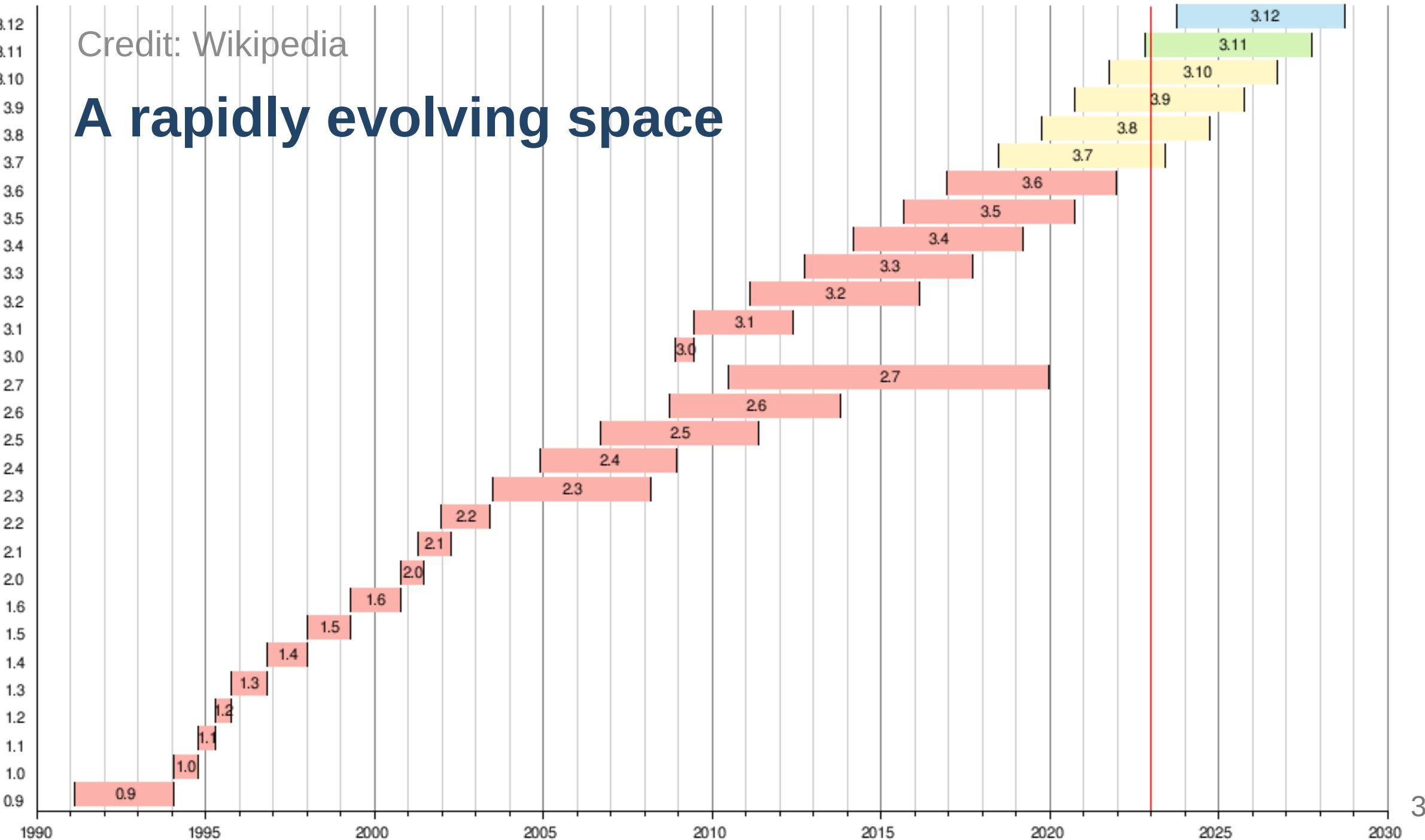
# The world is a diverse place

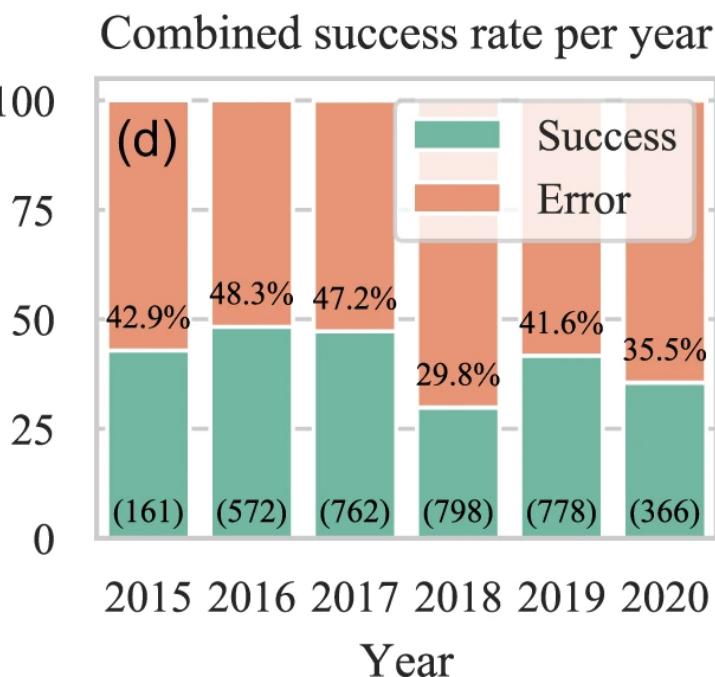
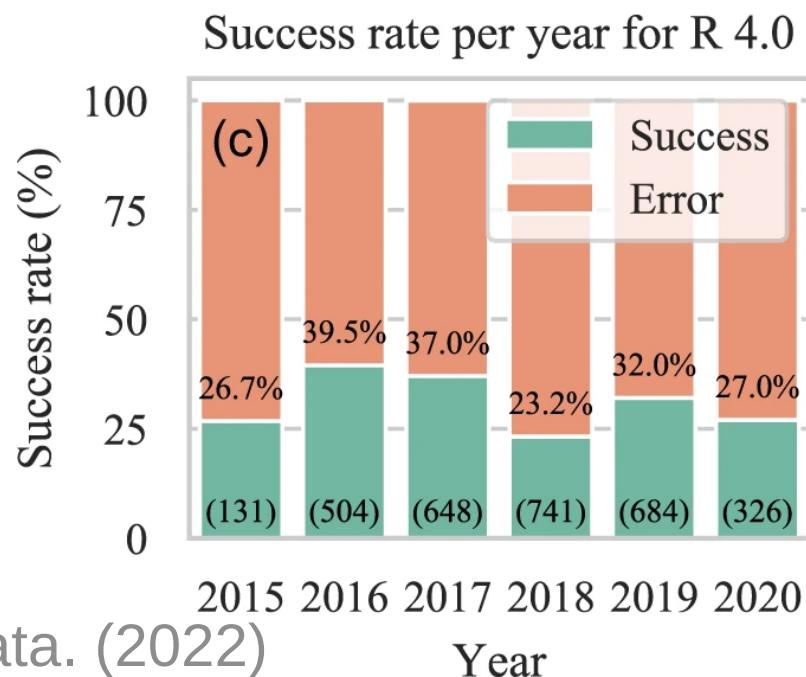
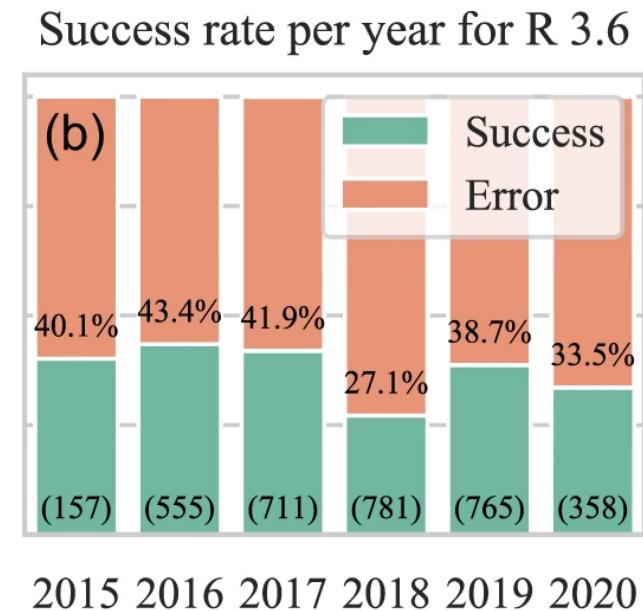
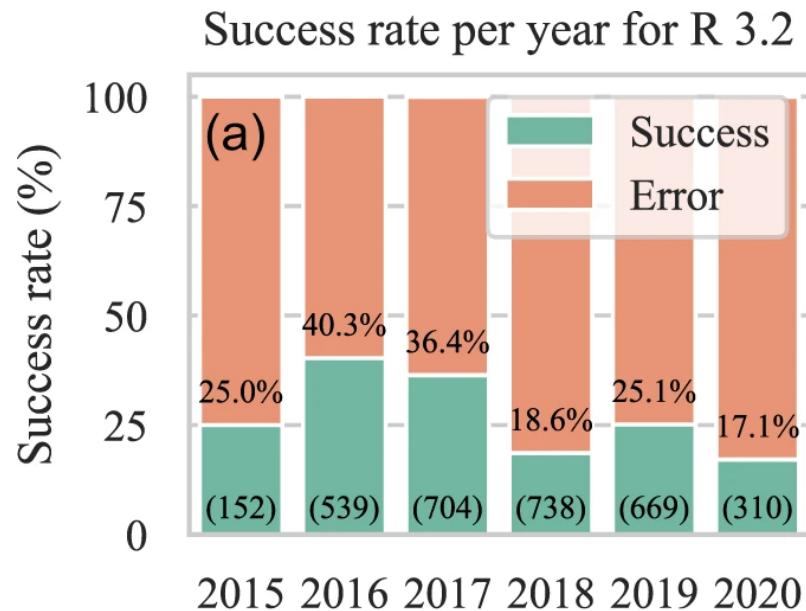


## Credit:

Credit: Wikipedia

# A rapidly evolving space





## Challenge

**Sharing and deploying reproducible code in dynamic and diverse environments**

# Solution

A host-independent format to package and deploy software components

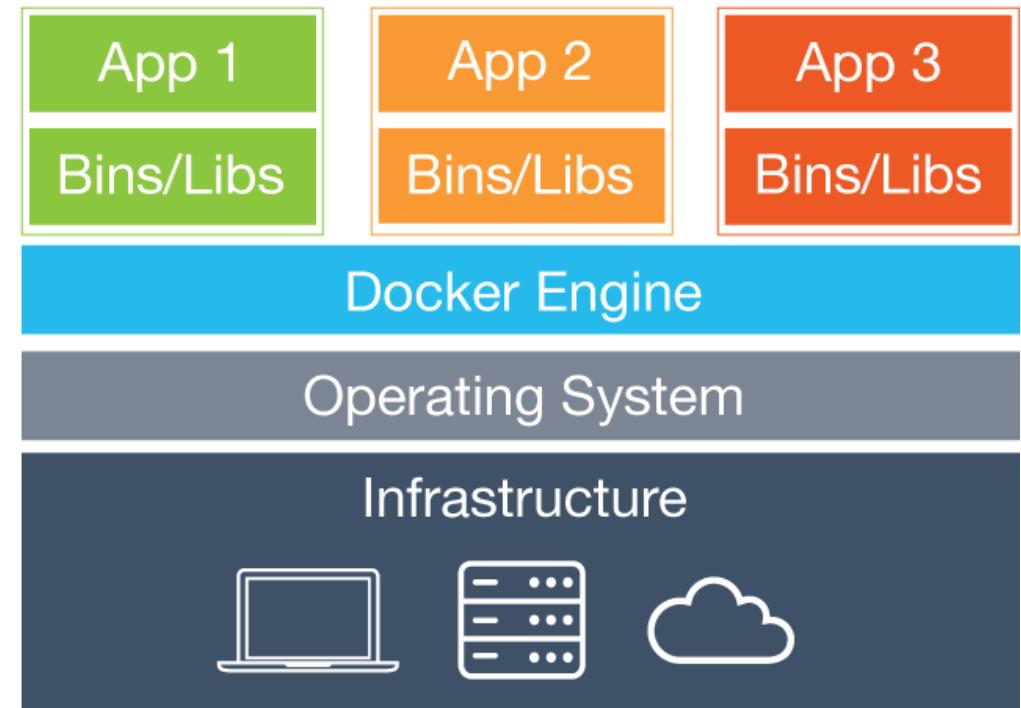
Credit: Google Images





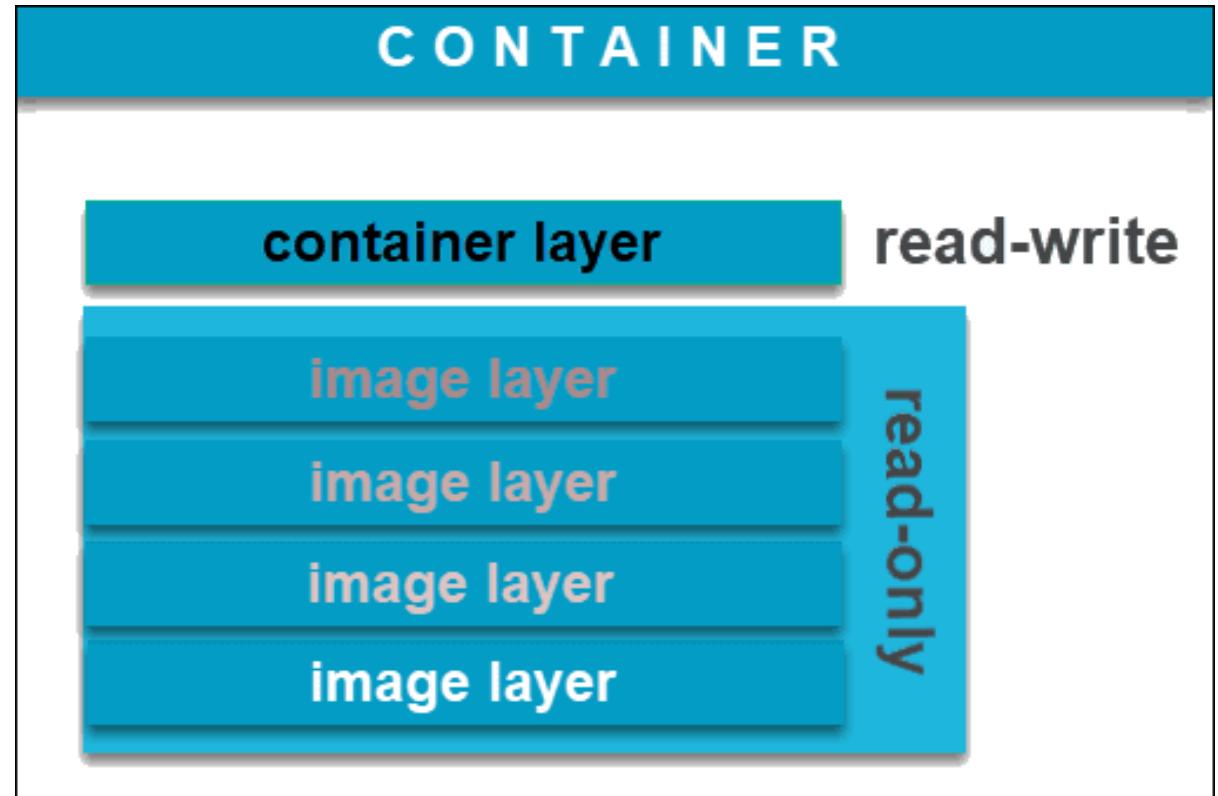
# Docker Architecture

- Can virtualize multiple OS on any host infrastructure
- Source code, libraries, dependencies are packaged in immutable objects called `images`
- Mutable running instances of `images` are called `containers`



# A container is simply another layer on top

- New images are built by adding layers to existing images
- Each layer encodes tracked changes



# Demo: Writing a Dockerfile

Directive	Description	Example
FROM	Base image	FROM python:3.9.16
RUN	Command(s) to execute	RUN pip install pandas
ARG	Define variables within Dockerfile	ARG script=".src/parse.py"
ADD	Import files from the host system	ADD \$script /src/
ENV	Define environment variables accessible within containers	ENV BLAST_DB="/data/ncbi.db"

# Demo: Writing a Dockerfile (10 minutes)

1. Build a custom image using `biocontainers/blast:2.2.31` as base image
2. Add the query sequence to the image under `/data`
3. Add the BLAST database to the image under `/blast_db`

# Demo: Building the Docker image

## Command structure

```
docker build -t [image_name]:[image_tag] [Path to Dockerfile]
```

## Example command

```
docker build -t blast:[username] .
```

# Demo: Running BLAST in Docker containers

## Command structure

```
docker run [image_name] [cmd]
```

## Example command

```
docker run blast blastn \  
  -db /blast_db/plasmids \  
  -query /data/query.fasta \  
  -out blast.out \  
  -outfmt 6 \  
  -word_size 7 \  
  -evalue 1e-5
```

# Demo: Pushing Docker image to Container Registry

## Log into DockerHub

- Username: cidgoh
- Password: See [spreadsheet](#)

```
docker login -u [username] -p [password]
```

## Tag image

```
docker tag blast cidgoh/blast:[username]
```

## Push image to DockerHub

```
docker push cidgoh/blast:[username]
```

# Advanced Topics

- Automated builds with CI/CD
- Persistent volumes
- Multi-stage builds
- Multi-container applications ( docker-compose )