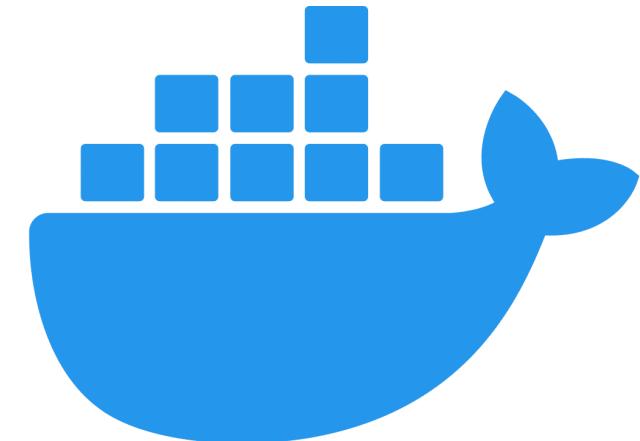




jimmyliu1326/cidgoh_docker_2023

Software Containerization with Docker

Jimmy Liu
Feb 14th 2023



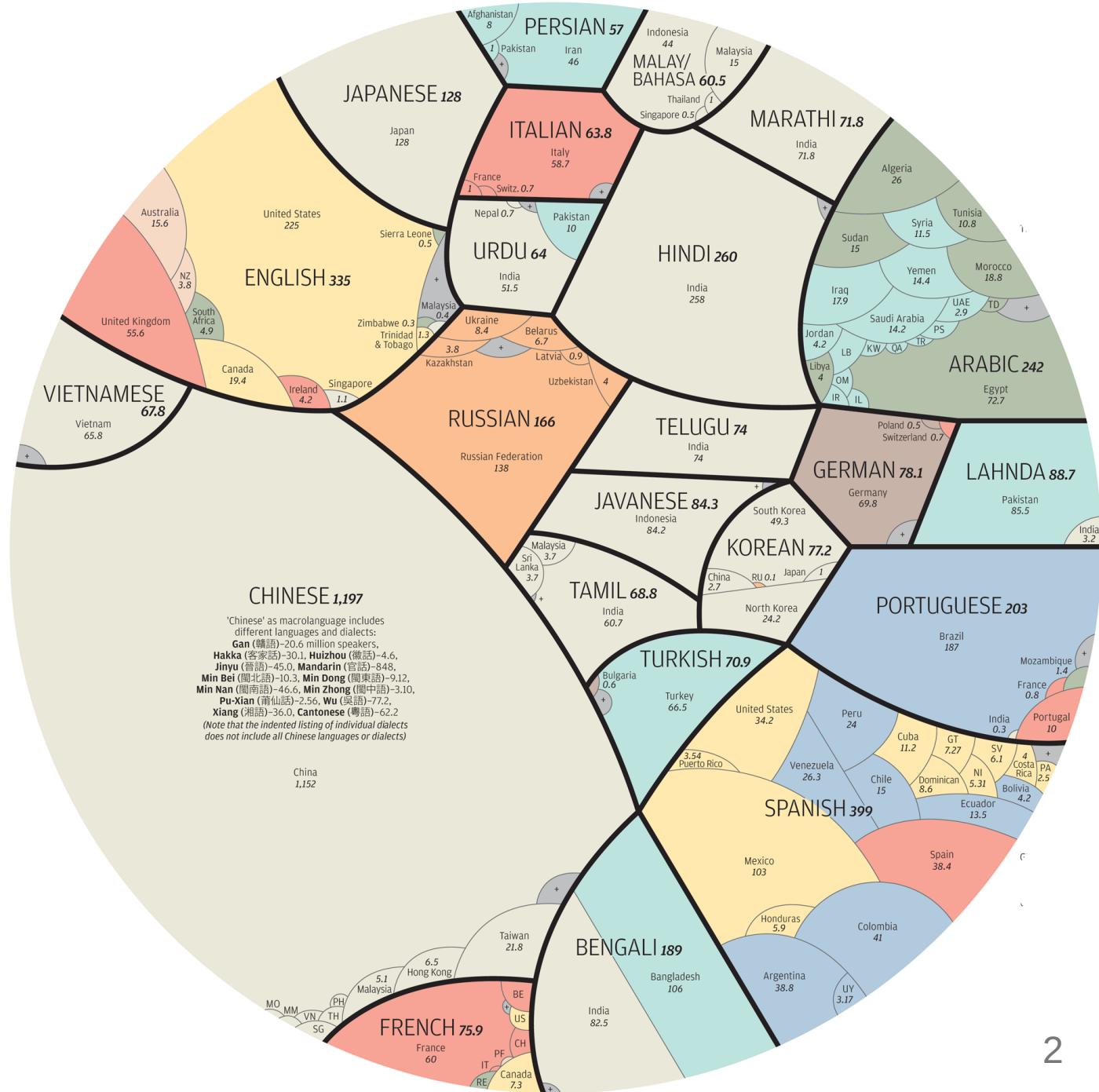
docker®



CENTRE FOR
INFECTIOUS DISEASE
GENOMICS AND
ONE HEALTH

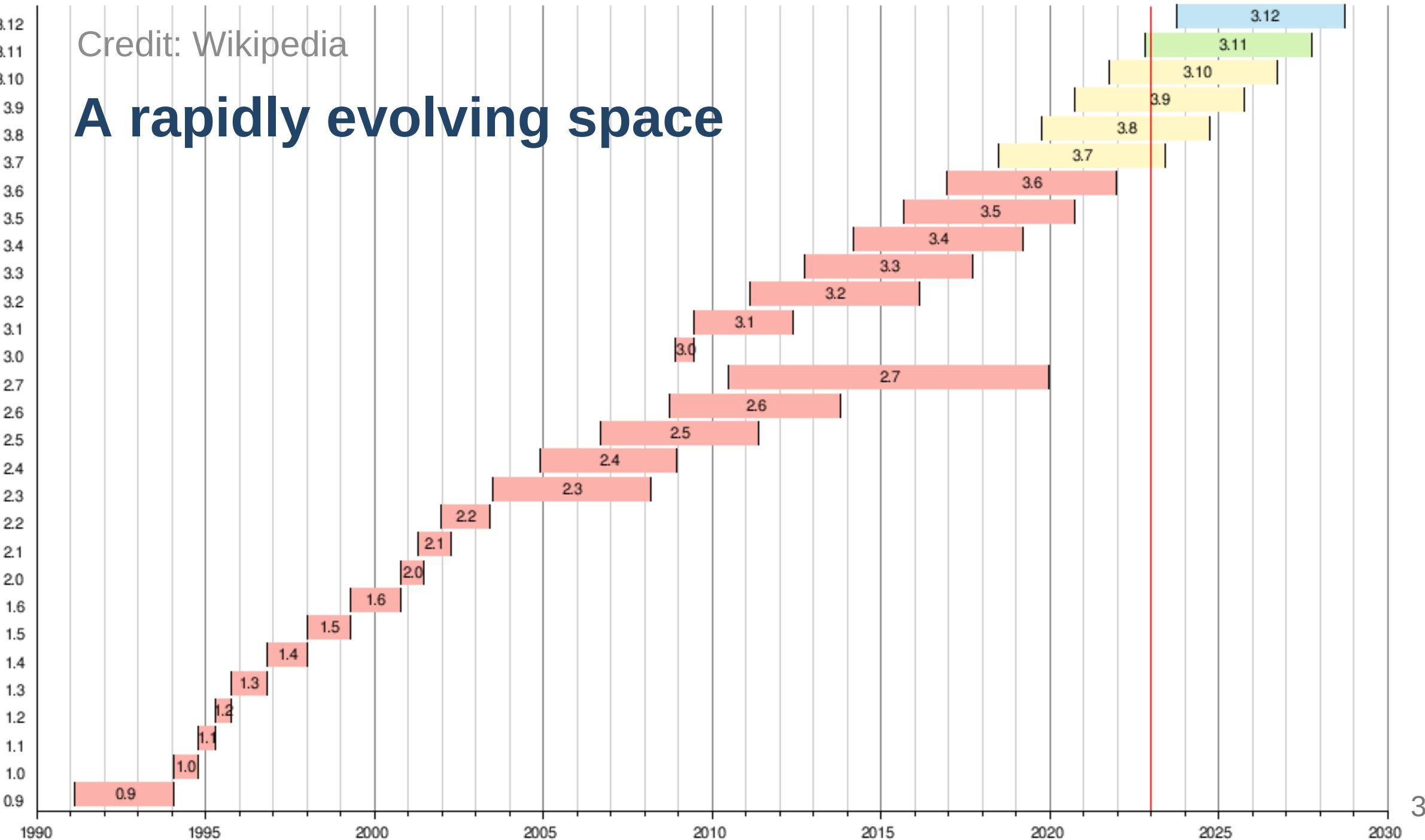
The world is a diverse place

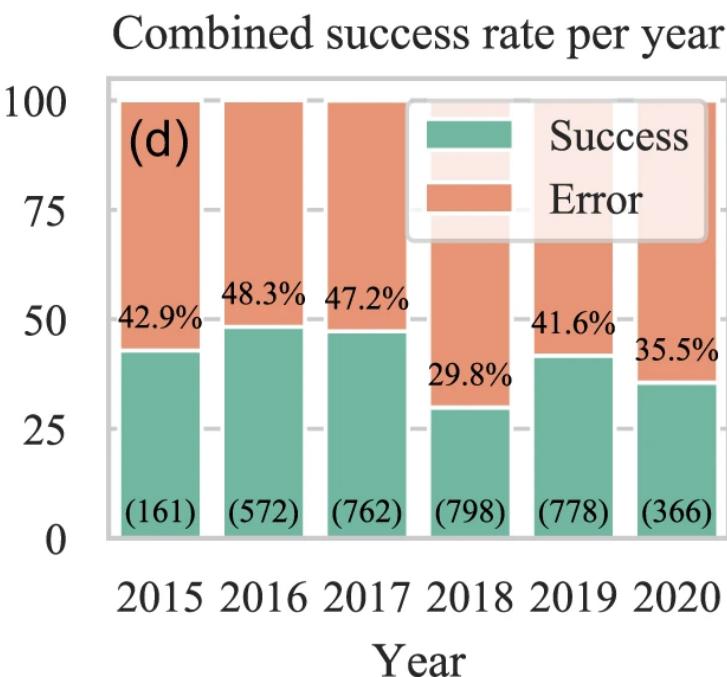
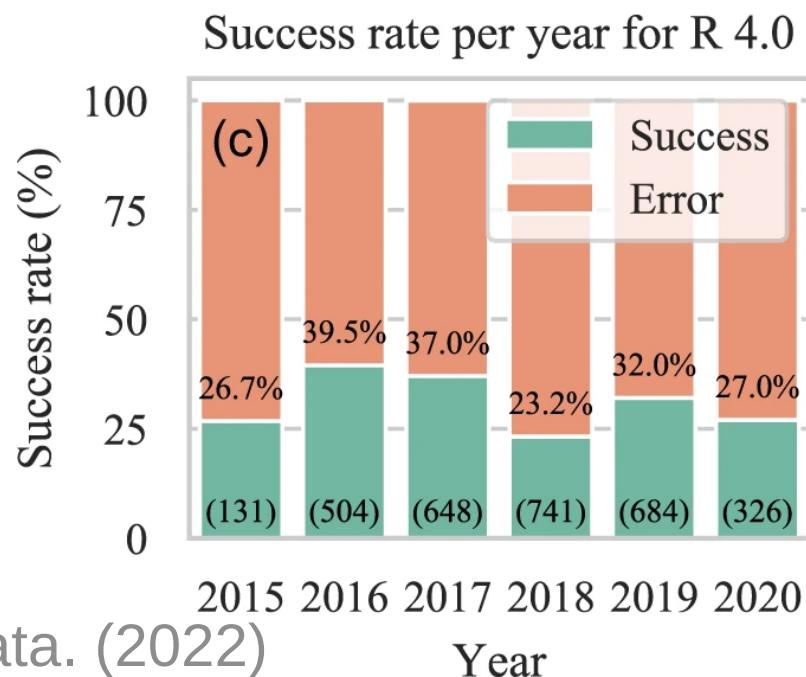
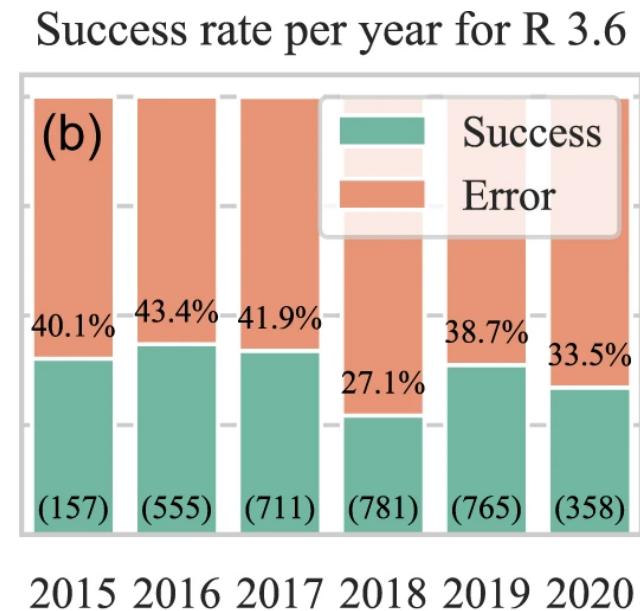
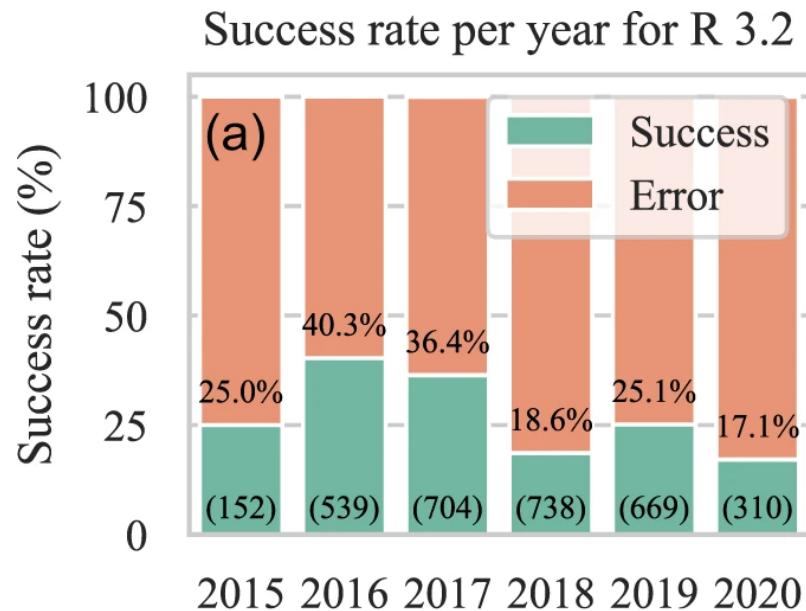
Credit: Lopez (2015)



Credit: Wikipedia

A rapidly evolving space





Challenge

Sharing and deploying reproducible code in dynamic and diverse environments

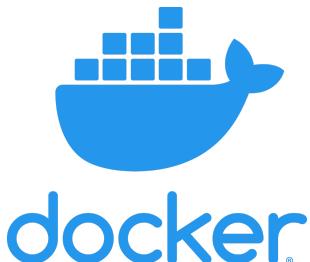
Solution

A host-independent format to package and deploy software components

Credit: Google Images

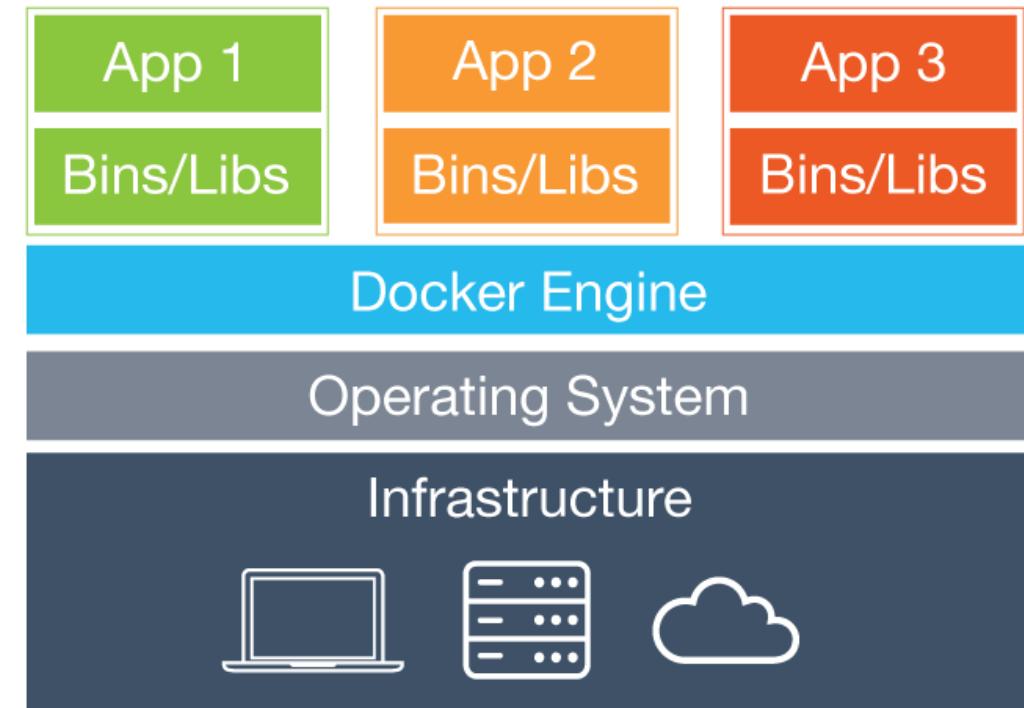






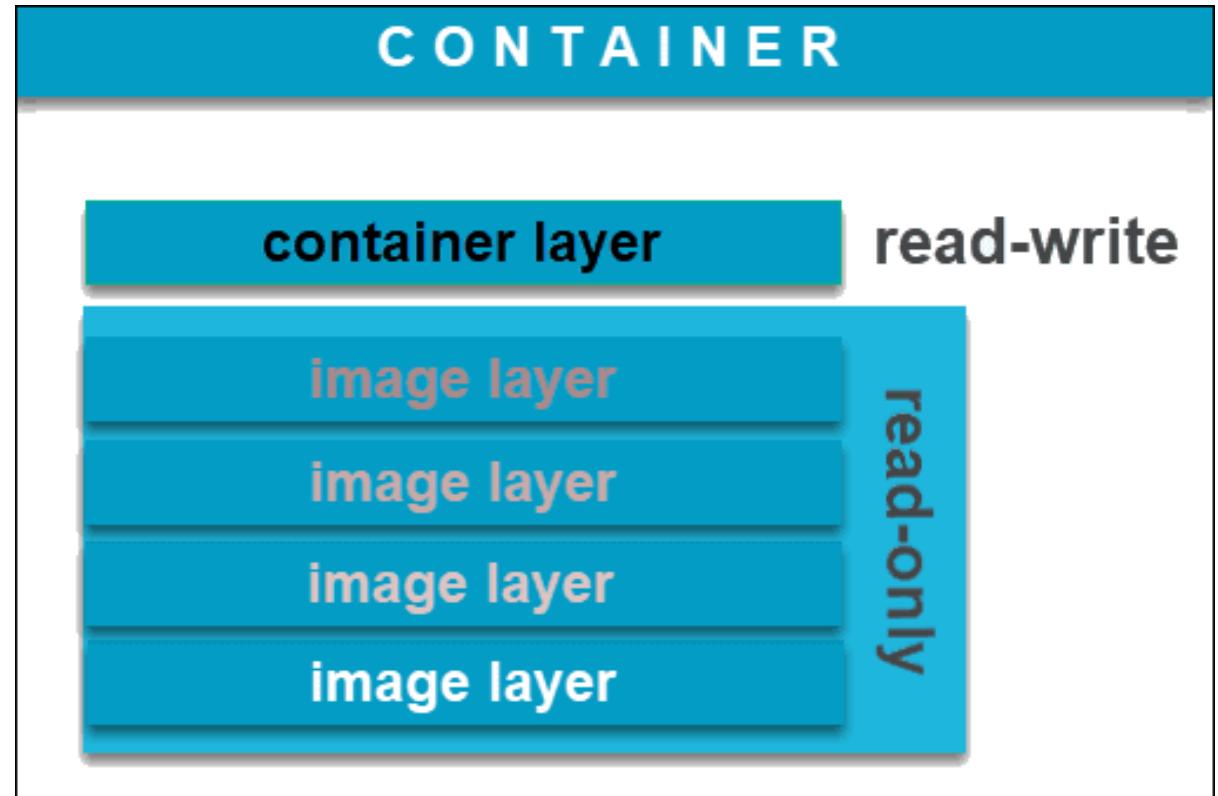
Docker Architecture

- A client-server application powered by Docker Engine
- 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 `staphb/blast:2.13.0` 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 [options] [image_name] [cmd]
```

Example command

```
docker run -w $(pwd) -v $(pwd):$(pwd) \
blast:[username] \
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:[username] 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)