REINVENTING HPC

ISC High Performance

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Containers and container orchestration systems

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Outline

- Containers
- Docker
- Security of containers
- Container orchestration
- Hands-on I

Timeline of Containerization

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- 2001—Linux VServer
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- 2013—Docker

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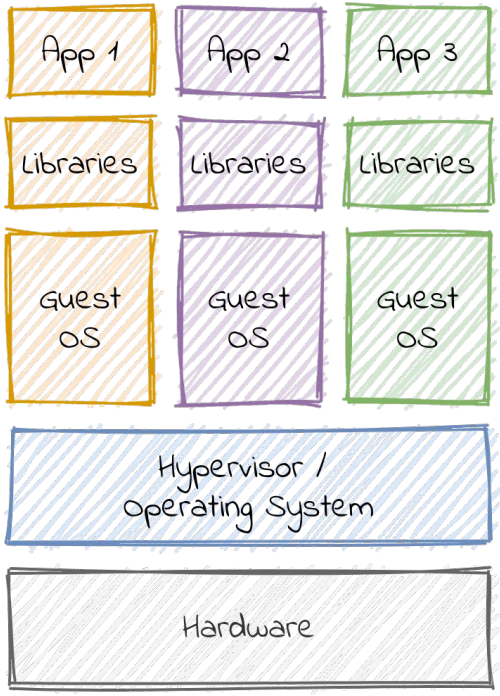
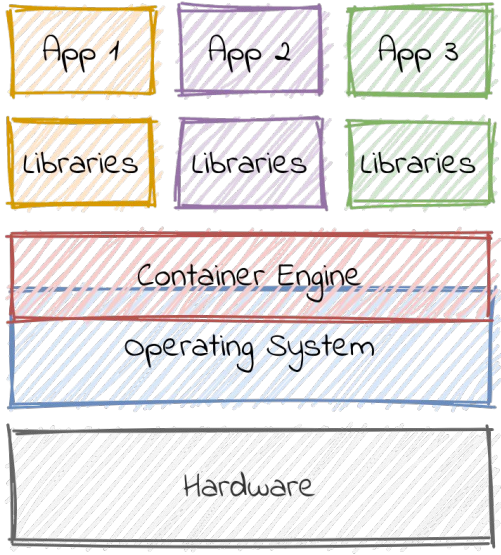
- 2008—LXC
- 2013—Docker
- 2015—OCI

Containers vs VMs



Virtualization



Containers

What Docker implemented

- A container image format
- A method for building container images (Dockerfile/docker build)
- A way to manage container images (docker images, docker rm , etc.)
- A way to manage instances of containers (docker ps, docker rm , etc.)
- A way to share container images (docker push/pull)
- A way to run containers (docker run)

Container

- cgroups + namespaces
- filesystem implementation

Running a container

```
$ docker run hello-world
```

Running a container

```
$ docker run hello-world
```

```
Unable to find image 'hello-world:latest' locally
latest: Pulling from library/hello-world
c1ec31eb5944: Pull complete
Digest: sha256:a26bff933ddc26d5cdf7faa98b4ae1e3ec20c4985e6f87ac0973052224d24302
Status: Downloaded newer image for hello-world:latest

Hello from Docker!
This message shows that your installation appears to be working correctly.

To generate this message, Docker took the following steps:
 1. The Docker client contacted the Docker daemon.
 2. The Docker daemon pulled the "hello-world" image from the Docker Hub.
       (amd64)
 3. The Docker daemon created a new container from that image which runs the
       executable that produces the output you are currently reading.
 4. The Docker daemon streamed that output to the Docker client, which sent it
       to your terminal.

To try something more ambitious, you can run an Ubuntu container with:
 $ docker run -it ubuntu bash

Share images, automate workflows, and more with a free Docker ID:
 https://hub.docker.com/

For more examples and ideas, visit:
 https://docs.docker.com/get-started/
```

Running a container

```
$ docker ps -a
CONTAINER ID   IMAGE         COMMAND    CREATED          STATUS                      PORTS   NAMES
559c1857f440   hello-world   "/hello"   5 seconds ago    Exited (0) 5 seconds ago            festive_benz
```

Running a container

```
$ docker ps -a
CONTAINER ID   IMAGE         COMMAND    CREATED         STATUS                     PORTS   NAMES
559c1857f440   hello-world   "/hello"   5 seconds ago   Exited (0) 5 seconds ago           festive_benz
```

```
$ docker images
REPOSITORY    TAG       IMAGE ID       CREATED          SIZE
hello-world   latest    d2c94e258dcb   12 months ago    13.3kB
```

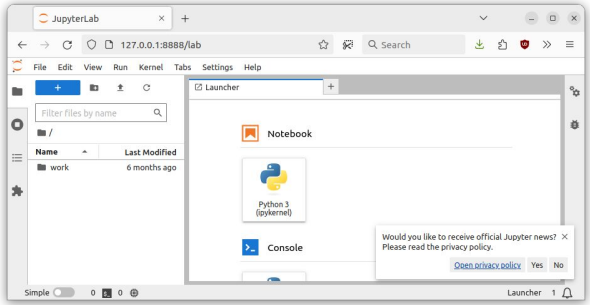
Running a container

```
$ docker ps -a
CONTAINER ID   IMAGE         COMMAND    CREATED          STATUS                      PORTS   NAMES
559c1857f440   hello-world   "/hello"   5 seconds ago    Exited (0) 5 seconds ago            festive_benz
```

```
$ docker images
REPOSITORY    TAG       IMAGE ID       CREATED          SIZE
hello-world   latest    d2c94e258dcb   12 months ago    13.3kB
```

```
$ docker run -it --rm -p 127.0.0.1:8888:8888 jupyter/base-notebook
```

```
…
To access the server, open this file in a browser:
file:///home/jovyan/.local/share/jupyter/runtime/jpserver-7-open.html
Or copy and paste one of these URLs:
http://7836f62fb4bc:8888/lab?token=d1073f1feb67beb0b90fe6051e9610a6d08ed23f9cde4c2b
http://127.0.0.1:8888/lab?token=d1073f1feb67beb0b90fe6051e9610a6d08ed23f9cde4c2b
```



Dockerfile

```
FROM python:3.8

WORKDIR /home

ENV PYTHONUNBUFFERED=1

RUN apt update && apt install -y curl
RUN rm -rf /var/lib/apt/lists/*
RUN pip install "paho-mqtt<2.0.0"

COPY publisher.py /home/

ENTRYPOINT ["python3"]
CMD ["publisher.py"]
```

Dockerfile

```
FROM python:3.8

WORKDIR /home

ENV PYTHONUNBUFFERED=1

RUN apt update && apt install -y curl
RUN rm -rf /var/lib/apt/lists/*
RUN pip install "paho-mqtt<2.0.0"

COPY publisher.py /home/

ENTRYPOINT ["python3"]
CMD ["publisher.py"]
```

Check Best Practices from the Dockerfile documentation

Security

Security

```
$ docker run -it --rm ubuntu
root@8c65593bdbf3:/# id
uid=0(root) gid=0(root) groups=0(root)
root@8c65593bdbf3:/# hostname
8c65593bdbf3
root@8c65593bdbf3:/# ll /home/
total 8
drwxr-xr-x 2 root root 4096 Apr 18  2022 ./
drwxr-xr-x 1 root root 4096 Apr 28 22:20 ../
```

Security

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uid=0(root) gid=0(root) groups=0(root)
root@8c65593bdbf3:/# hostname
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root@8c65593bdbf3:/# ll /home/
total 8
drwxr-xr-x 2 root root 4096 Apr 18  2022 ./
drwxr-xr-x 1 root root 4096 Apr 28 22:20 ../
```

```
$ docker run -it --rm -v /:/host_root ubuntu
root@68bf8ffda46e:/# ll /host_root/home/
total 32
drwxr-xr-x  5 root root  4096 Aug 25  2023 ./
drwxr-xr-x 21 root root  4096 Apr  8 08:17 ../
drwxr-xr-x  4 root root  4096 Aug 25  2023 VMs/
drwxr-x--- 41 1000 1000  4096 Apr 26 13:24 myuser/
drwx------  2 root root 16384 Aug 23  2023 lost+found/
```

Security (continued)

- User namespaces

Security (continued)

- User namespaces
  - CVE-2009-1338, CVE-2014-4014, CVE-2016-8655, CVE-2017-7184, CVE-2018-18955, CVE-2019-5736, CVE-2021-22555, CVE-2022-0185, CVE-2022-0492
- Other related CVEs
  - CVE-2020-14386 - CAP_NET_RAW
  - CVE-2021-32635 - Singularity
  - CVE-2021-29657 - KVM
  - CVE-2022-25636 - network_namespaces
  - CVE-2022-32250, CVE-2022-34918 - network_namespaces + nf_tables
  - CVE-2022-4378 - network_namespaces
  - CVE-2023-30549 - Apptainer
  - CVE-2024-1753 - Podman/Buildah
  - CVE-2024-21626 - runc
  - CVE-2024-23651, CVE-2024-23652, CVE-2024-23653, CVE-2024-23650, CVE-2024-24557 - Docker

Advanced topics

- Security
  - Containers are designed for dependencies isolation, not for users isolation
  - Most runtimes have binaries with setuid and/or rely on namespaces
  - This might be problematic on shared systems like HPC
- Hardware optimization
  - Images are usually generic
  - Builds for different architectures might be needed
  - Use of hardware acceleration
- Reproducibility
  - Two consequent builds may produce different images
  - Caching

Container orchestration

Orchestration tasks

- Deployment and scheduling
- Networking
- Load balancing, traffic routing and service discovery
- Health monitoring and self-healing
- Scaling

Orchestration systems

- **Kubernetes**
- Docker Swarm
- (Docker-compose)
- Apache Mesos
- Nomad
- xOpera

Questions?

Tutorial: Compute Continuum

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The Numerical Algorithms Group (NAG) Ltd.

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HAICGU cluster

HAICGU : Huawei AI and Computing at Frankfurt’s Goethe University (HAICGU)

28 X TaiShan 200 (Standard compute node)

ARM architecture

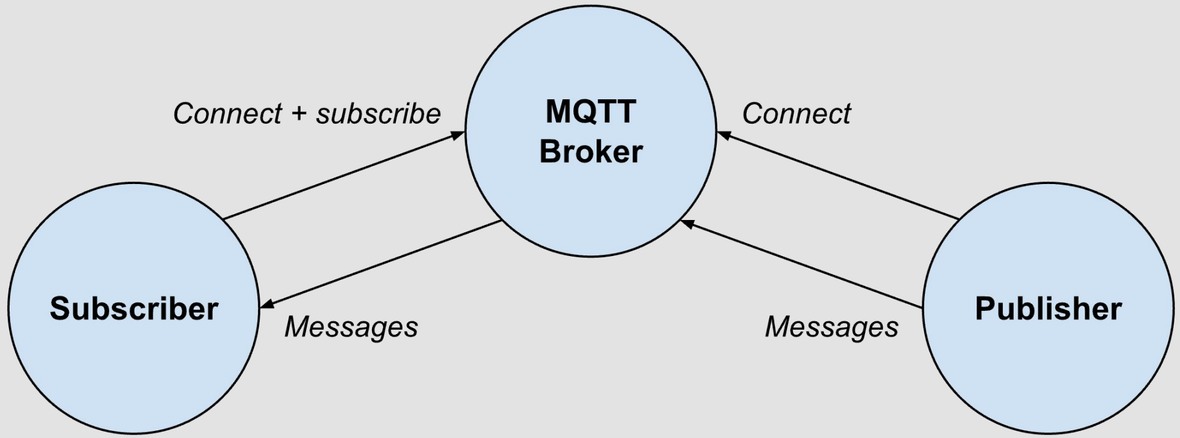
Maintained by Open Edge and HPC initiative (OEHI).

More details at https://haicgu.github.io/index.html

Compute Continuum tutorial – Hands on 1
Build and Push MQTT Application

MQTT (mosquito)**:** Light weight messaging protocol

Goal: Deploy on the cluster a MQTT publisher and subscriber and check that they can write/read on a predefined topic.



In the GitHub repository, you will find:

- Python scripts for the publisher and subscriber.
- Dockerfiles to build the images for publisher and subscriber.
- YAML files to deploy the containers on the k8s cluster.

SSH Access to Training Cluster

1. Collect account name and passphrase
2. Download ZIP archive with SSH key pairs
   from https://shorturl.at/qBKTW
3. Unzip archive and select key pair that corresponds
   the assigned account
4. Use this key pair to connect to login server:

   ```
   ssh -i <path_to_private_key> -l <account_name> 141.2.112.17
   ```

5. From login server connect to development server:

   ```
   ssh dev
   ```

Tutorial materials: https://github.com/haicgu/HPC_compute_continuum