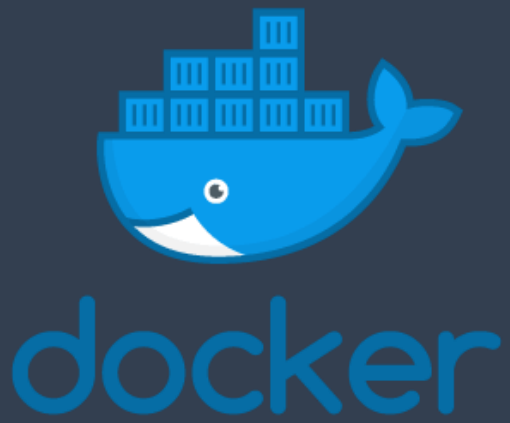

Basic usage of Docker containers in scientific research

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About me

- **MSc in Computer Science (AGH UST Kraków)**
- **Works in Sybilla Technologies**
  - **Robotization of astronomical observatories**
  - **Creating networks of astronomical sensors and scheduling them**
  - **Providing data products and services in SST for ESA and PAK (Polish Space Agency)**

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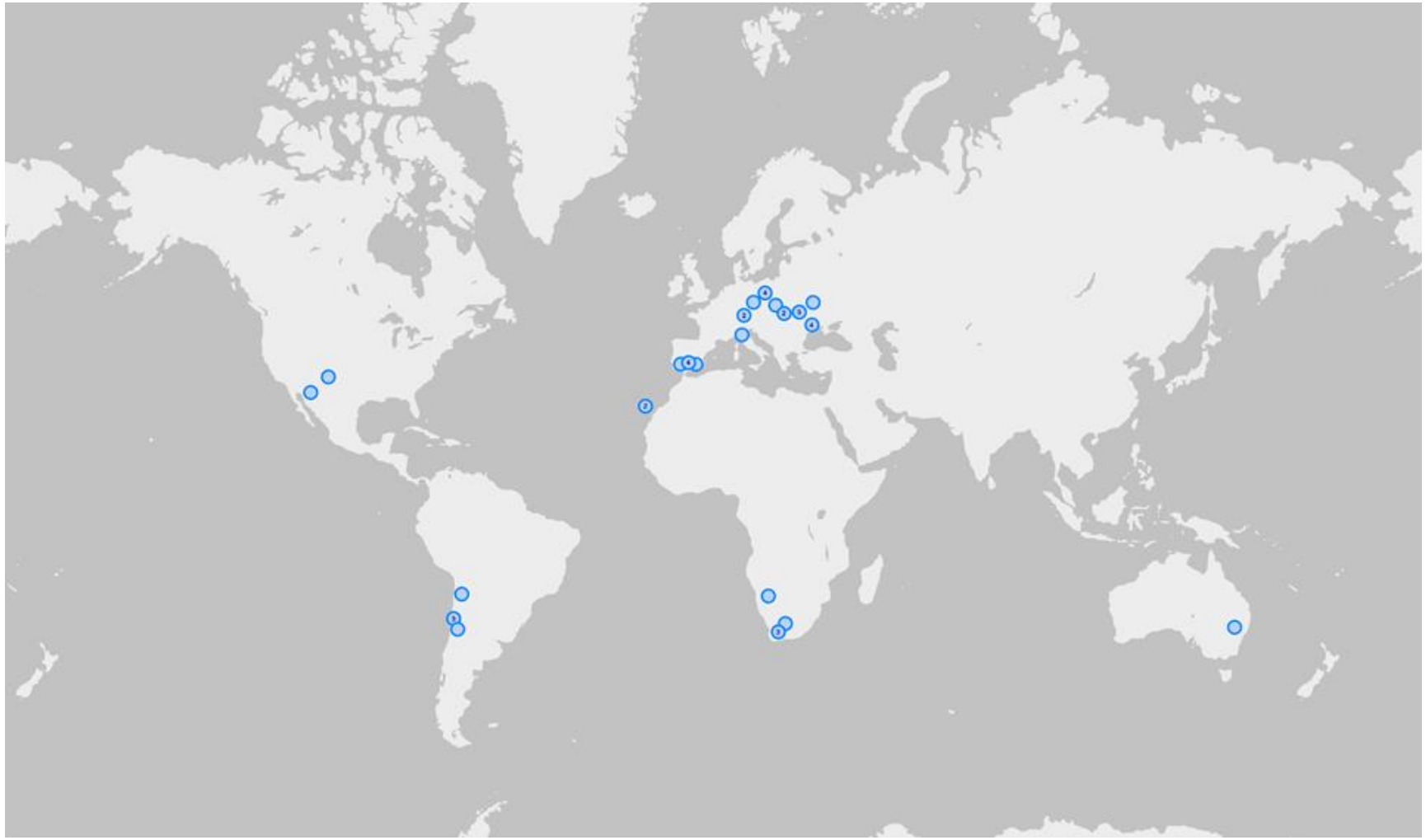
Sensor network



40 sensors running under control of company's scheduling system, largest European network used for ESA and POLSA projects

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What is Docker?

What is Docker container?

A container is a standard unit of software that packages up code and all its dependencies so the application runs quickly and reliably **from one computing environment to another**. A Docker container image is a lightweight, standalone, executable package of software **that includes everything needed to run an application: code, runtime, system tools, system libraries and settings.**

Source: https://www.docker.com/resources/what-container

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How is Docker different than VirtualBox?

- Virtual machines are running a guest OSes with their own kernels and this virtualization requires preallocating resources, bootstraping kernels
- Docker containers use host kernel and separate between the containers via kernel-level feature called namespaces
- No need to boot the system and kernel – just run the code
- Docker provide also mechanisms for managing networking and sharing directories between containers
- How then Windows and MacOS can use container using Linux Kernel?
  - Both systems use just enough virtualization to have a Linux kernel available for Docker (HyperV/WSL on Windows and Hypervisor on MacOS)

Source: https://stackoverflow.com/questions/16047306/how-is-docker-different-from-a-virtual-machine

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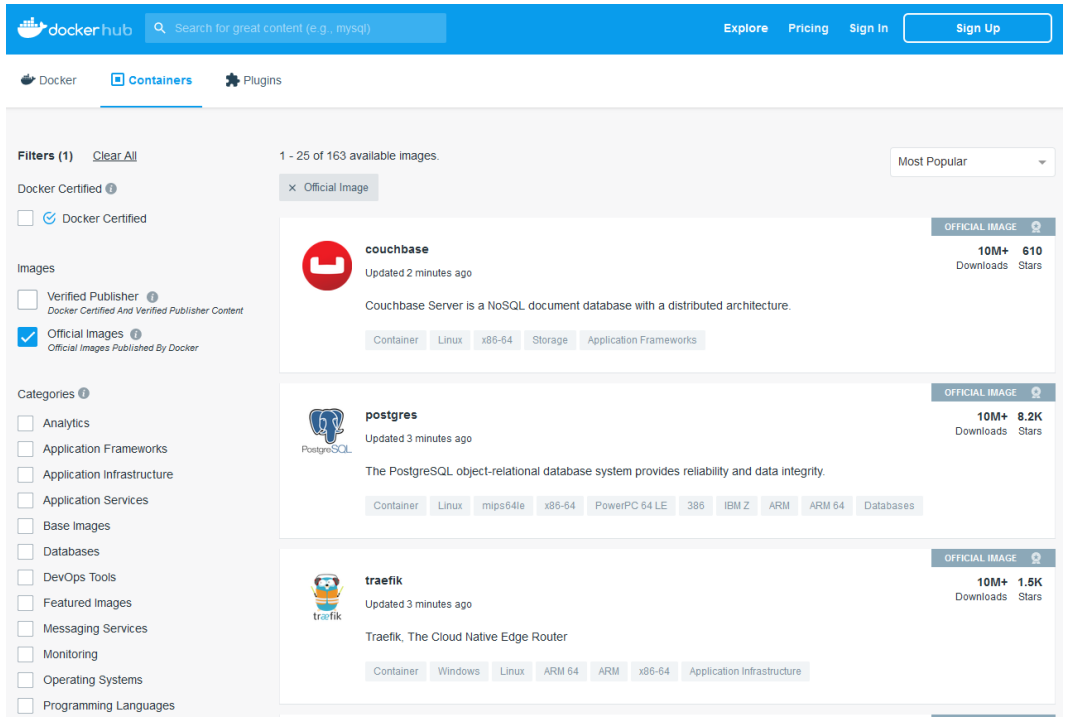
Building and running containers

Downloading images from Docker Hub

- Wide selection of ready to use databases, application servers and other ready to download and run container images
- We will focus on jupyter/scipy-notebook

Source: https://hub.docker.com/search?q=&type=image



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Running containers from Docker Hub

```
docker run -p 8888:8888 jupyter/scipy-notebook:latest
```

- Interaction with docker is done via docker command with different subcommands
- -p publishes container's port (on the right) to host port (one the left)
- Jupyter is the name of the image publisher
- scipy-notebook is the name the image
- latest is the tag which is mostly used for versioning
- Right now container has no persistence – after restart it will lose any files saved internally
  - Fix that with `-v D:/test:/home/jovyan/work` now everything saved in work directory will also be preserved on host system

Source: https://docs.docker.com/engine/reference/commandline/docker/

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Creating and building Dockerfile

- Dockerfile is recipe for building container image
- Basically a bash build script with extra syntax
  - https://hub.docker.com/r/jupyter/scipy-notebook/dockerfile
- Designed to be reused

```
FROM jupyter/scipy-notebook
RUN pip install --upgrade pip
COPY requirements.txt requirements.txt
RUN pip install -r requirements.txt
WORKDIR $HOME
```

- To build and run:
  - docker build -t custom_notebook .
  - docker run -p 8888:8888 custom_notebook

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Creating Dockerfile from scratch

- Select base distribution closest to your needs
  - https://hub.docker.com/search?q=&type=image&operating_system=linux&category=base
  - Debian/Ubuntu are a good first choice - you can select older versions (helpful with legacy) and you get apt-get package manager
  - Alpine is a distro designed with being used within Docker container – good choice when optimizing for smaller container footprint
- Follow exactly same procedure as previously but this time you have to remember about setting entrypoint command
  - CMD specifies the process that is being run inside container
- Simplest Ubuntu-based Dockerfile

```
FROM ubuntu:bionic
CMD ["/bin/bash"]
```

  - Good for wrapping commandline utilities – containers don't have to be long-lived

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Composing multiple containers

docker-compose.yml

Docker Compose allows for creating a single YAML file with all configuration that can be done via Docker CLI

- Convenient for storage in GIT repository
- Allows for simultaneous building and running of multiple containers at once
- After docker-compose.yml is created starting containers is simply:

```
docker-compose up
```

- And stopping them is:

```
docker-compose down
```

Source: https://docs.docker.com/compose/

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docker-compose.yml

- Services section defines Docker containers to run
- Volumes section allows for creation of named volumes
- Configuration of containers (mounting configuration files, injecting environment variables)
- Services names are also their hostnames and they by default are put in the same bridge network
  - Access from the host machine is done thanks to port publishing – otherwise network is separated

```
from sqlalchemy import create_engine
db  = create_engine('postgresql://postgres:changeme@db:5432/postgres')
result_set = db.execute("SHOW ALL")
for r in result_set:
    print(r)
```

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Summary of benefits of using Docker in science and education

- repeatable environment
- easily resetable environment
- reduction in work required for distribution of student assignments
  - Difficult configuration can be done once and everyone else can focus on assignment
- ability to wrap legacy code or code available only for specific linux distribution
- separation from environment
- composing small service ecosystems

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Thank you

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