2nd CCU Workshop on GPU Computing

Today’s Schedule

- 09:00 to 10:30 - Docker containers
- 10:30 to 11:00 - Coffee break - No coffee unfortunately
- 11:00 to 11:30 - Baden Württemberg High Performance Computing (bwHPC)
- 11:30 to 12:30 - Introduction to CPU and GPU computing
- 12:30 to 14:00 – Lunch break
- 14:00 to 15:00 - Kubernetes and the CASCB Cluster

You might remember me from ...

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Data analysis meetings began in 2022 with Jacob Davidson and myself as organizers

Jacob Davidson

Daniel S. Calovi

IMPRS – Introduction to Scientific Coding workshop

The Data Science Consultancy

Join our Slack channel

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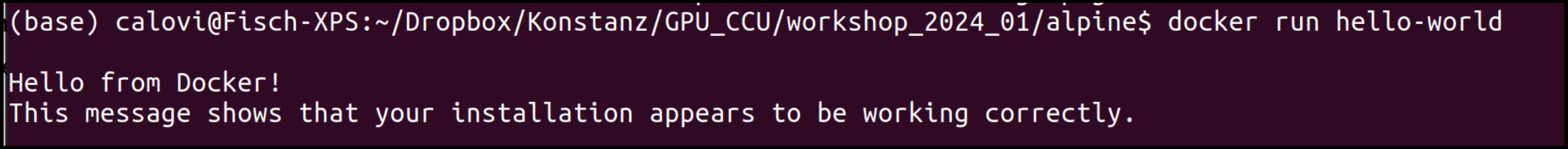
Docker

- Docker is a virtualization software
  - It creates a standalone VM (container) that is able to run cross platform with little efficiency loss (depends on the application, but fair approximation)
- Think of Conda environments, but completely separated from your system
  - Had you ever had to run a software that only runs in Ubuntu xx and uses an outdated package that conflicts with other libraries and software?
- Docker containers are versionable
  - Each new addition just gets added to the last version instead of having to redo it
- Docker containers are stateless
  - Once created, your container is frozen in time in that state. One can change it while it’s running, but once closed, it reverts to the original state

Learning by doing it

- First thing to check is if docker is running properly in your machine

  docker run hello-world



```
(base) calovi@Fisch-XPS:~/Dropbox/Konstanz/GPU_CCU/workshop_2024_01/alpine$ docker run hello-world

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

  After, type

  docker images

- To delete, type

  docker rmi hello-world

- Most likely it failed, try:

  docker rmi -f hello-world

How to create a docker image?

- Extract folder Alpine into an appropriate location
- Open the file Dockerfile
- Within a terminal, go inside that folder
- Type:

```
docker build -f Dockerfile -t alpine .
```

Running a container

- Type:

```
docker run alpine
```

- Open the file Dockerfile_2
  - What are the differences?
  - What do you imagine it will happen when we run it?
- Now build it and run it:

```
docker build -f Dockerfile_2 -t alpine2 .
docker run alpine2
```

- Was it what you expected?

Running a container

- Type:

```
docker run alpine
```

- Open the file Dockerfile_2
  - What are the differences?
  - What do you imagine it will happen when we run it?
- Now build it and run it:

```
docker build -f Dockerfile_2 -t alpine2 .
docker run alpine2
```

- Was it what you expected?
  - Aren’t containers stateless?

RUN/CMD commands

- Run commands are performed during the building of the image
  - The base state of our container already contained the 2 files
- Only the last CMD command will be run
  - The first one in the Dockerfile_2 was ignored

Stateless version

- Open file Dockerfile_3, and then build it and run it

  ```
  docker build -f Dockerfile_3 -t alpine3 .
  docker run alpine3
  ```

- Note the difference between the CMD syntax of the first container to this one
  - Exec form (CMD ["command", "param"]) Directly executes commands without a shell, enhancing signal responsiveness and process control
  - Shell form (CMD command) Executes commands via a shell, enabling complex scripting such as command chaining and variable expansion
- For complex commands, better to create a bash script and use CMD to run it, e.g.

  ```
  CMD ["/usr/local/bin/start-notebook.sh"]
  ```

Docker is versionable

- Open file Dockerfile_4, examine it and build it

  ```
  docker build -f Dockerfile_4 -t apine4 .
  ```

- Quite a few more packages were added, now uncomment line 7 (`RUN apk --no-cache add git`) and build the file again
  - Not everything was rebuilt, git was just appended to the image

Docker is versionable

- Open file Dockerfile_4, examine it and build it

  `docker build -f Dockerfile_4 -t apine4 .`
- Quite a few more packages were added, now uncomment line 7 (`RUN apk --no-cache add git`) and build the file again
  - Not everything was rebuilt, git was just appended to the image
- Now move line 7 before line 6 and build it again
  - It now had to rebuild package “feh” as well

Docker is versionable

- When building complex containers it is worth to using RUN many times in order to have more saved states
- If building crashes midway through, all completed iterations of RUN are already cached
  - imagine having to install opencv multiple times because something at the end of your container crashed?

Versioning your containers

- In Docker :latest is just the default version, not exactly the latest version
- Instead of creating multiple images (alpine, alpine2, alpine3), we can create different versions of them
- Type:

```
docker build -f Dockerfile -t alpine:1.0  -t alpine:latest .
docker build -f Dockerfile_3 -t alpine:2.0  .
docker run alpine
docker run alpine:2.0
```

- Tags can be anything and are case sensitive, latest and Latest would refer to different versions

More complex example

- Open file Dockerfile_Jupyter
  - (I did some last minute trimming, might not work from scratch)

Logging in the container

- You have a container, and you want to get inside that VM, type:

  ```
  docker run -d --name running_alpine alpine tail -f /dev/null
  ```

  - -d is to keep the terminal free (detached)
  - --name is to ensure you give an specific name
- Type

  ```
  docker ps
  docker exec -it running_alpine /bin/sh
  ```

- Now you are actually inside the pod, and while it is active you can perform changes to it

Mouting folders in your container

- Very often you need your container to be able to see folders from your local machine
- To mount a specific folder type:

```
docker run -d --name local_folder  -v $(pwd):/workspace alpine tail -f /dev/null
```

  - -v is to mount a specific folder
    - In this case we used the current folder
  - :/workspace is the location and name of the folder to be created in the container

Uploading your container

- To upload your container you need to be logged in a repository and have permission to push (upload) it
- Before pushing, one needs to update the image name to have the address of the repository, i.e.

```
docker tag ccu-workshop-jupyter
ccu-k8s.inf.uni-konstanz.de:32250/daniel.calovi/ccu-workshop-jupyter

docker push ccu-k8s.inf.uni-konstanz.de:32250/daniel.calovi/ccu-workshop-jupyter
```

- This will not run for you, just an example for later

Repositories

- When building an image you can use default packages like
  - FROM alpine:latest
  - FROM quay.io/jupyter/base-notebook
  - FROM docker pull nvcr.io/nvidia/pytorch:21.10-py3
- But you can also download a pre-packaged container

This will download a ~13GB container if not downloaded already

- For the next part of the workshop type:

```
docker run --gpus all -p 2000:8888 -v $(pwd):/workspace
nvcr.io/nvidia/pytorch:21.10-py3 jupyter lab --ip 0.0.0.0 --allow-root --
NotebookApp.token=''
```

  - Where the port syntax is: -p localhost:container

Questions/Coffee Break?