4th CCU Workshop on Docker and GPU Computing

Today's Schedule

- 09:00 to 10:30 - Docker containers

- 10:30 to 11:00 – Intermission and questions

- 11:00 to 12:30 - Introduction to CPU and GPU computing

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

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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

- 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  - Had you ever had to run a software that only runs in Ubuntu xx and uses an outdated package that conflicts with other libraries and software?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

- Open a terminal

- In Windows, open the WSL terminal (Ubuntu most likely)

- Create a folder where we will work today

  - In Windows, open the file explorer and create the folder inside the Ubuntu/Linux icon on the left bar

- Unzip the alpine folder into the working directory you created

- In the terminal access the folder you are going to work on

  - In case you want to work inside the Windows folder structure, access normal windows folder in: /mnt/c/

```
calovi@DESKTOP-M1LE1C2:~$ cd /mnt/c/Users/Calovi/Downloads/
calovi@DESKTOP-M1LE1C2:/mnt/c/Users/Calovi/Downloads$ ls
 BoseUpdaterInstaller_7.1.13.5138.exe   'Docker Desktop Installer.exe'    SteamSetup.exe
 Cellects                                Example                          ZoomInstaller.exe
'ChromeSetup (1).exe'                    Example.zip                      ZoomInstallerFull.exe
 ChromeSetup.exe                         LibreOffice_24.8.4_Win_x86-64.msi  desktop.ini
calovi@DESKTOP-M1LE1C2:/mnt/c/Users/Calovi/Downloads$
```

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:~/DockerGpu-2025$ docker run hello-world
Unable to find image 'hello-world:latest' locally
latest: Pulling from library/hello-world
e6590344b1a5: Already exists
Digest: sha256:d715f14f9eca81473d9112df50457893aa4d099adeb4729f679006bf5ea12407
Status: Downloaded newer image for hello-world:latest

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?

- 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?
  - Why did it not list the files twice?

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

  - Shell form (CMD command) Executes commands via a shell

- For complex commands, better to create an executable 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

Logging in the container

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

  docker run -it --rm --name running_alpine alpine /bin/sh

  - -it is for interactive mode

  - --rm is to stop the running container after closing it

  - --name is to ensure you give an specific running name

  - /bin/sh is to run this command inside the container, which opens a shell

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

Mounting 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 -it --rm --name local_folder -v ~/DockerGpu_2025:/usr/src/app/ alpine /bin/sh

  - -v is to mount a specific folder

    - In this case we used my current folder

  - /usr/src/app/ is the location of the working directory set in the Dockerfile

More complex example

- Open file Dockerfile_DLC3.1

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

Removing old images

- At some point, you will want to remove old images

- docker rmi -f image_name will remove from the list, but not necessarily free hardisk space

- To clean any unused (unlabeled) containers, you can type:

  docker system prune

Repositories

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

This will download a ~20GB container if not downloaded already

- For the next part of the workshop type:

- docker build -f Dockerfile_pytorch23:.01 -t my-pytorch .

- If you have a GPU type:

- docker run --gpus all -it --rm -p 2000:8888 -v ~/DockerGpu_2025:/workspace --name pip_container my-pytorch
  - Where the port syntax is: -p localhost:container

Questions/Coffee Break?