Docker for Reproducible Research

Anastasiia Enne

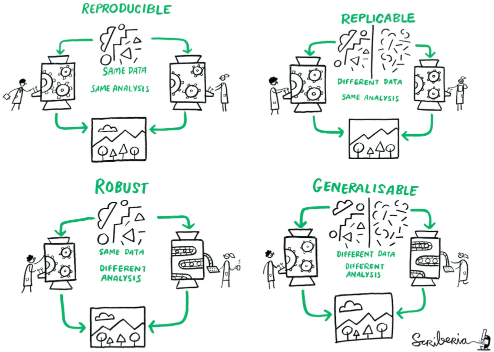
Group meeting, 14.01.2026

Overview

1. **Reproducibility crisis** — why just publishing your code is not enough
2. **What is Docker** and how can it help us with reproducibility
3. **Dockerizing an existing project** — a step-by-step guide if you want to try Docker

Reproducibility crisis

- Reminder: 4 definitions of reproducible research[1]



[1] The Turing Way Community. This illustration is created by Scriberia with The Turing Way community, used under a CC-BY 4.0 licence. DOI: 10.5281/zenodo.3332807

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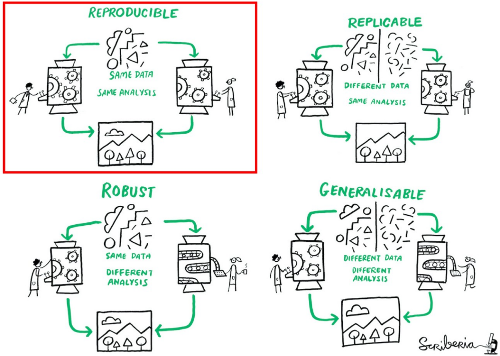

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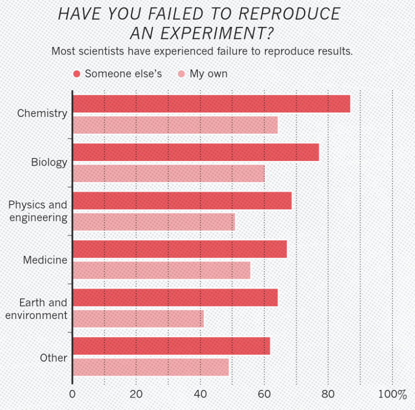

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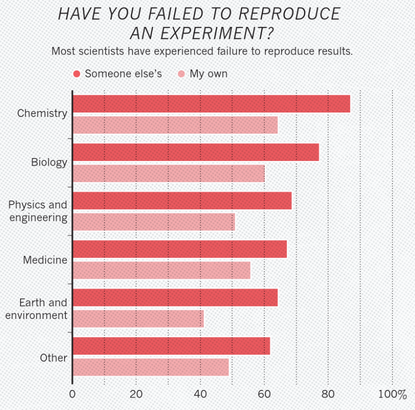
- But what about modelling?



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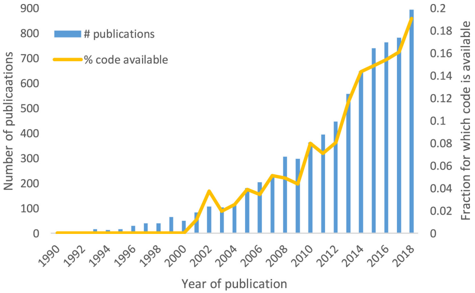

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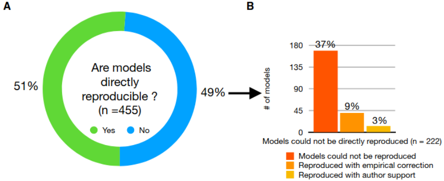

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[2] (Tiwari et al. 2021)

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- **Docker**
  - Lightweight and easily scalable
  - Clear list of dependencies
  - Open source
  - Linux functionality

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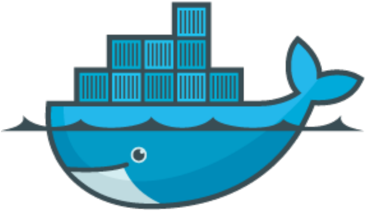

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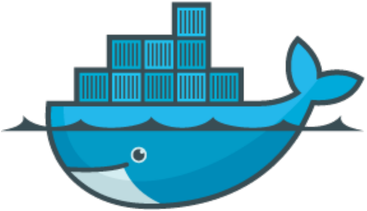

These slides are baked with Rmd and Dockerized! Go to github.com/enne-anastasia/docker-for-reproducible-research and see how I used Docker!

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- If Bob doesn't want to be bothered with using Docker he still can read the file and install all the dependencies on his own device manually.
- Alice is certain that she provided all the dependencies, because she tested this file with the Docker software.

What is Docker?

`docker build` ⇒ `docker run` ⇒

Docker file

- Text file with "source code" of the image:
  - Instructions on how to build the image
  - Commands to run your project

Docker image

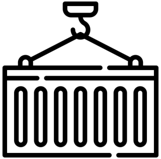
- An executable snapshot of a container
- Includes all dependencies needed to run a container

Docker container

- A running instance of the image
- Your "pocket Ubuntu"
- Self-contained

What is Docker?

More about Docker containers



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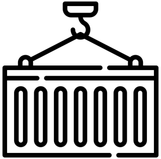

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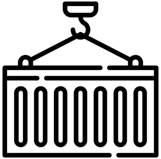

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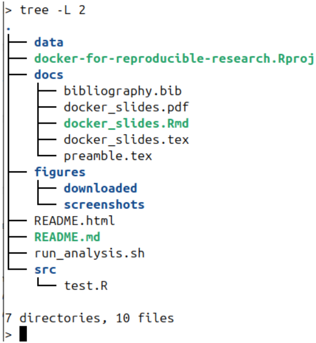
- Consequently, you need to either
  - copy your files into the image (with a command in your Docker file), or
  - mount a folder to a container (during `docker run`)
- The rule of thumb is:
  - We MOUNT everything that takes plenty of space: e.g., data
  - We MOUNT everything that we want to be changed: e.g., figures
  - We COPY source code

Dockerizing an existing project

What project are we going to Dockerize?

- We will Dockerize the R project that I used to prepare this presentation
- It has a very common structure for a code supplementary:
    - data — folder containing all the data used in this project (empty in this case)
    - docs — folder with Rmd file that generates these slides
    - figures — folder with all the figures I used
    - README file
    - run_analysis.sh — one script to execute this project
    - src — source code (1 test R script in this case)



```
> tree -L 2
.
├── data
├── docker-for-reproducible-research.Rproj
├── docs
│   ├── bibliography.bib
│   ├── docker_slides.pdf
│   ├── docker_slides.Rmd
│   ├── docker_slides.tex
│   └── preamble.tex
├── figures
│   ├── downloaded
│   └── screenshots
├── README.html
├── README.md
├── run_analysis.sh
└── src
    └── test.R

7 directories, 10 files
> 
```

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- Verify that the installation is successful:

  ```
  sudo systemctl status docker
  sudo docker run hello-world
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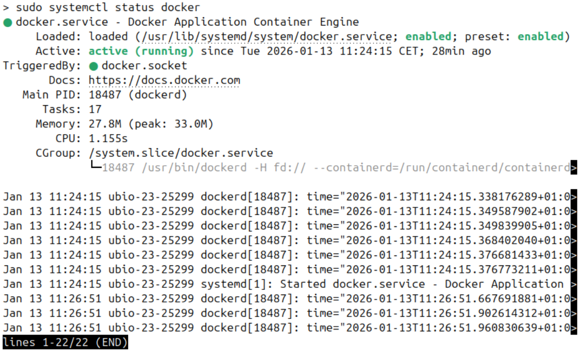

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TriggeredBy: ● docker.socket
       Docs: https://docs.docker.com
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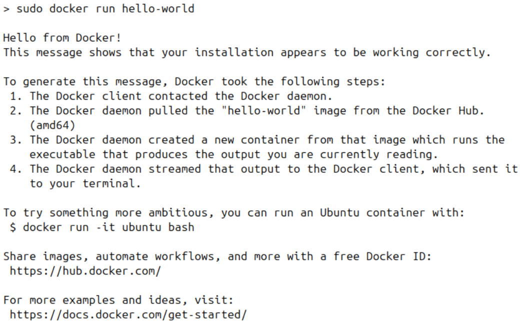

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> sudo docker run hello-world

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/
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STEP 2: Trying the basic Docker commands

- **Starting Docker:**

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  (Docker is running in the background waiting for you to use it)

- **Stopping Docker:**

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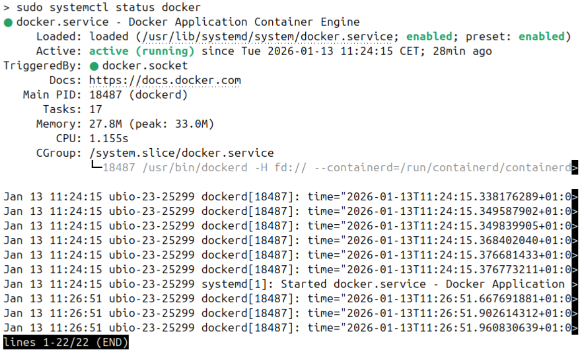

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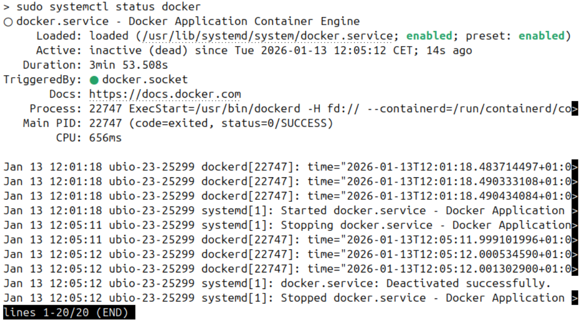

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     Loaded: loaded (/usr/lib/systemd/system/docker.service; enabled; preset: enabled)
     Active: inactive (dead) since Tue 2026-01-13 12:05:12 CET; 14s ago
   Duration: 3min 53.508s
TriggeredBy: ● docker.socket
       Docs: https://docs.docker.com
    Process: 22747 ExecStart=/usr/bin/dockerd -H fd:// --containerd=/run/containerd/co>
   Main PID: 22747 (code=exited, status=0/SUCCESS)
        CPU: 656ms

Jan 13 12:01:18 ubio-23-25299 dockerd[22747]: time="2026-01-13T12:01:18.483714497+01:0>
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- To kill `docker.socket` use
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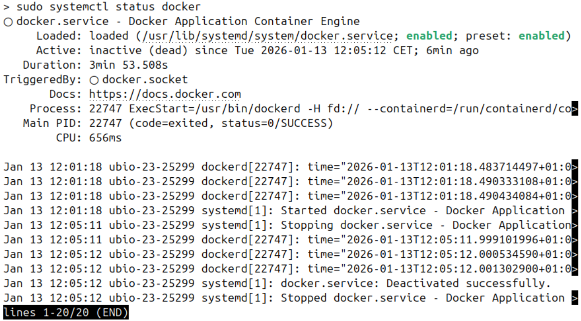

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   Main PID: 22747 (code=exited, status=0/SUCCESS)
        CPU: 656ms

Jan 13 12:01:18 ubio-23-25299 dockerd[22747]: time="2026-01-13T12:01:18.483714497+01:0>
Jan 13 12:01:18 ubio-23-25299 dockerd[22747]: time="2026-01-13T12:01:18.490333108+01:0>
Jan 13 12:01:18 ubio-23-25299 dockerd[22747]: time="2026-01-13T12:01:18.490434084+01:0>
Jan 13 12:01:18 ubio-23-25299 systemd[1]: Started docker.service - Docker Application >
Jan 13 12:05:11 ubio-23-25299 systemd[1]: Stopping docker.service - Docker Application>
Jan 13 12:05:11 ubio-23-25299 dockerd[22747]: time="2026-01-13T12:05:11.999101996+01:0>
Jan 13 12:05:12 ubio-23-25299 dockerd[22747]: time="2026-01-13T12:05:12.000534590+01:0>
Jan 13 12:05:12 ubio-23-25299 dockerd[22747]: time="2026-01-13T12:05:12.001302900+01:0>
Jan 13 12:05:12 ubio-23-25299 systemd[1]: docker.service: Deactivated successfully.
Jan 13 12:05:12 ubio-23-25299 systemd[1]: Stopped docker.service - Docker Application >
lines 1-20/20 (END)
```
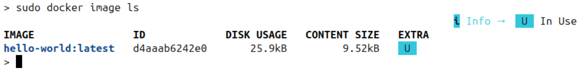

Dockerizing an existing project

STEP 2: Trying the basic Docker commands

- **Listing all available Docker images:**

  `sudo docker image ls`

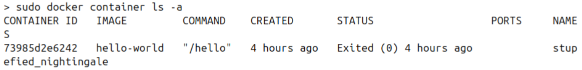


```
> sudo docker image ls
                                                                 i Info → U In Use
IMAGE                ID             DISK USAGE   CONTENT SIZE   EXTRA
hello-world:latest   d4aaab6242e0       25.9kB         9.52kB   U
> 
```

Dockerizing an existing project

STEP 2: Trying the basic Docker commands

- **Listing all available Docker images:**
  `sudo docker image ls`
- **Listing all containers that are currently running:**
  `sudo docker container ls -a`



```
> sudo docker container ls -a
CONTAINER ID   IMAGE         COMMAND    CREATED       STATUS                   PORTS     NAME
S
73985d2e6242   hello-world   "/hello"   4 hours ago   Exited (0) 4 hours ago             stup
efied_nightingale
```

Dockerizing an existing project

STEP 2: Trying the basic Docker commands

- **Listing all available Docker images:**

  `sudo docker image ls`

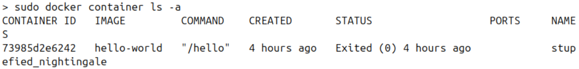
- **Listing all containers that are currently running:**

  `sudo docker container ls -a`

- **Deleting a container:**

  `sudo docker container rm <ID>`

  `sudo docker container rm <NAME>`



```
> sudo docker container ls -a
CONTAINER ID   IMAGE         COMMAND    CREATED         STATUS                     PORTS     NAME
S
73985d2e6242   hello-world   "/hello"   4 hours ago     Exited (0) 4 hours ago               stup
efied_nightingale
```

Dockerizing an existing project

STEP 2: Trying the basic Docker commands

- **Listing all available Docker images:**

  `sudo docker image ls`
- **Listing all containers that are currently running:**

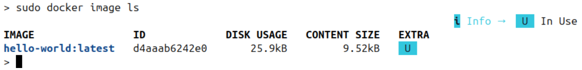
  `sudo docker container ls -a`
- **Deleting a container:**

  `sudo docker container rm <ID>`

  `sudo docker container rm <NAME>`
- **Deleting an image:**

  `sudo docker image rm <ID>`

  `sudo docker image rm <IMAGE>`

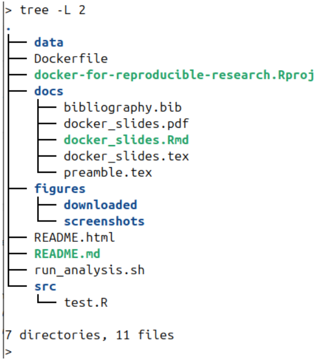


```
> sudo docker image ls
                                                                          i Info → U In Use
IMAGE                ID             DISK USAGE   CONTENT SIZE   EXTRA
hello-world:latest   d4aaab6242e0       25.9kB         9.52kB   U
> 
```

Dockerizing an existing project

STEP 3: Writing the Docker file

1. Create an empty `Dockerfile` in the root directory of you project

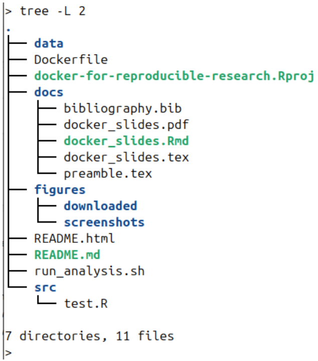


```
> tree -L 2
.
├── data
├── Dockerfile
├── docker-for-reproducible-research.Rproj
├── docs
│   ├── bibliography.bib
│   ├── docker_slides.pdf
│   ├── docker_slides.Rmd
│   ├── docker_slides.tex
│   └── preamble.tex
├── figures
│   ├── downloaded
│   └── screenshots
├── README.html
├── README.md
├── run_analysis.sh
└── src
    └── test.R

7 directories, 11 files
>
```

Dockerizing an existing project

STEP 3: Writing the Docker file

1. Create an empty `Dockerfile` in the root directory of you project
2. Pick the base image
   - Writing your Docker file from scratch is like setting a new work laptop from scratch
   - Thankfully, we do not have to do that because there are Docker images we can build upon!

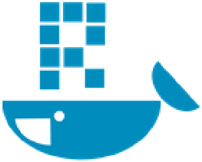


```
> tree -L 2
.
├── data
├── Dockerfile
├── docker-for-reproducible-research.Rproj
├── docs
│   ├── bibliography.bib
│   ├── docker_slides.pdf
│   ├── docker_slides.Rmd
│   ├── docker_slides.tex
│   └── preamble.tex
├── figures
│   ├── downloaded
│   └── screenshots
├── README.html
├── README.md
├── run_analysis.sh
└── src
    └── test.R

7 directories, 11 files
>
```

Dockerizing an existing project

STEP 3: Writing the Docker file

1. Create an empty `Dockerfile` in the root directory of you project
2. Pick the base image
   - Writing your Docker file from scratch is like setting a new work laptop from scratch
   - Thankfully, we do not have to do that because there are Docker images we can build upon!
   - For this project I will use `rocker` — Docker image with pre-installed R



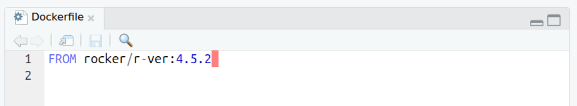
The Rocker Project

Docker Containers for the R Environment

Dockerizing an existing project

STEP 3: Writing the Docker file

3. Write the first line in your `Dockerfile`:
   - We build our image starting from Docker image with pre-installed R
   - I specify the version 4.5.2 of R since this is the version that I currently have on my laptop
   - There can be only one `FROM` image!



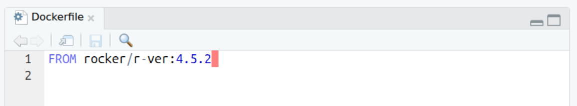
```
FROM rocker/r-ver:4.5.2
```

Dockerizing an existing project

STEP 3: Writing the Docker file

3. Write the first line in your `Dockerfile`:
   - We build our image starting from Docker image with pre-installed R
   - I specify the version 4.5.2 of R since this is the version that I currently have on my laptop
   - There can be only one `FROM` image!

- Congratulations! This is the the minimal Docker file we can use to build and run a Docker image (atlhough, not very usefull one)

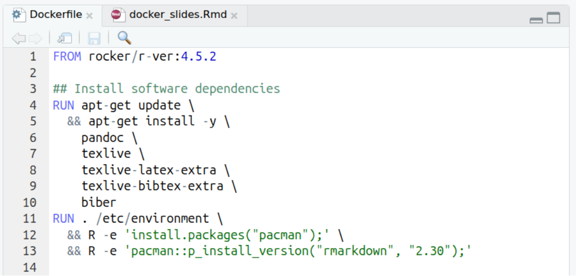


```
FROM rocker/r-ver:4.5.2
```

Dockerizing an existing project

STEP 3: Writing the Docker file

4. Specify software dependencies
   - It is okay to do that in iterations. When you think you got all the dependencies, go to the next step and see if you can run your project in the Docker container.
   - Here I have 2 types of dependencies: OS-level and R-level.

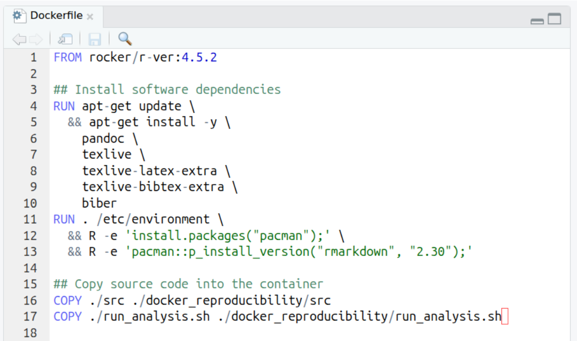


```
FROM rocker/r-ver:4.5.2

## Install software dependencies
RUN apt-get update \
  && apt-get install -y \
    pandoc \
    texlive \
    texlive-latex-extra \
    texlive-bibtex-extra \
    biber
RUN . /etc/environment \
  && R -e 'install.packages("pacman");' \
  && R -e 'pacman::p_install_version("rmarkdown", "2.30");'

```

Dockerizing an existing project

STEP 3: Writing the Docker file

5. Copy the source code into the image
   - The inside of the container is an Ubuntu file system with installed dependencies, therefore I copy everything into a separate folder to keep things neat.

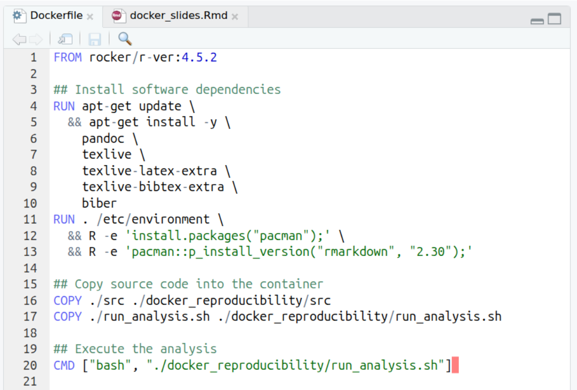


```
FROM rocker/r-ver:4.5.2

## Install software dependencies
RUN apt-get update \
  && apt-get install -y \
    pandoc \
    texlive \
    texlive-latex-extra \
    texlive-bibtex-extra \
    biber
RUN . /etc/environment \
  && R -e 'install.packages("pacman");' \
  && R -e 'pacman::p_install_version("rmarkdown", "2.30");'

## Copy source code into the container
COPY ./src ./docker_reproducibility/src
COPY ./run_analysis.sh ./docker_reproducibility/run_analysis.sh

```

Dockerizing an existing project

STEP 3: Writing the Docker file

5. Copy the source code into the image
   - The inside of the container is an Ubuntu file system with installed dependencies, therefore I copy everything into a separate folder to keep things neat.
6. Write the last line with the command to execute the analysis
   - There can be only one `CMD` line in your Docker file!

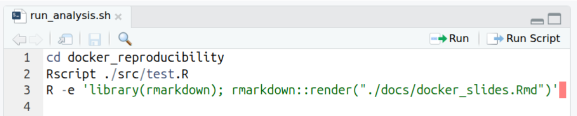


```
FROM rocker/r-ver:4.5.2

## Install software dependencies
RUN apt-get update \
  && apt-get install -y \
    pandoc \
    texlive \
    texlive-latex-extra \
    texlive-bibtex-extra \
    biber
RUN . /etc/environment \
  && R -e 'install.packages("pacman");' \
  && R -e 'pacman::p_install_version("rmarkdown", "2.30");'

## Copy source code into the container
COPY ./src ./docker_reproducibility/src
COPY ./run_analysis.sh ./docker_reproducibility/run_analysis.sh

## Execute the analysis
CMD ["bash", "./docker_reproducibility/run_analysis.sh"]
```

Dockerizing an existing project

STEP 3: Writing the Docker file

5. Copy the source code into the image
   - The inside of the container is an Ubuntu file system with installed dependencies, therefore I copy everything into a separate folder to keep things neat.
6. Write the last line with the command to execute the analysis
   - There can be only one CMD line in your Docker file!



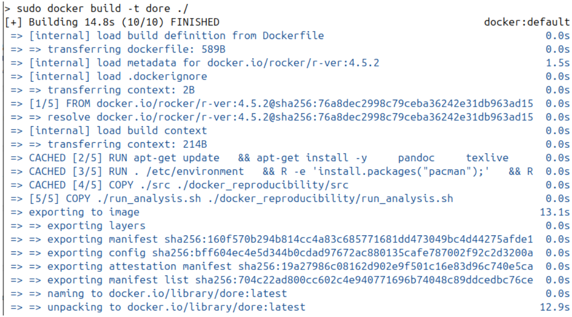
```
cd docker_reproducibility
Rscript ./src/test.R
R -e 'library(rmarkdown); rmarkdown::render("./docs/docker_slides.Rmd")'

```

Dockerizing an existing project

STEP 4: Building the image

```
sudo docker build -t <TAG_NAME> ./
```

- It probably will take a while to install all dependencies
- When you change one layer of your image and build again, Docker will execute only starting from layers that were changed



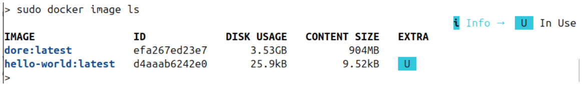
```
> sudo docker build -t dore ./
[+] Building 14.8s (10/10) FINISHED                                           docker:default
 => [internal] load build definition from Dockerfile                                    0.0s
 => => transferring dockerfile: 589B                                                    0.0s
 => [internal] load metadata for docker.io/rocker/r-ver:4.5.2                           1.5s
 => [internal] load .dockerignore                                                       0.0s
 => => transferring context: 2B                                                         0.0s
 => [1/5] FROM docker.io/rocker/r-ver:4.5.2@sha256:76a8dec2998c79ceba36242e31db963ad15  0.0s
 => => resolve docker.io/rocker/r-ver:4.5.2@sha256:76a8dec2998c79ceba36242e31db963ad15  0.0s
 => [internal] load build context                                                       0.0s
 => => transferring context: 214B                                                       0.0s
 => CACHED [2/5] RUN apt-get update   && apt-get install -y     pandoc     texlive      0.0s
 => CACHED [3/5] RUN . /etc/environment   && R -e 'install.packages("pacman");'   && R  0.0s
 => CACHED [4/5] COPY ./src ./docker_reproducibility/src                                0.0s
 => [5/5] COPY ./run_analysis.sh ./docker_reproducibility/run_analysis.sh               0.0s
 => exporting to image                                                                 13.1s
 => => exporting layers                                                                 0.0s
 => => exporting manifest sha256:160f570b294b814cc4a83c685771681dd473049bc4d44275afde1  0.0s
 => => exporting config sha256:bff604ec4e5d344b0cdad97672ac880135cafe787002f92c2d3200a  0.0s
 => => exporting attestation manifest sha256:19a27986c08162d902e9f501c16e83d96c740e5ca  0.0s
 => => exporting manifest list sha256:704c22ad800cc602c4e940771696b74048c89ddcedbc76ce  0.0s
 => => naming to docker.io/library/dore:latest                                          0.0s
 => => unpacking to docker.io/library/dore:latest                                      12.9s
```

Dockerizing an existing project

STEP 4: Building the image

```
sudo docker build -t <TAG_NAME> ./
```

- It probably will take a while to install all dependencies
- When you change one layer of your image and build again, Docker will execute only starting from layers that were changed



```
> sudo docker image ls
                                                                        i Info →  U  In Use
IMAGE                ID             DISK USAGE   CONTENT SIZE   EXTRA
dore:latest          efa267ed23e7       3.53GB          904MB
hello-world:latest   d4aaab6242e0       25.9kB         9.52kB   U
>
```

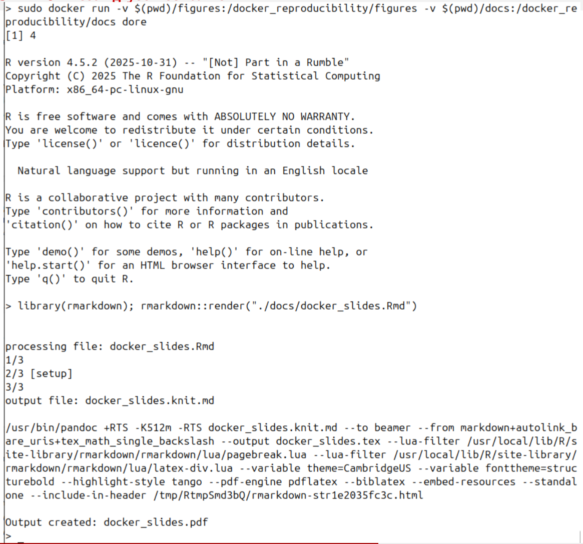
Dockerizing an existing project

STEP 5: Testing your container

```
sudo docker run -v $(pwd)/figures:/docker_reproducibility/figures -v
$(pwd)/docs:/docker_reproducibility/docs <TAG_NAME>
```

Dockerizing an existing project

STEP 5: Testing your container



```
> sudo docker run -v $(pwd)/figures:/docker_reproducibility/figures -v $(pwd)/docs:/docker_re
producibility/docs dore
[1] 4

R version 4.5.2 (2025-10-31) -- "[Not] Part in a Rumble"
Copyright (C) 2025 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu

R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.

  Natural language support but running in an English locale

R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

> library(rmarkdown); rmarkdown::render("./docs/docker_slides.Rmd")


processing file: docker_slides.Rmd
1/3
2/3 [setup]
3/3
output file: docker_slides.knit.md

/usr/bin/pandoc +RTS -K512m -RTS docker_slides.knit.md --to beamer --from markdown+autolink_b
are_uris+tex_math_single_backslash --output docker_slides.tex --lua-filter /usr/local/lib/R/s
ite-library/rmarkdown/rmarkdown/lua/pagebreak.lua --lua-filter /usr/local/lib/R/site-library/
rmarkdown/rmarkdown/lua/latex-div.lua --variable theme=CambridgeUS --variable fonttheme=struc
turebold --highlight-style tango --pdf-engine pdflatex --biblatex --embed-resources --standal
one --include-in-header /tmp/RtmpSmd3bQ/rmarkdown-str1e2035fc3c.html

Output created: docker_slides.pdf
> _
```

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