Software Environments, Notebooks and Containers

(for Bioinformatics and Computational Biology)

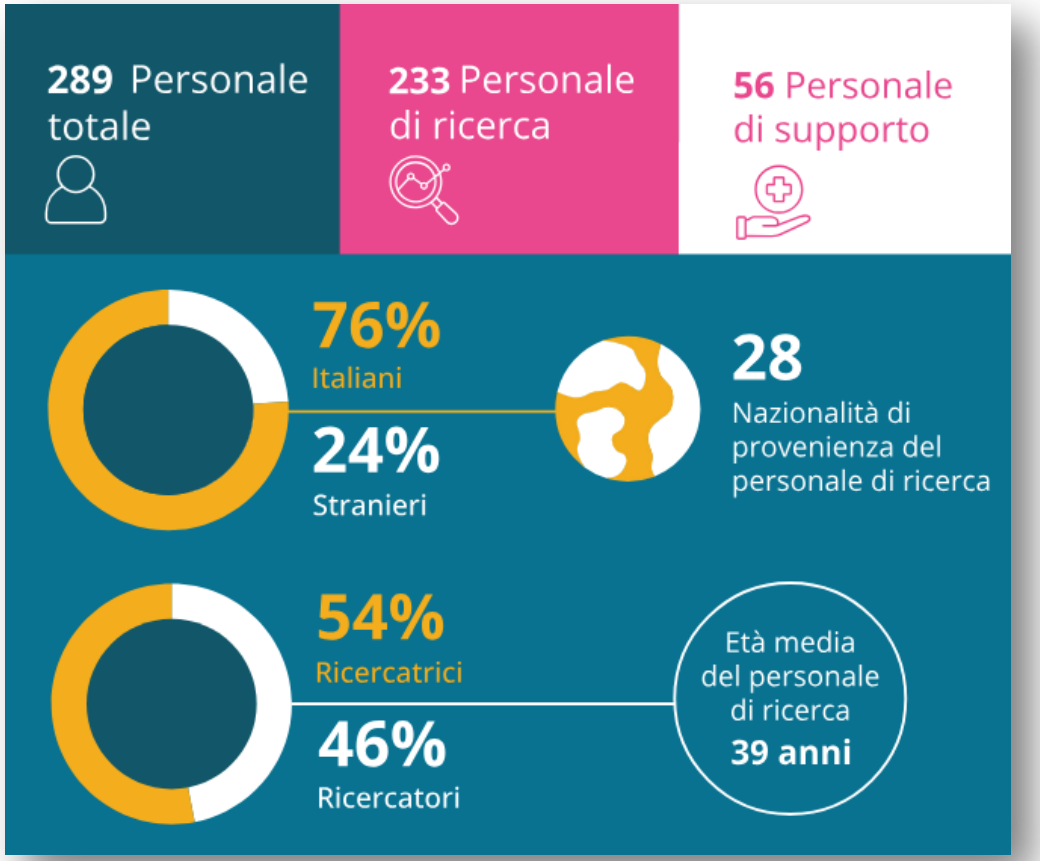
Naples, November 26th, 2024

Overview

- Let’s get introduced
- Reproducibility in (computational) Science
- Software environments: Conda
- Go interactive with Jupyter Notebook
- Freeze across space and time with Containers
- Best practices & collaboration

- hands on through out the presentation

IFOM - ETS
The AIRC Institute of Molecular Oncology



Research Computing & Data Science

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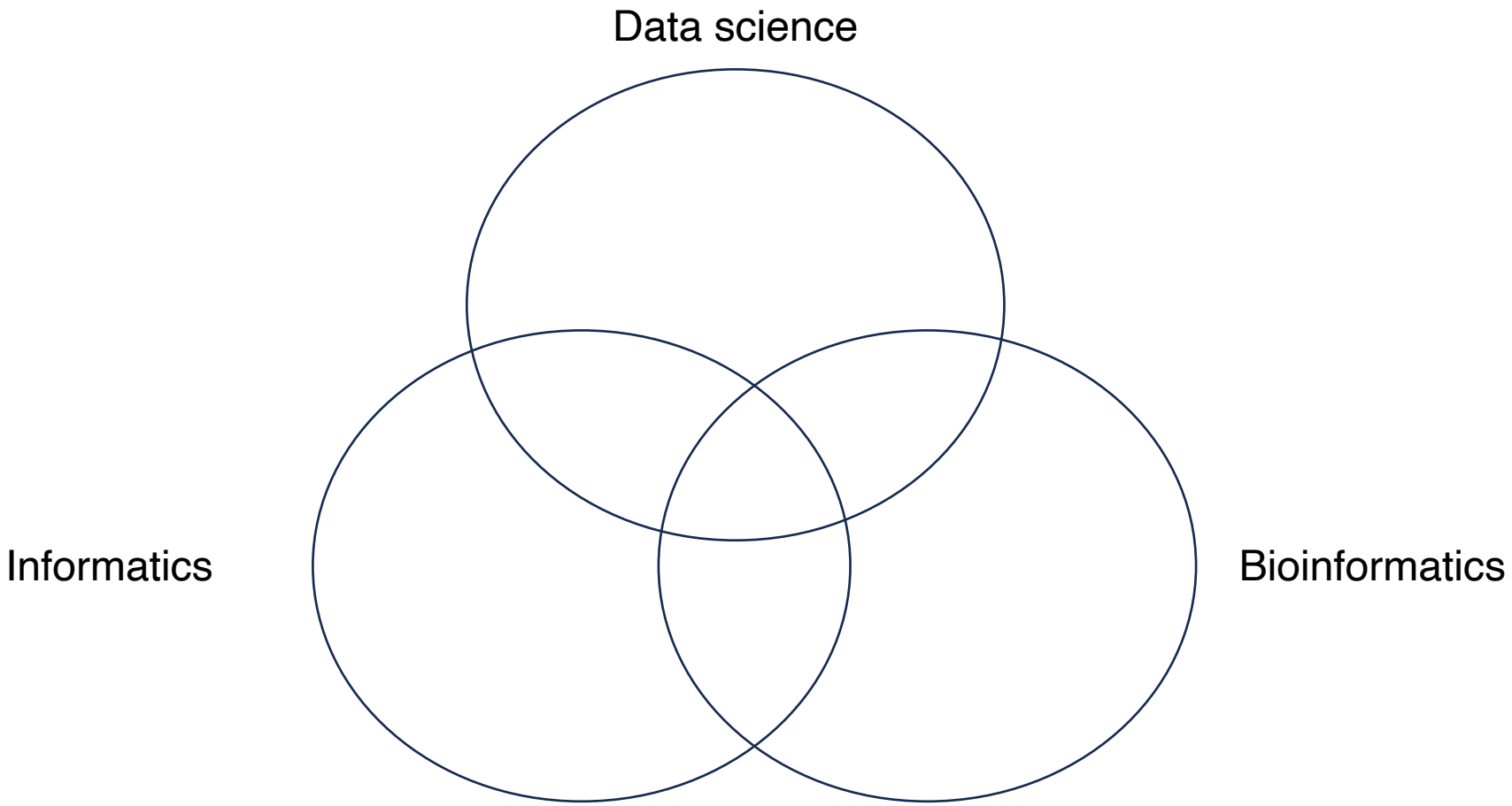
Bioinformatics Scientist

@ricrossi

Tell us about you and where you are!



Reproducibility in *(computational)* Science

The challenge of reproducible research

Napoli, 26/11/2024

Reproducible research

The term reproducible research refers to **the idea that scientific results should be documented in such a way that their deduction is fully transparent**. This requires a detailed description of the methods used to obtain the data and making the full dataset and the code to calculate the results easily accessible.

Wikipedia
https://en.wikipedia.org › wiki › Reproducibility

Reproducibility - Wikipedia

Your research is reproducible if - and only if - you can repeatedly and easily reproduce it

(and you are *another* person in 6 months time)

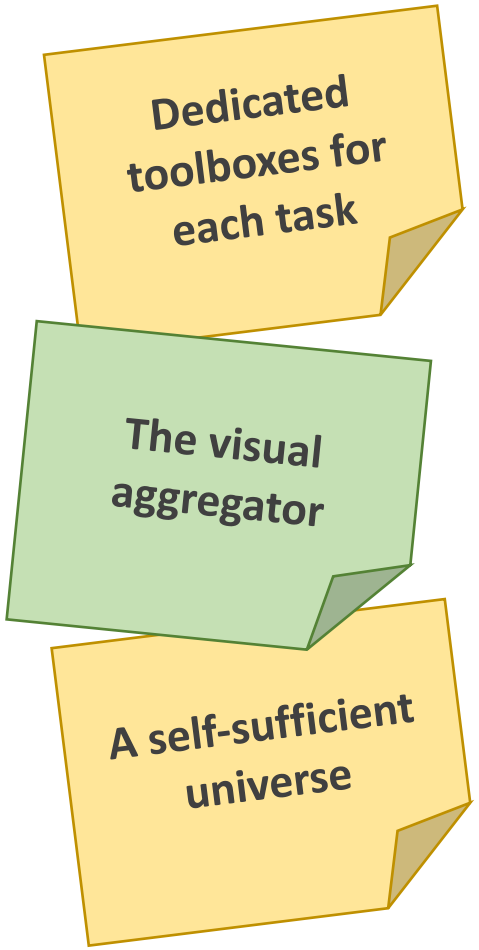
Reproducibility in Computational Science

- Unique Challenges of Code and Algorithms: Complex workflows that may **not be adequately documented**.
- Reproducibility as a Computational Requirement: Need for consistent outputs given **identical inputs**.
- **Software Environment Variability**: Differences in libraries, dependencies, tools, OS, hardware,…

Software Environment Variability

1. **Operating System Differences**
   - Scripts and tools often behave differently across operating systems (Linux, macOS, Windows).
   - This variability introduces challenges when sharing workflows between researchers using different platforms.
2. **Dependency Management Issues**
   - Software tools and workflows depend on specific versions of libraries, frameworks, and dependencies.
   - Variations in versions can lead to differences in outputs, even with the same dataset and code.
3. **Hardware-Specific Variability**
   - Computational performance and precision may depend on the hardware used.
   - Some analyses might fail or provide inconsistent results if moved to a less or differently capable system.
4. **Network and Access Issues**
   - Cloud services or remote dependencies may change over time, making workflows break without notice.
   - External API calls or dependency links can become unavailable or version-incompatible.

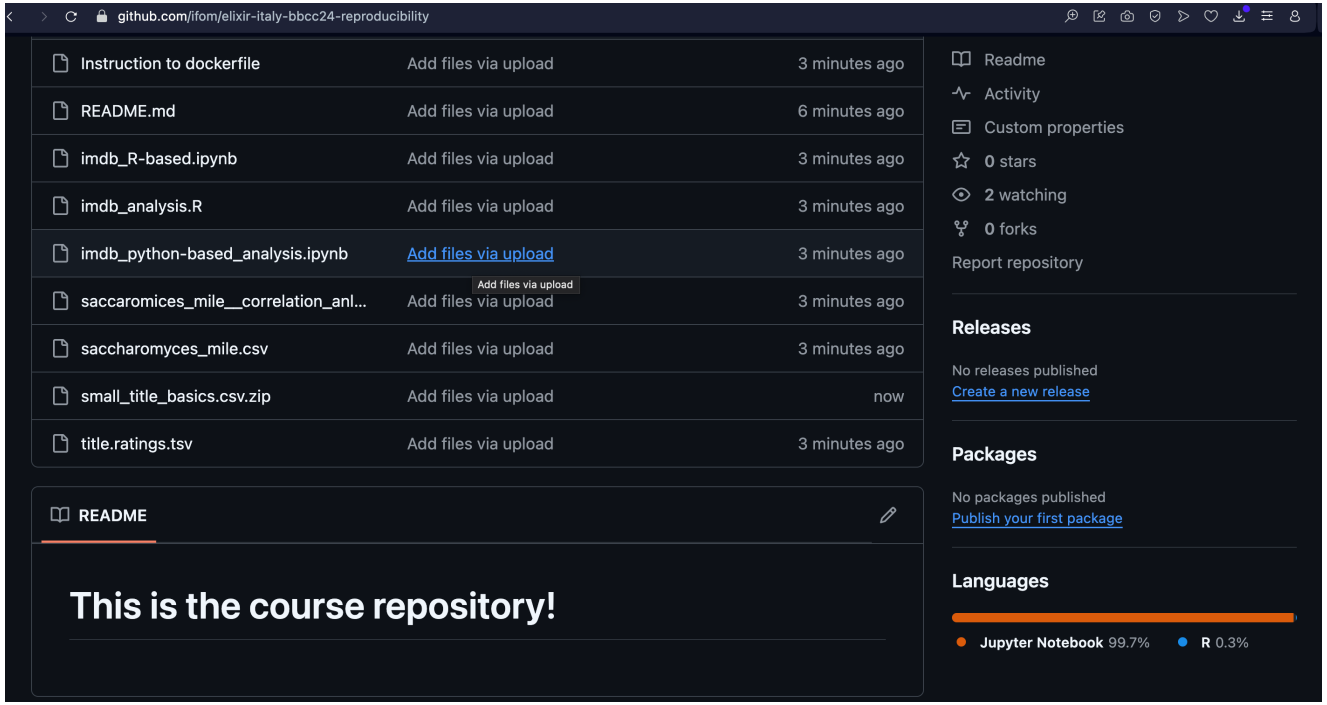
Tools to mitigate variability

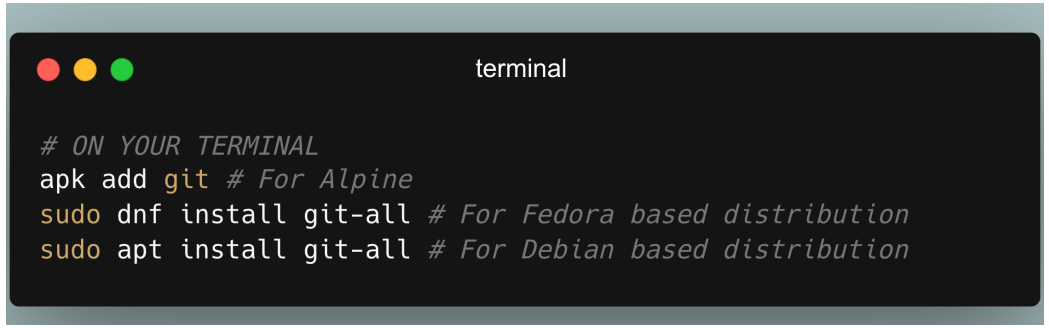


- **Software environments**
  - Tools like **Conda** and virtual environments ensure dependency versions are pinned and reproducible.
  - Configuration files like `requirements.txt` or `environment.yml` standardize environment setup.
- **Notebook Environments**
  - Platforms like **Jupyter** provide a controlled, shareable, and interactive environment, reducing variability.
- **Containerization**
  - Tools like **Docker** encapsulate the complete software environment, including dependencies, operating systems, and configurations.

GitHub, get the workshop material

https://github.com/ifom/elixir-italy-bbcc24-reproducibility





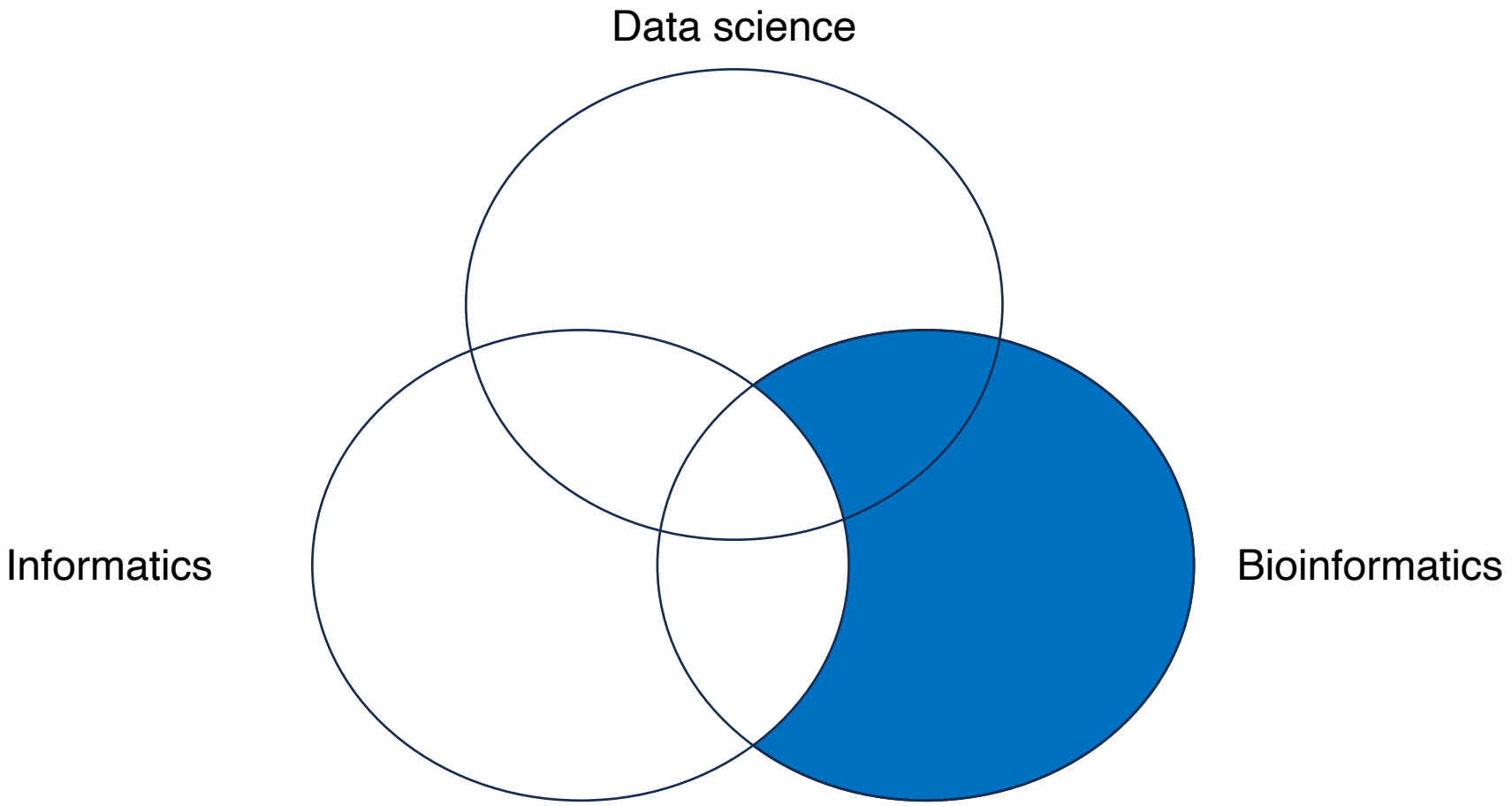
Conda environments

Conda & companions

Install and organize software

BBCC2024, RCDS

Topic domain: bioinformatics



Bioinformaticians are not system engineers!

- Bioinformaticians need software
- Software do not need bioinformaticians

Bioinformaticians are not system engineers!

- Bioinformaticians need software
- Software *should* ~~do~~ not need bioinformaticians

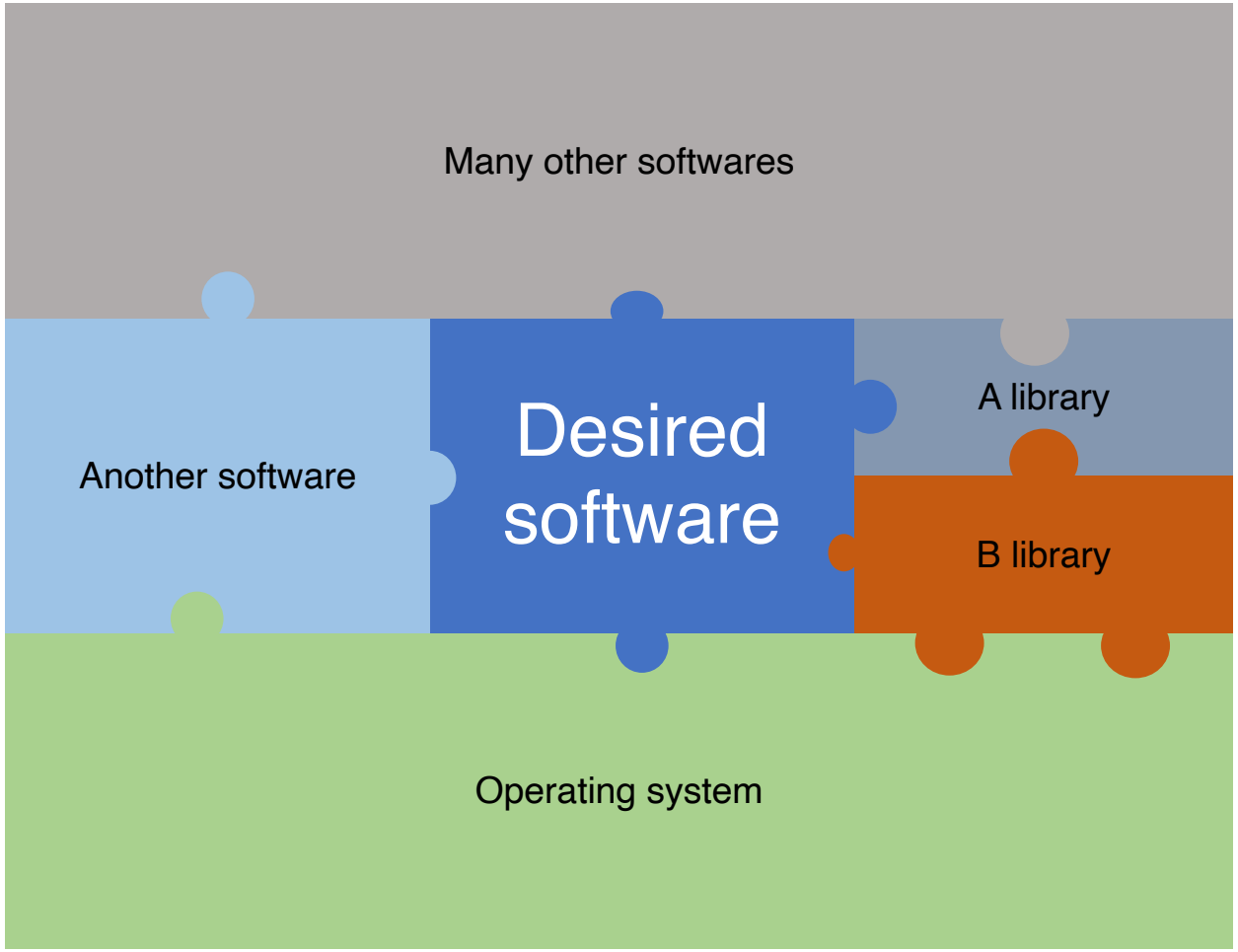
Languages often have their own repos

CRAN, Bioconductor, GitHubs,…

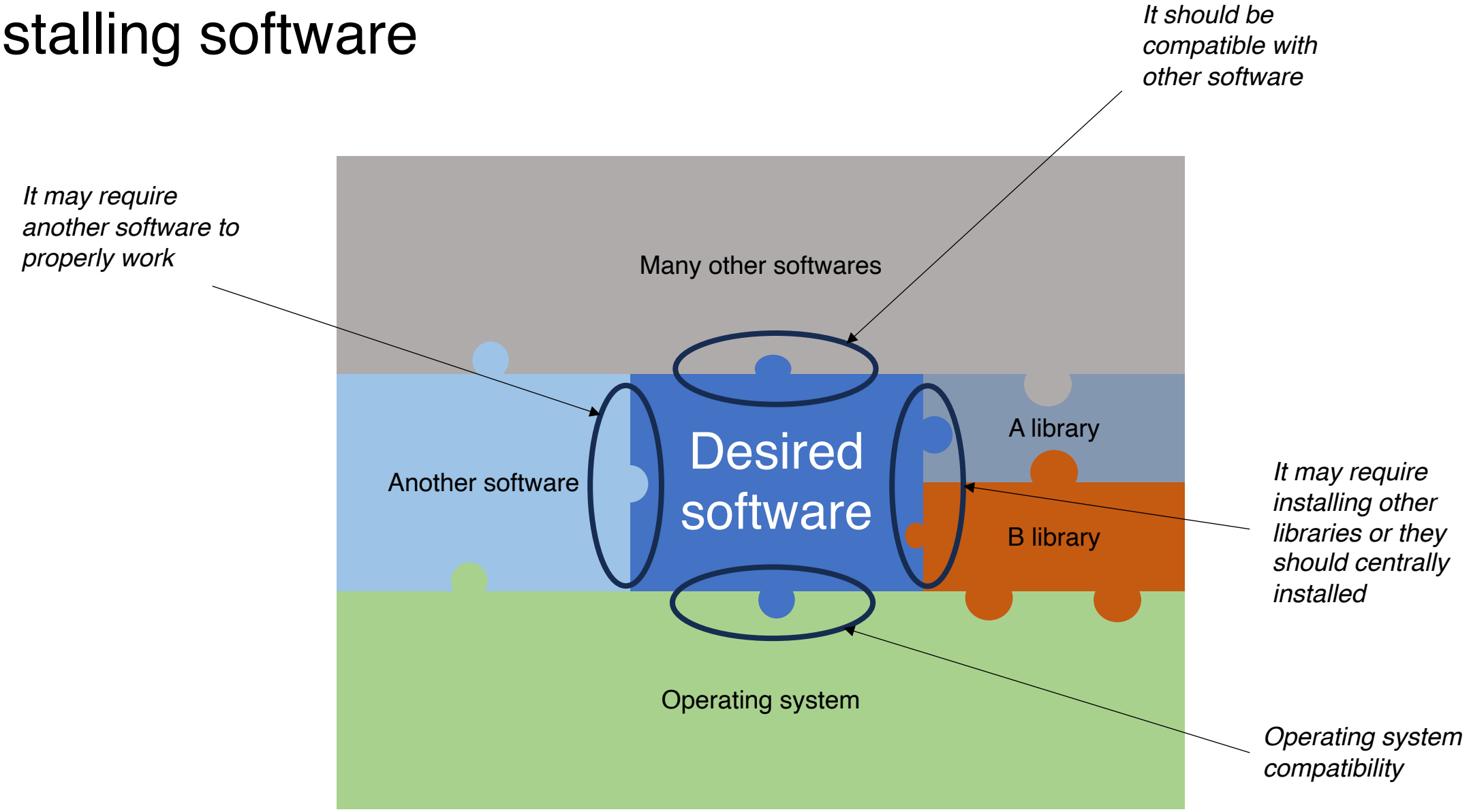
Pip, GitHubs, …

Installing software

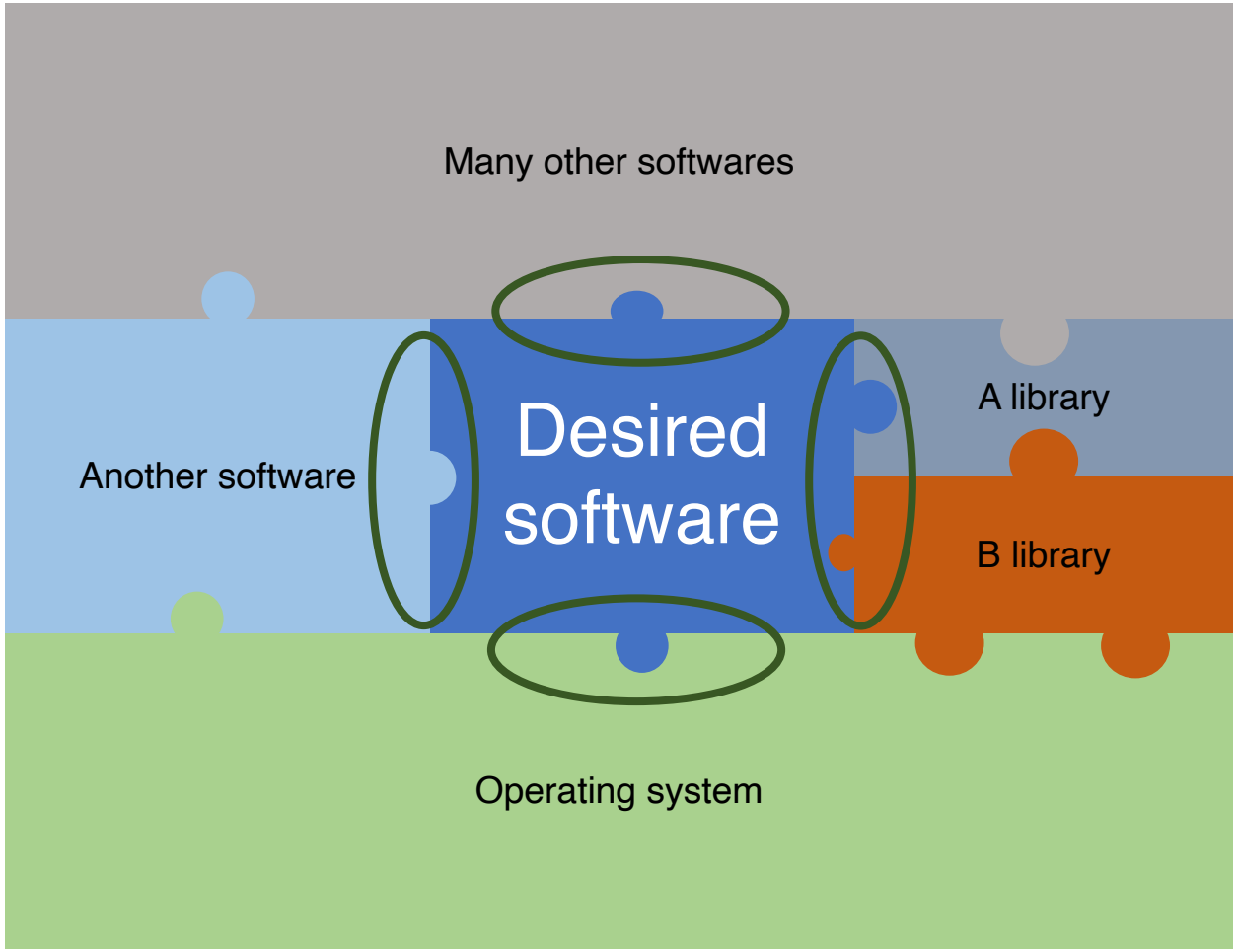
Installing software



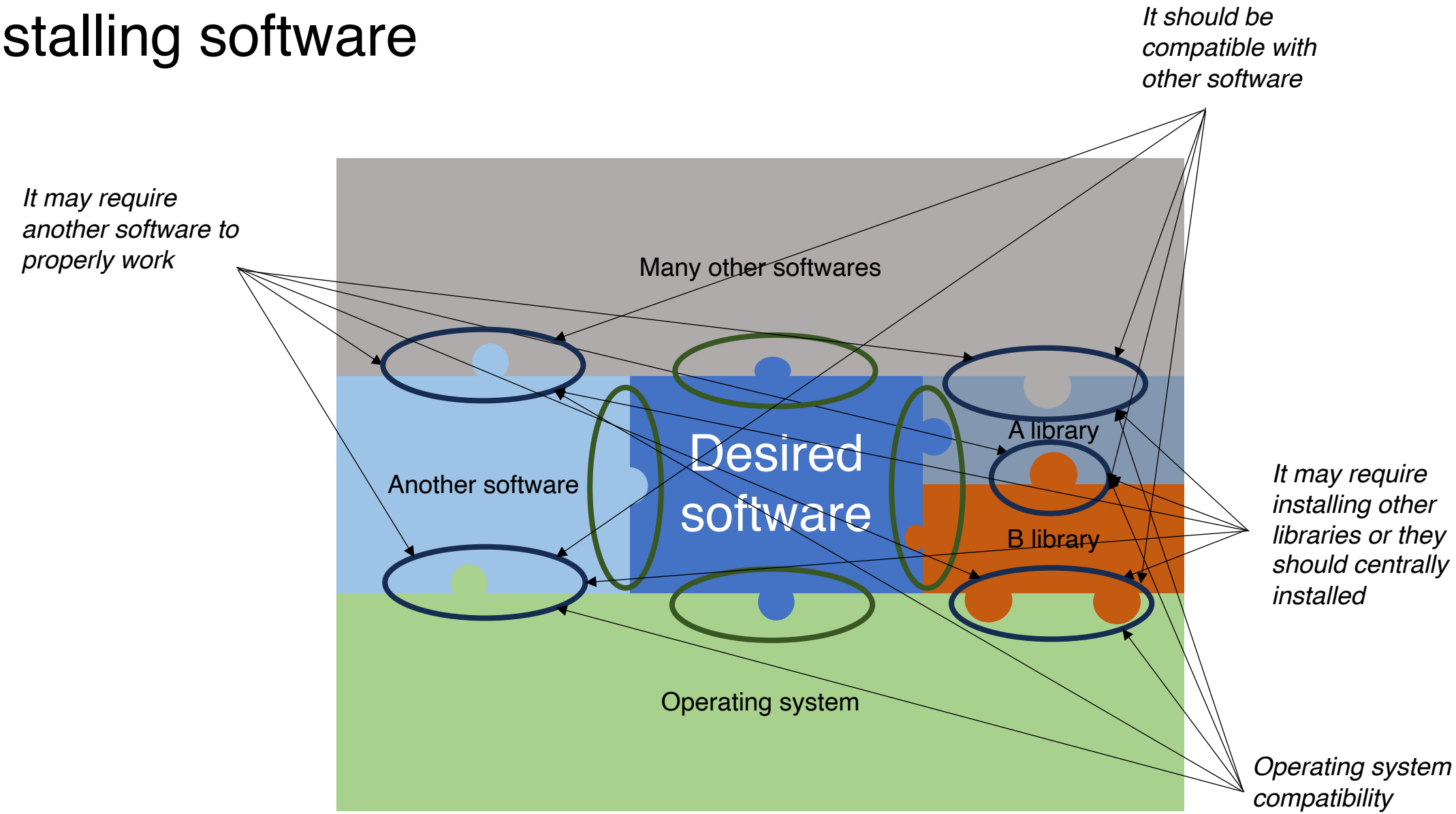
Installing software



Installing software



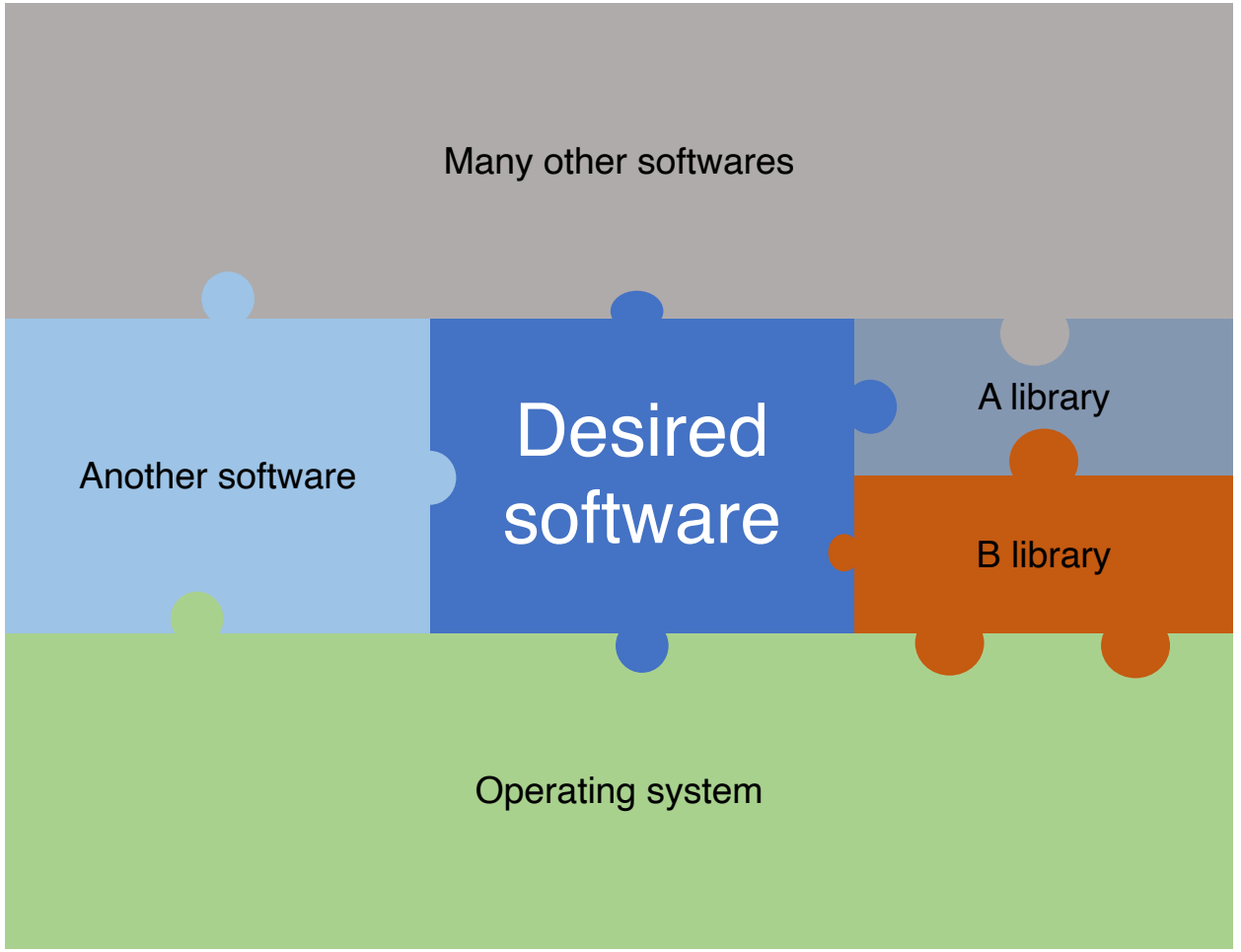
Installing software



Installing software: conda

Conda is an open source **package management** system and **environment management** system for installing multiple versions of software packages and their dependencies and switching easily between them.

It works on Linux, OS X and Windows, and was created for Python programs but can package and distribute any software.



Conda:

- *solves software compatibilities*
- *installs missing softwares*
- *installs required libraries*

Conda description from: https://anaconda.org/anaconda/conda

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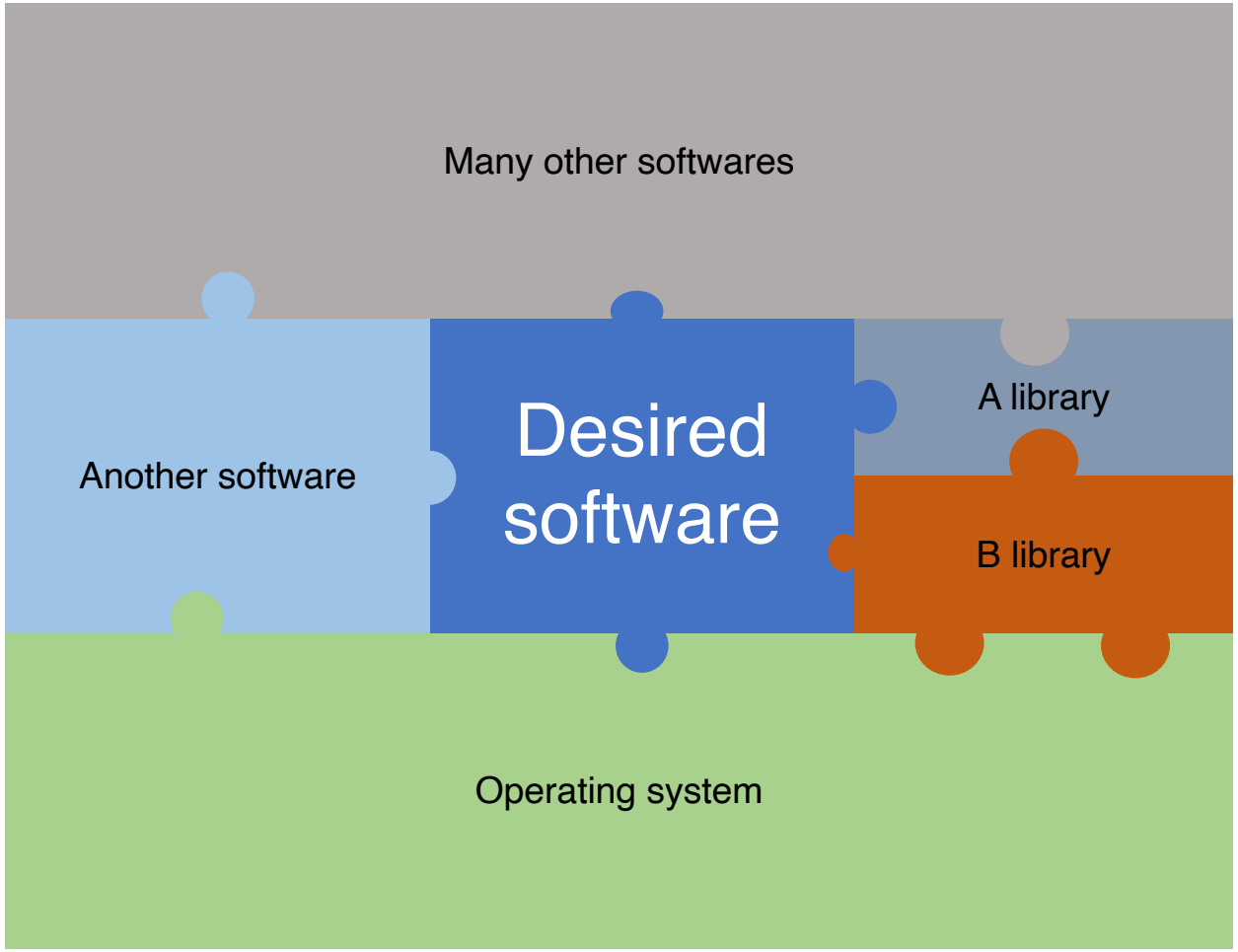


Conda:

- *solves software compatibilities*
- *installs missing softwares*
- *installs required libraries*

In other words, it is like the Appstore or Playstore for bioinformatics!

Conda is a ***package manager***

- **Why Conda Was Created**
  - Managing dependencies for Python and scientific libraries was challenging.
  - Anaconda Inc. (formerly Continuum Analytics) introduced Conda in 2012 to address this issue.

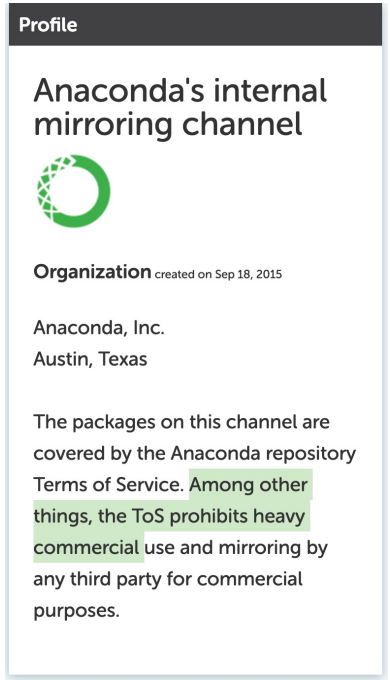
- **Goals of Conda**
  - Provide a cross-platform package manager.
  - Handle complex dependencies and allow reproducible environments.

Evolution and Development of Conda

- Expansion Beyond Python
  - Initially Python-focused, now supports R, Ruby, Lua, and other languages.
- Integration of Data Science Tools
  - Became the backbone for scientific computing environments.
  - Widely adopted in bioinformatics and computational biology.
- Key Milestones in Development
  - Introduction of the **Conda Forge** repository.
  - Development of tools like **Miniconda** for lightweight installations.

Then there are ***package repositories***

- **Anaconda**
  - https://anaconda.org/anaconda
- **Bioconda**
  - https://anaconda.org/bioconda
- **Conda-forge**
  - https://anaconda.org/conda-forge



Correspondence | Published: 02 July 2018

Bioconda: sustainable and comprehensive software distribution for the life sciences

Björn Grüning, Ryan Dale, Andreas Sjödin, Brad A. Chapman, Jillian Rowe, Christopher H. Tomkins-Tinch, Renan Valieris, Johannes Köster ✉ & The Bioconda Team

Nature Methods **15**, 475–476 (2018) |

BIOCONDA®

Bioconda lets you install thousands of software packages related to biomedical research using the conda package manager.

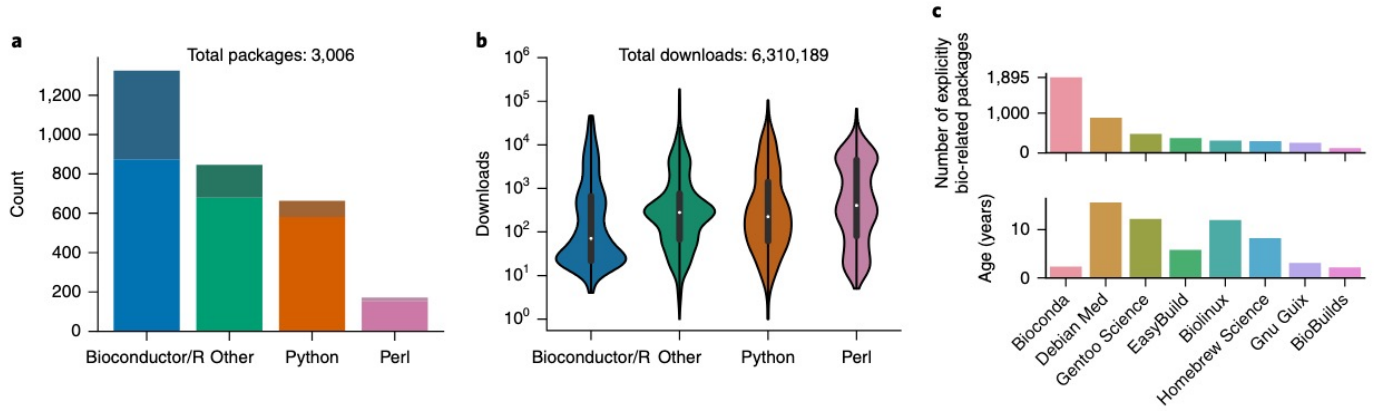
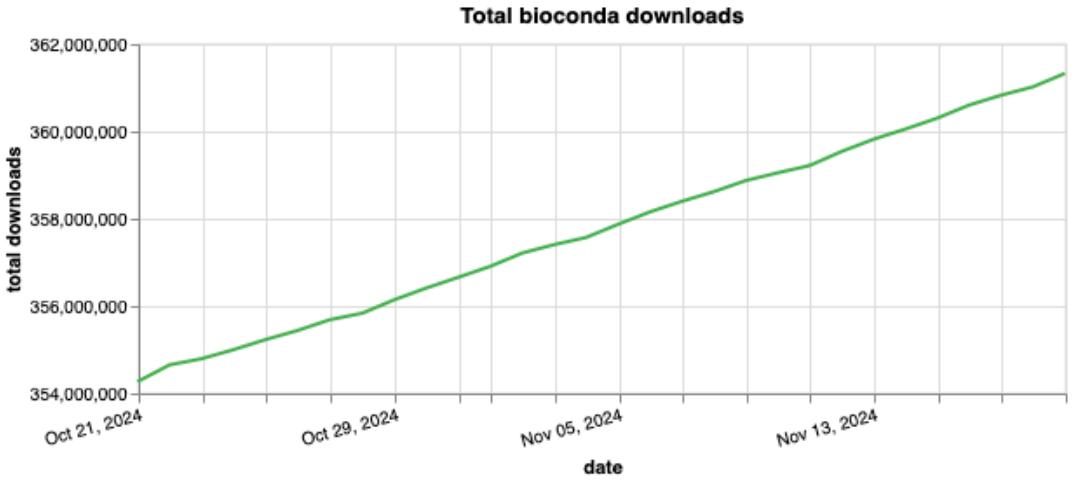
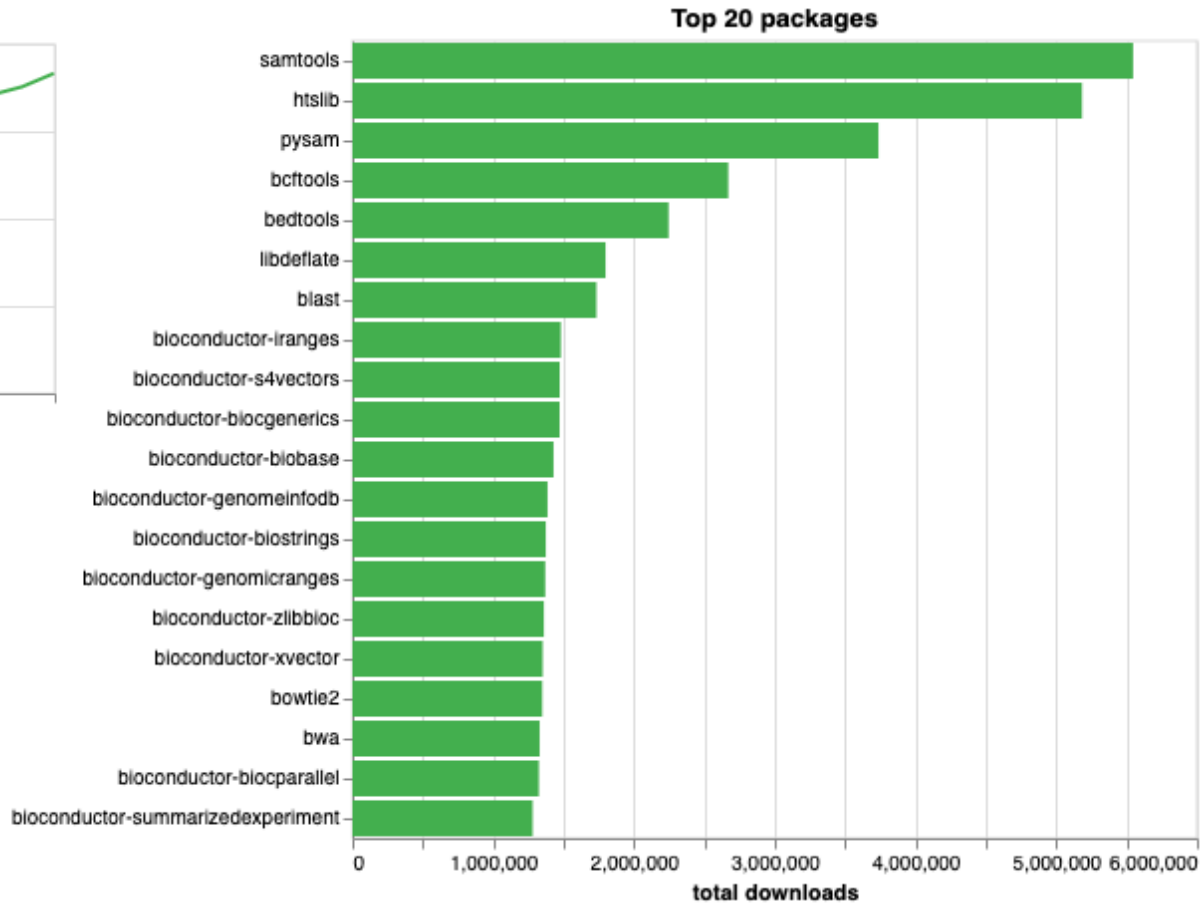
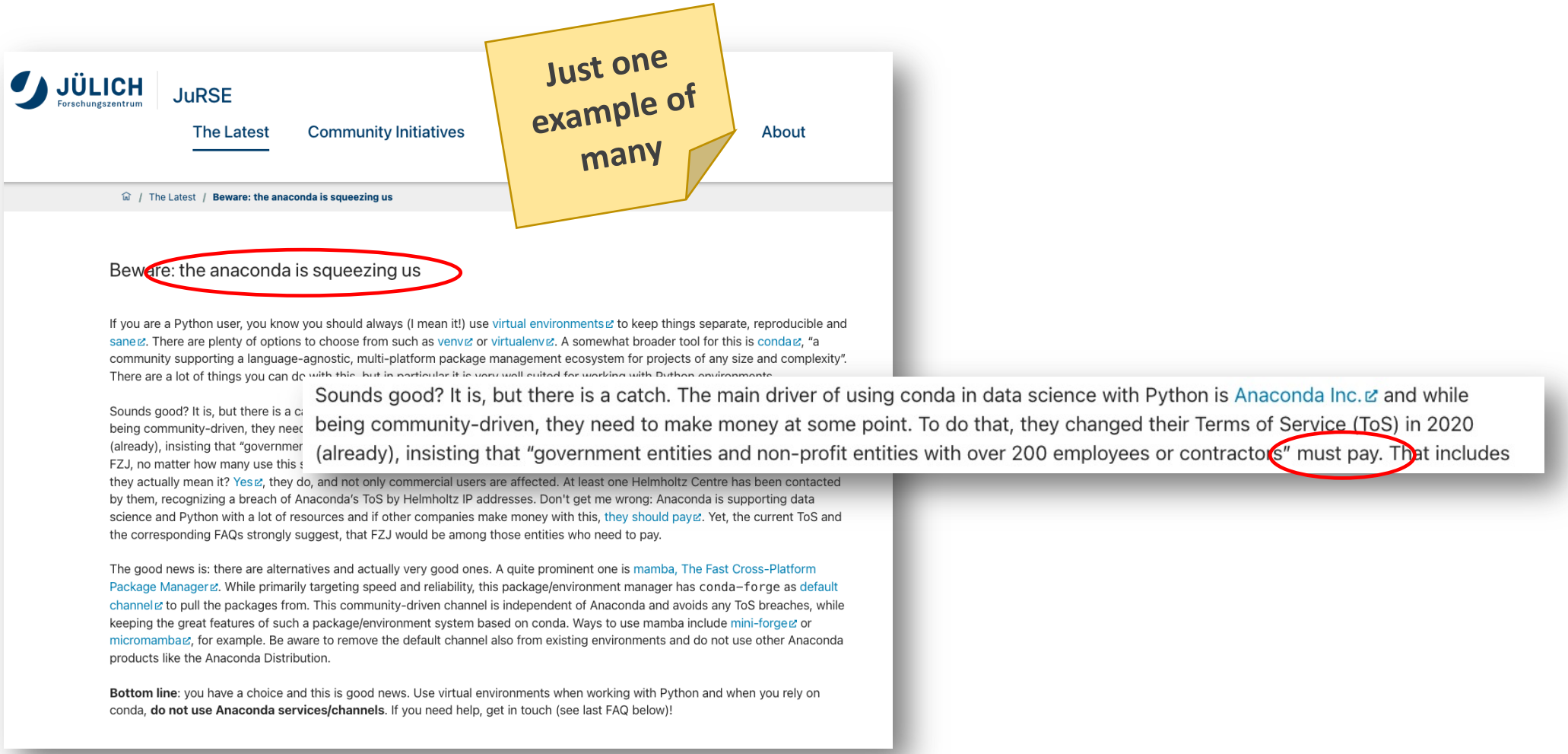


Fig. 1 | Package numbers and usage. a, Package count per language ecosystem (saturated colors on the lower portions of the bars represent explicitly life-science-related packages). **b**, Distribution of per-package downloads, separated by language ecosystem. The term "other" encompasses all packages that do not fall into one of the specific categories named. White dots represent the mean; dark bars represent the interval between upper and lower quartiles. **c**, Comparison of the number of explicitly life-science-related packages in Bioconda with that in Debian Med (https://www.debian.org/devel/debian-med), Gentoo Science Overlay (category sci-biology; https://github.com/gentoo/sci), EasyBuild (module bio; https://easybuilders.github.io/easybuild), Biolinux[6], Homebrew Science (tag bioinformatics; https://brew.sh), GNU Guix (category bioinformatics; https://www.gnu.org/s/guix), and BioBuilds (https://biobuilds.org). The lower graph shows the project age since the first release or commit. Statistics obtained 25 October 2017.


Total bioconda downloads
362,000,000
360,000,000
358,000,000
356,000,000
354,000,000
total downloads
Oct 21, 2024
Oct 29, 2024
Nov 05, 2024
Nov 13, 2024
date


Top 20 packages
samtools
htslib
pysam
bcftools
bedtools
libdeflate
blast
bioconductor-iranges
bioconductor-s4vectors
bioconductor-biocgenerics
bioconductor-biobase
bioconductor-genomeinfodb
bioconductor-biostrings
bioconductor-genomicranges
bioconductor-zlibbioc
bioconductor-xvector
bowtie2
bwa
bioconductor-biocparallel
bioconductor-summarizedexperiment
0
1,000,000
2,000,000
3,000,000
4,000,000
5,000,000
6,000,000
total downloads

Always read the fine print (TOS)



CDO TRENDS
Digital & Data Insights for Business Leaders

DATA SCIENCE | MACHINE LEARNING

Anaconda Threatens Legal Action Over Licensing Terms

By **Paul Mah** August 21, 2024

https://www.cdotrends.com/story/4173/anaconda-threatens-legal-action-over-licensing-terms

The Register

Anaconda puts the squeeze on data scientists now deemed to be terms-of-service violators

Academic, non-profit organizations told to start paying up – or else

Thomas Claburn Thu 8 Aug 2024 // 12:26 UTC

UPDATED Research and academic organizations are just now finding out that they will have to pay for software made by Anaconda, when for years these groups were under the impression it could be used at no cost.

https://www.theregister.com/2024/08/08/anaconda_puts_the_squeeze_on/

IN THE UNITED STATES DISTRICT COURT
FOR THE DISTRICT OF DELAWARE

ANACONDA, INC., Plaintiff,	)	C.A. No. _____
v.	)	**DEMAND FOR JURY TRIAL**
INTEL CORPORATION, Defendant.	)	

COMPLAINT

Plaintiff Anaconda, Inc. ("Anaconda" or "Plaintiff") brings this complaint against Defendant Intel Corporation ("Intel" or "Defendant") and alleges as follows:

NATURE OF THE ACTION

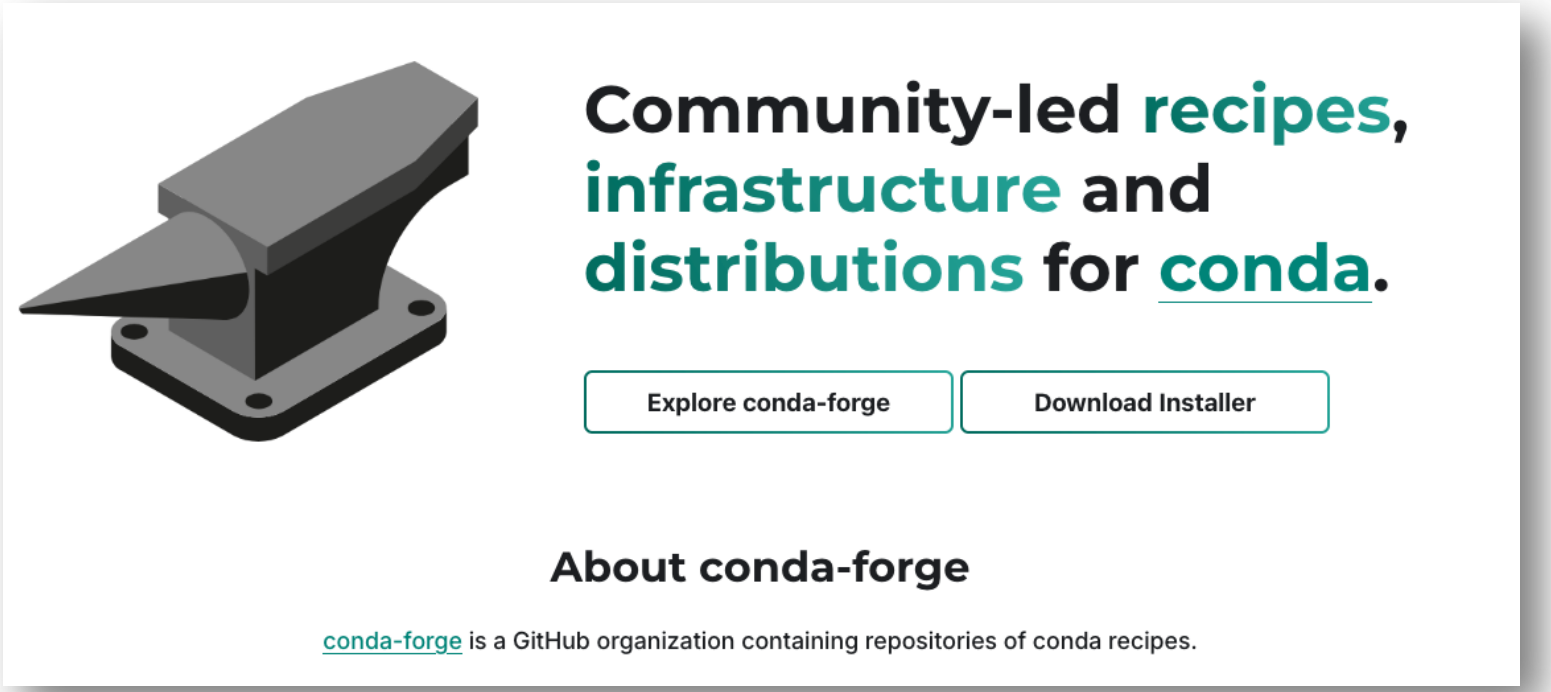
1. This is a civil action for the infringement, under the copyright laws of the United States, 17 U.S.C. § 101, *et seq.*, of proprietary material registered under U.S. Copyright No. TX 9-407-381 ("Asserted Copyright") in violation of 17 U.S.C. § 501.

2. Anaconda developed a technology that has become critical to the booming artificial intelligence ("AI") industry—one that is used by over 40 million users at over one million companies worldwide. Intel is one of those companies. For years, Intel bought licenses allowing

elixir ITALY | IFOM

Alternatives exist

- Community led
- Free to use
- Latest (*dev* also) releases



Hands-on: install miniforge3*

terminal

```
curl -L -O "https://github.com/conda-forge/miniforge/releases/latest/download/Miniforge3-$(uname)-$(uname -m).sh"
bash Miniforge3-$(uname)-$(uname -m).sh
```

**Why miniforge3 after all the slides on conda?*

After 2020, **Anaconda Inc.** (the company that owns conda) **set up a fee** on all the companies/non-academic institutes that use their repositories. The access to the conda **miniforge** repositories **instead** is still **free**.

Installing miniforge3 instead of miniconda3 (conda) we guarantee that the Anaconda Inc. repositories are not in the default repositories used to download software.

Miniforge3 installing code from: https://github.com/conda-forge/miniforge

Hands-on: install *software with* miniforge3

Hands-on: install *software with* miniforge3

terminal

```
conda install conda-forge::numpy
```

```
(base) cpetrini@ ~ % conda install conda-forge::numpy
Channels:
 - conda-forge
Platform: osx-64
Collecting package metadata (repodata.json): done
Solving environment: done

## Package Plan ##

  environment location: /Users/cpetrini/miniforge3

  added / updated specs:
    - conda-forge::numpy


The following packages will be downloaded:

    package                    |            build
    ---------------------------|-----------------
    libcblas-3.9.0             |25_osx64_openblas          15 KB  conda-forge
    numpy-2.1.3                |  py312hfc93d17_0         7.2 MB  conda-forge
    ------------------------------------------------------------
                                           Total:         7.2 MB

The following NEW packages will be INSTALLED:

  libcblas           conda-forge/osx-64::libcblas-3.9.0-25_osx64_openblas
  numpy              conda-forge/osx-64::numpy-2.1.3-py312hfc93d17_0


Proceed ([y]/n)?
```

Hands-on: install *software with* miniforge3

terminal

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conda install conda-forge::numpy
```

Repository collecting the required softwares

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    ------------------------------------------------------------
                                           Total:         7.2 MB

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  numpy              conda-forge/osx-64::numpy-2.1.3-py312hfc93d17_0


Proceed ([y]/n)?
```

Packages info

Hands-on: install *software with* miniforge3, specific version

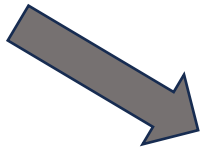
Hands-on: install *software with* miniforge3, specific version

Requested a specific version

Hands-on: install *software with* miniforge3, specific version

terminal

```
conda install conda-forge::r-base=4.3.2
```



```
The following packages will be DOWNGRADED:

  cairo                                1.18.0-h37bd5c4_3 ⟶ 1.18.0-h99e66fa_0
  harfbuzz                              9.0.0-h098a298_1 ⟶ 8.3.0-hf45c392_0
  icu                                    75.1-h120a0e1_0 ⟶ 73.2-hf5e326d_0
  libglib                           2.82.2-hb6ef654_0 ⟶ 2.78.4-hab64008_0
  libxml2                           2.13.4-h12808cf_2 ⟶ 2.12.7-hc603aa4_3
  pcre2                                10.44-h7634a1b_2 ⟶ 10.42-h0ad2156_0
  texlive-core                  20230313-hca7b749_15 ⟶ 20230313-ha022968_11


Proceed ([y]/n)?
```

Hands-on: install *software with* miniforge3, R libraries

terminal

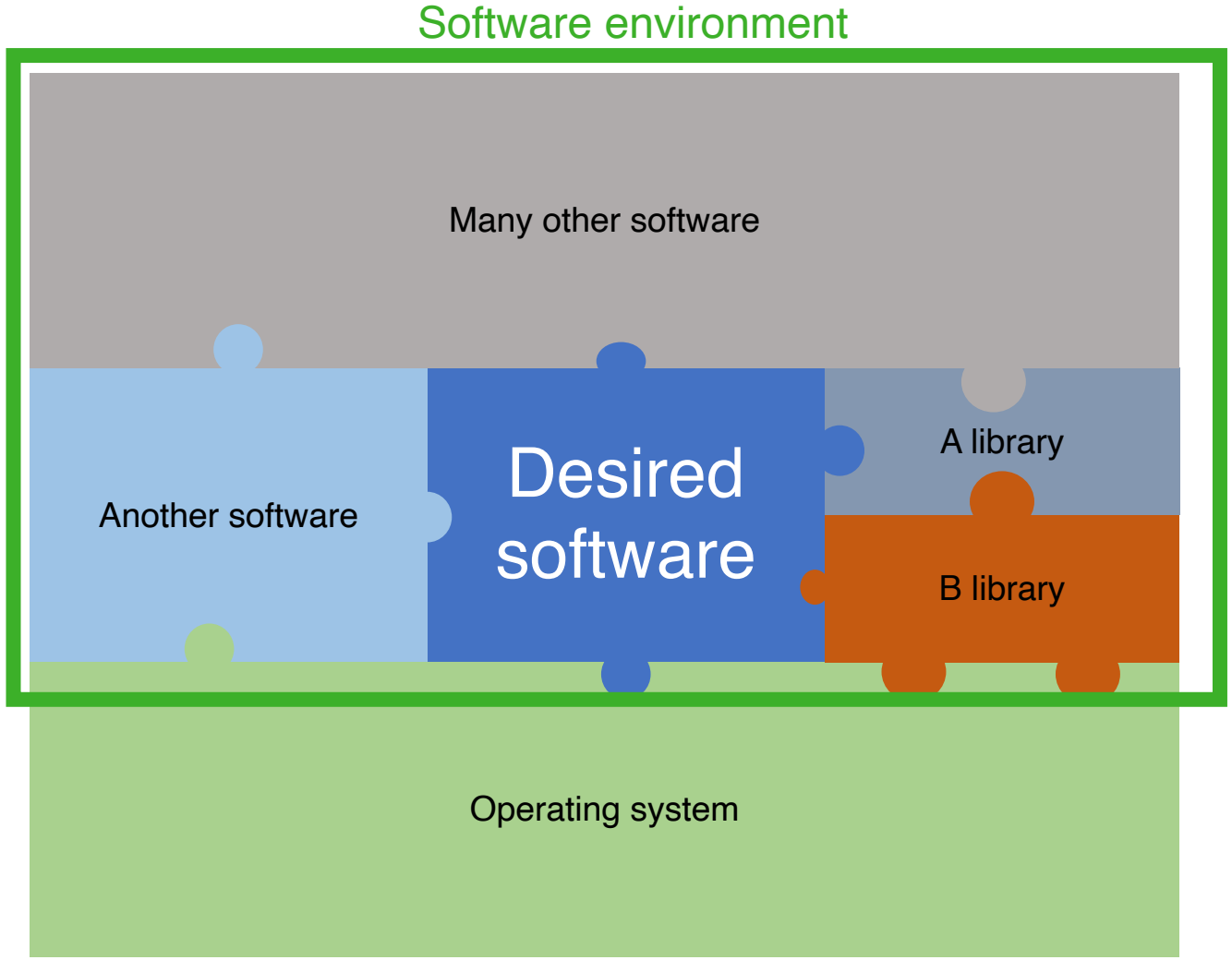
```
conda install conda-forge::r-tidyverse
```

or

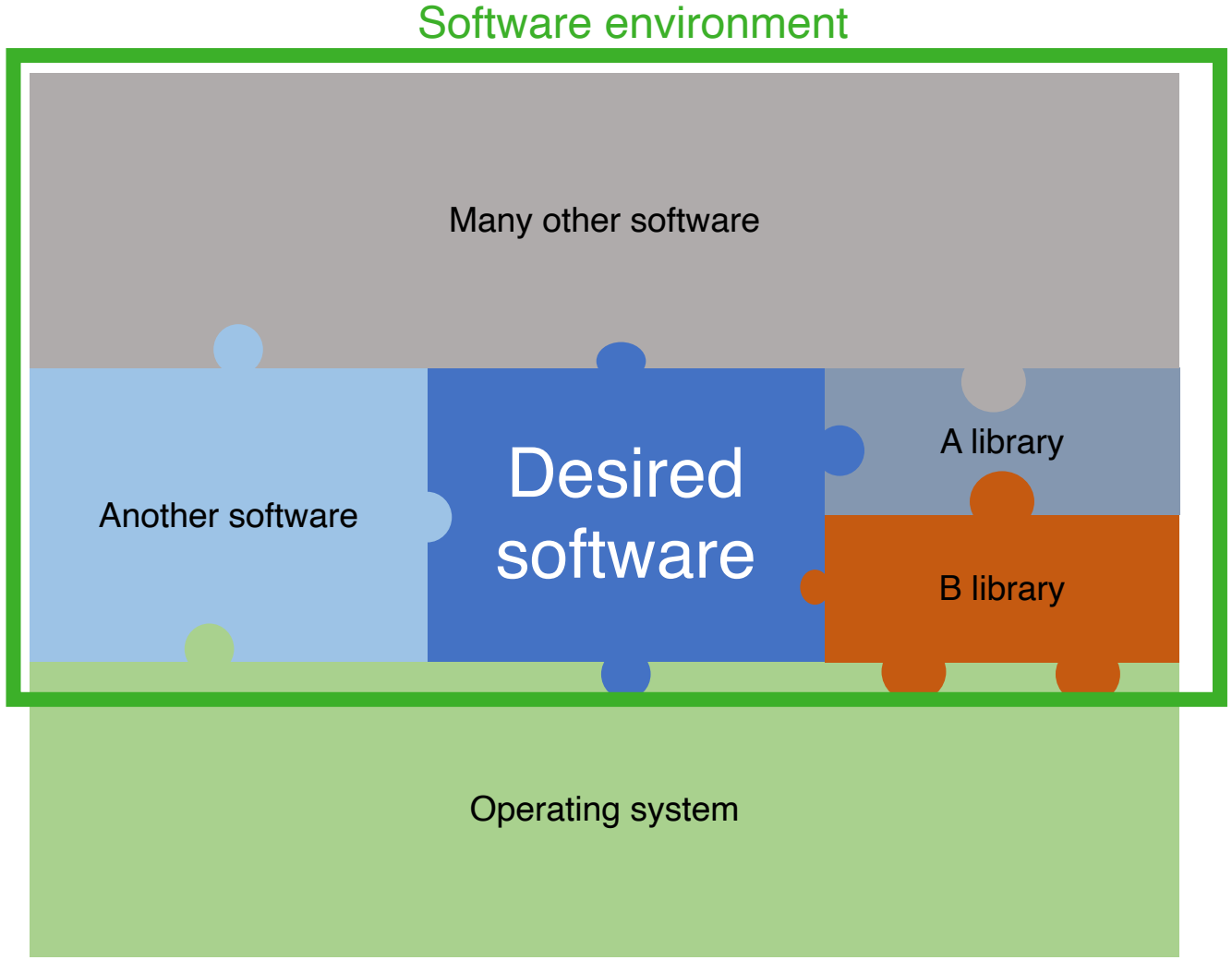
```
# Install from CRAN
install.packages("tidyverse")
```

What's the best strategy to install an R library?

Software environments with ~~conda~~ miniforge

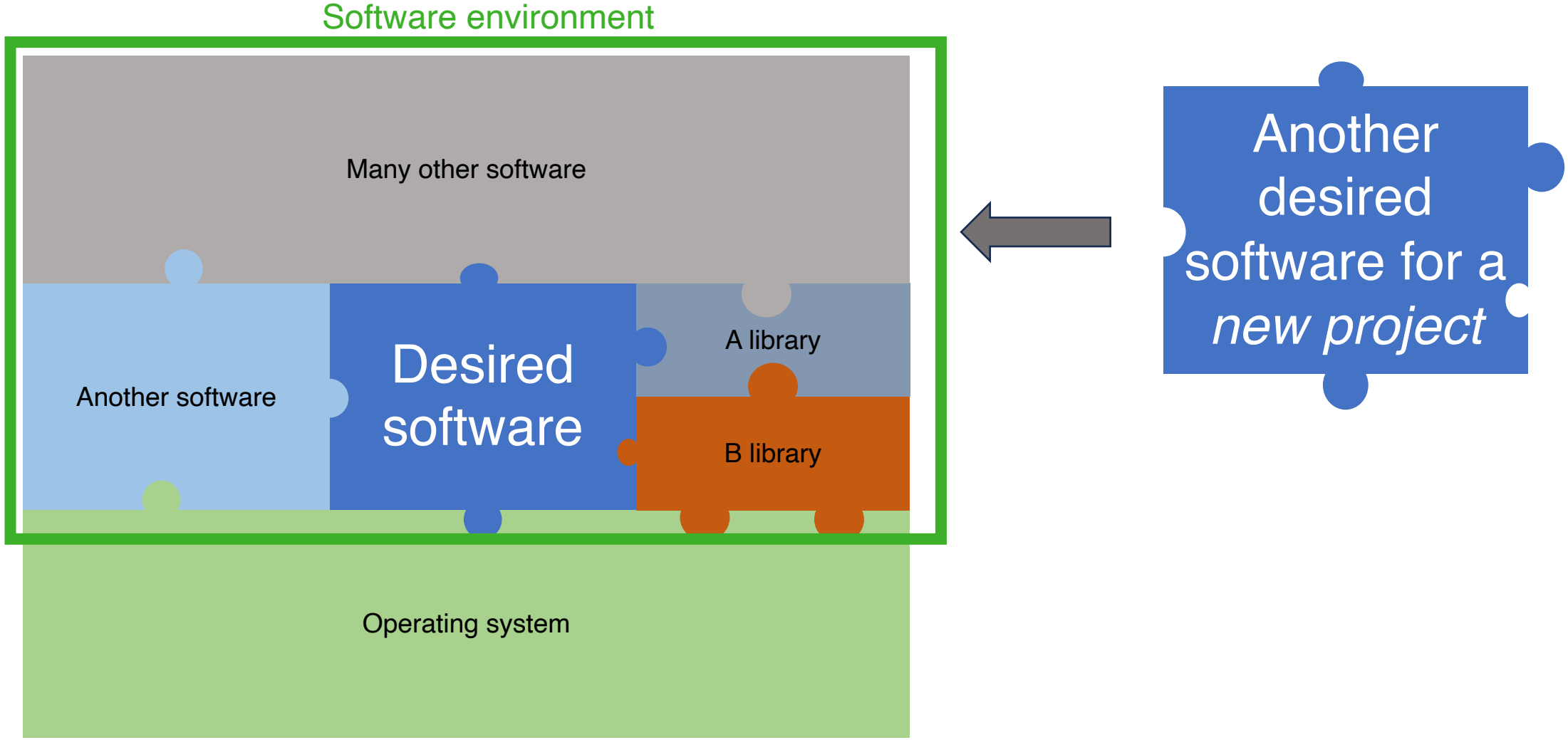


Software environments with ~~conda~~ miniforge

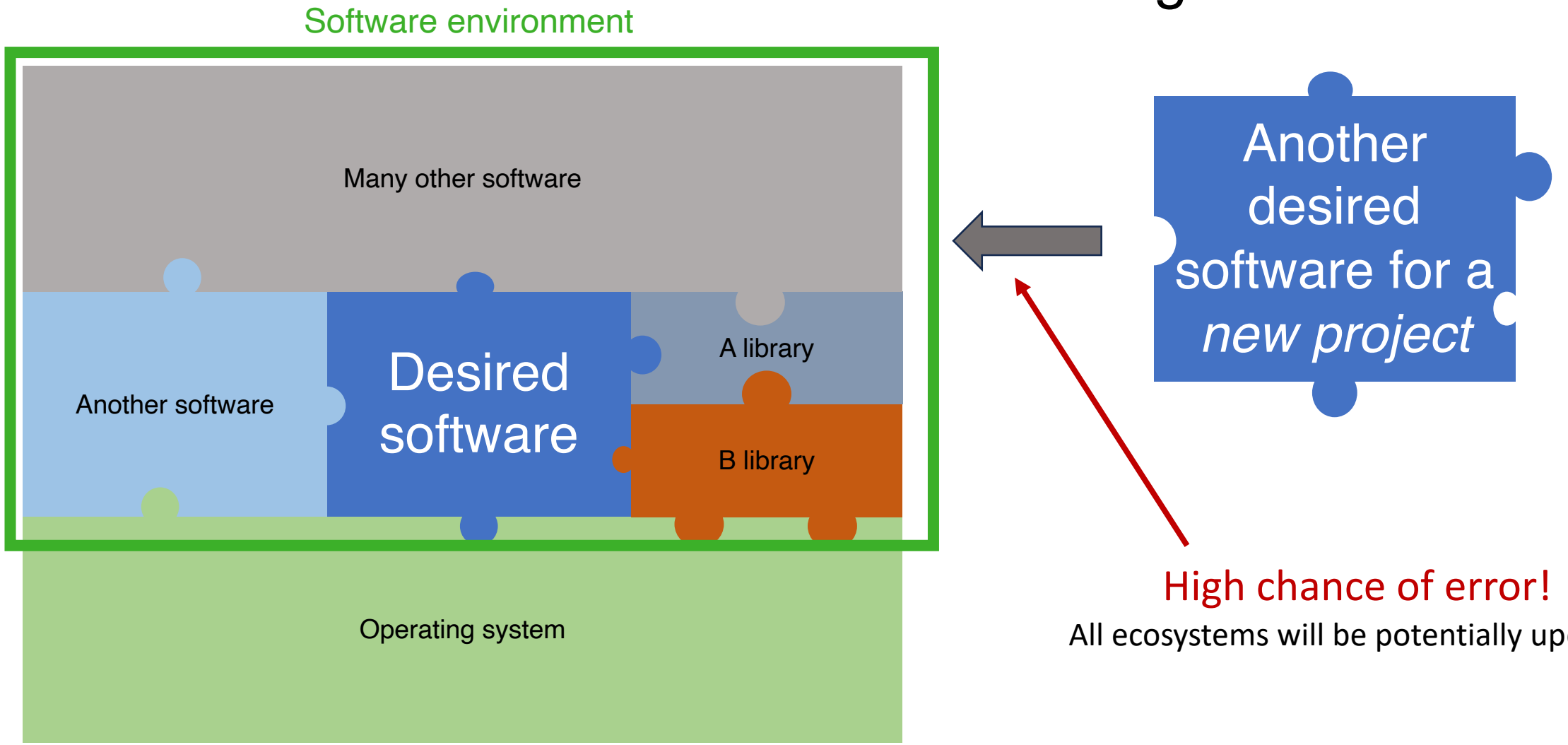


Another desired software for a *new project*

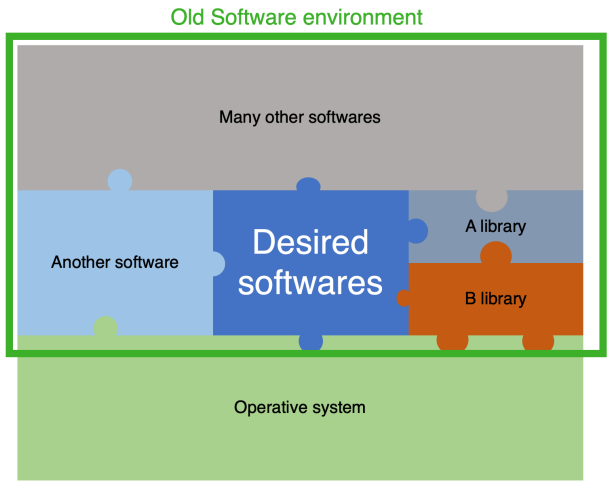
Software environments with ~~conda~~ miniforge

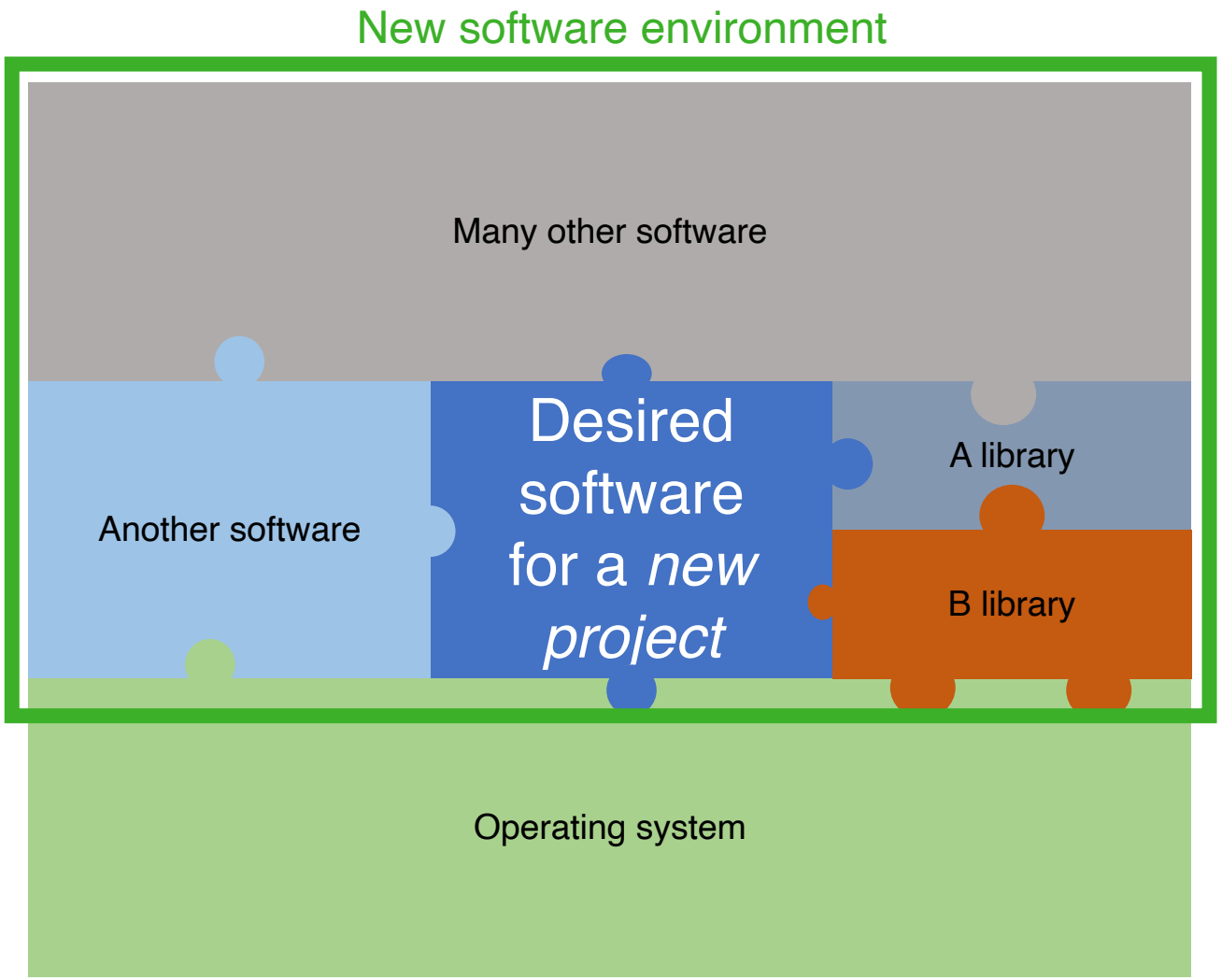


Software environments with ~~conda~~ miniforge



Software environments with ~~conda~~ miniforge





Hands-on: environments miniforge3

Hands-on: environments miniforge3

terminal

```
cpetrini@p-cpetrini ~ %
cpetrini@p-cpetrini ~ % echo "This is my prompt"
This is my prompt
(base) cpetrini@p-cpetrini ~ %
(base) cpetrini@p-cpetrini ~ % echo "This is my prompt after installing miniforge"
This is my prompt after installing miniforge
```

Give information about the environment in use

Hands-on: create a new environment


```
(base) cpetrini@p-cpetrini ~ % conda create -n a_new_env_for_projX
Channels:
 - conda-forge
Platform: osx-64
Collecting package metadata (repodata.json): done
Solving environment: done

## Package Plan ##

  environment location: /Users/cpetrini/miniforge3/envs/a_new_env_for_projX



Proceed ([y]/n)? y

Preparing transaction: done
Verifying transaction: done
Executing transaction: done
#
# To activate this environment, use
#
#     $ conda activate a_new_env_for_projX
#
# To deactivate an active environment, use
#
#     $ conda deactivate
```

Hands-on: create a new environment

Hands-on: create a new environment

You are not in “base” anymore

Hands-on: create a new environment

Hands-on: create a new environment

terminal

```
(base) cpetrini@p-cpetrini ~ % conda create -n a_new_env_for_projX
(base) cpetrini@p-cpetrini ~ % conda activate a_new_env_for_projX
(a_new_env_for_projX) cpetrini@p-cpetrini ~ %
(a_new_env_for_projX) cpetrini@p-cpetrini ~ % conda install bioconda::samtools
```

```
(a_new_env_for_projX) cpetrini@p-cpetrini ~ % conda install bioconda::samtools

Channels:
 - conda-forge
 - bioconda
Platform: osx-64
Collecting package metadata (repodata.json): done
Solving environment: done

## Package Plan ##

  environment location: /Users/cpetrini/miniforge3/envs/a_new_env_for_projX

  added / updated specs:
    - bioconda::samtools


The following packages will be downloaded:

    package                    |            build
    ---------------------------|-----------------
    htslib-1.21                |       hec81eee_0         2.8 MB  bioconda
    libdeflate-1.21            |       hfdf4475_0          69 KB  conda-forge
    samtools-1.21              |       h94387ee_0         457 KB  bioconda
    ------------------------------------------------------------
                                           Total:         3.3 MB

The following NEW packages will be INSTALLED:
```

Hands-on: create a new environment

terminal

```
(base) cpetrini@p-cpetrini ~ % conda create -n a_new_env_for_projX
(base) cpetrini@p-cpetrini ~ % conda activate a_new_env_for_projX
(a_new_env_for_projX) cpetrini@p-cpetrini ~ %
(a_new_env_for_projX) cpetrini@p-cpetrini ~ % conda install bioconda::samtools
```

```
(a_new_env_for_projX) cpetrini@p-cpetrini ~ % conda install bioconda::samtools

Channels:
 - conda-forge
 - bioconda
Platform: osx-64
Collecting package metadata (repodata.json): done
Solving environment: done

## Package Plan ##

  environment location: /Users/cpetrini/miniforge3/envs/a_new_env_for_projX

  added / updated specs:
    - bioconda::samtools


The following packages will be downloaded:

    package                    |            build
    ---------------------------|-----------------
    htslib-1.21                |       hec81eee_0         2.8 MB  bioconda
    libdeflate-1.21            |       hfdf4475_0          69 KB  conda-forge
    samtools-1.21              |       h94387ee_0         457 KB  bioconda
    ------------------------------------------------------------
                                           Total:         3.3 MB

The following NEW packages will be INSTALLED:
```

```
(a_new_env_for_projX) cpetrini@p-cpetrini ~ % samtools

Program: samtools (Tools for alignments in the SAM format)
Version: 1.21 (using htslib 1.21)

Usage:   samtools <command> [options]

Commands:
  -- Indexing
     dict           create a sequence dictionary file
     faidx          index/extract FASTA
     fqidx          index/extract FASTQ
     index          index alignment
```

Hands-on: create a new environment

Hands-on: create a new environment

```
(base) cpetrini@p-cpetrini ~ % samtools
zsh: command not found: samtools
```

Hands-on: create a new environment on a specific path

Hands-on: create a new environment on a specific path

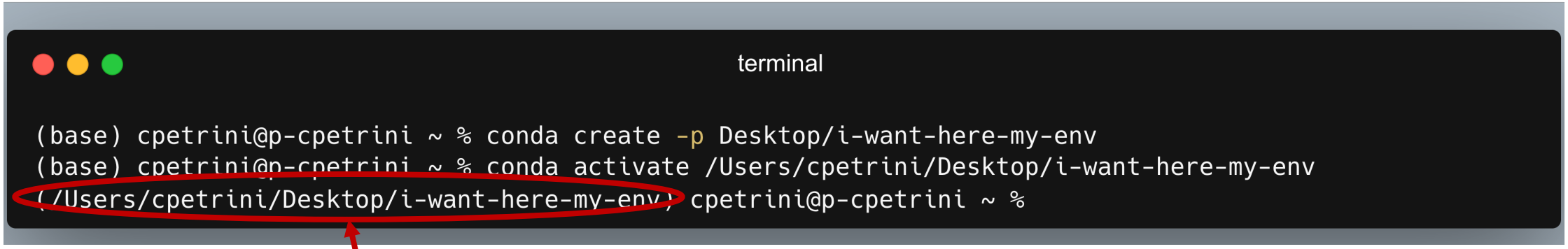
terminal

```
(base) cpetrini@p-cpetrini ~ % conda create -p Desktop/i-want-here-my-env
(base) cpetrini@p-cpetrini ~ % conda activate /Users/cpetrini/Desktop/i-want-here-my-env
(/Users/cpetrini/Desktop/i-want-here-my-env) cpetrini@p-cpetrini ~ %
```

Now all the software installed for this environment will be located here

Hands-on: create a new environment on a specific path

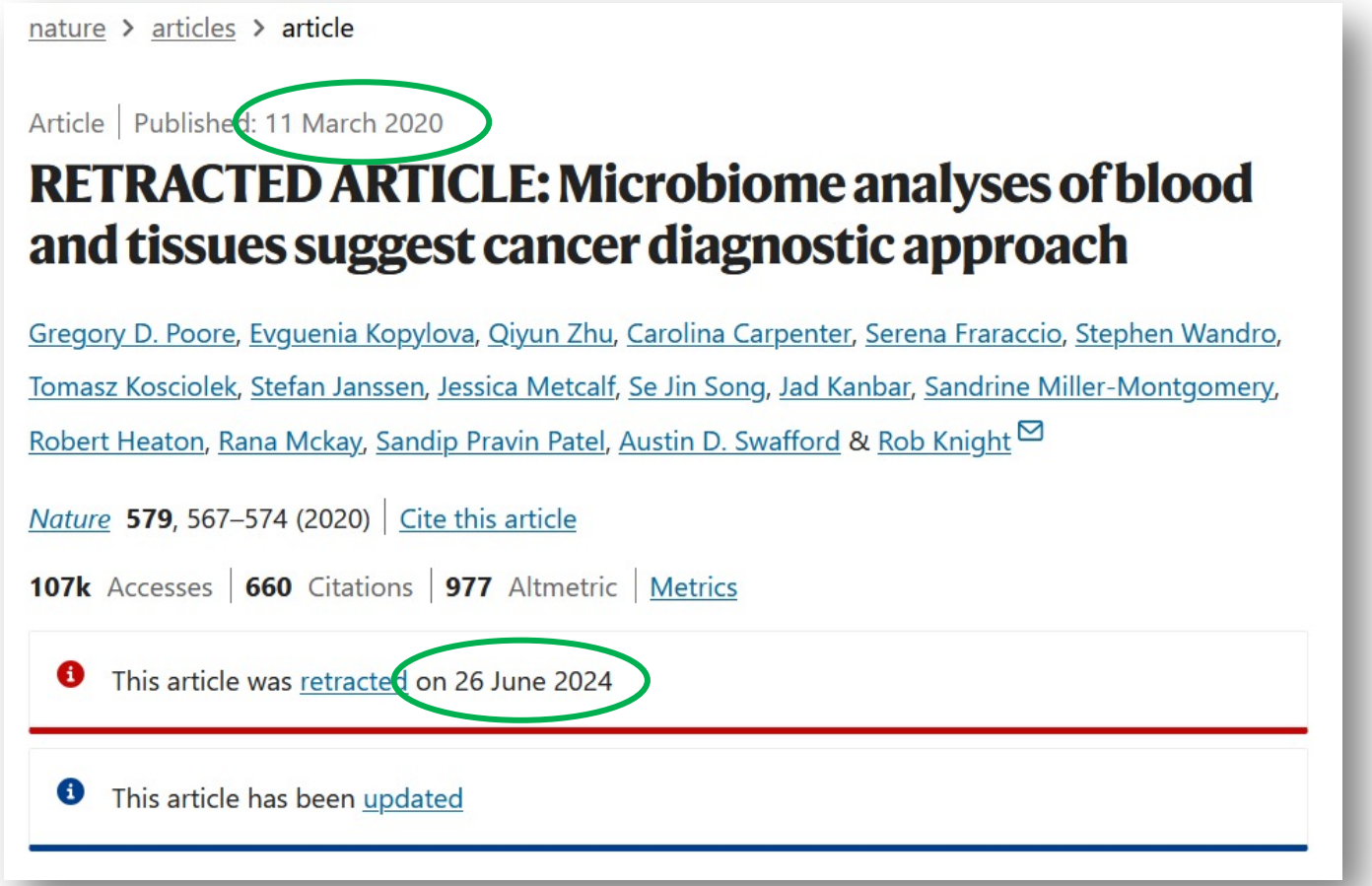
Environments in a specific path is the key for reproducibility, stay tuned!



Now all the software installed for this environment will be located here

Back to reproducibility

The case of brain's microbiome



nature > articles > article

Article | Published: 11 March 2020

RETRACTED ARTICLE: Microbiome analyses of blood and tissues suggest cancer diagnostic approach

Gregory D. Poore, Evguenia Kopylova, Qiyun Zhu, Carolina Carpenter, Serena Fraraccio, Stephen Wandro, Tomasz Kosciolek, Stefan Janssen, Jessica Metcalf, Se Jin Song, Jad Kanbar, Sandrine Miller-Montgomery, Robert Heaton, Rana Mckay, Sandip Pravin Patel, Austin D. Swafford & Rob Knight

Nature **579**, 567–574 (2020) | Cite this article

107k Accesses | **660** Citations | **977** Altmetric | Metrics

This article was retracted on 26 June 2024

This article has been updated

A **controversial** paper that generated much buzz in the field notwithstanding the high-impact journal.

Was later retracted **by the editors** (not by the authors) after the buzz substantiated into data **irreproducibility**

> 900 citations

Retraction came after…

- Steven Salzberg, one of the most influential bioinformatics scientists took on a multi year battle
- Salzberg and team spent massive computational resources/time to re-analyse the whole data.

The biggest problem with reproducibility

Since there is a **stigma** that comes with not being reproducible

=>

- Hi pressure in not **admitting** errors
- Huge effort to **prove** something is wrong

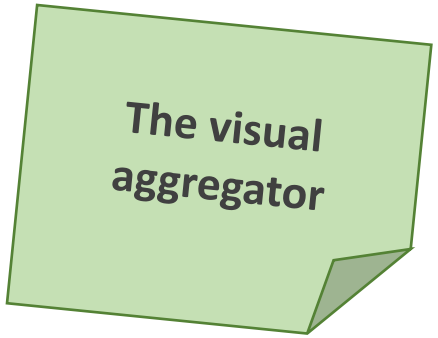
The Reproducibility Crisis in Science

- **Reproducibility**: The ability to replicate the results of a study using the same methods, data, and analysis.
- **Challenges in traditional research:** Issues like incomplete documentation, inaccessible datasets, and variability in methods.
- **Impact on scientific progress:** Loss of trust, slower advancement, and difficulties in building on previous research

Lesson learnt

- Exaggerated claims are the new norm!
- We have **a credibility problem in science**: there is NO COST to being wrong, so people are wrong more often than ever

- As a scientist you should be extraordinarily careful
- Don't build a career on nonsense
- Redo the analysis in papers you want to build upon



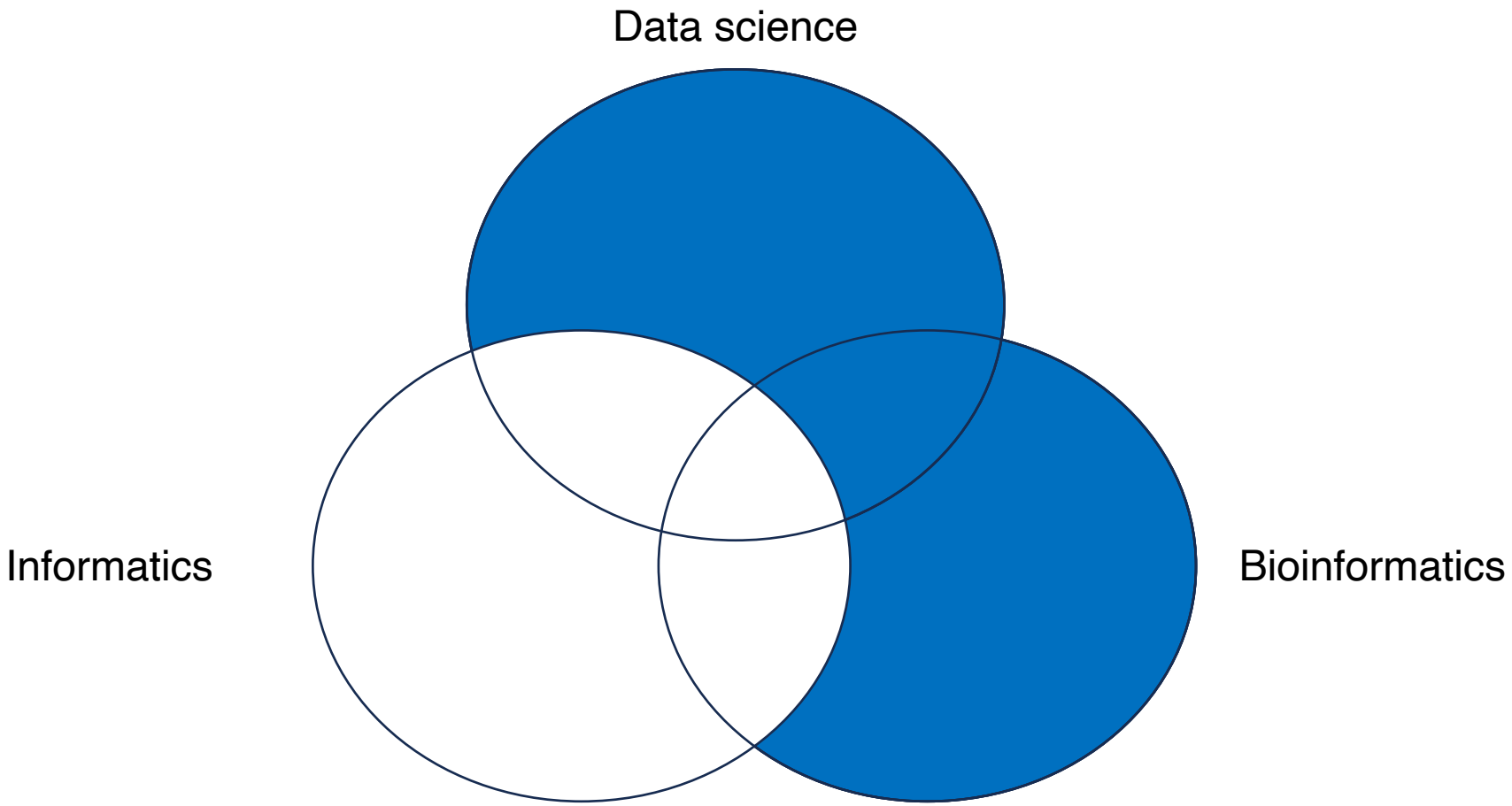
Notebooks

Is seeing believing? Go interactive with Jupyter Notebooks

Work reports and data visualization

BBCC2024, RCDS

Topic domain: bioinformatics



The problem: keep constantly track of what you are doing!

Bioinformaticians are required to **be conscious** of the work they perform and performed in the past

That means:

- Create detailed and easily accessible **reports** of analyses
- **Be aware** of the data processed and managed

Why creating a report?

The analyses are usually based on:

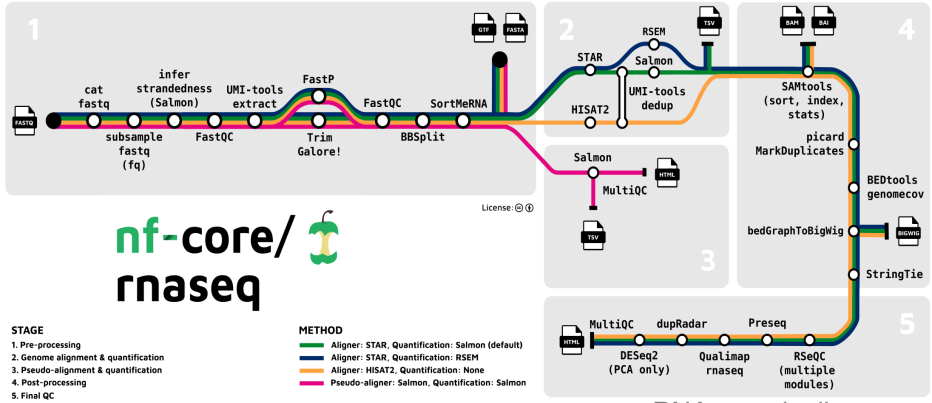
- many parameters
- many steps

remembering everything after days/months/years could be completely unreliable.

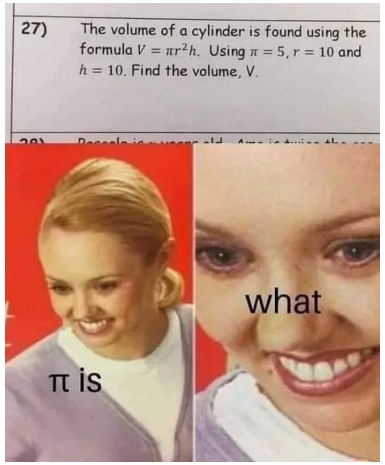
At the same time:

- PI
- colleague
- collaborator
- reviewer
- a random interested person

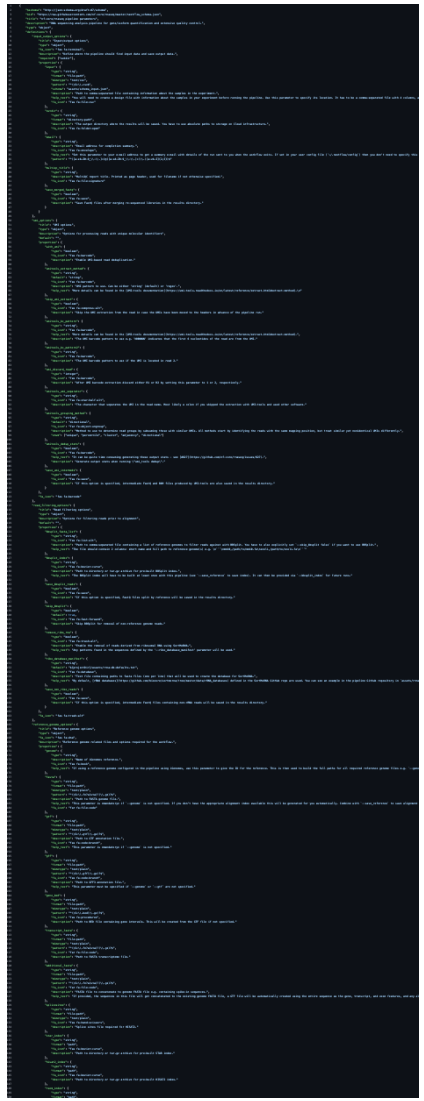
could ask you about it and you should be able to answer correctly and quickly



RNA-seq pipeline steps



Your PI after you attempt to guess a parameter you forgot

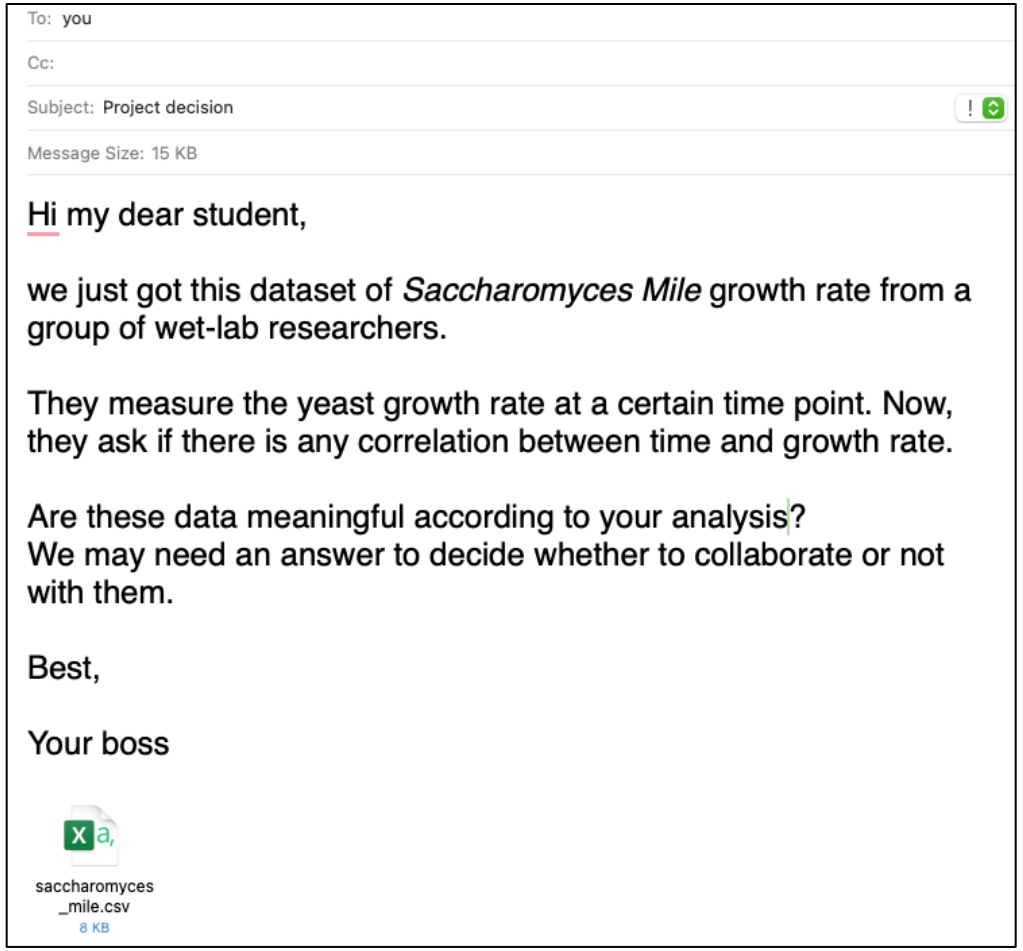


A portion of JSON describing RNA-seq required parameters

Pipeline presented: https://nf-co.re/rnaseq/3.12.0

Why be aware of data managed?

An example:



To: you

Cc:

Subject: Project decision

Message Size: 15 KB

Hi my dear student,

we just got this dataset of *Saccharomyces Mile* growth rate from a group of wet-lab researchers.

They measure the yeast growth rate at a certain time point. Now, they ask if there is any correlation between time and growth rate.

Are these data meaningful according to your analysis?
We may need an answer to decide whether to collaborate or not with them.

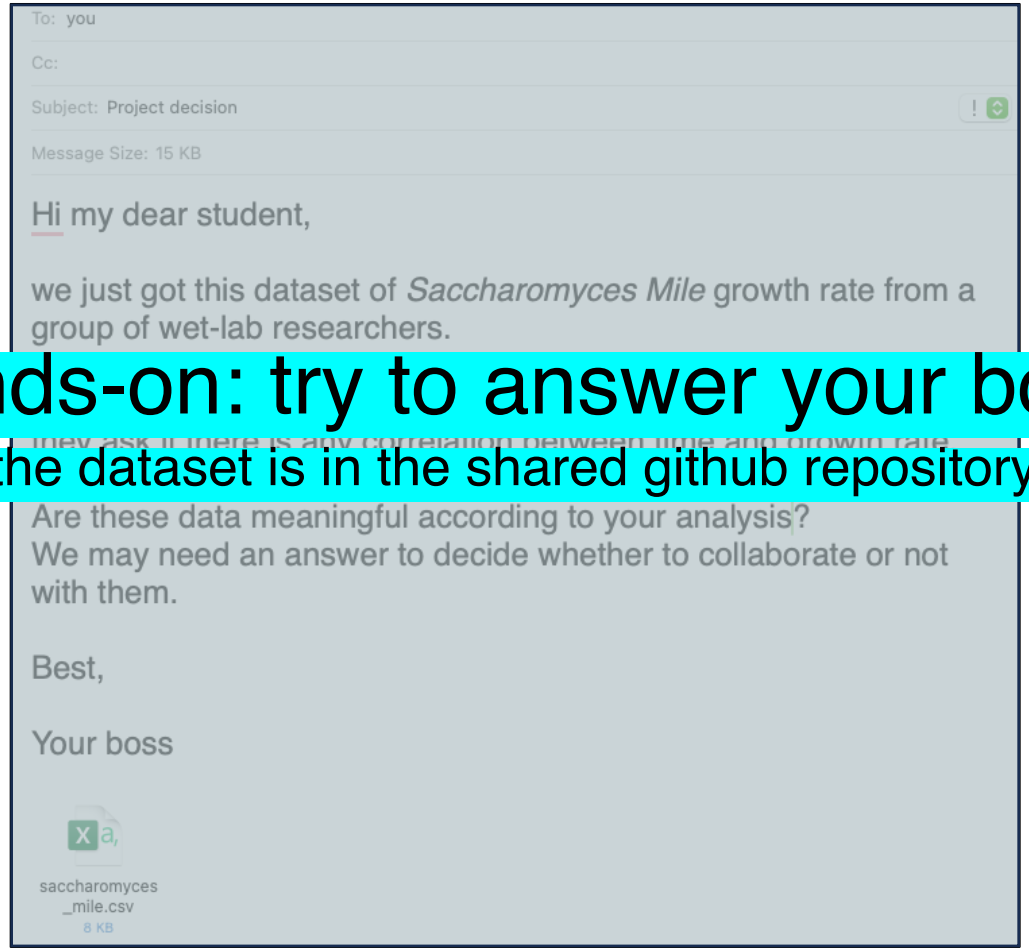
Best,

Your boss

saccharomyces_mile.csv
8 KB

Why be aware of data managed?

An example:



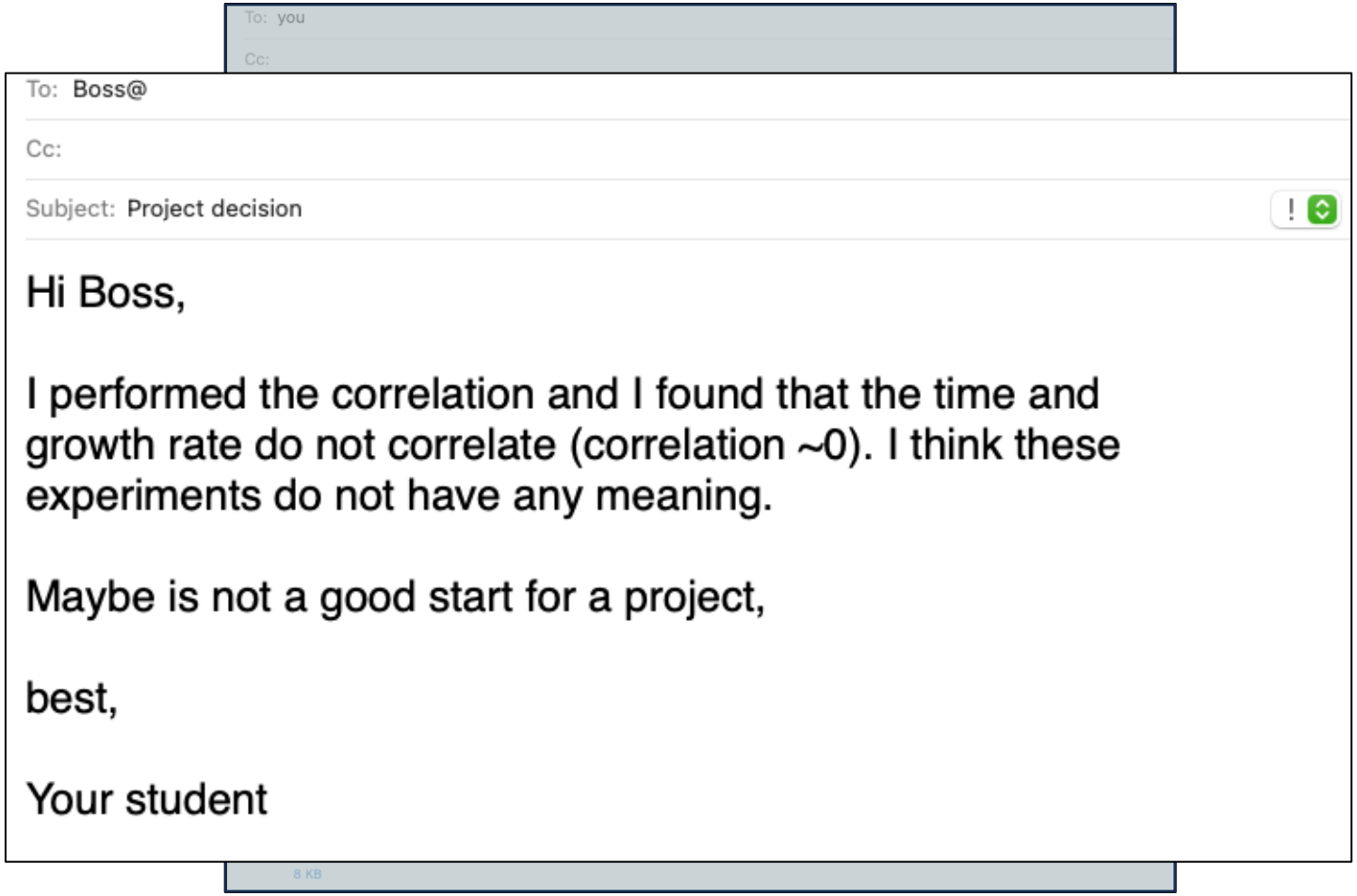
Hands-on: try to answer your boss!

(the dataset is in the shared github repository)

R correlation function: `cor()`; python correlation function `corrcoef()` from Numpy library

Why be aware of data managed?

An example:



Why be aware of data managed? Did you plot the data?

An example:

To: you

Cc:

To: Boss@

Cc:

Subject: Project decision

Hi Boss,

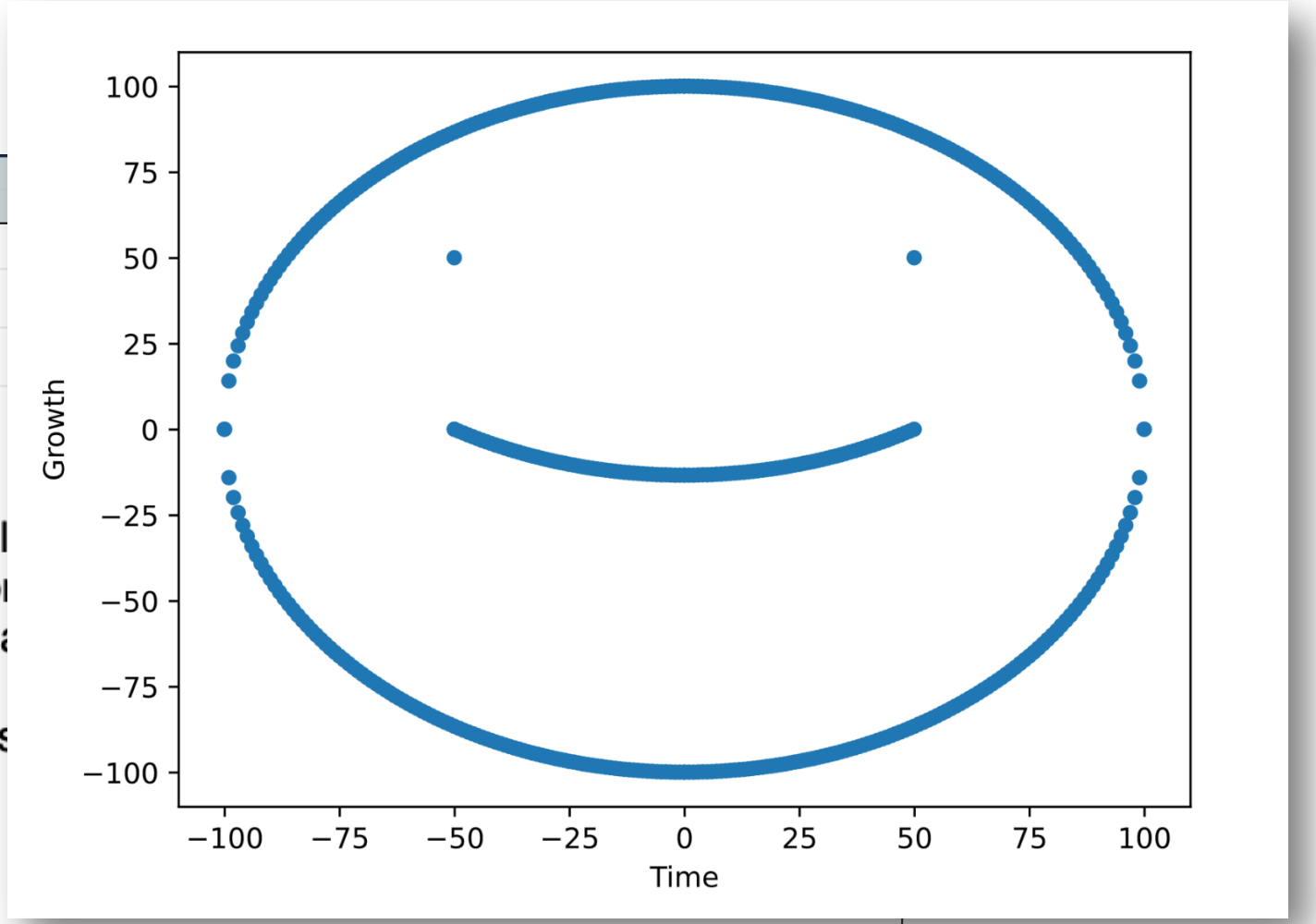
I performed the correl
growth rate do not co
experiments do not ha

Maybe is not a good s

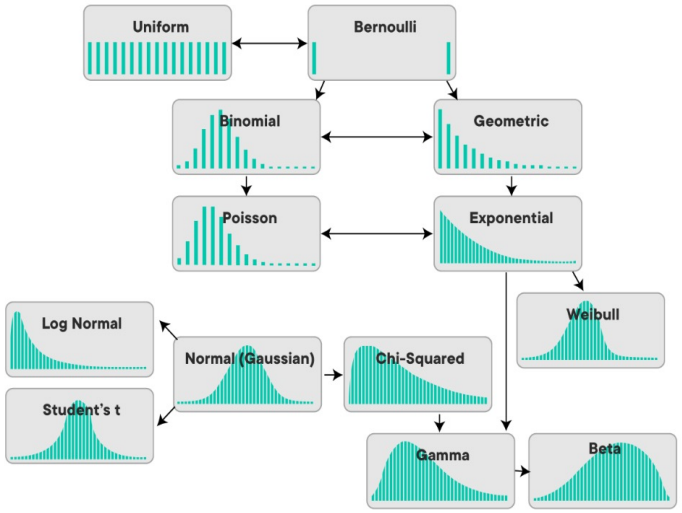
best,

Your student

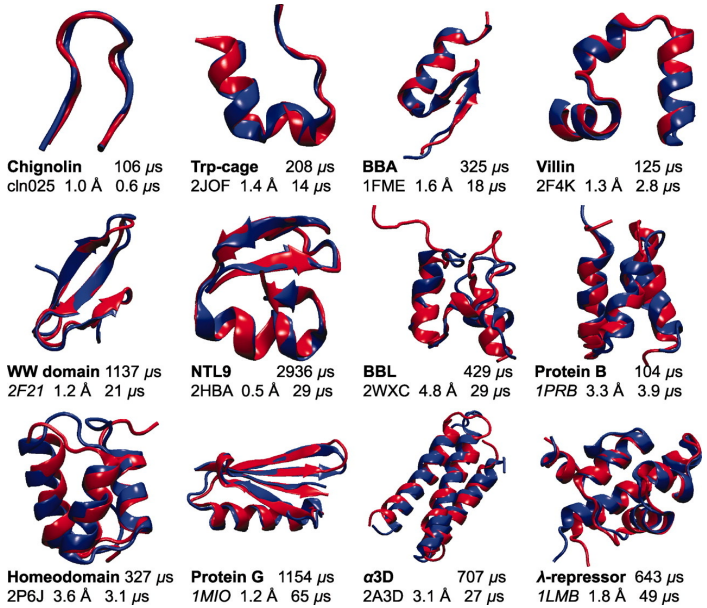
8 KB



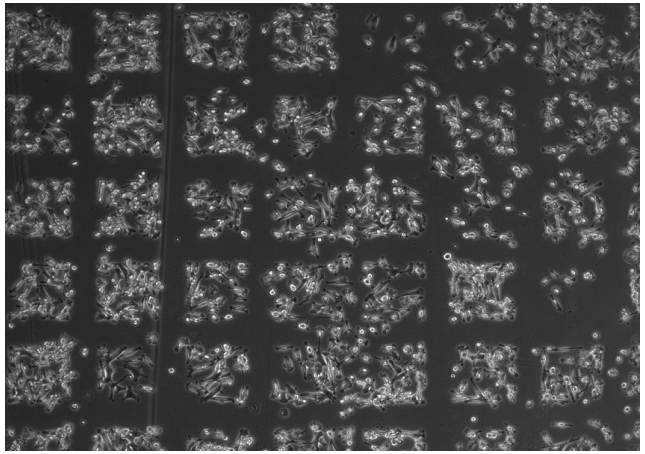
Why be aware of data managed? Other examples



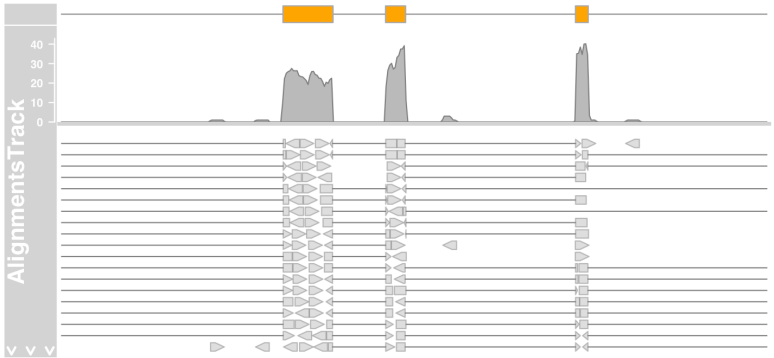
Data distributions



Protein structures



Cell images



Sequenced reads distribution

Introducing JupyterLab & notebooks

https://jupyter.org/

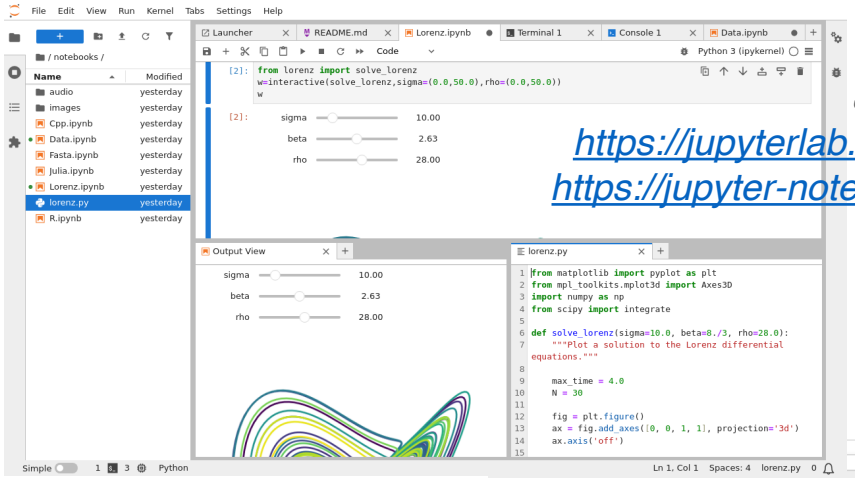
Free software, open standards, and web services for **interactive** computing **across all programming languages**

The problems solver: JupyterLab

JupyterLab is an IDE that combines

- coding,
- code processing,
- work reports
- data visualization

in a single file (called a Jupyter Notebook).

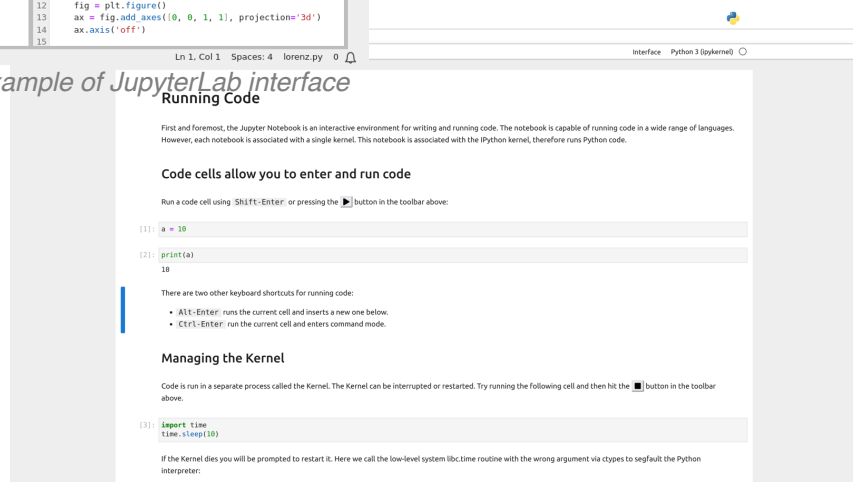


Jupyter official documentation: https://jupyterlab.readthedocs.io/en/latest/# and https://jupyter-notebook.readthedocs.io/en/latest/

Example of JupyterLab interface

Extra features features:

- plugins (*e.g.* to convert the notebook into a pdf)
- many languages supported (*e.g.* python, R, Perl, ruby, etc.)
- server-integrated solution (allows you to work directly on your cluster server)
- Interactivity

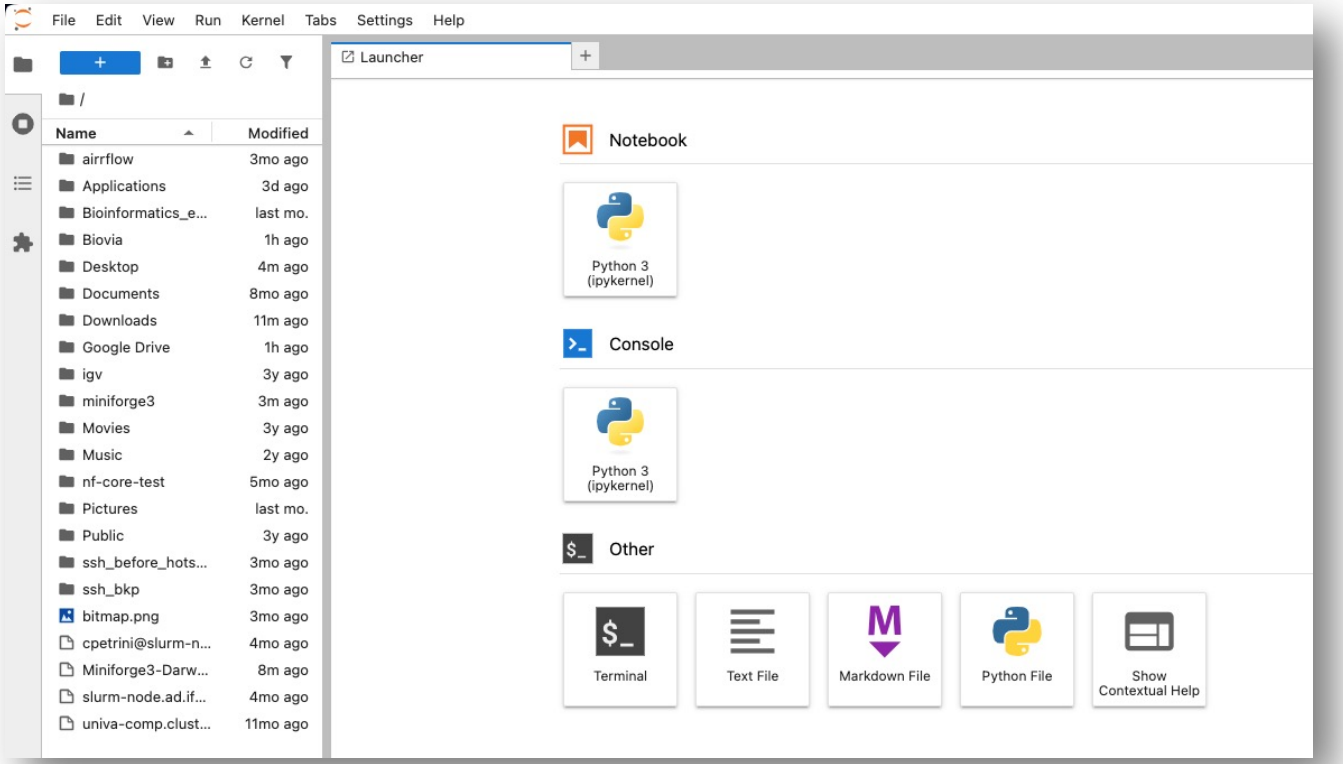


Example of Jupyter Notebook

Hands-on: install JupyterLab

Hands-on: run JupyterLab

*It automatically opens the browser**



**Officially supported browsers are:* Firefox, Chrome, Safari and Edge

Hands-on: install R kernel

Hands-on: install jupyter git extension

Hands-on: install jupyter with R and Jupyter lab

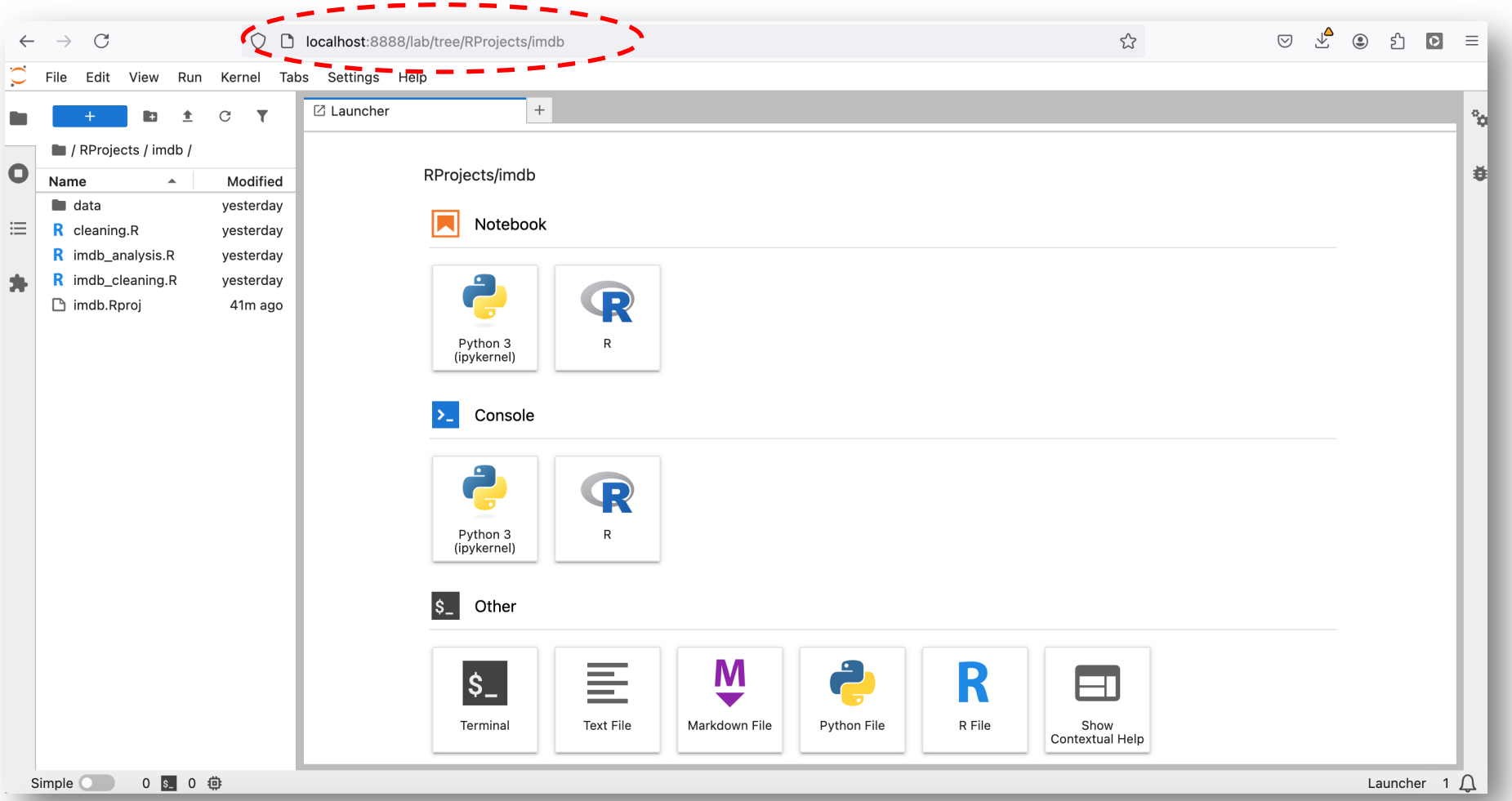
```
conda create --name tidyR
conda activate tidyR
conda install conda-forge::r-dplyr
conda install conda-forge::r-readr
conda install conda-forge::r-ggplot2
conda install conda-forge::r-irkernel
conda install conda-forge::jupyterlab
```

Launch JupyterLab after activating the conda env

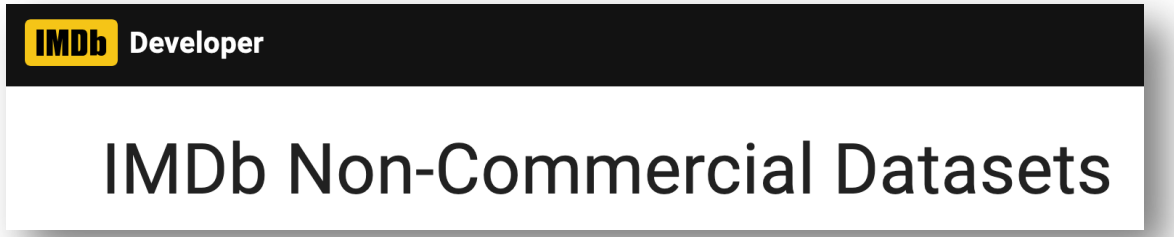
```
conda activate tidyR
jupyter lab
```

Hands-on: launch the jupyter lab environment

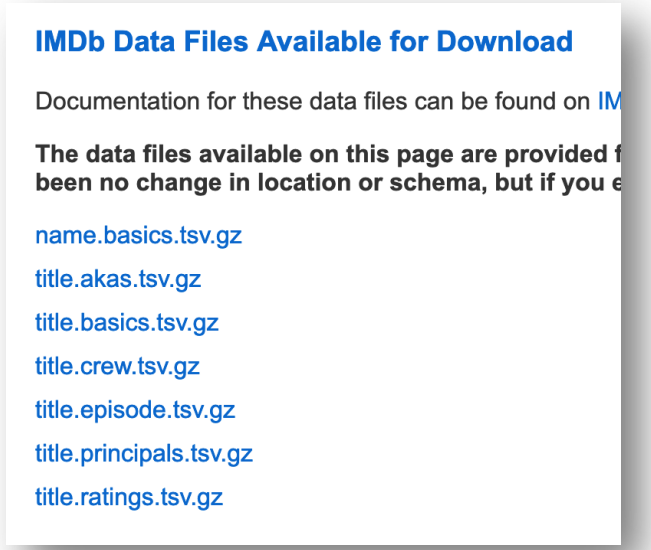
Hands-on: shift to the browser and start working



Exercise: analyze the IMDB data

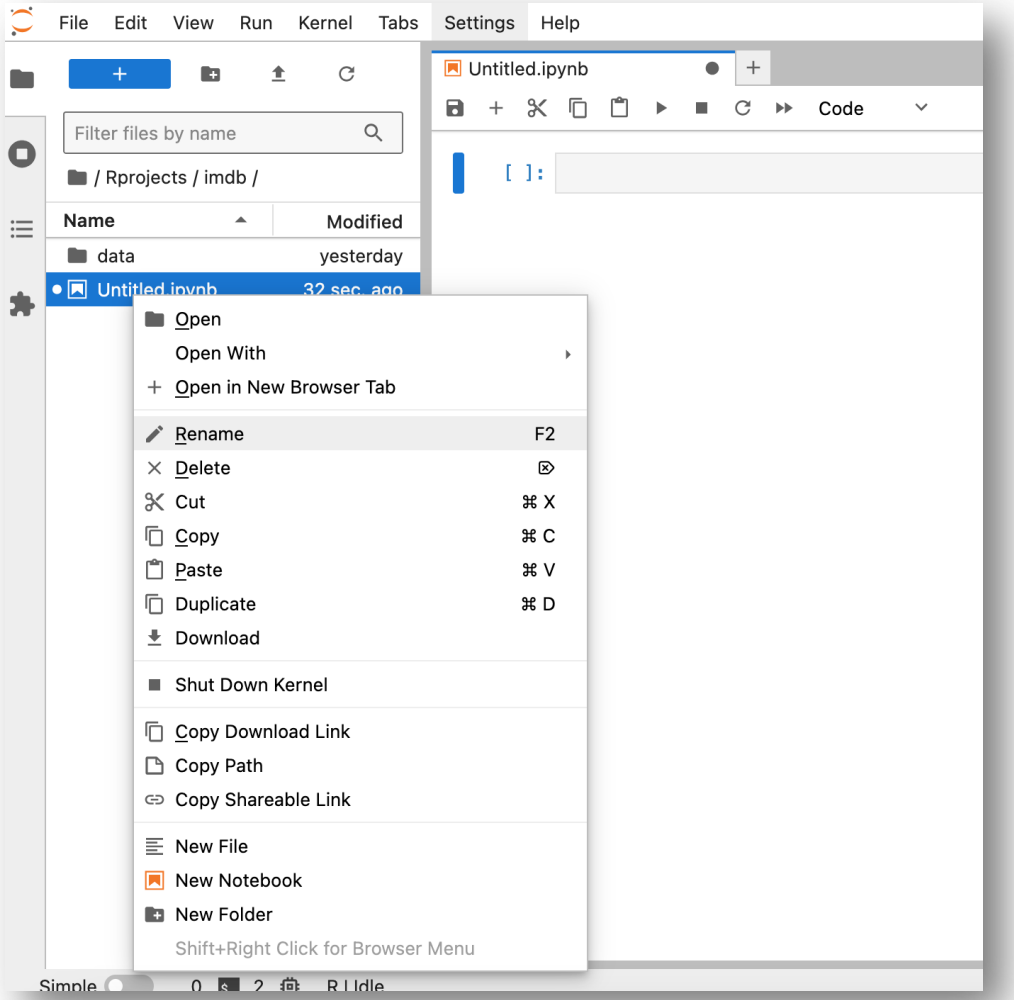


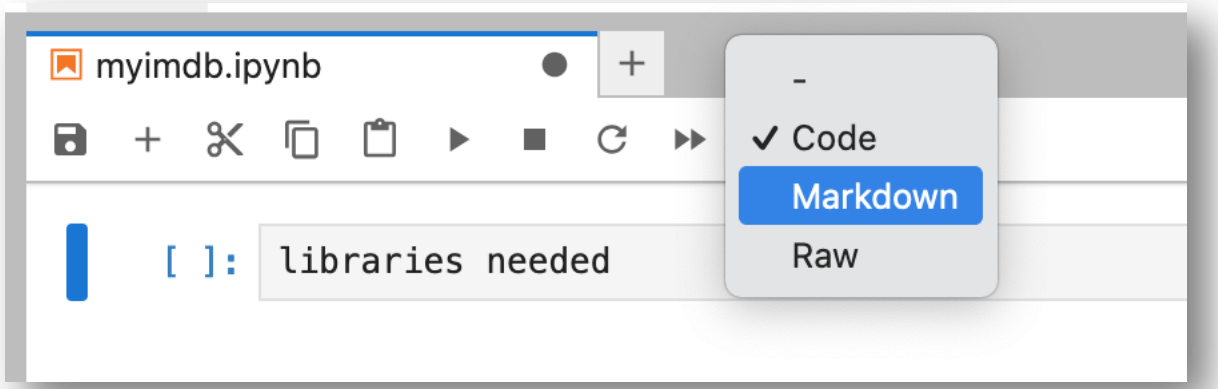
https://developer.imdb.com/non-commercial-datasets/

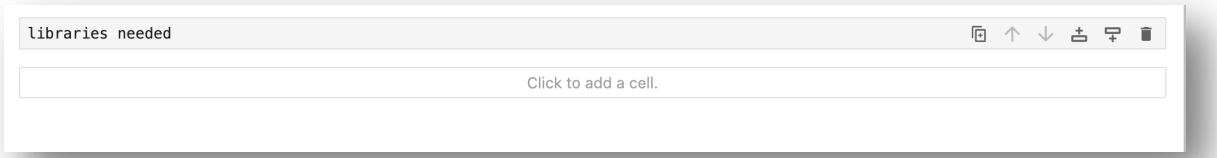


You will use the simplified data on the workshop GitHub repo instead

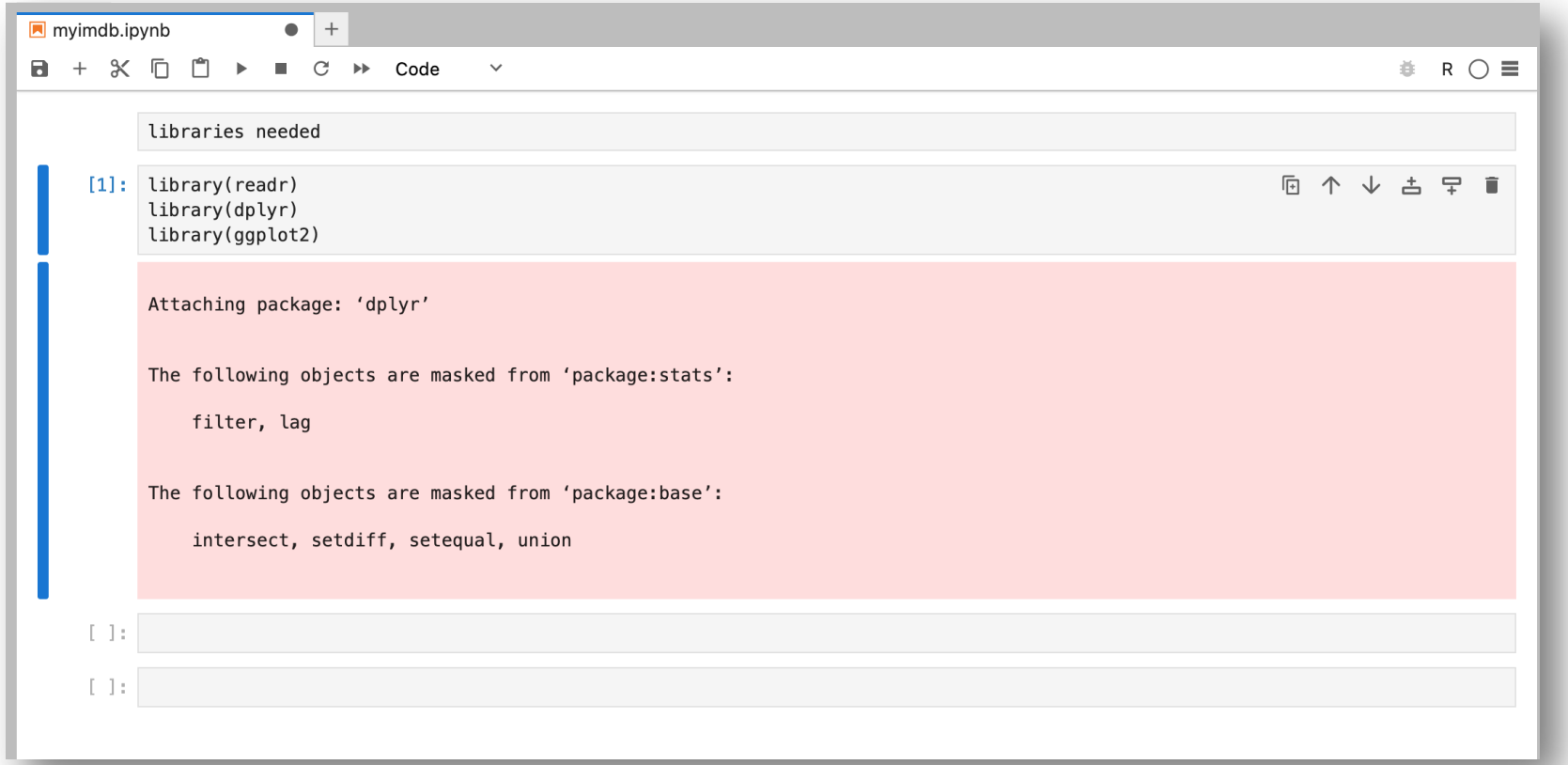
Hands-on: opening and renaming, code/markdown chunks







Hands-on: load libraries



Hands-on: read-in data files and inspect them

myimdb.ipynb

Code

```
READING FILES
please change reading path accordingly
```

[2]:

```
# read the main title table (reduced and cleaned)
title_basics <- read_csv("data/small_title_basics.csv")
head(title_basics)
```

```
Rows: 333760 Columns: 9
── Column specification ────────────────────────────────────────────────────────
Delimiter: ","
chr (5): tconst, titleType, primaryTitle, originalTitle, genres
dbl (3): isAdult, startYear, runtimeMinutes
lgl (1): endYear

ℹ Use `spec()` to retrieve the full column specification for this data.
ℹ Specify the column types or set `show_col_types = FALSE` to quiet this message.
```

A tibble: 6 × 9

tconst	titleType	primaryTitle	originalTitle	isAdult	startYear	endYear	runtimeMinutes	genres
<chr>	<chr>	<chr>	<chr>	<dbl>	<dbl>	<lgl>	<dbl>	<chr>
tt0011801	movie	Tötet nicht mehr	Tötet nicht mehr	0	2019	NA	NA	Action,Crime
tt0035423	movie	Kate & Leopold	Kate & Leopold	0	2001	NA	118	Comedy,Fantasy,Romance
tt0062336	movie	The Tango of the Widower and Its Distorting Mirror	El tango del viudo y su espejo deformante	0	2020	NA	70	Drama
tt0067758	movie	Simón, contamos contigo	Simón, contamos contigo	0	2015	NA	81	Comedy,Drama
tt0069049	movie	The Other Side of the Wind	The Other Side of the Wind	0	2018	NA	122	Drama

Hands-on: errors or warnings

myimdb.ipynb

Code

R

```
[3]: # read the ratings table
title_ratings <- read_tsv("data/title.ratings.tsv")
```

```
Rows: 1501791 Columns: 3
── Column specification ────────────────────────────────────────────────────────
Delimiter: "\t"
chr (1): tconst
dbl (2): averageRating, numVotes

ℹ Use `spec()` to retrieve the full column specification for this data.
ℹ Specify the column types or set `show_col_types = FALSE` to quiet this message.
```

```
[4]: head(title_ratings)
```

A tibble: 6 × 3

tconst	averageRating	numVotes
<chr>	<dbl>	<dbl>
tt0000001	5.7	2102
tt0000002	5.6	282
tt0000003	6.5	2121
tt0000004	5.4	182
tt0000005	6.2	2852
tt0000006	5.0	200

```
[ ]:
```

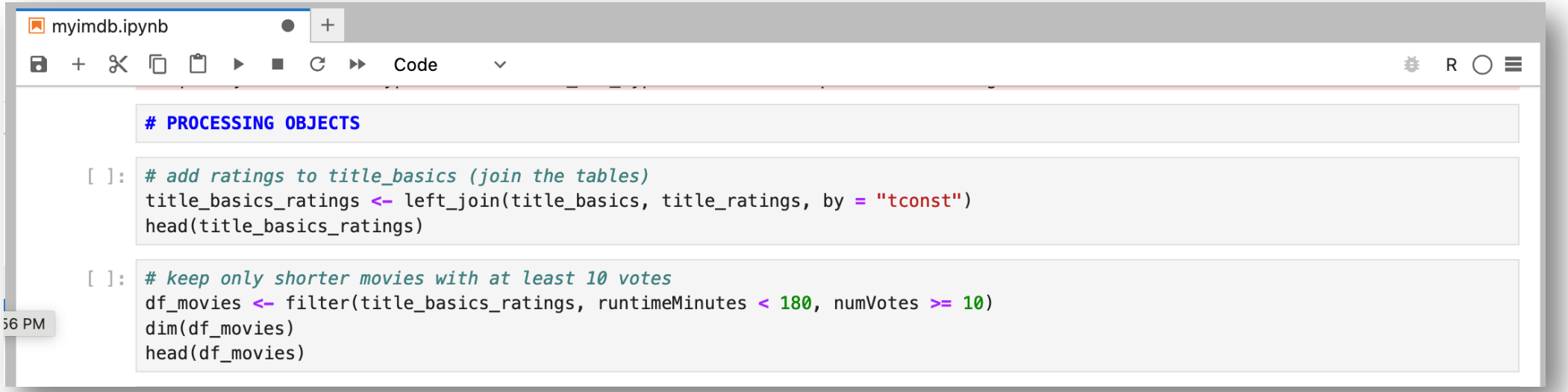
```
[ ]:
```

```
[5]: # read the principals table (containing data about actors, reduced and cleaned version)
title_principals <- read_csv("data/small_title_principals.csv")
# head(title_principals)
```

```
Error: 'data/small_title_principals.csv' does not exist in current working directory ('/storage/home/rrossi/Rprojects/imdb').
Traceback:

1. read_csv("data/small_title_principals.csv")
2. vroom::vroom(file, delim = ",", col_names = col_names, col_types = col_types,
 .     col_select = {
 .         {
```

Hands-on: processing objects



Hands-on: plotting

myimdb.ipynb

Code

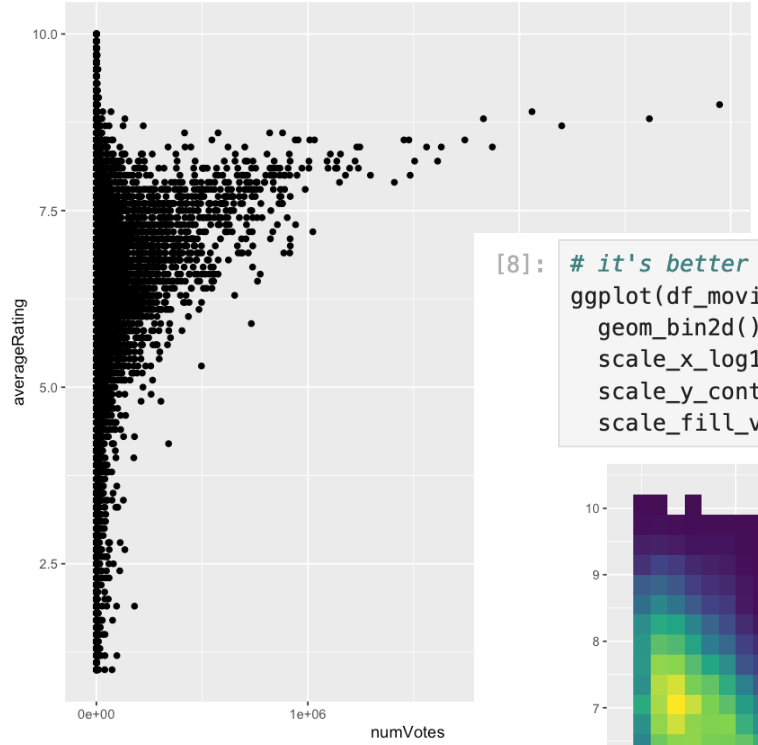
```
# PLOTTING FILES
```

```
[ ]: # Let's see the ratings vs number of votes distribution
ggplot(df_movies, aes(x = numVotes, y = averageRating)) +
  geom_point()
```

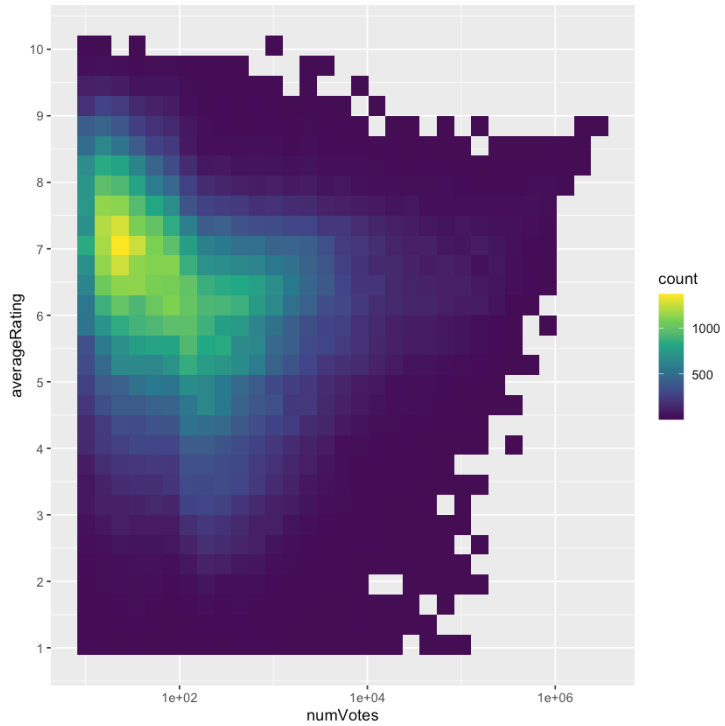
```
[ ]: # it's better to look at it with a heatmap on log10 scale
ggplot(df_movies, aes(x = numVotes, y = averageRating)) +
  geom_bin2d() +
  scale_x_log10() +
  scale_y_continuous(breaks = 1:10) +
  scale_fill_viridis_c()
```

```
[ ]: # what about the rating as a function of lenght of the movie?
ggplot(df_movies, aes(x = runtimeMinutes, y = averageRating)) +
  geom_bin2d() +
  scale_x_continuous(breaks = seq(0, 180, 60), labels = 0:3) +
  scale_y_continuous(breaks = 0:10) +
  scale_fill_viridis_c(option = "inferno") +
  theme_minimal() +
  labs(title = "Relationship between Movie Runtime and Average Movie Rating",
       subtitle = "Data from IMDb",
       x = "Runtime (Hours)",
       y = "Average User Rating",
       fill = "# Movies")
```

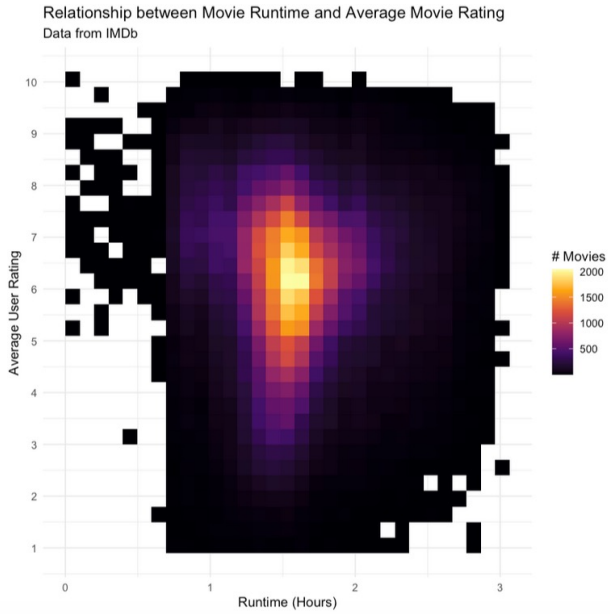
[7]:
```
# Let's see the ratings vs number of votes distribution
ggplot(df_movies, aes(x = numVotes, y = averageRating)) +
  geom_point()
```



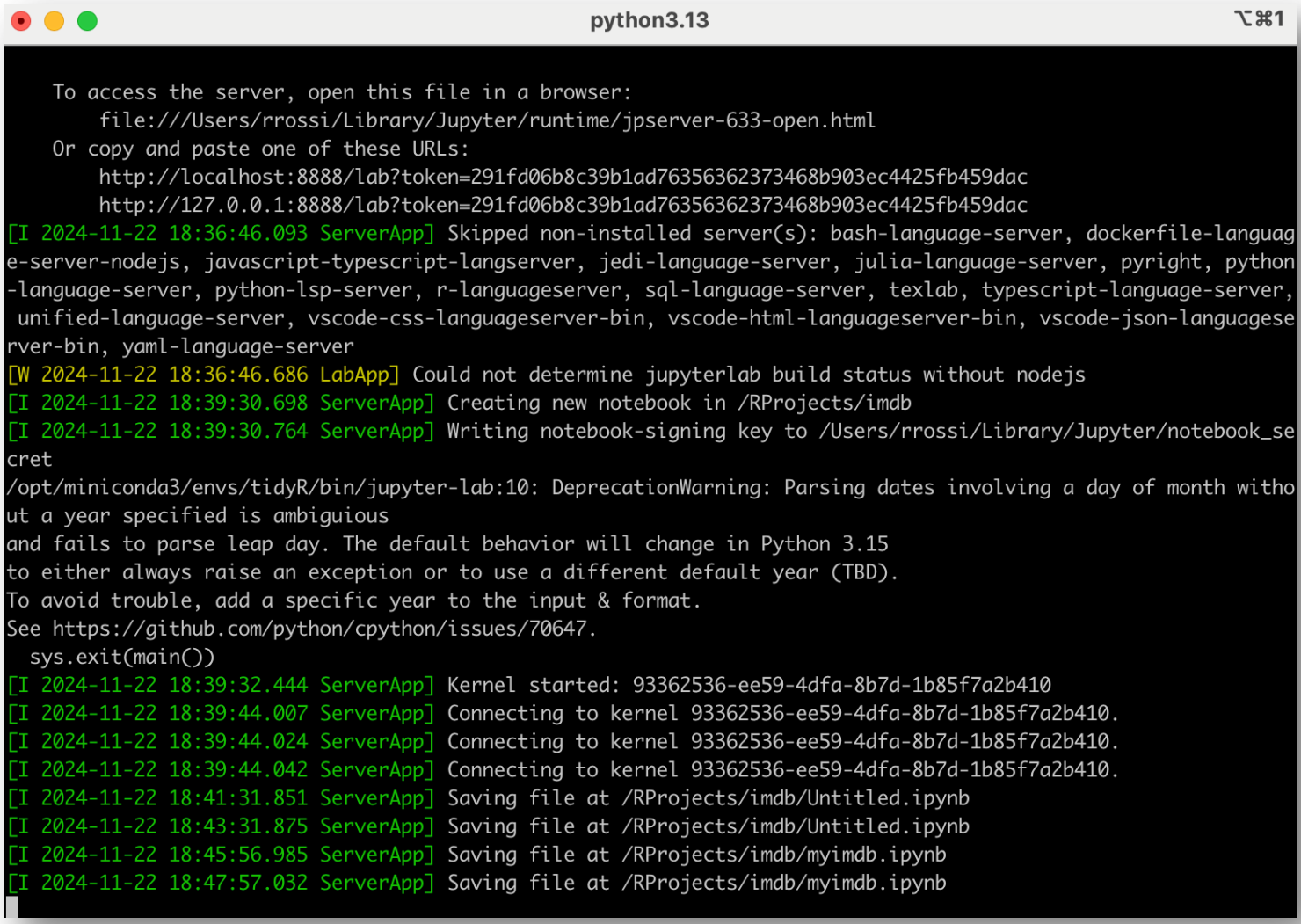
[8]:
```
# it's better to look at it with a heatmap on log10 scale
ggplot(df_movies, aes(x = numVotes, y = averageRating)) +
  geom_bin2d() +
  scale_x_log10() +
  scale_y_continuous(breaks = 1:10) +
  scale_fill_viridis_c()
```



[9]:
```
# what about the rating as a function of lenght of the movie?
ggplot(df_movies, aes(x = runtimeMinutes, y = averageRating)) +
  geom_bin2d() +
  scale_x_continuous(breaks = seq(0, 180, 60), labels = 0:3) +
  scale_y_continuous(breaks = 0:10) +
  scale_fill_viridis_c(option = "inferno") +
  theme_minimal() +
  labs(title = "Relationship between Movie Runtime and Average Movie Rating",
       subtitle = "Data from IMDb",
       x = "Runtime (Hours)",
       y = "Average User Rating",
       fill = "# Movies")
```



Hands-on: meanwhile, in the background…

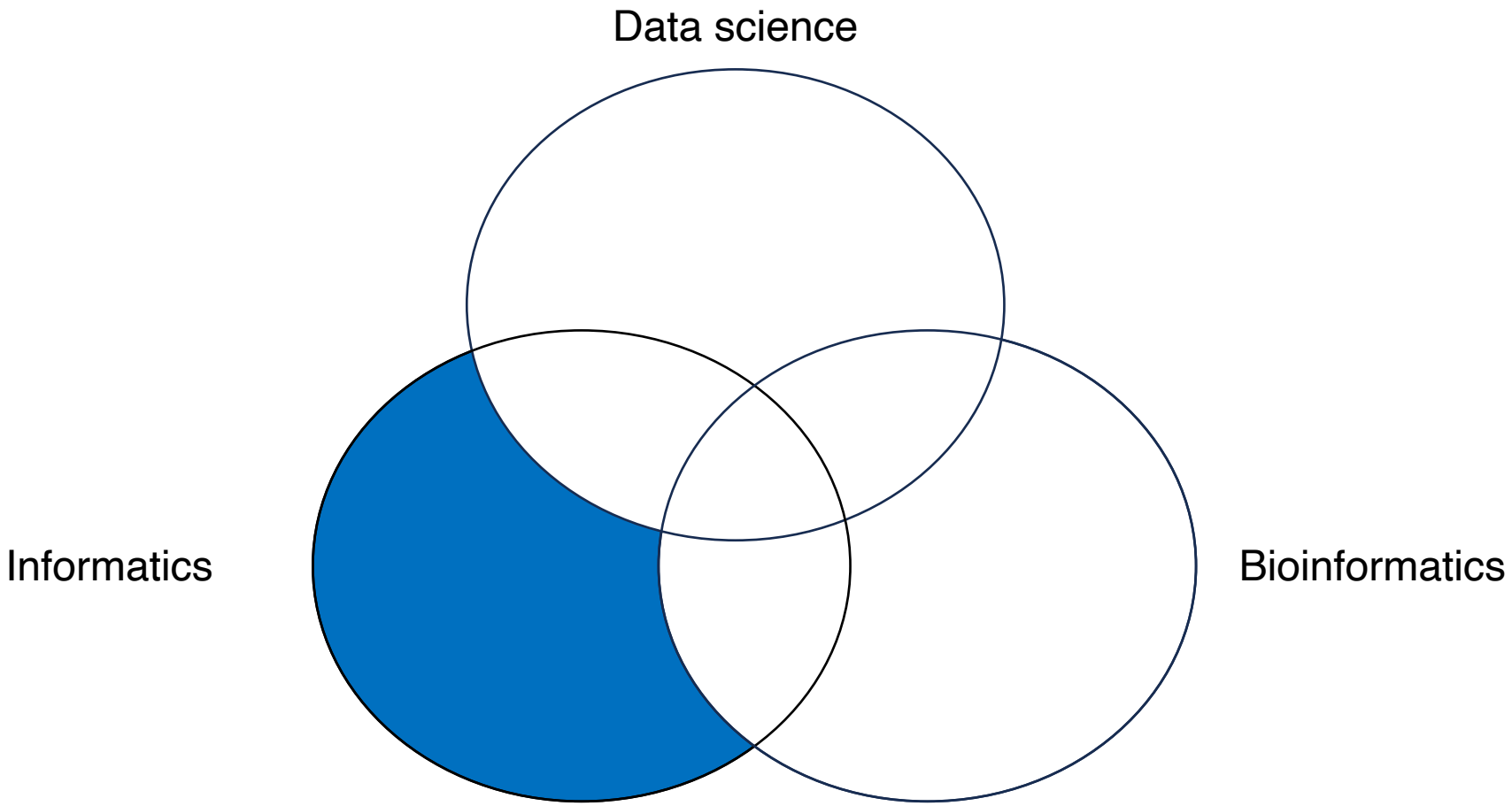


A self-sufficient universe

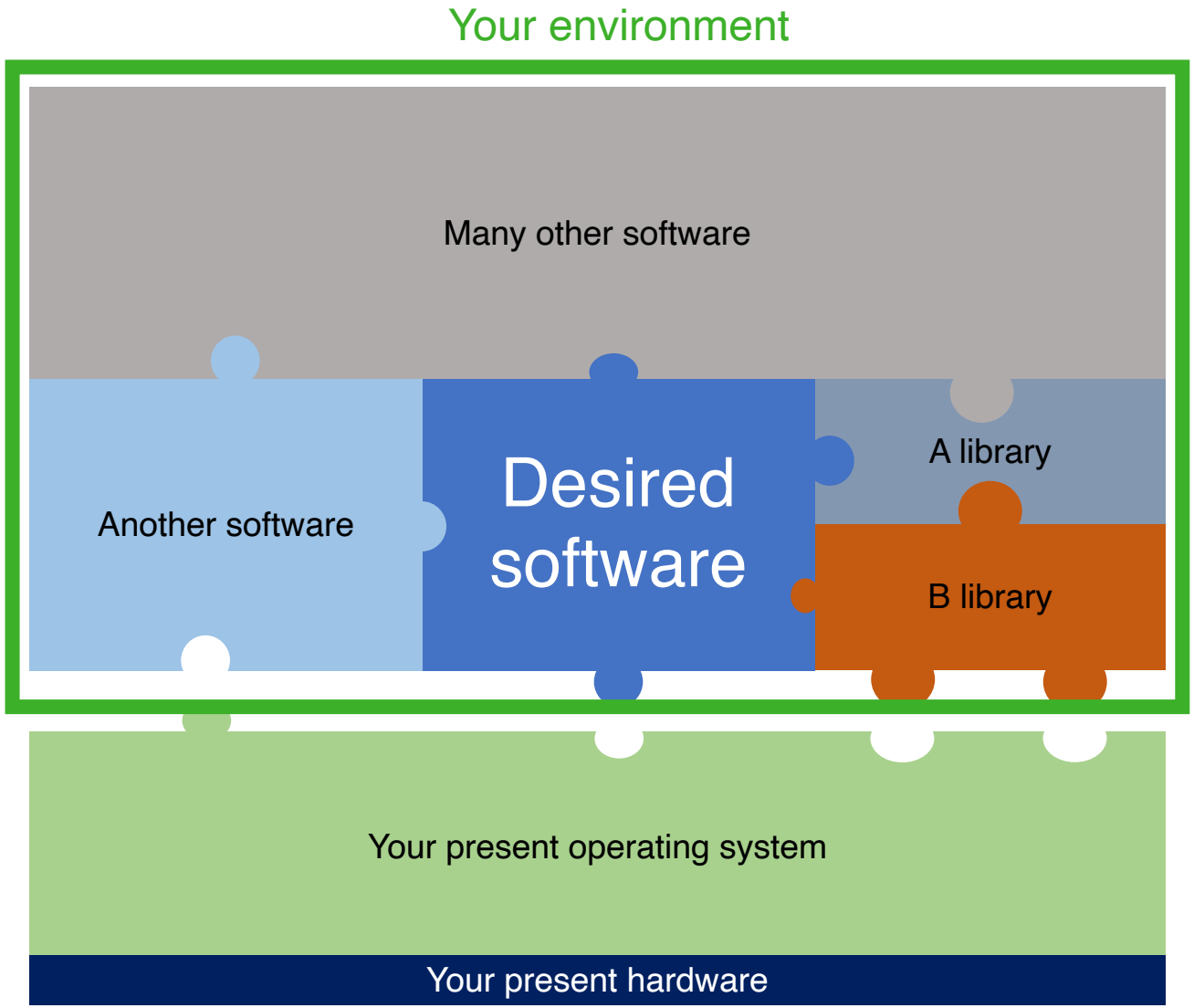
Containers

A step forward in reproducibility

Topic domain: informatics



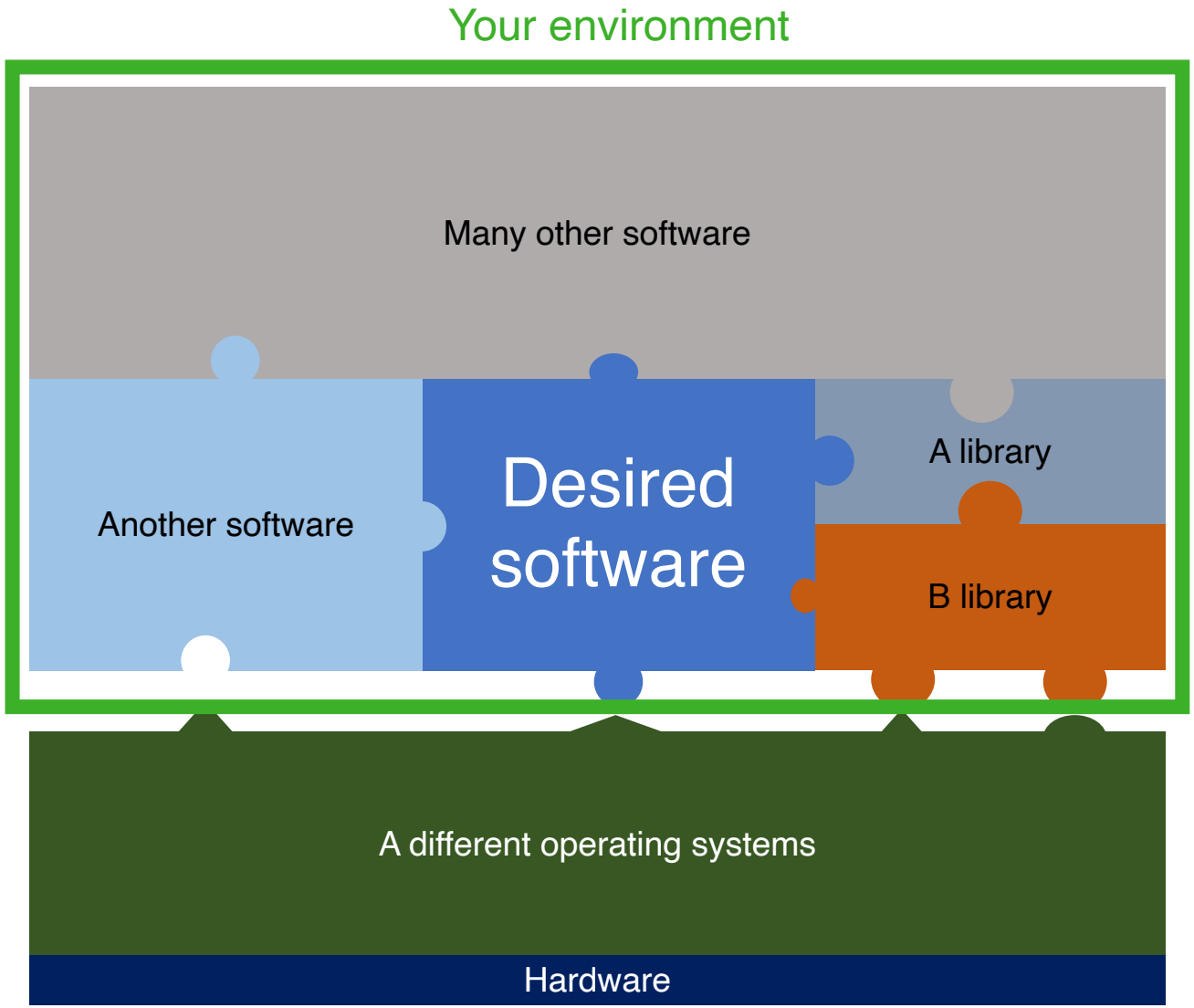
The problem: reproducibility across time and space!



The operative systems:

- could be updated
- could be changed
- are many

The problem: reproducibility across time and space!

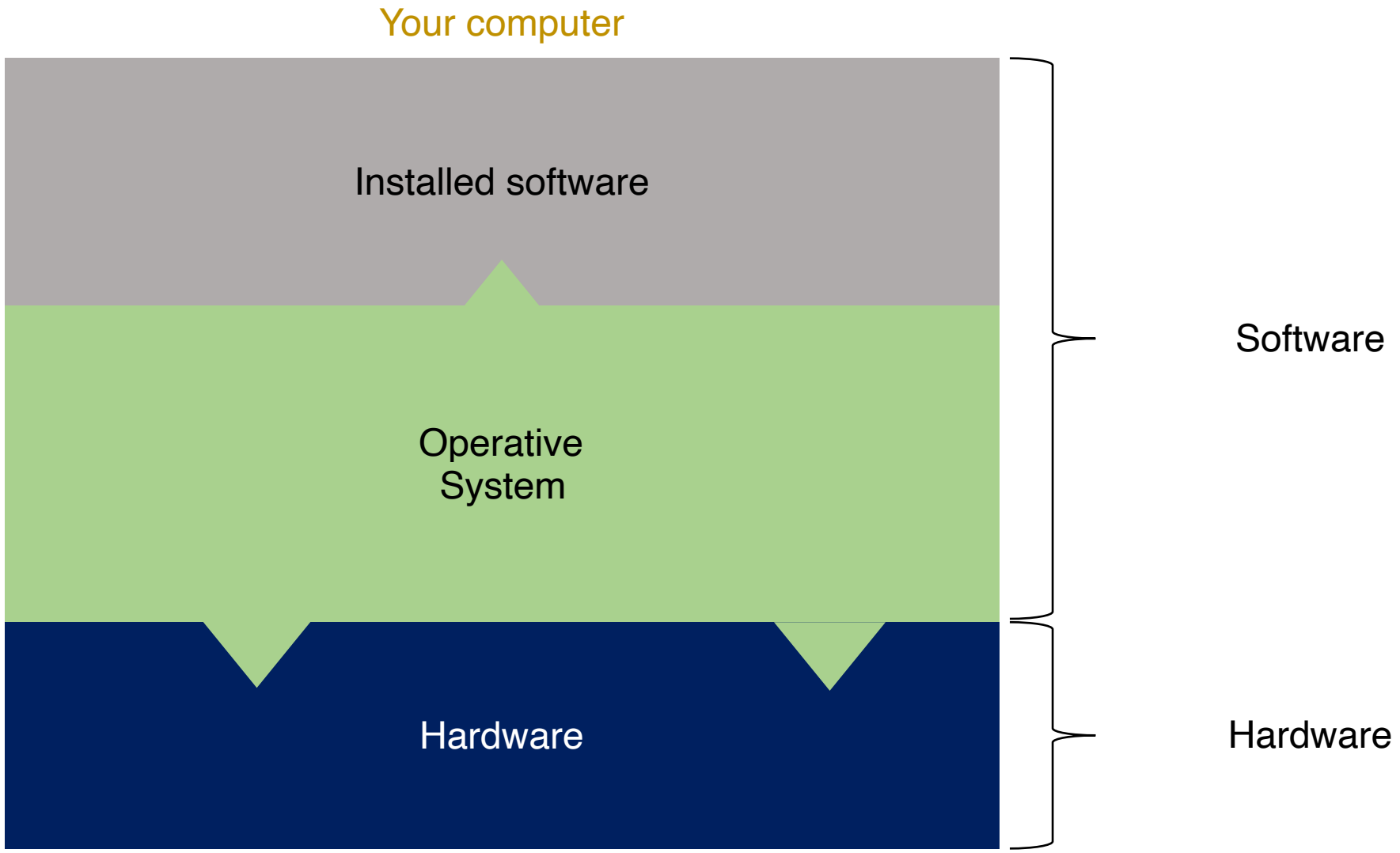


The operative systems:

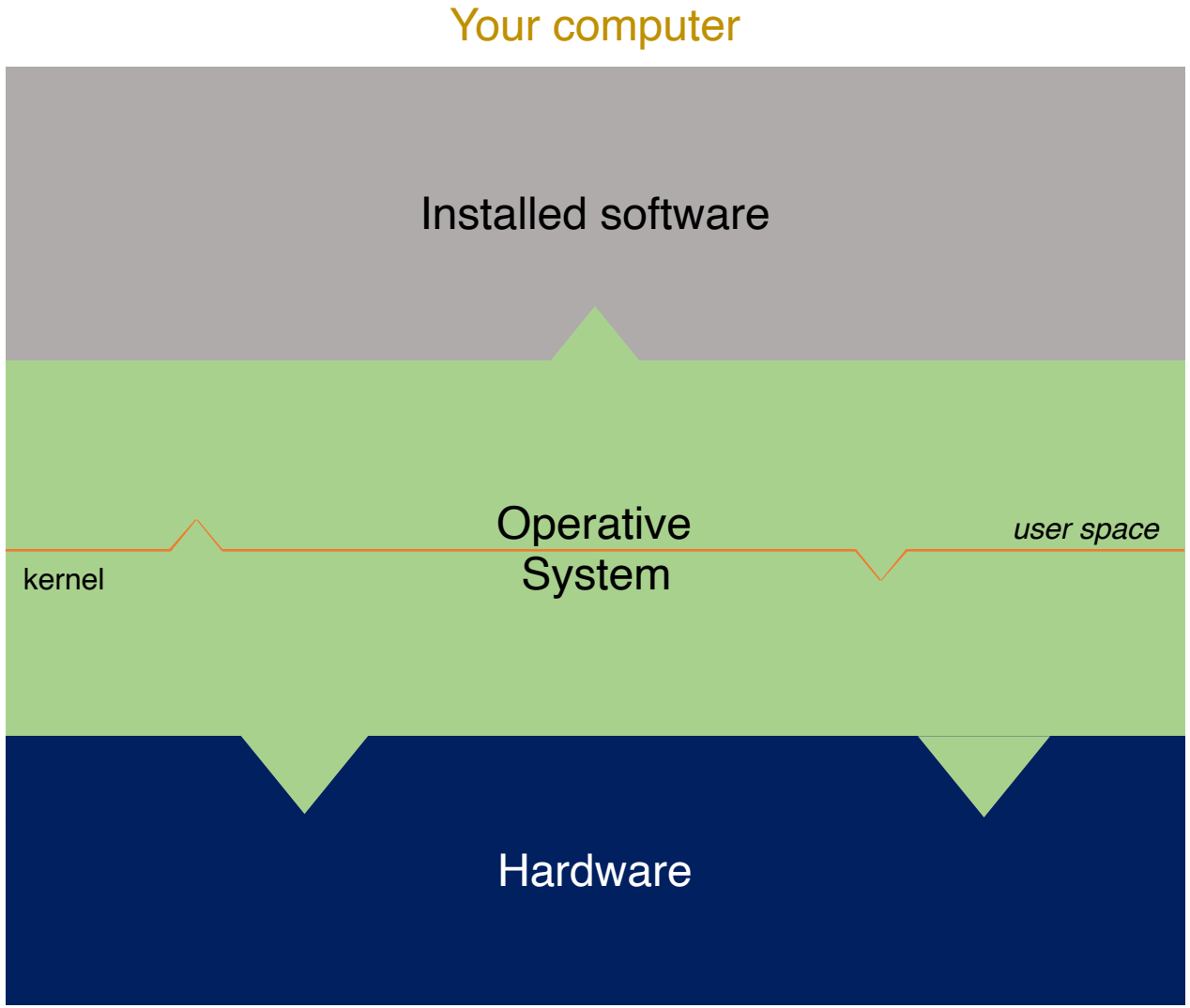
- could be updated
- could be changed
- are many

Compatibility issue!
Reproducibility compromised!

The solution: containers, freeze part of the operative system



The solution: containers, freeze part of the operative system



A Unix operating system is broken into two primary components:

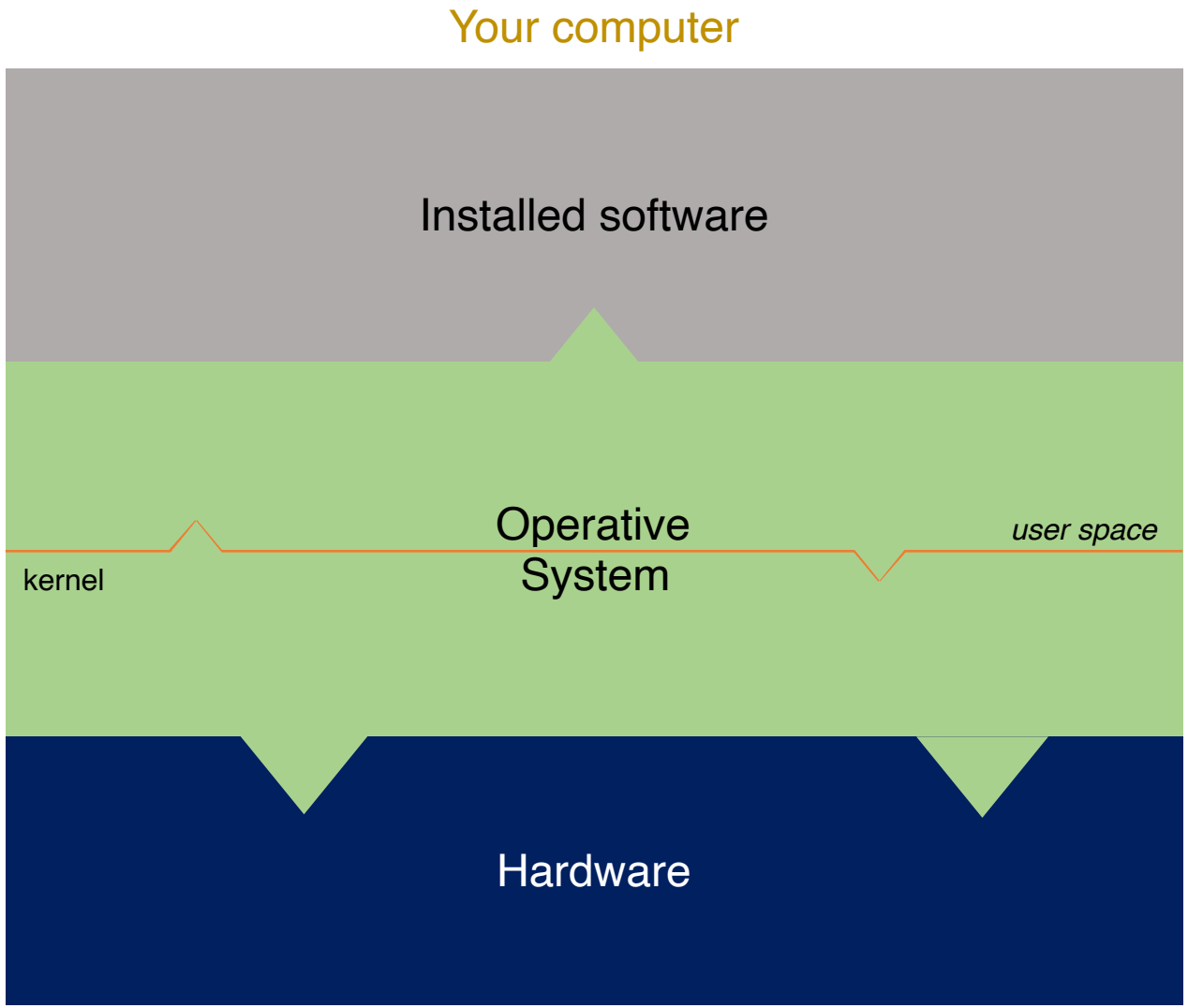
- the kernel space
- the user space.

The Kernel talks to the hardware, and provides core system features.

The user space is the environment that most people are most familiar with. It is where applications, libraries and system services run.

From Apptainer official documentation: https://apptainer.org/docs/user/latest/introduction.html

The solution: containers, freeze part of the operative system

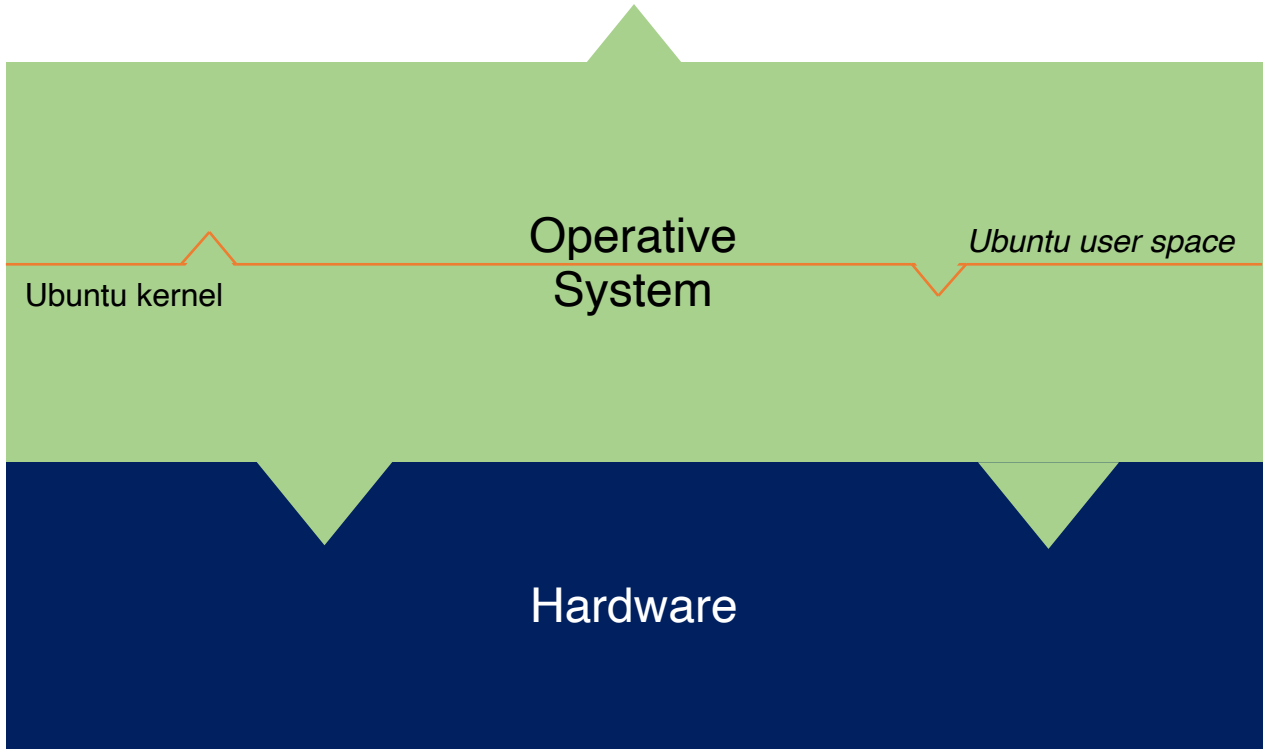


Containers change the user space into a swappable component.

This means that the entire user space portion of a Linux operating system, including programs, custom configurations, and environment can be independent of **whether your system is…**

An example

Your computer
with installed Ubuntu as OS



Your container
based on Fedora

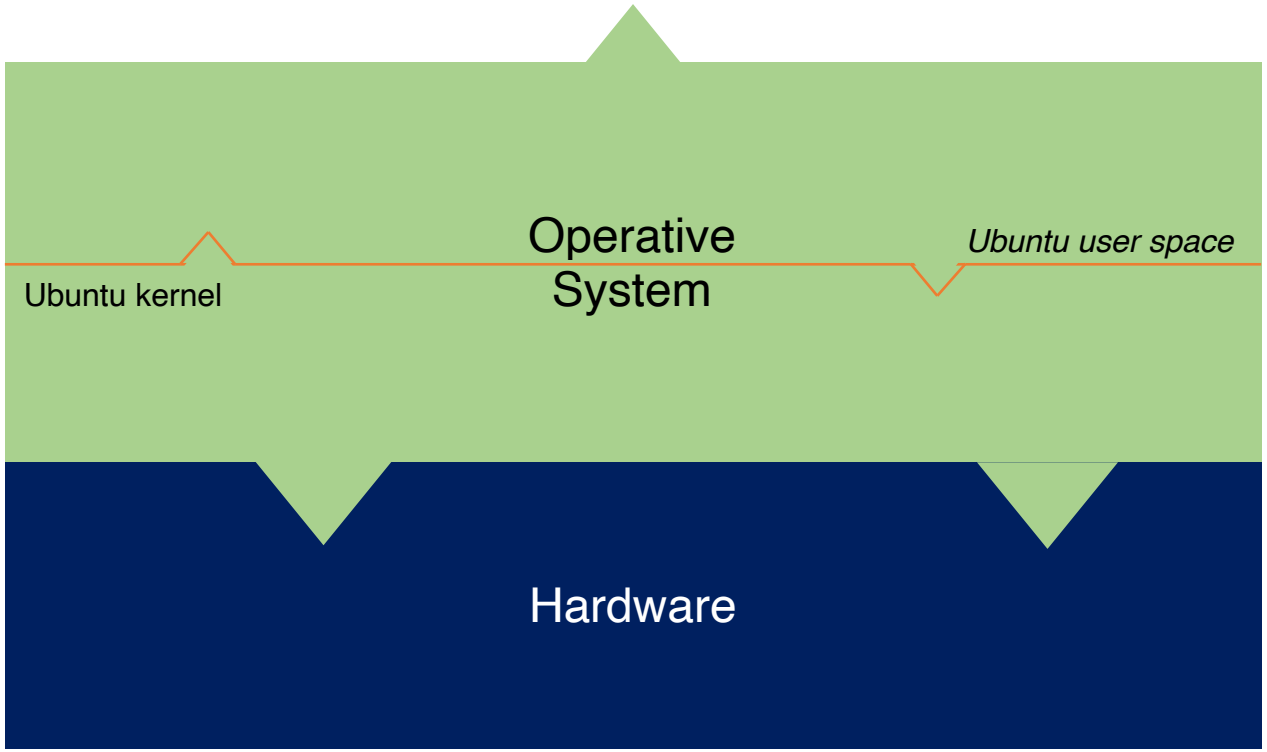
Fedora container image

An example

Your computer
with installed Ubuntu as OS

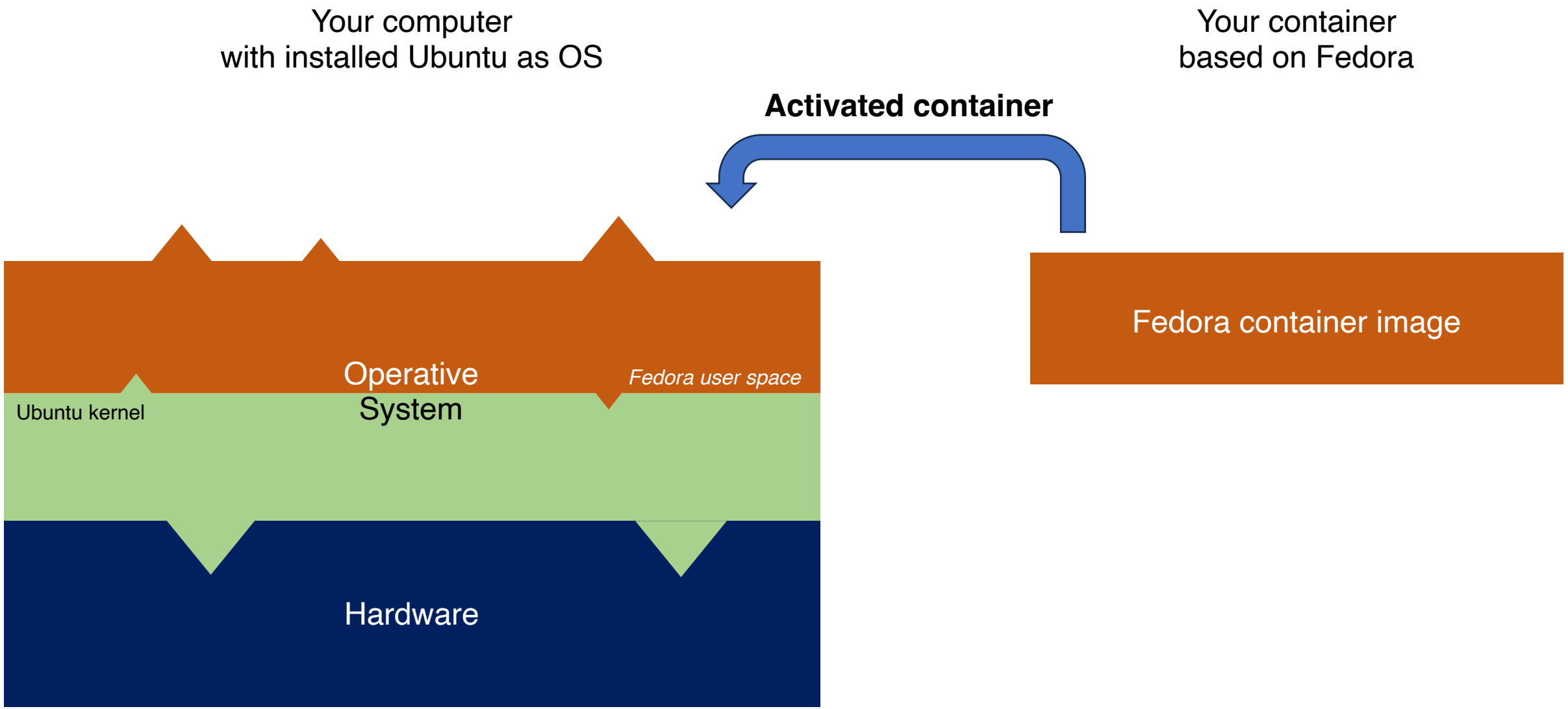
Your container
based on Fedora

Activate container!



Fedora container image

An example

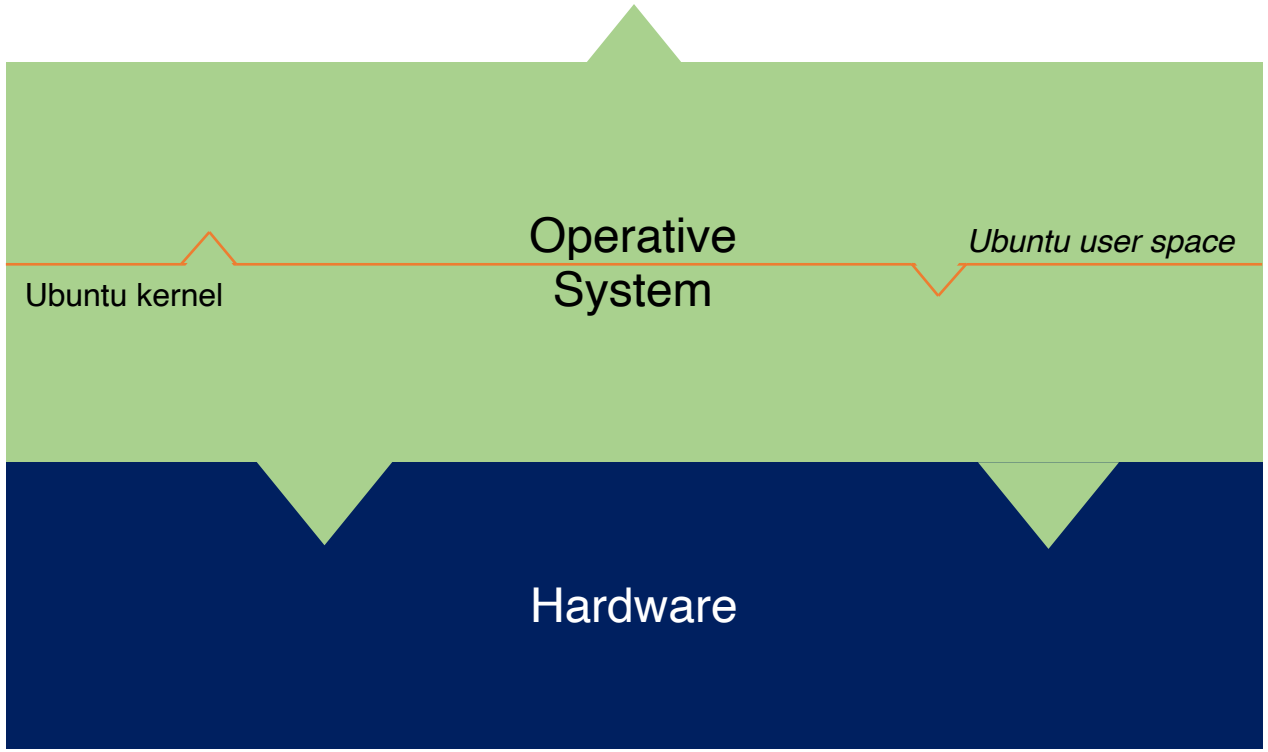

Your computer
with installed Ubuntu as OS
Your container
based on Fedora
Activated container
Fedora container image
Operative
System
Fedora user space
Ubuntu kernel
Hardware

An example

Your computer
with installed Ubuntu as OS

Your container
based on Fedora

Deactivate container



Fedora container image

An example, comments

Your computer
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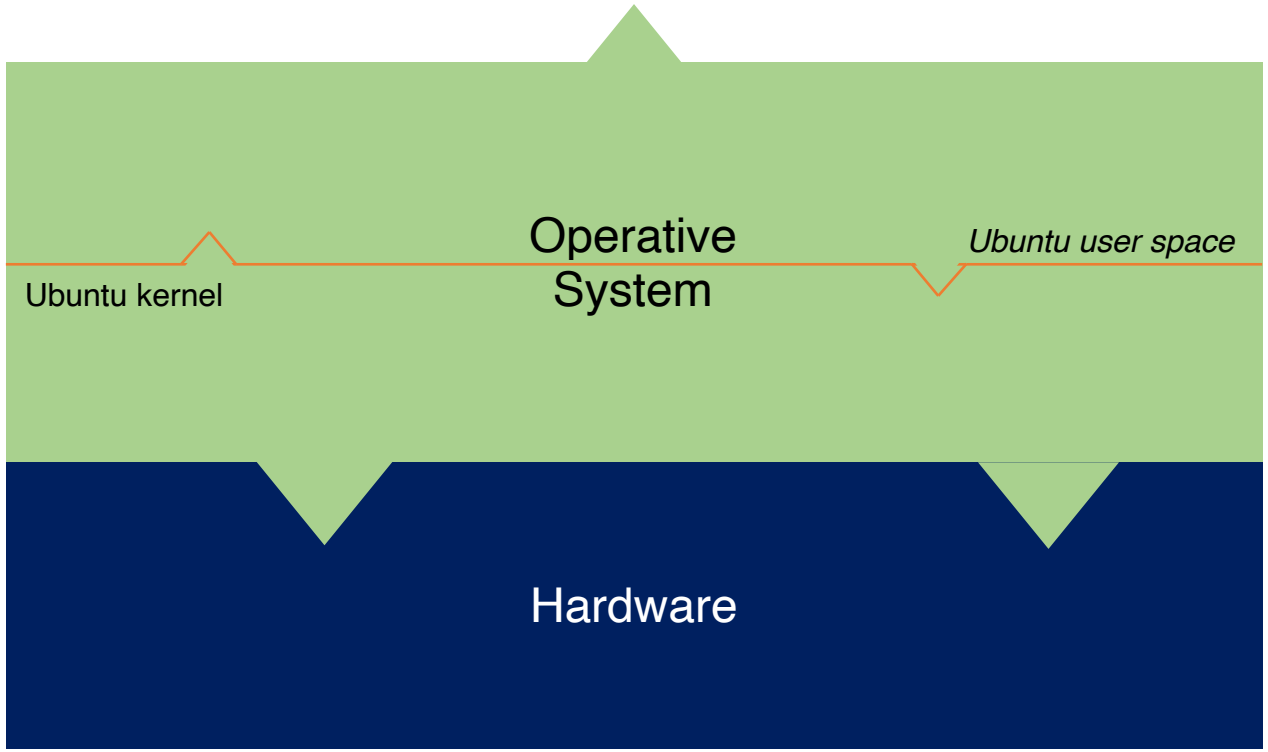
Your container
based on Fedora

Deactivate container



Fedora container image

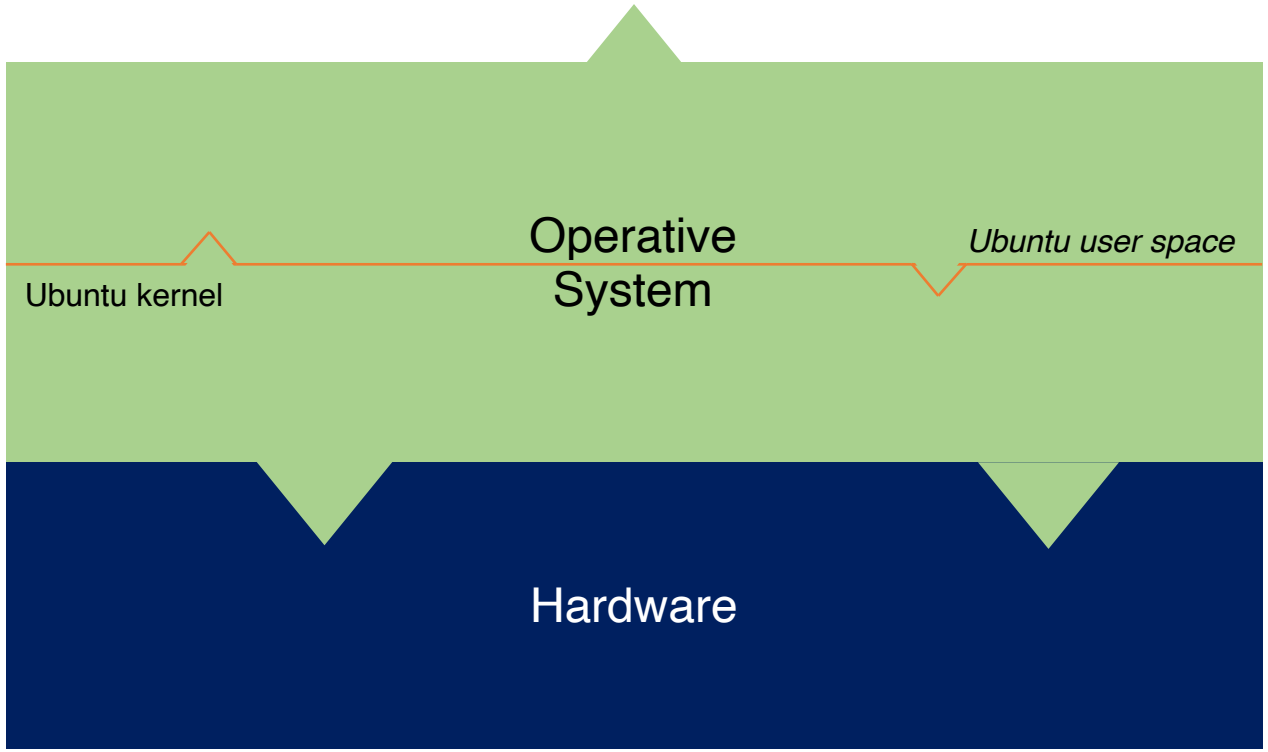
This is based on a file containing instructions
executed by a container manager

An example, comments

Your computer
with installed Ubuntu as OS

Your container
based on Fedora

Deactivate container



Fedora container image

Could be shared

This is based on a file containing instructions
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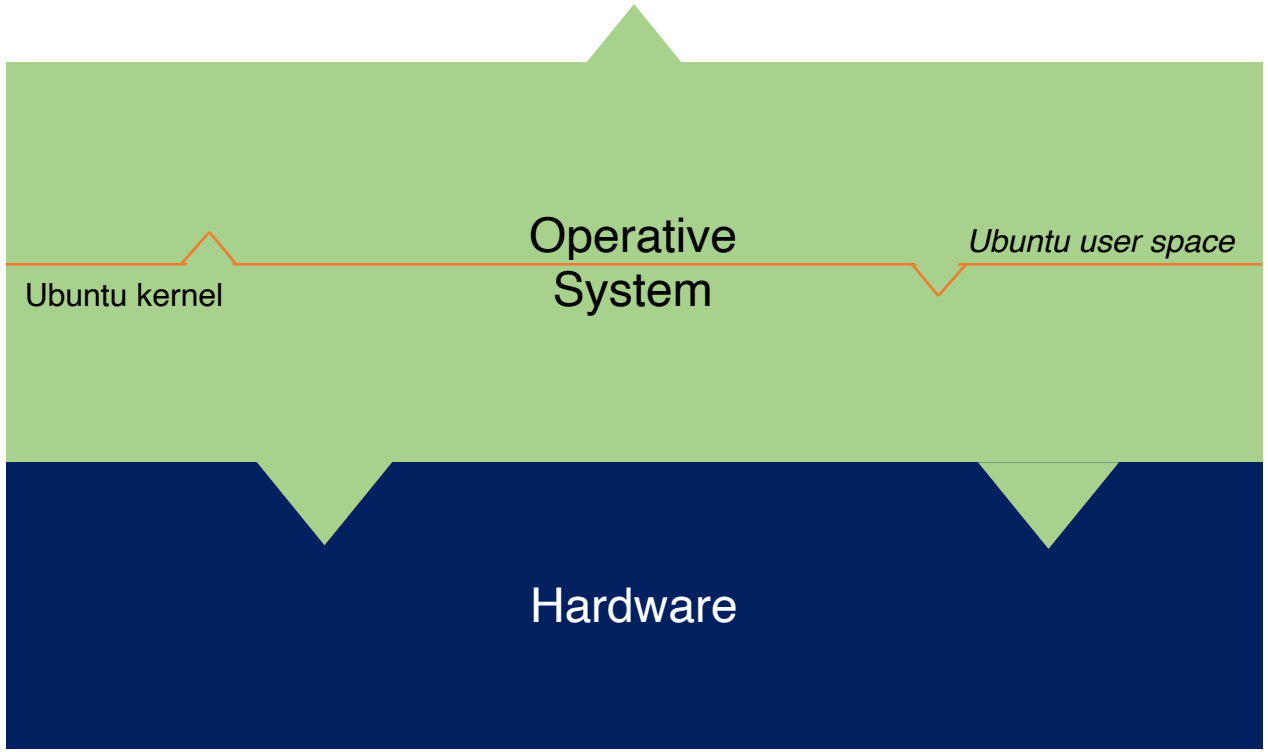
An example, comments

Your computer
with installed Ubuntu as OS

Your container
based on Fedora

Deactivate container

Could be convenient build an environment on top of a container instead of the real OS



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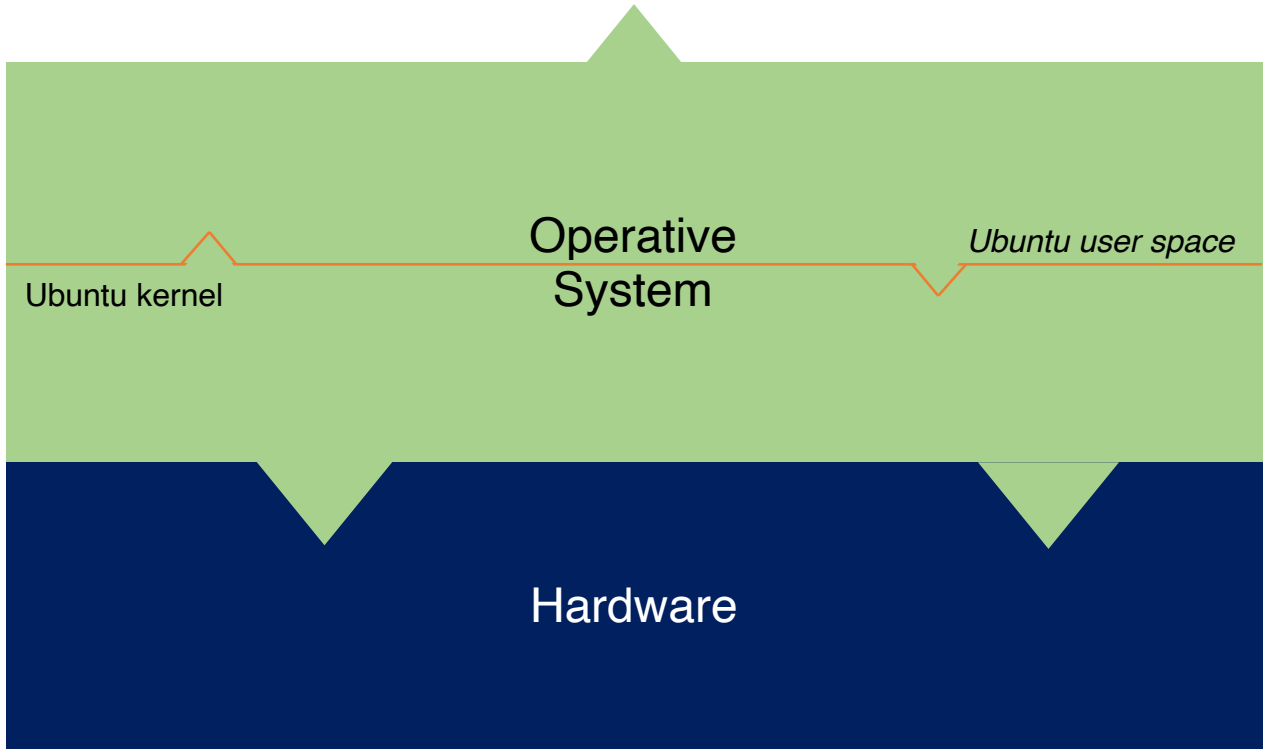
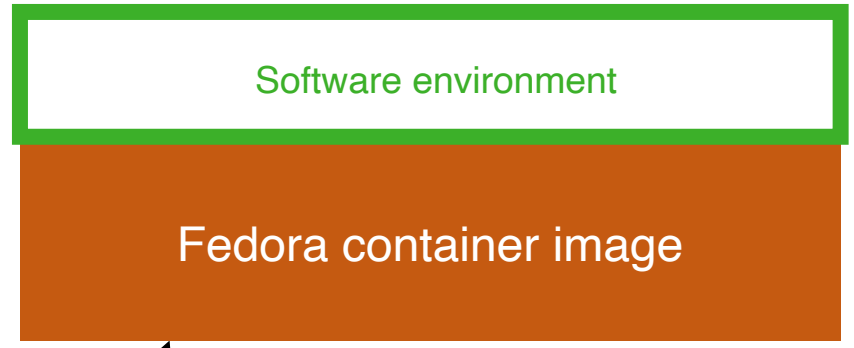


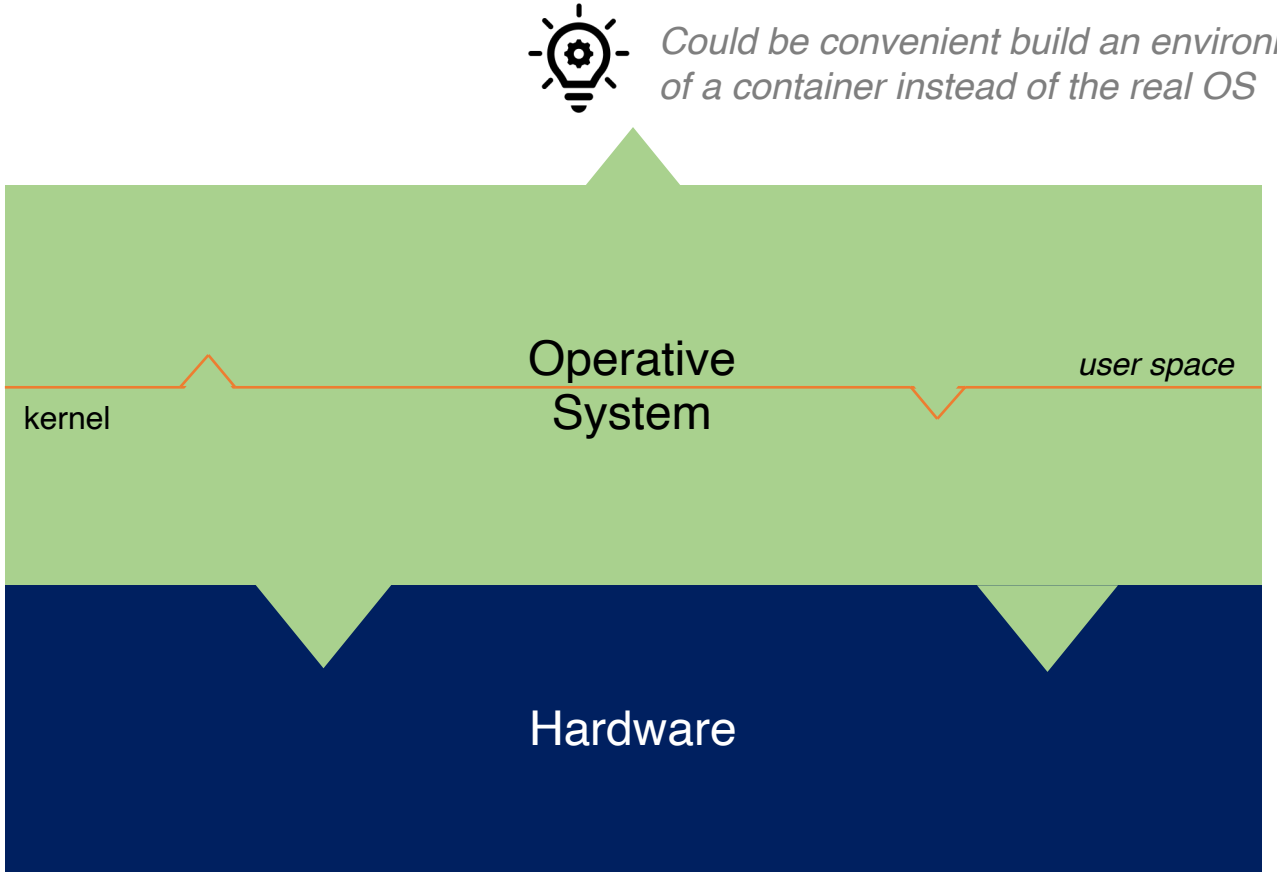


Could be shared

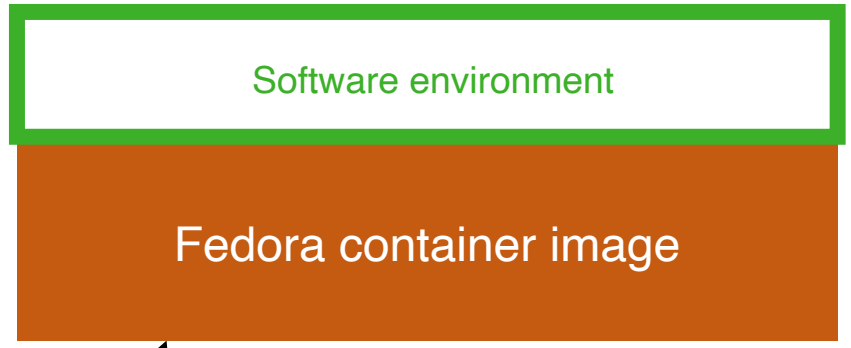
This is based on a file containing instructions executed by a container manager

You can run whatever container on whatever operative system

Your computer



Your container



Could be shared

This is based on a file containing instructions executed by a container manager

Recapitulating…

Conda environment on top of your OS

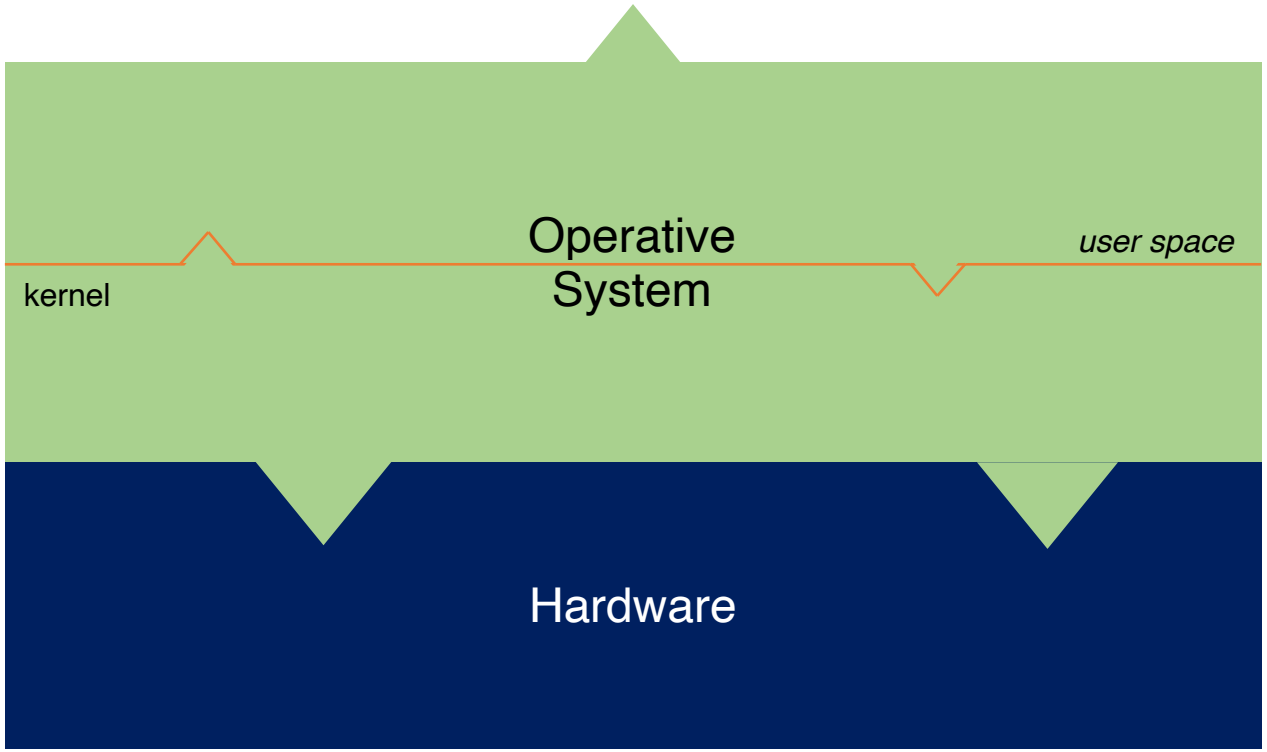
Dependent by:
- your present hardware
- your present operative system

Conda environment on top of a container

Reproducibility requires:
- instruction sharing
- container file

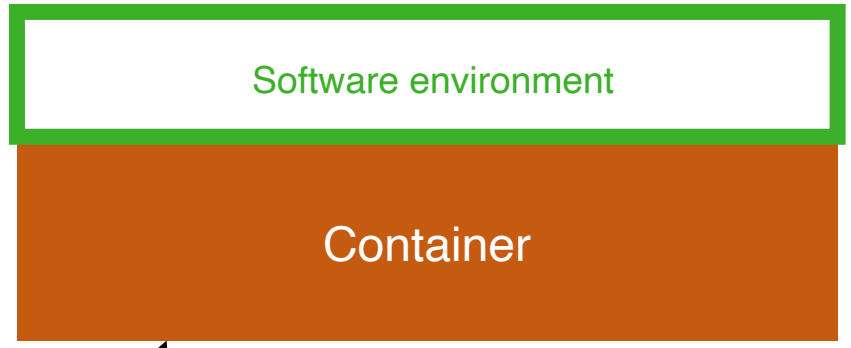
You can run whatever container on whatever operative system

Your computer



Could be convenient build an environment on top of a container instead of the real OS

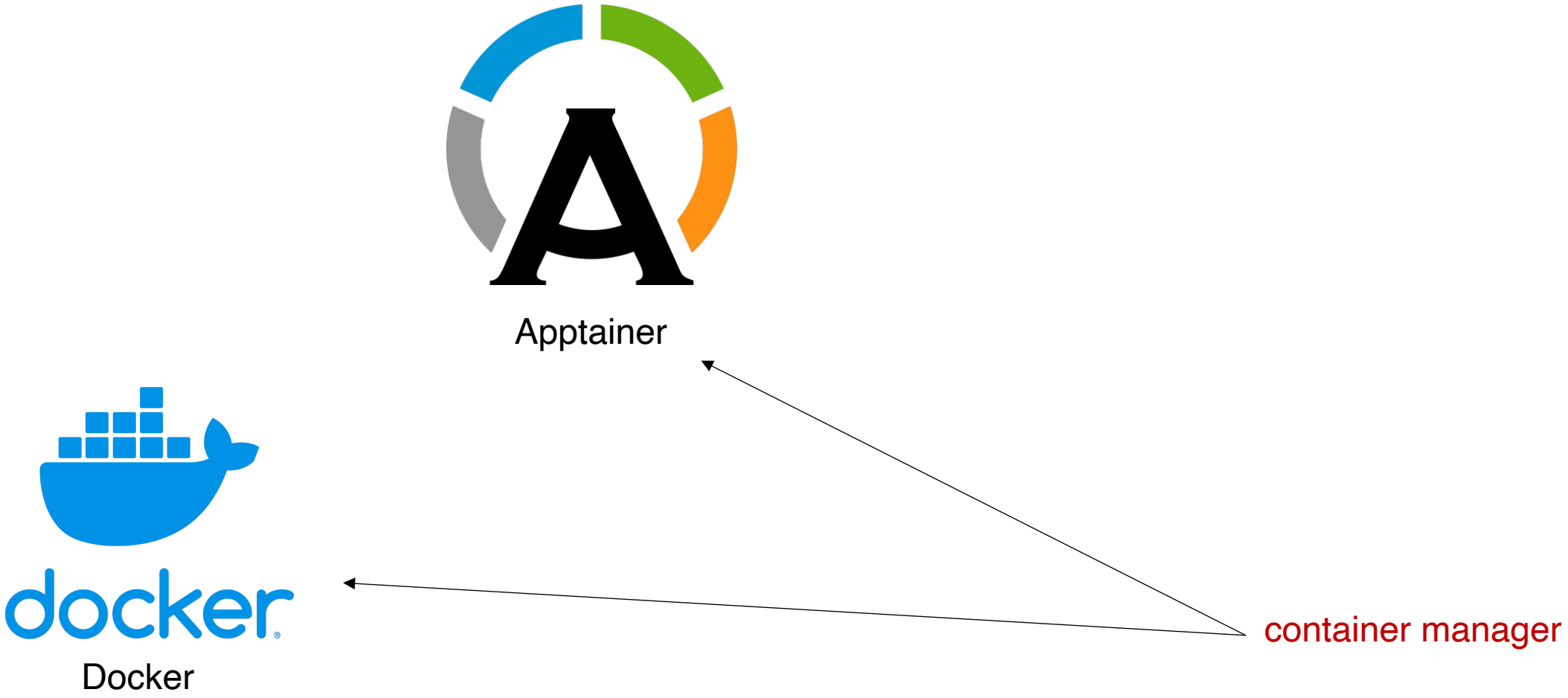
Your container



Could be shared

This is based on a file containing instructions executed by a container manager

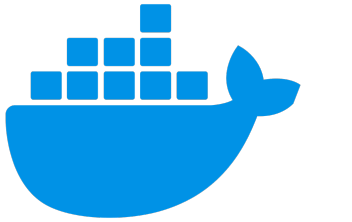
You can run whatever container on whatever operative system



You can run whatever container on whatever operative system

Apptainer

Normally used on High-Performance
Computers shared across multiple users



Docker

Used mostly in local or on cloud

container manager

Hands-on: build your RedHat based container

Hands-on: build your RedHat based container

0. Let's start creating our container instruction

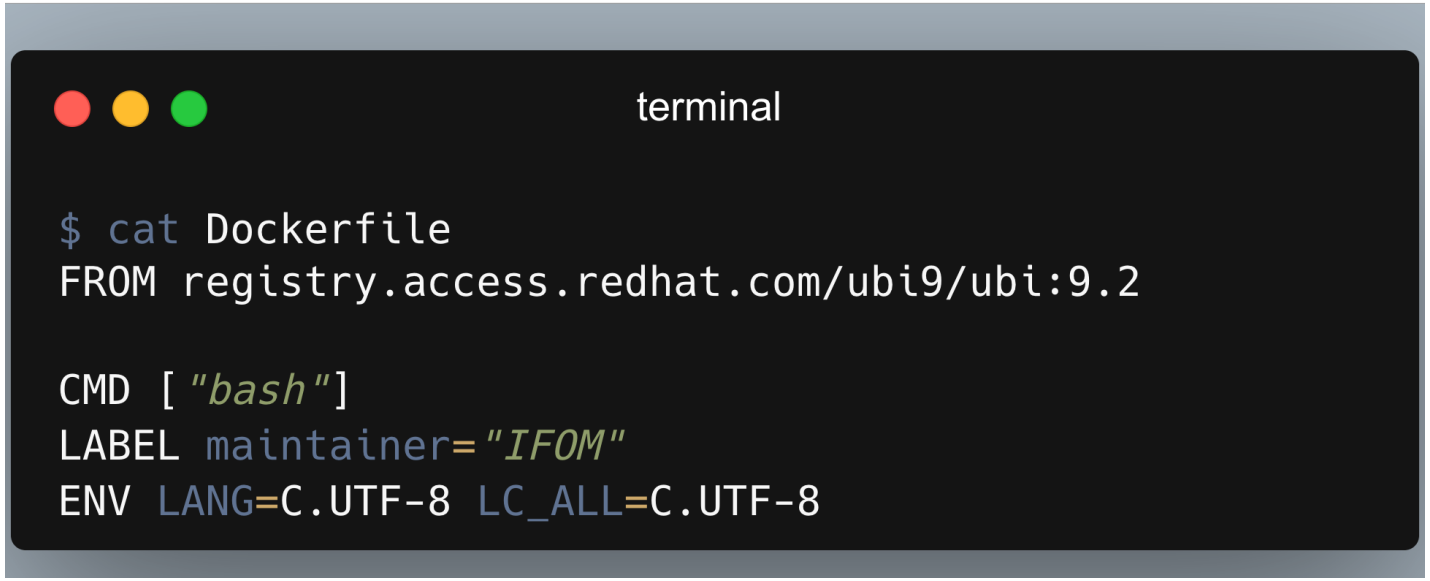
Hands-on: build your RedHat based container

terminal

```
mkdir -p containers # Create the folder where put your dockerfile
cd containers # Positionate yourself into the dockerfile folder
touch Dockerfile # Create the file containing the instruction to build your container
vi Dockerfile # Edit the Dockerfile, I am using vi, you can use whatever you like (e.g.nano, emacs, sublimetext)
```

0. Let's start creating our container instruction

Hands-on: build your RedHat based container



1. Define the operative system (we will use RedHat 9.2)

Hands-on: build your RedHat based container

terminal

```
$ cat Dockerfile
FROM registry.access.redhat.com/ubi9/ubi:9.2

CMD ["bash"]
LABEL maintainer="IFOM"
ENV LANG=C.UTF-8 LC_ALL=C.UTF-8
```

FROM Create a new build stage from a base image.

1. Define the operative system (we will use RedHat 9.2)

Hands-on: build your RedHat based container

terminal

```
$ cat Dockerfile
FROM registry.access.redhat.com/ubi9/ubi:9.2

CMD ["bash"]
LABEL maintainer="IFOM"
ENV LANG=C.UTF-8 LC_ALL=C.UTF-8
```

FROM Create a new build stage from a base image.

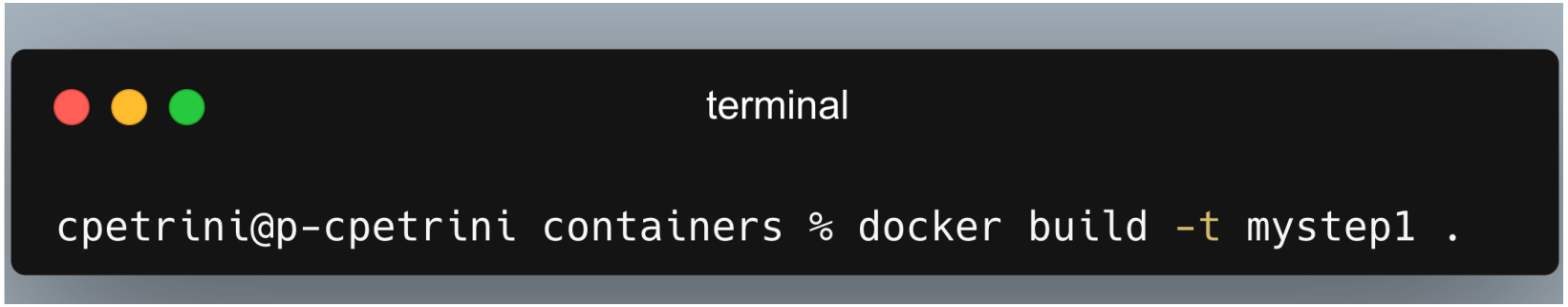
1. Define the operative system (we will use RedHat 9.2)

CMD Specify default commands.

LABEL Add metadata to an image.

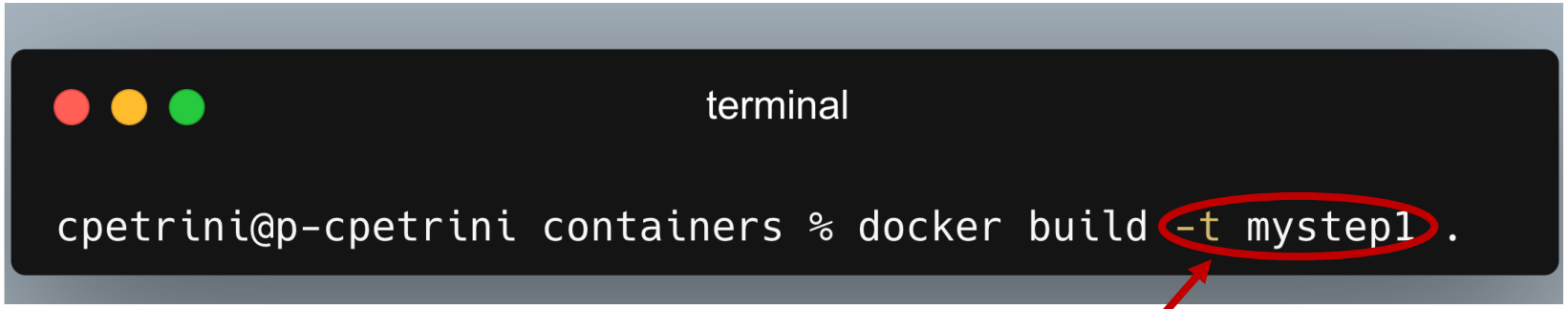
ENV Set environment variables.

Hands-on: build your RedHat based container



1. Define the operative system (we will use RedHat 9.2), build it

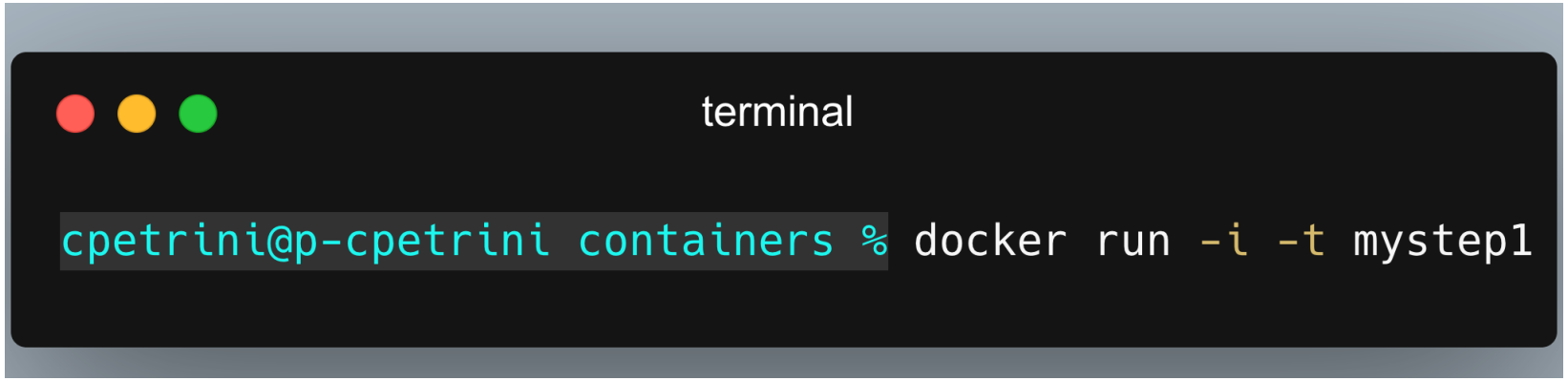
Hands-on: build your RedHat based container



Describe the name of the *user space* that will run on top of the kernel

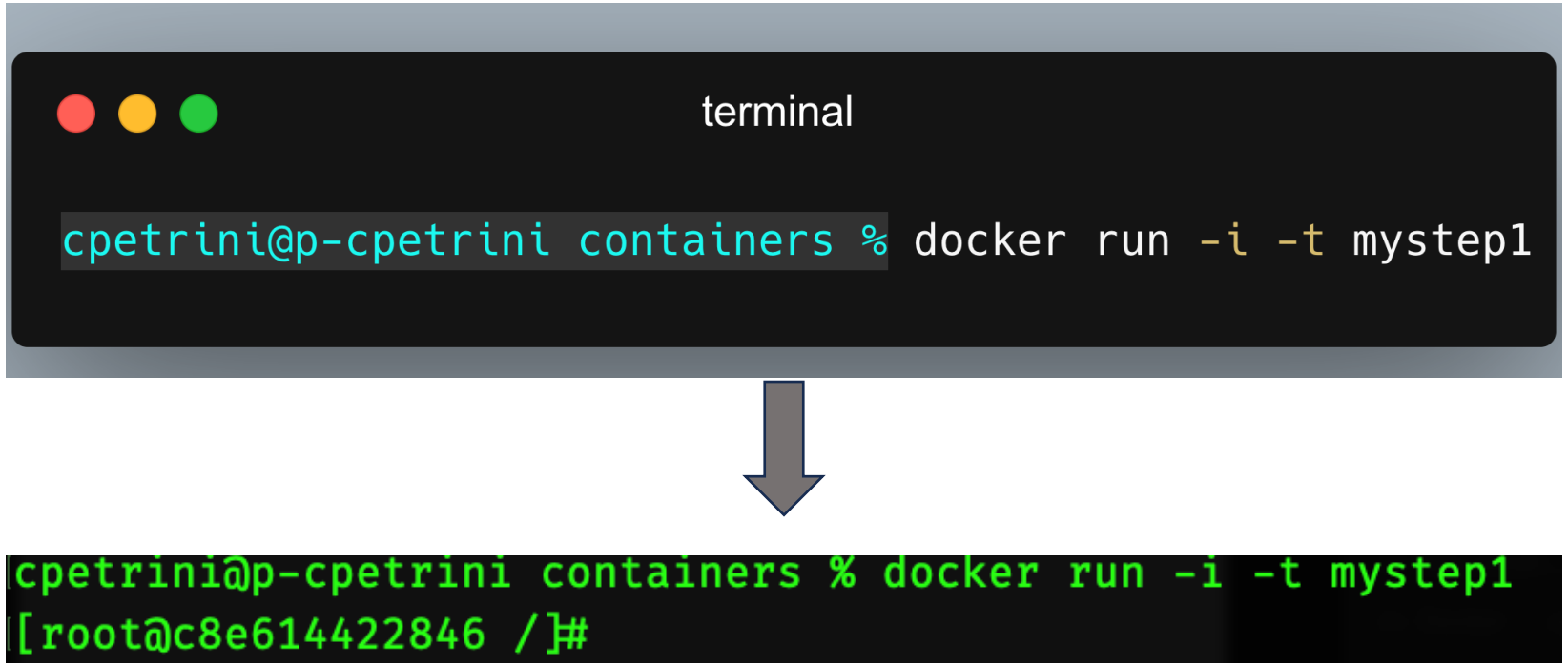
1. Define the operative system (we will use RedHat 9.2), build it

Hands-on: build your RedHat based container



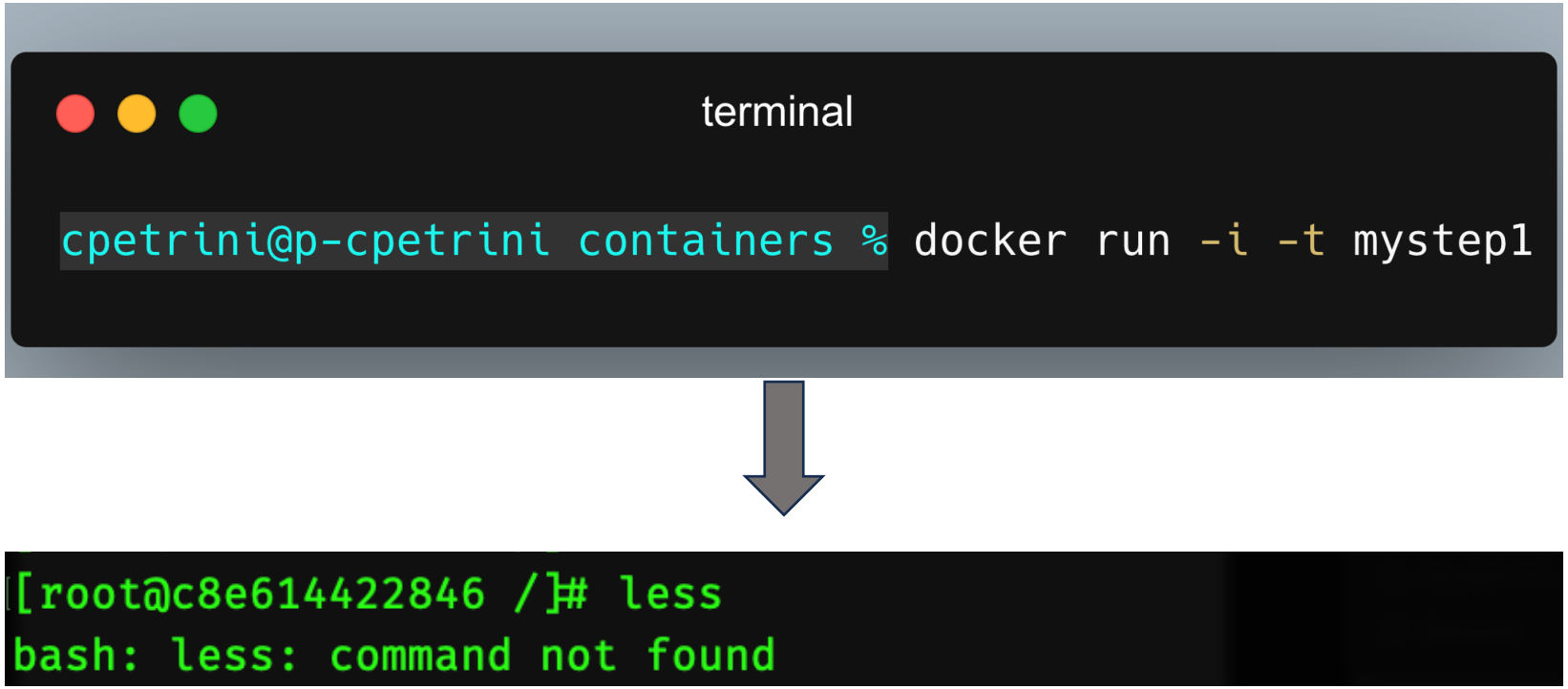
1. Define the operative system (we will use RedHat 9.2), build and run it

Hands-on: build your RedHat based container



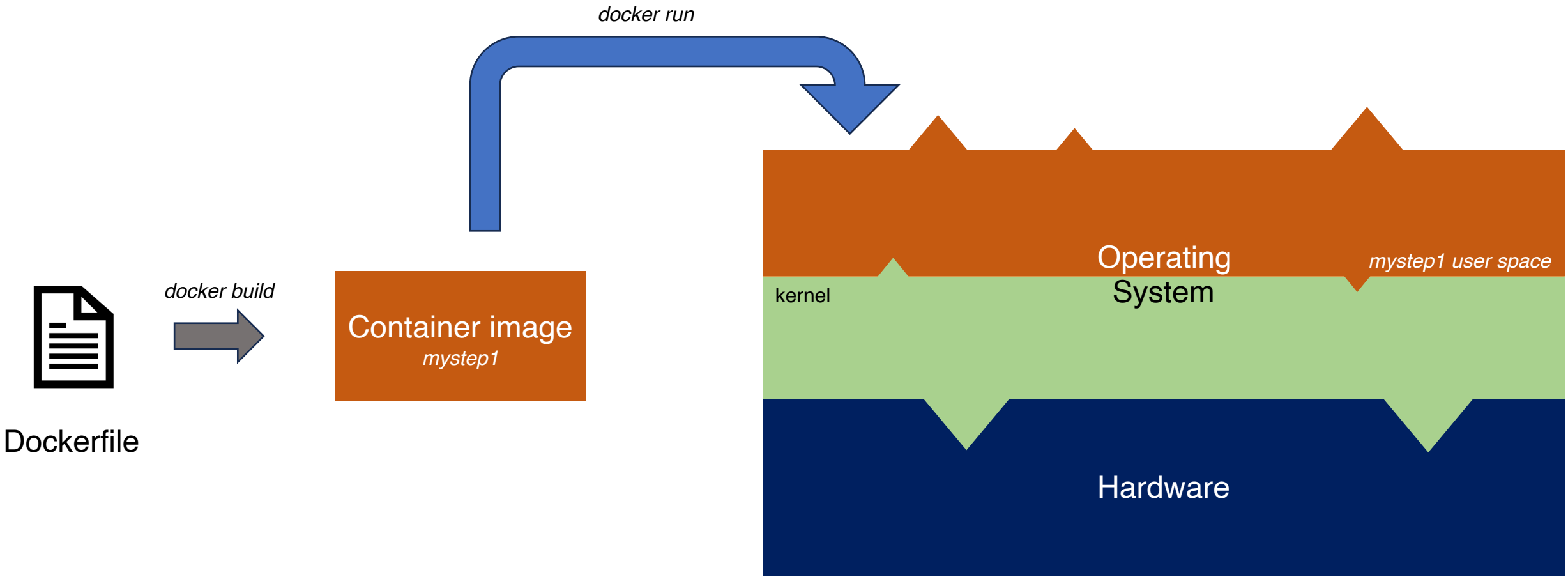
1. Define the operative system (we will use RedHat 9.2), build and run it

Hands-on: build your RedHat based container



1. Define the operative system (we will use RedHat 9.2), build and run it

What did it happen?!



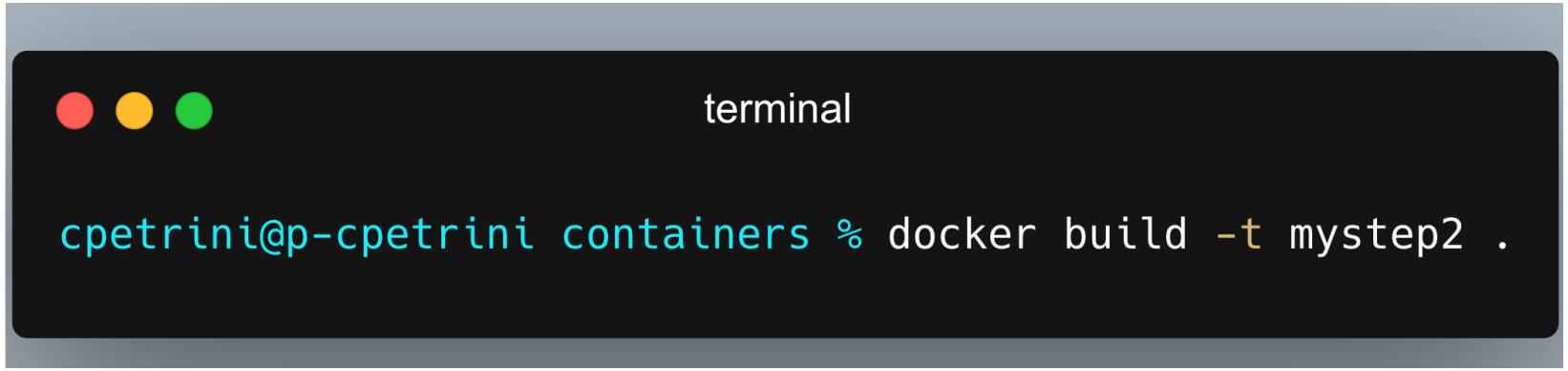
Hands-on: build your RedHat based container

2. Add some useful tools to our container (*e.g.* less)

terminal

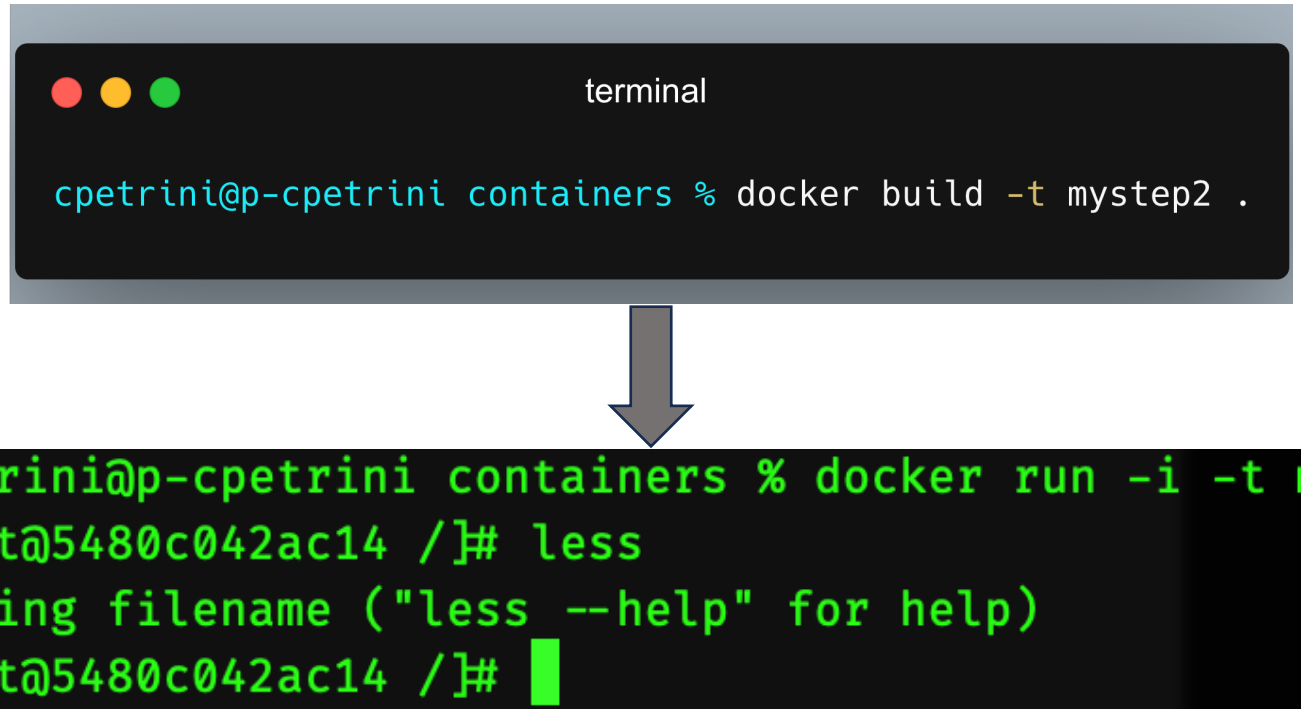
```
cpetrini@p-cpetrini containers % cat Dockerfile
FROM registry.access.redhat.com/ubi9/ubi:9.2

CMD ["bash"]
LABEL maintainer="IFOM"
ENV LANG=C.UTF-8 LC_ALL=C.UTF-8

# Install on your container some useful tools like "less" or "vim"
RUN \
    dnf -y install \
        https://dl.fedoraproject.org/pub/epel/epel-release-latest-9.noarch.rpm \
    && usr/bin/crb enable \
    && dnf -y update-minimal \
    && dnf -y install \
            bzip2 \
            ca-certificates \
            git \
            glib2 \
            hostname \
            libSM \
            libXext \
            libXrender \
            less \
            mercurial \
            openssh-clients \
            procps \
            procps-ng \
            subversion \
            time \
            vim \
            wget \
    && dnf clean all
```

Hands-on: build your RedHat based container



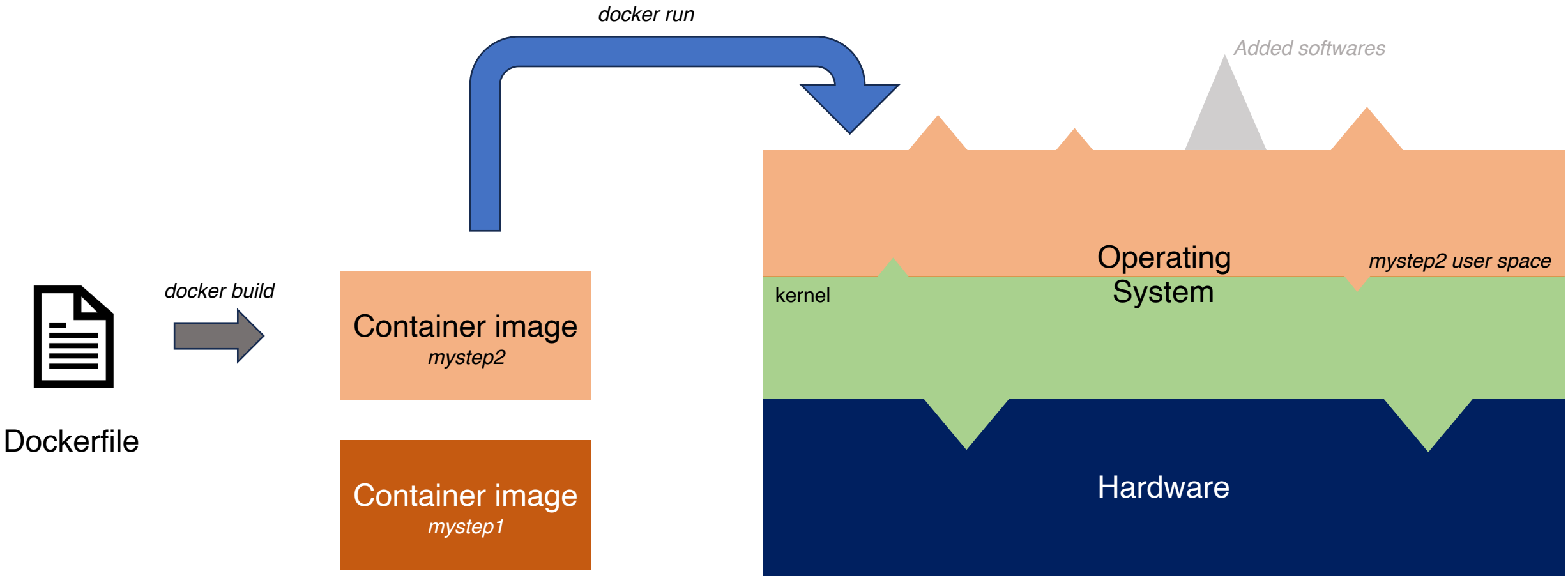
2. Add some useful tools to our container (*e.g.* less), build it

Hands-on: build your RedHat based container

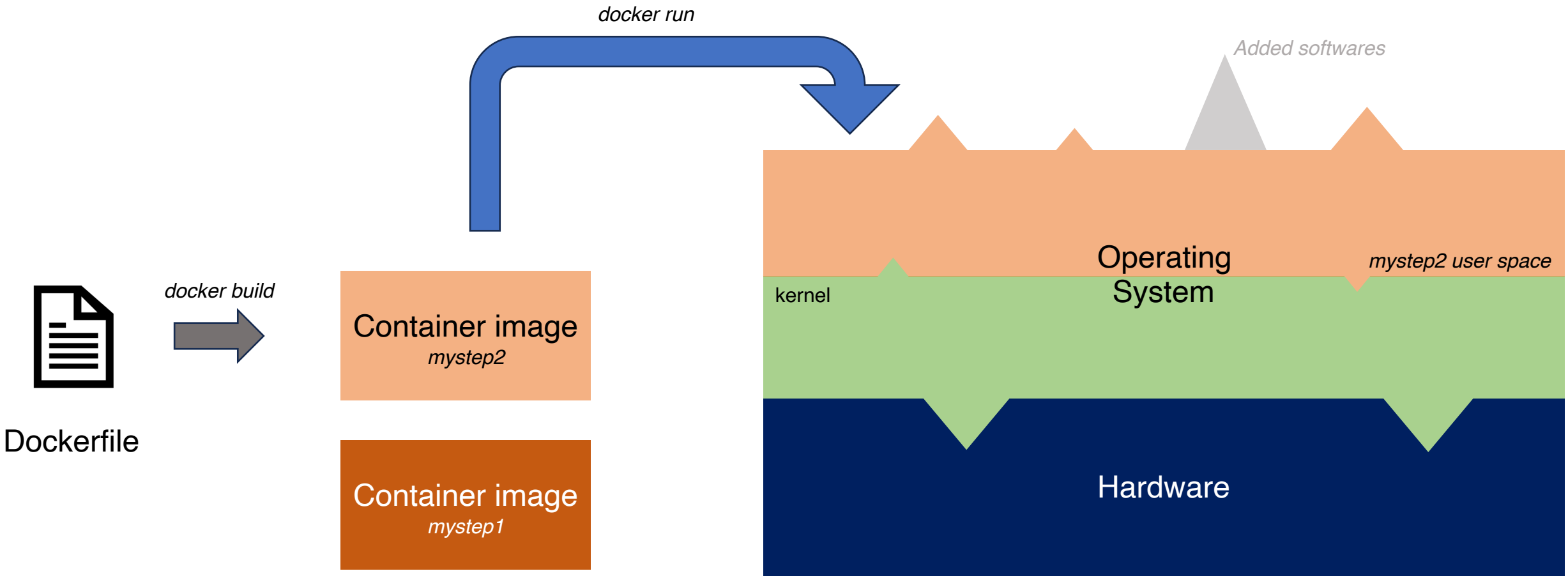


2. Add some useful tools to our container (*e.g.* less), build and run it

What did it happen?!

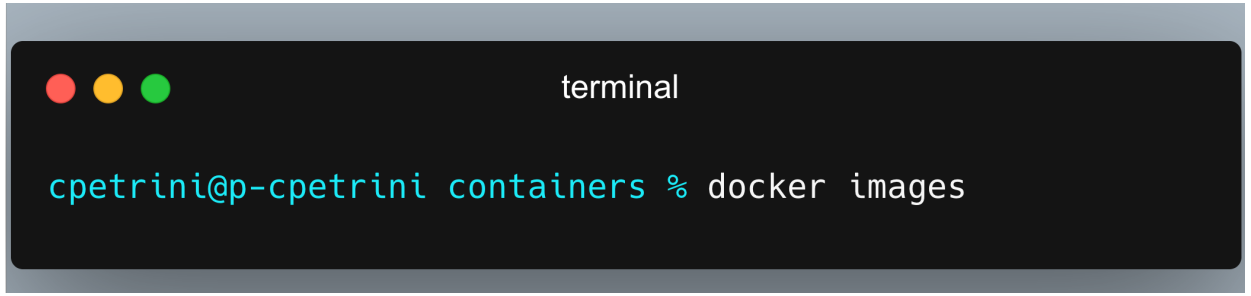


What about *mystep1*?!



It is still there and you can load it when you want!

Hands-on: build your RedHat based container




```
cpetrini@p-cpetrini containers % docker images
REPOSITORY   TAG       IMAGE ID       CREATED          SIZE
mystep2      latest    ec9b9409aa82   5 hours ago      578MB
mystep1      latest    b1dc540c596a   13 months ago    313MB
cpetrini@p-cpetrini containers %
```

2bis. Check the available containers

Hands-on: build your RedHat based container

3. Install miniforge inside container

terminal

```
cpetrini@p-cpetrini containers % cat Dockerfile
FROM ...
                ...
                           ...
                                       ...
RUN \
    /bin/sh -c set -x \
    && UNAME_M="$(uname -m)" \
    && MINIFORGE_URL="https://github.com/conda-
forge/miniforge/releases/download/${FORGE_VERSION}/Miniforge3-${FORGE_VERSION}-$(uname)-$(uname -m).sh" \
    && wget "${MINIFORGE_URL}" -O miniforge.sh -q \
    && mkdir -p /opt \
    && bash miniforge.sh -b -p /opt/conda \
    && rm miniforge.sh \
    && ln -s /opt/conda/etc/profile.d/conda.sh /etc/profile.d/conda.sh \
    && echo ". /opt/conda/etc/profile.d/conda.sh" >> ~/.bashrc \
    && echo "conda activate base" >> ~/.bashrc \
    && find /opt/conda/ -follow -type f -name '*.a' -delete \
    && find /opt/conda/ -follow -type f -name '*.js.map' -delete \
    && /opt/conda/bin/conda clean -afy
```

Hands-on: build your RedHat based container

3. Install miniforge inside container

terminal

```
cpetrini@p-cpetrini containers % cat Dockerfile
FROM ...
                ...
                            ...
                                        ...
RUN \
    /bin/sh -c set -x \
    && UNAME_M="$(uname -m)" \
    && MINIFORGE_URL="https://github.com/conda-
forge/miniforge/releases/download/${FORGE_VERSION}/Miniforge3-${FORGE_VERSION}-$(uname)-$(uname -m).sh" \
    && wget "${MINIFORGE_URL}" -O miniforge.sh -q \
    && mkdir -p /opt \
    && bash miniforge.sh -b -p /opt/conda \
    && rm miniforge.sh \
    && ln -s /opt/conda/etc/profile.d/conda.sh /etc/profile.d/conda.sh \
    && echo ". /opt/conda/etc/profile.d/conda.sh" >> ~/.bashrc \
    && echo "conda activate base" >> ~/.bashrc \
    && find /opt/conda/ -follow -type f -name '*.a' -delete \
    && find /opt/conda/ -follow -type f -name '*.js.map' -delete \
    && /opt/conda/bin/conda clean -afy
```

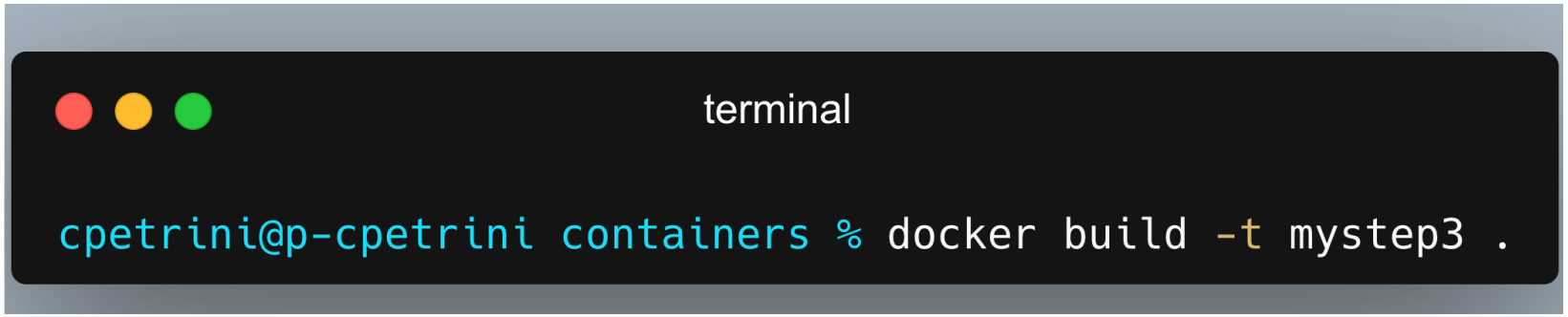
It is just a sophisticated version of

terminal

```
curl -L -O "https://github.com/conda-forge/miniforge/releases/latest/download/Miniforge3-$(uname)-$(uname -m).sh"
bash Miniforge3-$(uname)-$(uname -m).sh
```

saw on conda section

Hands-on: build your RedHat based container



3. Install miniforge inside container

Hands-on: create a conda environment on top of the container

terminal

```
cpetrini@p-cpetrini containers % mkdir -p ${HOME}/Desktop/my_prj_sw/ubi9.2/miniforge3.24-3/myproject_env
```

Hands-on: create a conda environment on top of the container

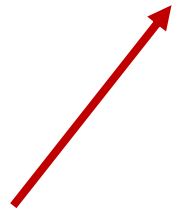
terminal

```
cpetrini@p-cpetrini containers % mkdir -p ${HOME}/Desktop/my_prj_sw/ubi9.2/miniforge3.24-3/myproject_env
cpetrini@p-cpetrini containers % docker run -i -v ${HOME}/Desktop/my_prj_sw/ubi9.2/miniforge3.24-3/myproject_env:/opt/myenv -t mystep3
```

Hands-on: create a conda environment on top of the container

terminal

```
cpetrini@p-cpetrini containers % mkdir -p ${HOME}/Desktop/my_prj_sw/ubi9.2/miniforge3.24-3/myproject_env
cpetrini@p-cpetrini containers % docker run -i -v ${HOME}/Desktop/my_prj_sw/ubi9.2/miniforge3.24-3/myproject_env:/opt/myenv -t mystep3
```



Mount a folder inside the container

Hands-on: create a conda environment on top of the container

terminal

```
cpetrini@p-cpetrini containers % mkdir -p ${HOME}/Desktop/my_prj_sw/ubi9.2/miniforge3.24-3/myproject_env
cpetrini@p-cpetrini containers % docker run -i -v ${HOME}/Desktop/my_prj_sw/ubi9.2/miniforge3.24-3/myproject_env:/opt/myenv -t mystep3
```

Mount a folder inside the container

Folder we want to mount

:

position where we want the folder inside the container

Hands-on: create a conda environment on top of the container

terminal

```
cpetrini@p-cpetrini containers % mkdir -p ${HOME}/Desktop/my_prj_sw/ubi9.2/miniforge3.24-3/myproject_env
cpetrini@p-cpetrini containers % docker run -i -v ${HOME}/Desktop/my_prj_sw/ubi9.2/miniforge3.24-3/myproject_env:/opt/myenv -t mystep3
(base) [root@970e6bb7e8f3 /]# conda create -p /opt/myenv
```

Hands-on: create a conda environment on top of the container

terminal

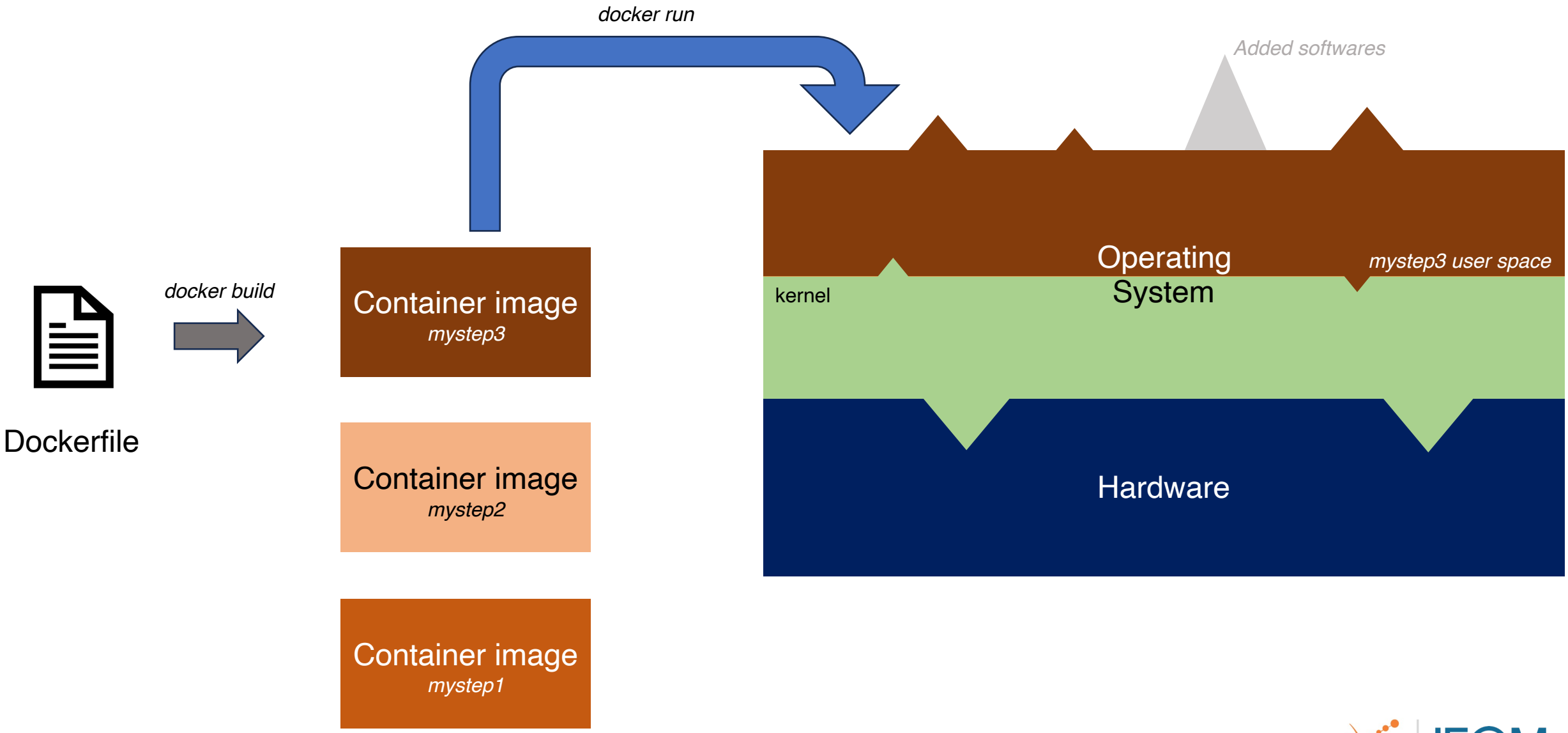
```
cpetrini@p-cpetrini containers % mkdir -p ${HOME}/Desktop/my_prj_sw/ubi9.2/miniforge3.24-3/myproject_env
cpetrini@p-cpetrini containers % docker run -i -v ${HOME}/Desktop/my_prj_sw/ubi9.2/miniforge3.24-3/myproject_env:/opt/myenv -t mystep3
(base) [root@970e6bb7e8f3 /]# conda create -p /opt/myenv
(base) [root@970e6bb7e8f3 /]# conda activate /opt/myenv/
```

Hands-on: create a conda environment on top of the container

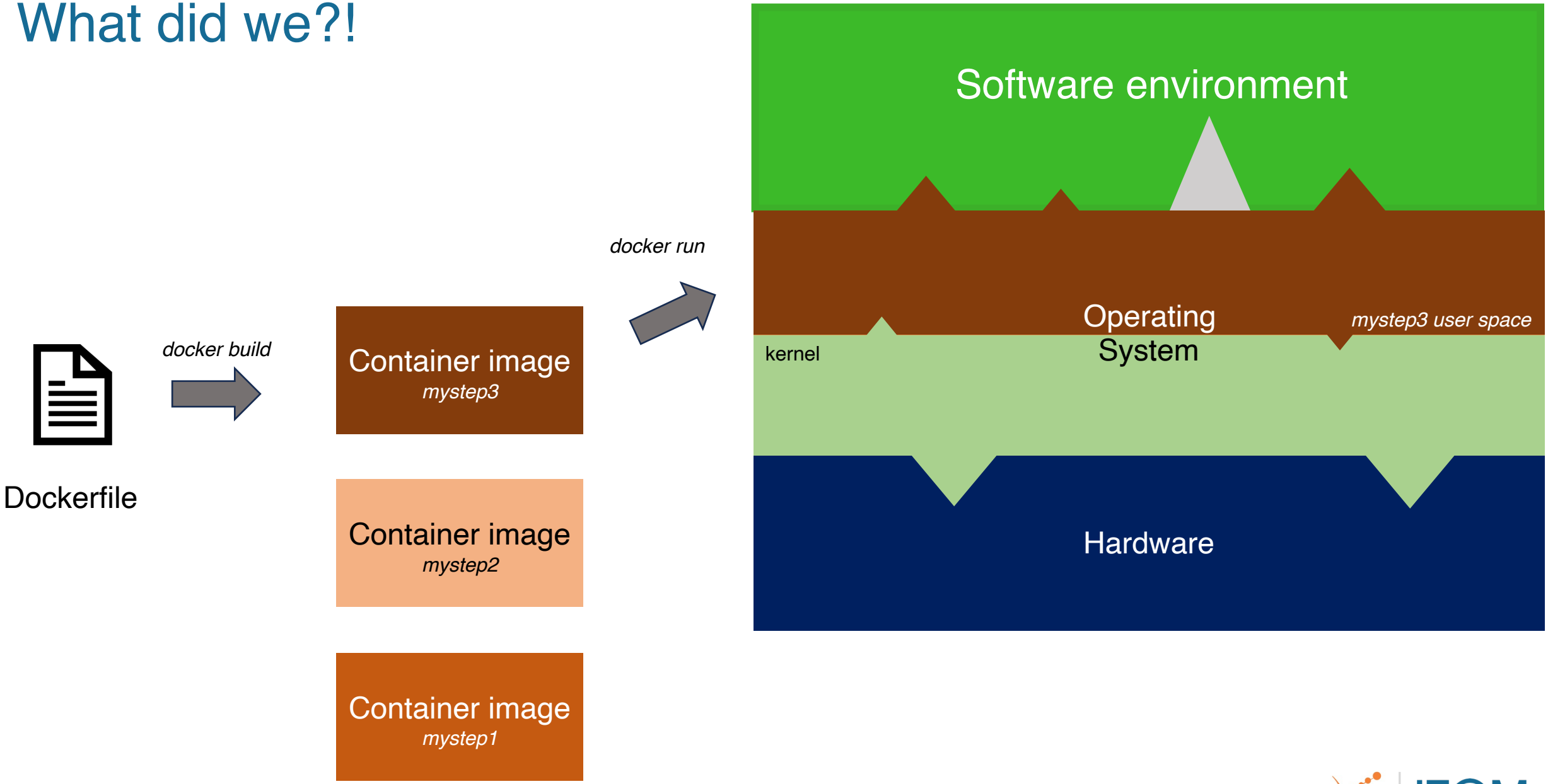
terminal

```
cpetrini@p-cpetrini containers % mkdir -p ${HOME}/Desktop/my_prj_sw/ubi9.2/miniforge3.24-3/myproject_env
cpetrini@p-cpetrini containers % docker run -i -v ${HOME}/Desktop/my_prj_sw/ubi9.2/miniforge3.24-3/myproject_env:/opt/myenv -t mystep3
(base) [root@970e6bb7e8f3 /]# conda create -p /opt/myenv
(base) [root@970e6bb7e8f3 /]# conda activate /opt/myenv/
(/opt/myenv) [root@970e6bb7e8f3 /]# conda install bioconda::samtools
```

What did we?!


docker run
Added softwares
Operating System
mystep3 user space
kernel
Hardware
docker build
Container image
mystep3
Container image
mystep2
Container image
mystep1
Dockerfile

What did we?!


Dockerfile
docker build
Container image
mystep3
Container image
mystep2
Container image
mystep1
docker run
Software environment
Operating System
mystep3 user space
kernel
Hardware

Hands-on: create a conda environment on top of the container

terminal

```
cpetrini@p-cpetrini containers % mkdir -p ${HOME}/Desktop/my_prj_sw/ubi9.2/miniforge3.24-3/myproject_env
cpetrini@p-cpetrini containers % docker run -i -v ${HOME}/Desktop/my_prj_sw/ubi9.2/miniforge3.24-3/myproject_env:/opt/myenv -t mystep3
(base) [root@970e6bb7e8f3 /]# conda create -p /opt/myenv
(base) [root@970e6bb7e8f3 /]# conda activate /opt/myenv/
(/opt/myenv) [root@970e6bb7e8f3 /]# conda install bioconda::samtools
```

Do some tests yourself!

Recreate the environment built before:

- can you have access it from outside the container?
- does it works?
- what about JupyterLab?

Git & GitHub

Collaboration best practices

Napoli, 26/11/2024

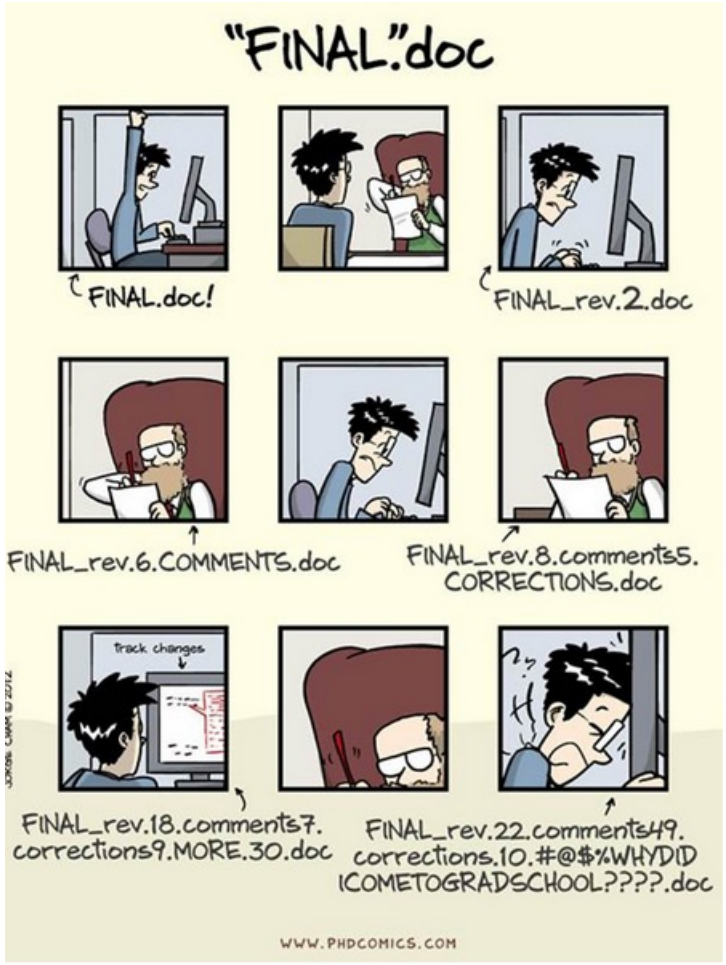
What is git?

A Version Control System for Everyone: Git is a free, open-source version control system that **tracks changes in files**, allowing multiple people to collaborate on projects efficiently.

- It keeps **a history of your project**.
- **Safely** experiment with new ideas (branching).
- **Collaborate** with others without overwriting each other's work

Real-Life Example: Think of it as "Track Changes" in Word but for code and complex projects.

Why Version Control is Essential?



Solve Collaboration and Tracking Issues (**i.e. files proliferation**)

It keeps a history of your project.

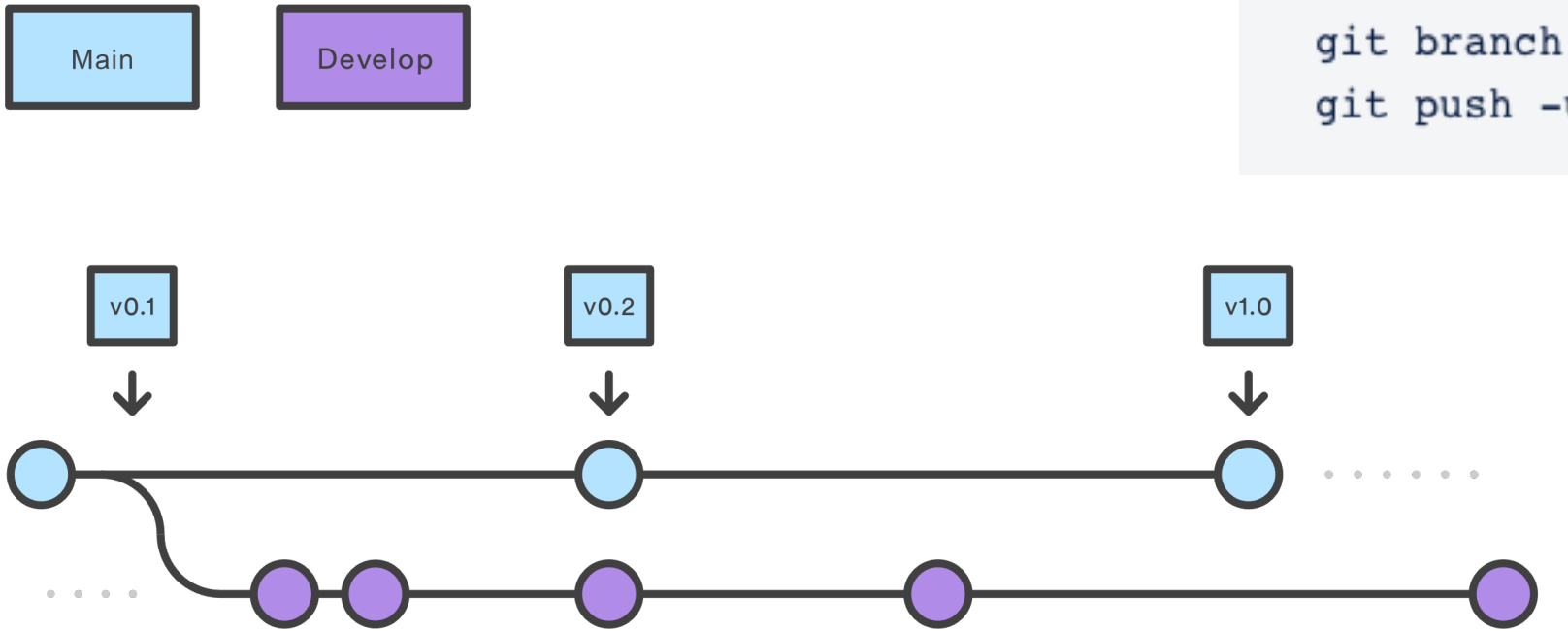
- Maintaining a history of changes.
- Enabling collaboration via branching and merging.
- Allowing **rollbacks** to any previous state.

Git & GitHub

- Git is a piece of free software living on your computer, where you develop/write code

- GitHub (and others) are remote (web) repositories that collect your code and organize your work lines according to the rules of Git

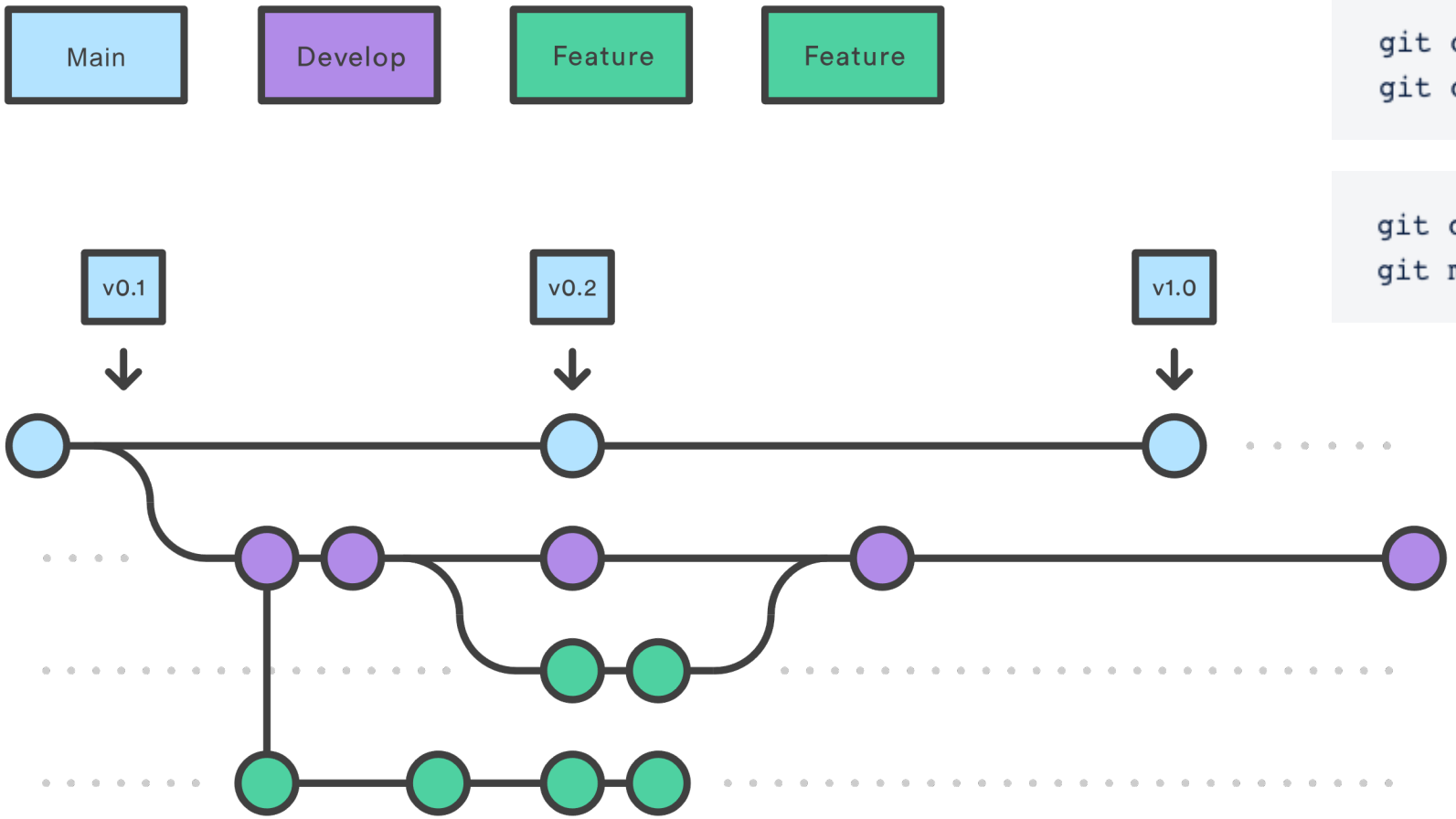
Branches: different worklines




```
git branch develop
git push -u origin develop
```

Credits: Atlassian, https://www.atlassian.com/it/git/tutorials/comparing-workflows/

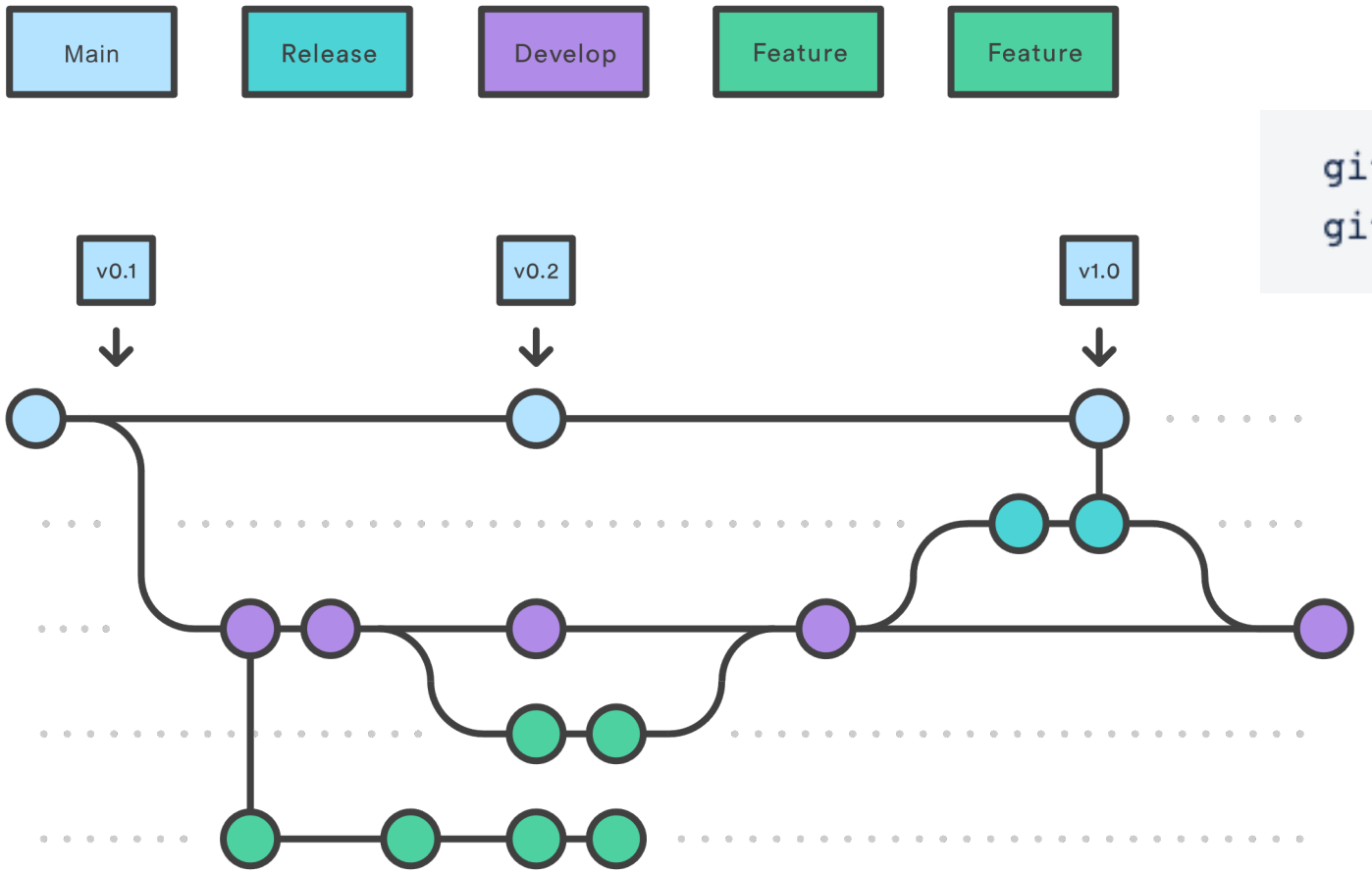
More features branches




```
git checkout develop
git checkout -b feature_branch
```

```
git checkout develop
git merge feature_branch
```

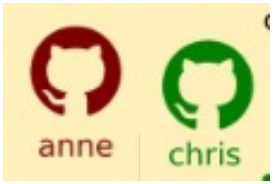
Release




```
git checkout develop
git checkout -b release/0.1.0
```

The actors in a collaboration

Colleagues in a lab



A collaborator in another lab

All the others

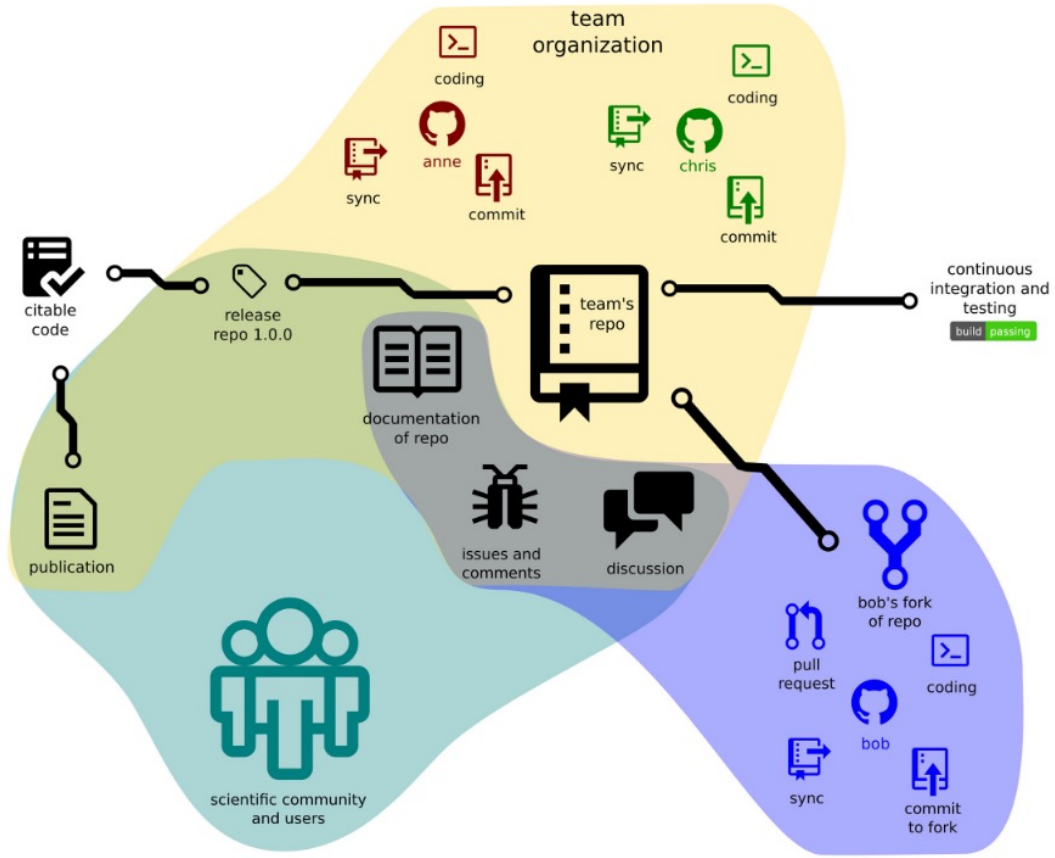


Fig 1. The structure of a GitHub-based project illustrating project structure and interactions with the community.

doi:10.1371/journal.pcbi.1004947.g001

PLOS COMPUTATIONAL BIOLOGY

EDITORIAL

Ten Simple Rules for Taking Advantage of Git and GitHub

Yasset Perez-Riverol[1]*, Laurent Gatto[2], Rui Wang[1], Timo Sachsenberg[3], Julian Uszkoreit[4], Felipe da Veiga Leprevost[5], Christian Fufezan[6], Tobias Ternent[1], Stephen J. Eglen[7], Daniel S. Katz[8], Tom J. Pollard[9], Alexander Konovalov[10], Robert M. Flight[11], Kai Blin[12], Juan Antonio Vizcaíno[1]*

Ten simple rules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- Rule 1: Use GitHub to Track Your Projects
- Rule 2: GitHub for Single Users, Teams, and Organizations
- Rule 3: Developing and Collaborating on New Features: Branching and Forking
- Rule 4: Naming Branches and Commits: Tags and Semantic Versions
- Rule 5: Let GitHub Do Some Tasks for You: Integrate
- Rule 6: Let GitHub Do More Tasks for You: Automate
- Rule 7: Use GitHub to Openly and Collaboratively Discuss, Address, and Close Issues
- Rule 8: Make Your Code Easily Citable, and Cite Source Code!
- Rule 9: Promote and Discuss Your Projects: Web Page and More
- Rule 10: Use GitHub to Be Social: Follow and Watch

Ten simple rules


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- Rule 10: Use GitHub to Be Social: Follow and Watch

“Acta est fabula plaudite”

Svetonio

(The play has been performed; applaud!)

https://www.latin-is-simple.com/en/vocabulary/phrase/40/

Credits & References

- *Code picture created using: https://carbon.now.sh/*
- *Conda description from: https://anaconda.org/anaconda/conda*
- *Miniforge3 installing code from: https://github.com/conda-forge/miniforge*
- *Jupyter official documentation: https://jupyterlab.readthedocs.io/en/latest/# and https://jupyter-notebook.readthedocs.io/en/latest/*
- *Apptainer official documentation: https://apptainer.org/docs/user/latest/introduction.html*