



# Reproducibility: an old friend, the laboratory notebook

Better reproducibility with documented code



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UNIVERSITÉ Clermont @uvergne







# Sommaire

- 1 The laboratory notebook
  - The aim

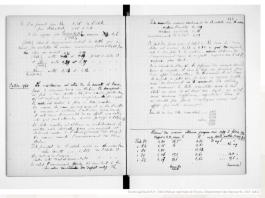
2 Notebook in bioinformatic

- 3 Practicial training
  - Build your own documentation

#### Laboratory notebook allow to:

■ Day-to-day recording each step in a process, experiments...





- Day-to-day recording each step in a process, experiments...
- Report on the progress, and scientific experimentations from the idea to final conclusions.

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- Report on the progress, and scientific experimentations from the idea to final conclusions.
- Keep track of knowledge in a lab
- Useful drafting a patent
- Proof of anteriority







This is a legal tool:

■ Page numbered in each notebook



- Page numbered in each notebook
- Cover page with the owner of the results



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- Each page contain a part to date, to sign for at least to people



At each research level:

# Paper version

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#### At each research level:

Researchers



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- Engineers

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- Researchers
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- Technicians

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- Researchers
- Engineers
- Technicians
- Students...

End what's happen for bioinformatic?

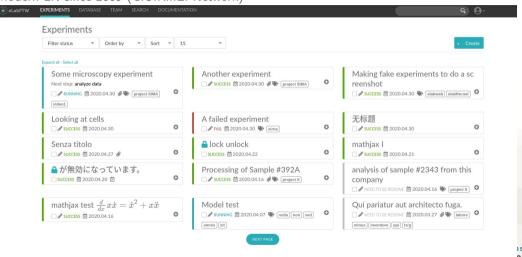


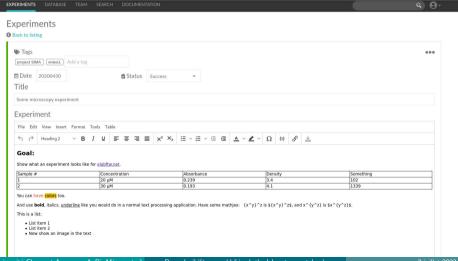


Electronic Laboratory Notebooks (ELN)

Modern LN since 2009 (C.U.R.I.E. Network)







- dematerialised
- archivable
- sharable
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But less and less adapted to recent evolutions of our work We need an electronic tool for individual traceability







Accueil > Bibliothèque de la science ouverte > Rapport du Groupe de travail sur les Cahiers de Laboratoire électroniques



Le rapport du groupe de travail « Cahier de laboratoire électronique » (ELN) présente une vision partagée sur la définition, le cadrage, les usages et le périmètre fonctionnel de l'ELN, qui doit pouvoir s'intégrer dans les environnements informatiques et institutionnels existants. Il émet un ensemble de recommandations sur les critères de choix d'un outil et intègre une liste comparative d'outils existants.

# Calendrier du projet











Janvier 2021

#### Mise en œuvre de la stratégie adoptée

- Mise en œuvre de la procédure d'achat (licences, etc.)
- Cahier des charges de la solution à Mars-Juillet développer

2021

Mise à disposition de ou des solutions sélectionnées

- Outils déployés sous licences CNRS
- Solution électronique développée en interne

I anvier 2022 \_ J uin 2023

Cabler de laboratoire électronique

17.11.20



What is literate programming?

<sup>1.</sup> Donald E. Knuth, Literate Programming, 1984

<sup>.</sup> https://en.wikipedia.org/wiki/Literate programming#Workflow

What is literate programming?

"Let us change our traditional attitude to the construction of programs :

Instead of imagining that our main task is to instruct a computer what to do, let us concentrate rather on explaining to humans what we want the computer to do." 1



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"Literate programming is a programming paradigm introduced by Donald Knuth in which a computer

program is given an explanation of its logic in a natural language, such as English, interspersed with snippets of macros and traditional source code, from which compilable source code can be generated."

. https://en.wikipedia.org/wiki/Literate\_programming#Workflow



<sup>1.</sup> Donald E. Knuth, Literate Programming, 1984

What does it look like?





#### This is an example title

I can add more infos about my code to explain to other users and aslo to rememb is doing

- · Cell with text to give informations
- · Cell with code to view what's happen
- · plot are also present in the output
- You can export the raw file in jupyter format but also in pdf. word, tex

#### Subtitle for configuration import

```
In [1]: import numpy as no
        import matplotlib.pyplot as plt
        %matplotlib inline
```

return vfit

#### Subtitle for my first plot

```
In [2]: def gaussian(x, a, b, c):
             return a * np.exp(-b * (x-c)**2)
        def noisy gaussian():
            # gaussian array v in interval -5 \le x \le 5
            nx = 100
            x = np.linspace(-5.0, 5.0, nx)
            v = gaussian(x, a=2.0, b=0.5, c=1.5)
            noise = np.random.normal(0.0, 0.2, nx)
            v += noise
            return x. v
        def fit(x, y, n):
            pfit = np.polyfit(x, y, n)
            vfit = np.polvval(pfit, x)
```

What does it look like? Interactive programming interface allowing to combine both natural and computer languages



What does it look like?
Interactive programming interface allowing to combine both natural and computer languages

- Explanation
- Code

In one file

- Results
- Graphs and plots



Why using literate programming frameworks?

Labbook



Why using literate programming frameworks?

- Labbook
- Day-to-day analysis

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- Day-to-day analysis
- Make automatic reports



Why using literate programming frameworks?

- Labbook
- Day-to-day analysis
- Make automatic reports
- Write scientific article



# Literate programming

Example of an article written using a notebook

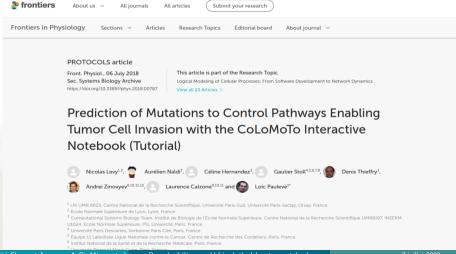


example



#### example





# Markup

A markup language uses tags to define elements within a document.

Three different types and usage :



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Presentational (used by traditional word-processing systems)

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Three different types and usage:

- Presentational (used by traditional word-processing systems)
- Procedural, provides instructions to process the text (e.g. TeX, PostScript)
- Descriptive, to label documents parts (e.g. LaTeX, HTML, XML...)

Markdown is a Lightweight markup language Designed to be :



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```
# Heading level 1
## Heading level 2
### Heading level 3
**Bold text**
*Italic*
~~strikethrough text~~
A [link](http://www.example.com)
Item list
    - one point
        - a subpoint
    - another point
    - last point
```



Markdown is a Lightweight markup language Designed to be :

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Used on Github to make the README.md
But how is this useful for literate programming?
When you want to weave both code (to be interpreted) and formatting information, you precisely need a lightweight language for the formatting part.



### R notebooks vs Jupyter(Lab) notebook





### R notebook

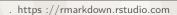
Sweave in 2002 Leisch, Friedrich (2002). "Sweave, Part I: Mixing R and LaTeX: A short introduction to the Sweave file format and corresponding R functions"

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- 2 knitR in 2011

"The knitr package was designed to be a transparent engine for dynamic report generation with R, solve some long-standing problems in Sweave, and combine features in other add-on packages into one package"

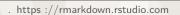
2012 Rmarkdown was born!





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When you run render, R Markdown feeds the .Rmd file to knitr, which executes all of the code chunks." and creates a new markdown (.md) document which includes the code and its output. The markdown file generated by knitR is then processed by pandoc which is responsible for creating the finished format."

. https://rmarkdown.rstudio.com



```
covid lineage analysis 3.5.3.Rmd* >
         ■ Knit on Save ABC ■ Knit - *
Source Visual B I () Normal - 📒 📜 🔗 🔛 Format - Insert - Table -
                                                                                                                                        Configuration de l'analyse
                                                                                                                                        Paramètres d'entrée de Covid-Seg depuis Basespace
                                                                                                                                        Import des données de la séquence S
                                                                                                                                        Création du jeu de données global
                                                                                                                                        Liste des mutations de reference des clades
                                                                                                                                        Analyse des patients et des contrôles
      author:
                                                                                                                                        Analyse des mutations dans S
                                                                                                                                        Rendu des résultats pour *GLIMS*
                                                                                                                                        Rendu des résultats pour *GISAID*
      output:
         rmdformats::readthedown
      editor options:
         chunk output type: console
   16 - # Configuration de l'analyse
                                                                                                                           8 ₹ 1
   18 # chemin absolu vers les fichiers, scripts de l'application
   19 lineage analysis dir <- "/home/pierre/Seafile/Seafile/lineage analysis/"
  20 #Sys.seteny(params = lineage analysis dir)
  21 source(paste0(lineage analysis dir."/conf R/initialize lineage.txt"))
  22 confR <- list.files(path = lineage analysis dir.pattern = conf lineage.full.names = T.recursive = T)</pre>
  23 # chargement du code R de configuration
  24 source(confR)
   25 # export for bash chunk the path of ANALYSE
  26 Sys.setenv(ANALYSE = ANALYSE)
   30 `r kable(config files input.col.names = "".caption = "Liste des fichiers de configurations")
```



#### Import des données de la séquence S

Nombre de séquences trouvées dans le fichier fasta depuis basespace : 93 Nombre de séquences trouvées dans le fichier fasta aligné via Nextclade : 93

#### Création du jeu de données global

Le fichier de fusion des données contient 96 entrées

#### Liste des mutations de reference des clades



RSITÉ

1 2011 : IPython (interactive Python shell) with notebook functionalities

. https://jupyter.org/

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  - "Jupyter will always be 100% open-source software, free for all to use and released under the liberal terms of the modified BSD license"
  - A reference to the three core programming languages supported by Jupyter (Julia, Python and R)



7 juillet 2023

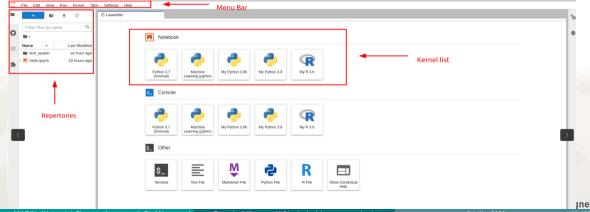
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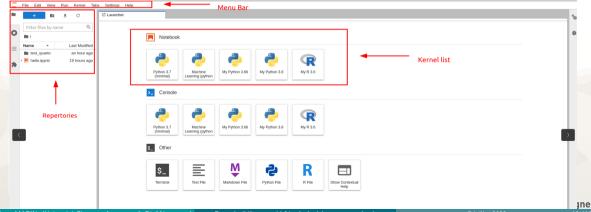
Web-based interactive computational environment

■ Web-based : client/server



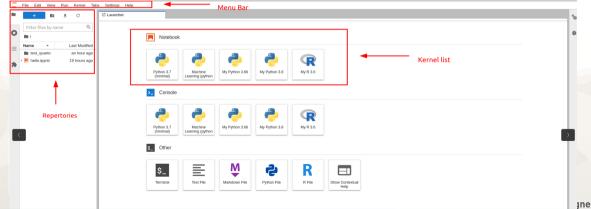
#### What is it exactly?

- Web-based : client/server
- Interactive : notebook system

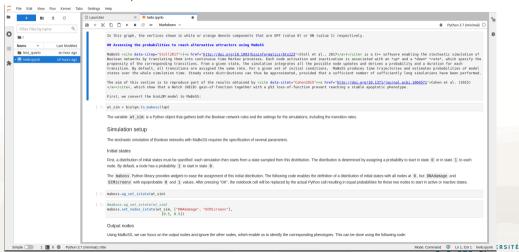


#### What is it exactly?

- Web-based : client/server
- Interactive : notebook system
- Computational environment : console, many kernels available...



### What is it exactly?



### PRACTICE

- Jupyter training link
- Rmarkdown training link

