



Reproducibility: an old friend, the laboratory notebook Better reproducibility with documented code



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23 novembre 2022



UNIVERSITÉ Clermont @uvergne





Sommaire

- 1 The laboratory notebook
 - The aim

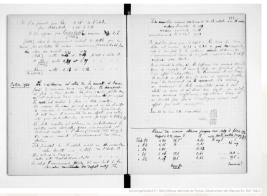
2 Notebook in bioinformatic

- 3 Practicial training
 - Build your own documentation

Laboratory notebook allow to:

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





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- Report on the progress, and scientific experimentations from the idea to final conclusions.

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- Keep track of knowledge in a lab
- Useful drafting a patent
- Proof of anteriority





This is a legal tool:



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■ Page numbered in each notebook



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- Cover page with the owner of the results



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At each research level :

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At each research level:

Researchers



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At each research level:

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- Engineers

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At each research level:

- Researchers
- Engineers
- Technicians
- Students...

End what's happen for bioinformatic?

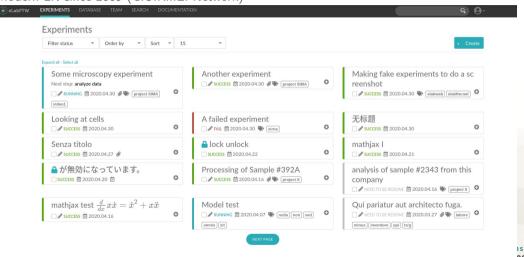


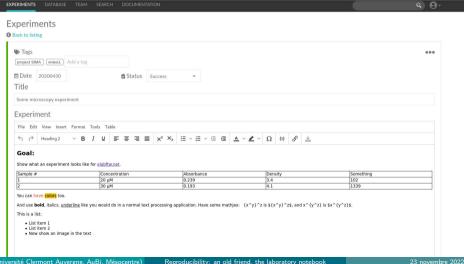


Electronic Laboratory Notebooks (ELN)

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







- dematerialised
- archivable
- sharable
- secure



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







ice! LA SC

OUVERTE NOS AC

ACTIONS RESSOU

CES A

QUI SOMMES N

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?



^{1.} Donald E. Knuth, Literate Programming, 1984 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

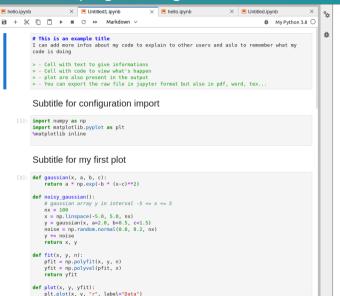


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^{1.} Donald E. Knuth, Literate Programming, 1984

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 In one file

- Explanation
- Code
- Results
- Graphs and plots

Why using literate programming frameworks?

Labbook



Why using literate programming frameworks?

- Labbook
- Day-to-day analysis



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- Labbook
- Day-to-day analysis
- Make automatic reports



Why using literate programming frameworks?

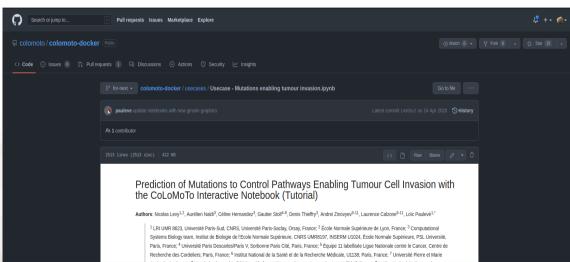
- Labbook
- Day-to-day analysis
- Make automatic reports
- Write scientific article

Literate programming

Example of an article written using a notebook



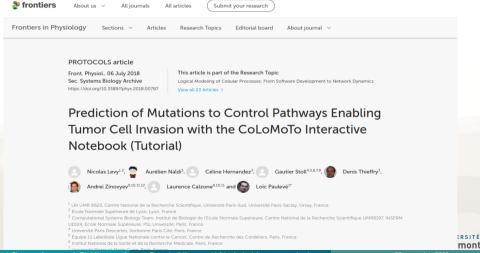
example



example



example



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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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"

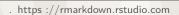
R notebook

- 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"
- 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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. https://rmarkdown.rstudio.com

2012 Rmarkdown was born!



"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(pasteO(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

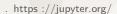
Le fichier de fusion des données contient 96 entrées

Liste des mutations de reference des clades

Copy	Excel PDF	Print Show 10 v entries Search:
ableau des mutations de références utilisées pour l'analyse des variants		
scorpio_clade 0	lineage.ref	synonymous_mutation_ref
All	A	All
20A.EU2	B.1.160	C4543T,G5629T,C11497T,T26876C
20A/S:126A	B.1.620	C241T,C3037T,C15324T,T20049C,A23416T,T27795-,T27796-,A27797-,A28271T
20A/S:439K	B.1.258	C8047T
20A/S:98F	B.1.221	C28651T
20B/S:1122L	B.1.1.302	
20B/S:626S	B.1.1.277	
20B/S:732A	B.1.1.519	C203T,C222T,C241T,C3037T,C10954T,T19839C,C21306T,C29197T
20C/S:80Y	B.1.367	G4960T.C6070T.C7303T.C7564T.C10279T.C10525T.C10582T.C27804T

ERSITÉ

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



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- 2 2014 : Spin-off project called Project Jupyter a non-profit, open-source project maintained by a strong community

. https://jupyter.org/

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- 1 2011 : IPython (interactive Python shell) with notebook functionalities
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 - A reference to the three core programming languages supported by Jupyter (Julia, Python and R)





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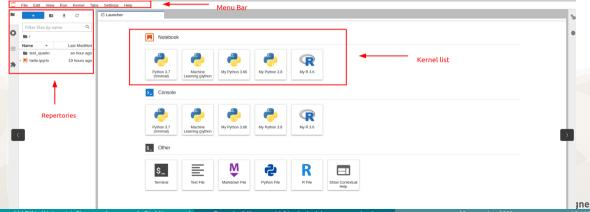
What is it exactly?



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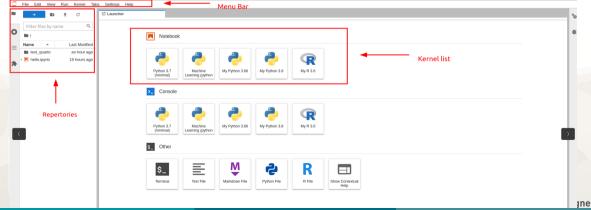
Web-based interactive computational environment

■ Web-based : client/server



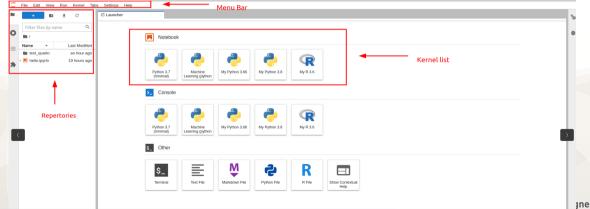
What is it exactly?

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

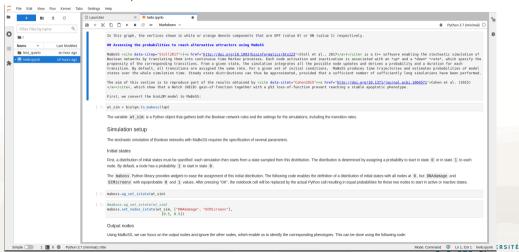


What is it exactly?

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



What is it exactly?



PRACTICE

- Jupyter training link
- Rmarkdown training link

