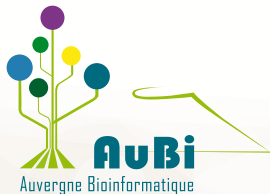


Reproducibility: an old friend, the laboratory notebook

Better reproducibility with documented code



P. Marin, M. Hiriart, P. Ruiz & N. Goué
aubi@uca.fr

Université Clermont Auvergne, AuBi, Mésocentre

4 juillet 2023

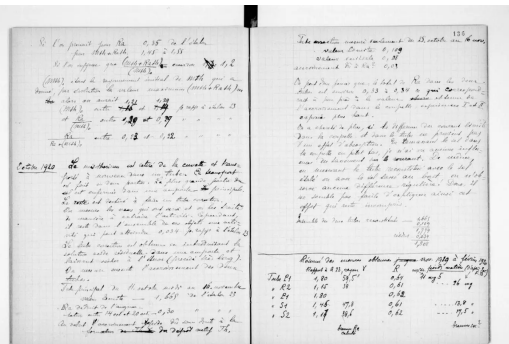


. This work is derived from the IFB and I2BC team members

Paper version

Laboratory notebook allow to :

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



Source gallica.bnf.fr / Bibliothèque nationale de France. Département des Manuscrits, NAF 18422

Paper version

Laboratory notebook allow to :

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

Paper version

Laboratory notebook allow to :

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- Keep track of knowledge in a lab

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- Useful drafting a patent

Paper version

Laboratory notebook allow to :

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

Paper version

Paper version

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 :

Paper version

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At each research level :

- Researchers

Paper version

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At each research level :

- Researchers
- Engineers

Paper version

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- Cover page with the owner of the results
- Each page contain a part to date, to sign for at least to people

At each research level :

- Researchers
- Engineers
- Technicians

Paper version

This is a legal tool :

- Page numbered in each notebook
- Cover page with the owner of the results
- Each page contain a part to date, to sign for at least to people

At each research level :

- Researchers
- Engineers
- Technicians
- Students...

End what's happen for bioinformatic ?

Electronic version

Electronic Laboratory Notebooks (ELN)
Modern LN since 2009 (C.U.R.I.E. Network)

Electronic version

Electronic Laboratory Notebooks (ELN)

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



eLabFTW

Electronic version

Electronic Laboratory Notebooks (ELN) Modern LN since 2009 (C.U.R.I.E. Network)

eLabFTW EXPERIMENTS DATABASE TEAM SEARCH DOCUMENTATION

Experiments

Filter status Order by Sort 15 Create

Expand all - Select all

<p>Some microscopy experiment</p> <p>Next step: analyze data</p> <p><input type="checkbox"/> RUNNING 2020.04.30 project SIMA</p> <p>video1</p>	<p>Another experiment</p> <p><input type="checkbox"/> SUCCESS 2020.04.30 project SIMA</p>	<p>Making fake experiments to do a screenshot</p> <p><input type="checkbox"/> SUCCESS 2020.04.30 elabweb elabftw.net</p>
<p>Looking at cells</p> <p><input type="checkbox"/> SUCCESS 2020.04.30</p>	<p>A failed experiment</p> <p><input type="checkbox"/> FAIL 2020.04.30 sirna</p>	<p>无标题</p> <p><input type="checkbox"/> SUCCESS 2020.04.30</p>
<p>Senza titolo</p> <p><input type="checkbox"/> SUCCESS 2020.04.27 </p>	<p>lock unlock</p> <p><input type="checkbox"/> SUCCESS 2020.04.22</p>	<p>mathjax I</p> <p><input type="checkbox"/> SUCCESS 2020.04.21</p>
<p>が無効になっています。</p> <p><input type="checkbox"/> SUCCESS 2020.04.20 </p>	<p>Processing of Sample #392A</p> <p><input type="checkbox"/> SUCCESS 2020.04.16 project X</p>	<p>analysis of sample #2343 from this company</p> <p><input type="checkbox"/> NEED TO BE REDONE 2020.04.16 project X</p>
<p>mathjax test $\frac{d}{dx} x\dot{x} = \dot{x}^2 + x\ddot{x}$</p> <p><input type="checkbox"/> SUCCESS 2020.04.16</p>	<p>Model test</p> <p><input type="checkbox"/> RUNNING 2020.04.07 nulla non sed</p> <p>omnis sit</p>	<p>Qui pariatur aut architecto fuga.</p> <p><input type="checkbox"/> NEED TO BE REDONE 2020.03.27 labore</p> <p>minus inventore qui ta'g</p>

NEXT PAGE

Electronic version

Electronic Laboratory Notebooks (ELN)
Modern LN since 2009 (C.U.R.I.E. Network)



Experiments

[← Back to listing](#)

Tags

project SIMA

video1

Add a tag

Date

20200430

Status

Success

Title

Some microscopy experiment

Experiment

FileEditViewInsertFormatToolsTable

<>

Heading 2

B I U

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Goal:

Show what an experiment looks like for [glabftw.net](#).

Sample #	Concentration	Absorbance	Density	Something
1	20 μM	0.239	3.4	102
2	30 μM	0.193	4.1	1339

You can have colors too.

And use bold, italics, underline like you would do in a normal text processing application. Have some mathjax: {x^y}^z is \${x^y}^z\$, and x^{y^z} is \$x^{y^z}\$.

This is a list:

- List item 1
- List item 2
- Now show an image in the text

Electronic version

Electronic Laboratory Notebooks (ELN)
Modern LN since 2009 (C.U.R.I.E. Network)

- dematerialised
- archivable
- sharable
- secure

Electronic version

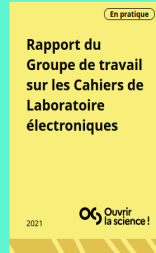
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But less and less adapted to recent evolutions of our work
We need an electronic tool for individual traceability

Electronic version

[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.

Electronic version

Calendrier du projet



Note de synthèse

- Caractéristiques techniques souhaitées
- Inventaire des solutions existantes sur le marché

J 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 développer

Mars-J uillet 2021

Mise à disposition de ou des solutions sélectionnées

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

J janvier 2022
– J uin 2023



Cahier de laboratoire électronique 17.11.20 PR96



UNIVERSITÉ
Clermont Auvergne

Literate programming

What is literate programming ?

-
1. Donald E. Knuth, Literate Programming, 1984
. https://en.wikipedia.org/wiki/Literate_programming#Workflow

Literate programming

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."

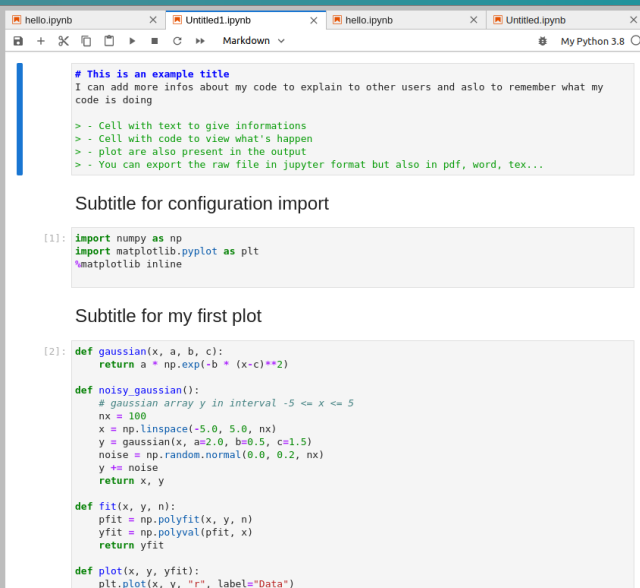
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Literate programming

What does it look like ?

Literate programming



hello.ipynb x Untitled1.ipynb x hello.ipynb x Untitled.ipynb x

My Python 3.8

This is an example title

I can add more infos about my code to explain to other users and aslo to remember what my code 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

```
[1]: import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
```

Subtitle for my first plot

```
[2]: def gaussian(x, a, b, c):
    return a * np.exp(-b * (x-c)**2)

def noisy_gaussian():
    # gaussian array y in interval -5 <= x <= 5
    nx = 100
    x = np.linspace(-5.0, 5.0, nx)
    y = gaussian(x, a=2.0, b=0.5, c=1.5)
    noise = np.random.normal(0.0, 0.2, nx)
    y += noise
    return x, y

def fit(x, y, n):
    pfit = np.polyfit(x, y, n)
    yfit = np.polyval(pfit, x)
    return yfit

def plot(x, y, yfit):
    plt.plot(x, y, "r", label="Data")
```

This is an example title

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Literate programming

What does it look like ?

Interactive programming interface allowing to combine both natural and computer languages

Literate programming

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

Literate programming

Why using literate programming frameworks ?

- Labbook

Literate programming

Why using literate programming frameworks ?

- Labbook
- Day-to-day analysis

Literate programming

Why using literate programming frameworks ?

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

Literate programming

Why using literate programming frameworks ?

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

Literate programming

example

Example of an article written using a notebook

. <https://www.frontiersin.org/articles/10.3389/fphys.2018.00787/full>

Literate programming

example

The screenshot shows the GitHub interface for the repository 'colomoto / colomoto-docker'. The repository is public and has 6 watchers, 6 forks, and 15 stars. The main content area displays a Jupyter Notebook file named 'Usecase - Mutations enabling tumour invasion.ipynb' by user 'pauleve'. The notebook has 2513 lines (2513 sloc) and is 422 KB in size. The notebook's title is 'Prediction of Mutations to Control Pathways Enabling Tumour Cell Invasion with the CoLoMoTo Interactive Notebook (Tutorial)'. The authors listed are Nicolas Levy^{1,2}, Aurélien Naldi³, Céline Hernandez³, Gautier Stoll⁴⁻⁶, Denis Thieffry³, Andrei Zinoviyev⁸⁻¹¹, Laurence Calzone⁹⁻¹¹, and Loïc Paulevé^{1,7}. The repository also shows a commit history and a list of contributors.

colomoto / colomoto-docker (Public)

Watch 6 Fork 6 Star 15

Code Issues 9 Pull requests 1 Discussions Actions Security Insights

for-next colomoto-docker / usecases / Usecase - Mutations enabling tumour invasion.ipynb Go to file

pauleve update notebooks with new ginsim graphics Latest commit 14905c2 on 24 Apr 2020 History

1 contributor

2513 lines (2513 sloc) 422 KB

Prediction of Mutations to Control Pathways Enabling Tumour Cell Invasion with the CoLoMoTo Interactive Notebook (Tutorial)

Authors: Nicolas Levy^{1,2}, Aurélien Naldi³, Céline Hernandez³, Gautier Stoll⁴⁻⁶, Denis Thieffry³, Andrei Zinoviyev⁸⁻¹¹, Laurence Calzone⁹⁻¹¹, Loïc Paulevé^{1,7}

¹ LRI UMR 8623, Université Paris-Sud, CNRS, Université Paris-Saclay, Orsay, France; ² École Normale Supérieure de Lyon, France; ³ Computational Systems Biology team, Institut de Biologie de l'École Normale Supérieure, CNRS UMR8197, INSERM U1024, École Normale Supérieure, PSL Université, Paris, France; ⁴ Université Paris Descartes/Paris V, Sorbonne Paris Cité, Paris, France; ⁵ Équipe 11 labellisée Ligue Nationale contre le Cancer, Centre de Recherche des Cordeliers, Paris, France; ⁶ Institut National de la Santé et de la Recherche Médicale, U1138; Paris, France; ⁷ Université Pierre et Marie

Literate programming

example



File Edit View Run Kernel Tabs Settings Help

Filter files by name

Name	Last Modified
test_quarto	7 hours ago
hello.ipynb	a minute ago

Prediction of Mutations to Control Pathways Enabling Tumour Cell Invasion with the CoLoMoTo Interactive Notebook (Tutorial)

Authors: Nicolas Levy^{1,2}, Aurélien Naldi³, Céline Hernandez³, Gautier Stoll⁴⁻⁸, Denis Thieffry³, Andrei Zinovyev⁹⁻¹¹, Laurence Calzone⁹⁻¹¹, Loïc Paulevé^{1,*}

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Abstract

Boolean and multi-valued logical formalisms are increasingly used to model complex cellular networks. To ease the development and analysis of logical models, a series of software tools have been proposed, often with specific assets. However, combining these tools typically implies a series of cumbersome software installation and model conversion steps. In this respect, the *CoLoMoTo Interactive Notebook* provides a joint distribution of several logical modelling software tools, along with an interactive web Python interface easing the chaining of complementary analyses.

Our computational workflow combines (1) the importation of a GiNsim model and its display, (2) its format conversion using the Java library BioLQM, (3) the formal prediction of mutations using the OCaml software Pint, (4) the model checking using the C++ software NuSMV, (5) quantitative stochastic simulations using the C++ software MaBoSS, and (6) the visualisation of results using the Python library matplotlib. We rely on the CoLoMoTo Interactive Notebook to provide a thoroughly documented and executable notebook of our computational analysis.

To illustrate our approach, we use a recent Boolean model of the signalling network controlling tumour cell invasion and migration. Our model analysis culminates with the prediction of sets of mutations presumably involved in a metastatic phenotype. Beyond the specific application considered here, the resulting Jupyter notebook constitutes a tutorial for the use and combination of several logical modelling tools, which can be easily adapted to analyse other models. Furthermore, the notebook web interface and the companion Docker distribution of logical modelling tools greatly facilitate the production of accessible and reproducible model analysis workflows.

Literate programming

example

The screenshot shows the Frontiers website interface. At the top, there's a navigation bar with the Frontiers logo, 'About us', 'All journals', 'All articles', and a 'Submit your research' button. Below this is a secondary navigation bar for 'Frontiers in Physiology' with links to 'Sections', 'Articles', 'Research Topics', 'Editorial board', and 'About journal'. The main content area features a 'PROTOCOLS article' section with the journal name 'Front. Physiol.', date '06 July 2018', and archive 'Sec. Systems Biology Archive'. It includes a DOI link and a link to 'View all 23 Articles'. The article title is 'Prediction of Mutations to Control Pathways Enabling Tumor Cell Invasion with the CoLoMoTo Interactive Notebook (Tutorial)'. The authors are listed with their profile pictures: Nicolas Levy, Aurélien Naldi, Céline Hernandez, Gautier Stoll, Denis Thieffry, Andrei Zinovyev, Laurence Calzone, and Loïc Paulevé. Below the authors are footnotes for their affiliations. The Frontiers logo is visible in the bottom right corner of the page.

frontiers

About us ▾ All journals All articles Submit your research

Frontiers in Physiology Sections ▾ Articles Research Topics Editorial board About journal ▾

PROTOCOLS article

Front. Physiol., 06 July 2018
Sec. Systems Biology Archive
<https://doi.org/10.3389/fphys.2018.00787>

This article is part of the Research Topic
Logical Modeling of Cellular Processes: From Software Development to Network Dynamics
[View all 23 Articles >](#)

Prediction of Mutations to Control Pathways Enabling Tumor Cell Invasion with the CoLoMoTo Interactive Notebook (Tutorial)

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⁷ Université Pierre et Marie Curie, Paris, France

FRONTIERS
mont Auvergne

Markup

A markup language uses tags to define elements within a document.
Three different types and usage :

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Three different types and usage :

- Presentational (used by traditional word-processing systems)

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Markup

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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

Markdown is a Lightweight markup language
Designed to be :



Markdown

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- easy to write using any generic text editor (plain-text-formatting syntax)



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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
```


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- easy to read in the raw format



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



vs



www.educba.com

R notebook

1 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

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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"

RMarkdown



2012 Rmarkdown was born !

. <https://rmarkdown.rstudio.com>

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RMarkdown

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."

RMarkdown

```

1 ---
2 title: |
3   <center> Rapport d'analyse séquençage NGS </center>
4   <center> Détection de variants SARS-CoV-2 </center>
5 author: |
6   <center> Service de Virologie </center>
7   <center> Laboratoire de Biologie du CHU de Clermont-Ferrand </center>
8
9 date: "r format(Sys.time(), '%d %B %Y')""
10 output:
11   rmdformats::readthedown|
12 editor_options:
13   chunk_output_type: console
14 ---
15
16 # Configuration de l'analyse
17 ```{r config, engine.opts='-l',echo=F}
18 # chemin absolu vers les fichiers, scripts de l'application
19 lineage_analysis_dir <- "/home/pierre/Seafle/Seafle/lineage_analysis/"
20 #Sys.setenv(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)
23 # chargement du code R de configuration
24 source(confR)
25 # export for bash chunk the path of ANALYSE
26 Sys.setenv(ANALYSE = ANALYSE)
27 ```
28
29 ```
30 `r kable(config_files_input,col.names = "",caption = "Liste des fichiers de configurations")`
  
```

Configuration de l'analyse
 Paramètres d'entrée de Covid-Seq depuis Basespace
 Import des données de la séquence S
 Création du jeu de données global
 Liste des mutations de référence des clades
 Analyse des patients et des contrôles
 Analyse des mutations dans S
 Rendu des résultats pour *GLIMS*
 Rendu des résultats pour *GISAID*

RMarkdown

Rapport d'analyse séquençage NGS Détection de variants SARS- CoV-2

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Rendu des résultats pour GISAIID



Service de Virologie
Laboratoire de Biologie du CHU de
Clermont-Ferrand

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 référence des clades

Copy

CSV

Excel

PDF

Print

Show

10

entries

Search:

Tableau des mutations de références utilisées pour l'analyse des variants

scorpio_clade	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

Jupyter

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

. <https://jupyter.org/>

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 - A reference to the three core programming languages supported by Jupyter (Julia, Python and R)

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Jupyter

What is it exactly ?

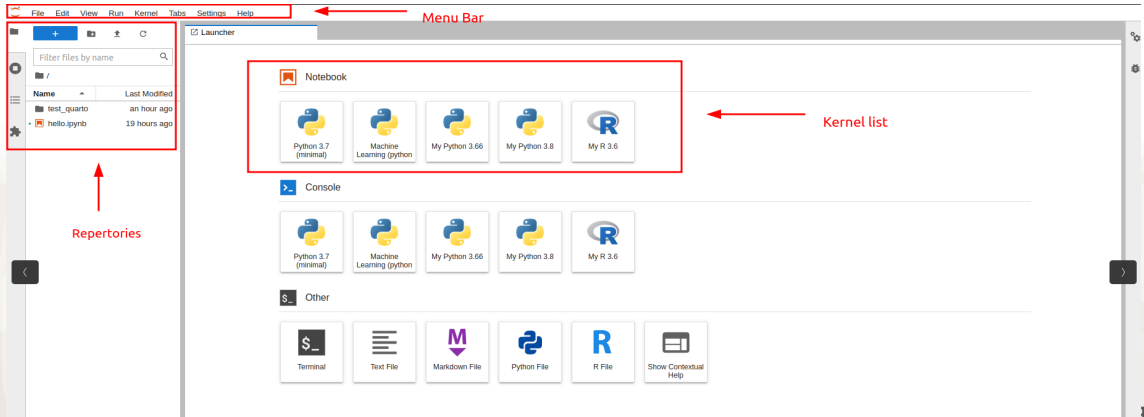
Web-based interactive computational environment

Jupyter

What is it exactly ?

Web-based interactive computational environment

- Web-based : client/server

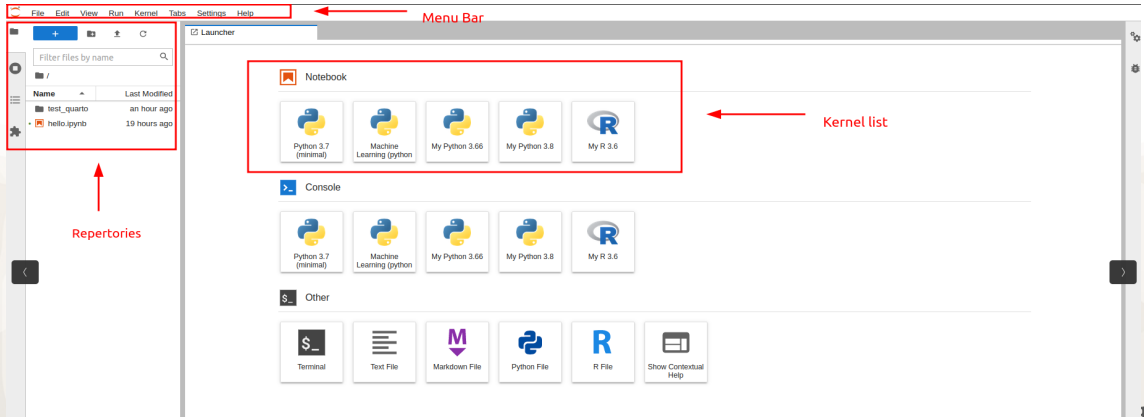


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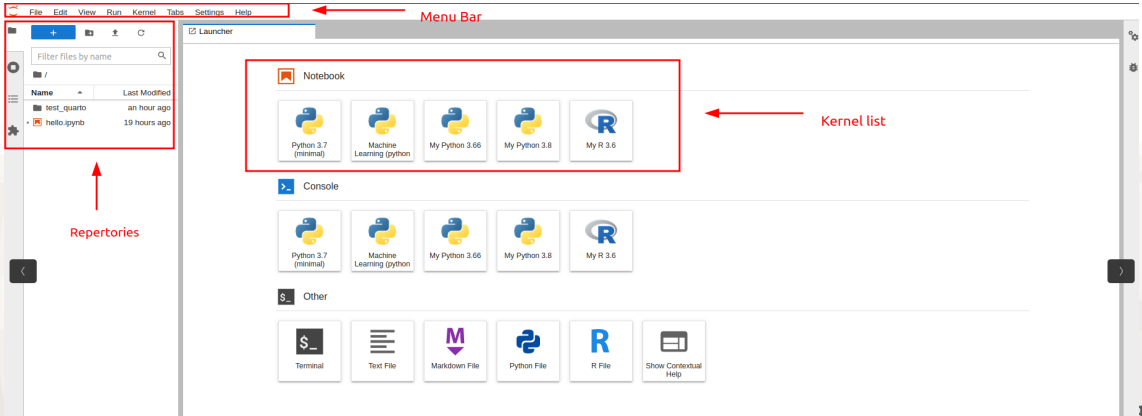


Jupyter

What is it exactly ?

Web-based interactive computational environment

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



Jupyter

What is it exactly ?

Web-based interactive computational environment

The screenshot displays the Jupyter Notebook web interface. On the left is a file browser sidebar with a search bar and a table of files:

Name	Last Modified
test_quarto	an hour ago
hello.ipynb	19 hours ago

The main area shows a notebook cell with the following content:

In this graph, the vertices shown in white or orange denote components that are OFF (value 0) or ON (value 1) respectively.

Assessing the probabilities to reach alternative attractors using MaBoSS

MaBoSS [Stoll2017](https://doi.org/10.1093/bioinformatics/btx123) is a C++ software enabling the stochastic simulation of Boolean networks by translating them into continuous time Markov processes. Each node activation and inactivation is associated with an "up" and a "down" rate, which specify the propensity of the corresponding transitions. From a given state, the simulation integrates all the possible node updates and derives a probability and a duration for each transition. By default, all transitions are assigned the same rate. For a given set of initial conditions, MaBoSS produces time trajectories and estimates probabilities of model states over the whole simulation time. Steady state distributions can thus be approximated, provided that a sufficient number of sufficiently long simulations have been performed.

The aim of this section is to reproduce part of the results obtained by [Cohen2015](https://doi.org/10.1371/journal.pcbi.1004571), which show that a Notch (NICD) gain-of-function together with a p53 loss-of-function prevent reaching a stable apoptotic phenotype.

First, we convert the bioQM model to MaBoSS:

```
[ ]: wt_sim = biolqm.to_maboss(lqm)
```

The variable `wt_sim` is a Python object that gathers both the Boolean network rules and the settings for the simulations, including the transition rates.

Simulation setup

The stochastic simulation of Boolean networks with MaBoSS requires the specification of several parameters.

Initial states

First, a distribution of initial states must be specified: each simulation then starts from a state sampled from this distribution. The distribution is determined by assigning a probability to start in state 0 or in state 1 to each node. By default, a node has a probability 1 to start in state 0.

The `maboss` Python library provides widgets to ease the assignment of this initial distribution. The following code enables the definition of a distribution of initial states with all nodes at 0, but `DNADamage` and `ECMicroenv` with equiprobable 0 and 1 values. After pressing "OK", the notebook cell will be replaced by the actual Python call resulting in equal probabilities for these two nodes to start in active or inactive states.

```
[ ]: maboss.wg_set_istate(wt_sim)

[ ]: #maboss.wg_set_istate(wt_sim)
maboss.set_nodes_istate(wt_sim, ["DNADamage", "ECMicroenv"],
                        [0.5, 0.5])
```

Output nodes

Using MaBoSS, we can focus on the output nodes and ignore the other nodes, which enable us to identify the corresponding phenotypes. This can be done using the following code:

PRACTICE

- Jupyter training link
- Rmarkdown training link