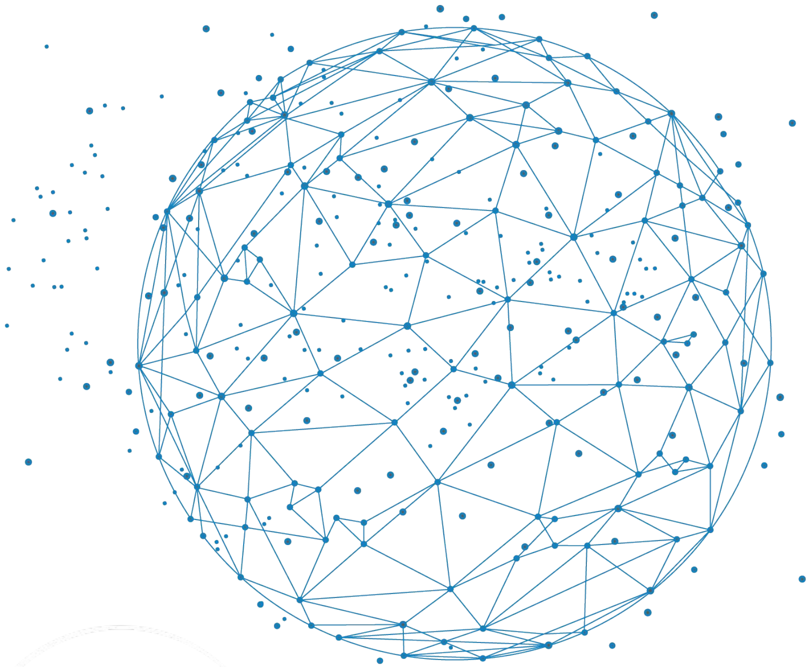
FAIR Bioinfo 2023

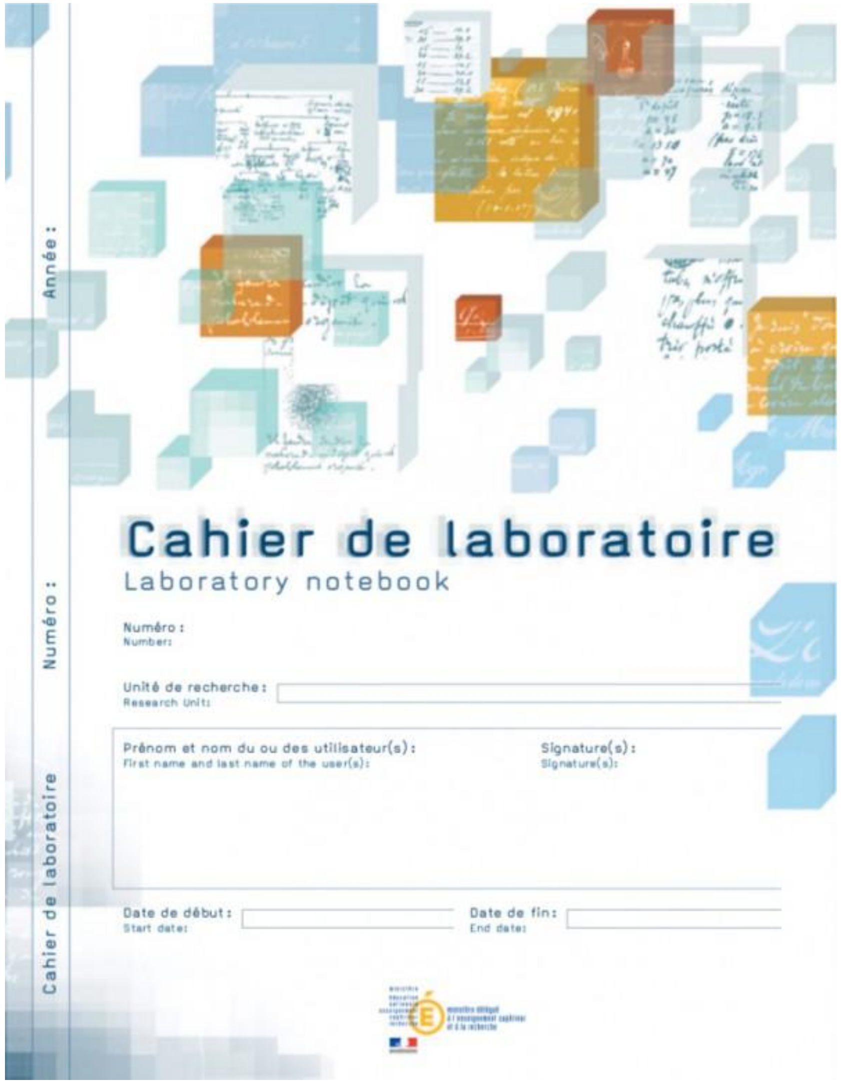


Usecase 1

Laboratory Notebooks

T. Denecker, IFB, https://orcid.org/0000-0003-1421-7641

What is this?



Année :

Numéro :

Cahier de laboratoire

Cahier de laboratoire

Laboratory notebook

Numéro :
Number:

Unité de recherche :
Research Unit:

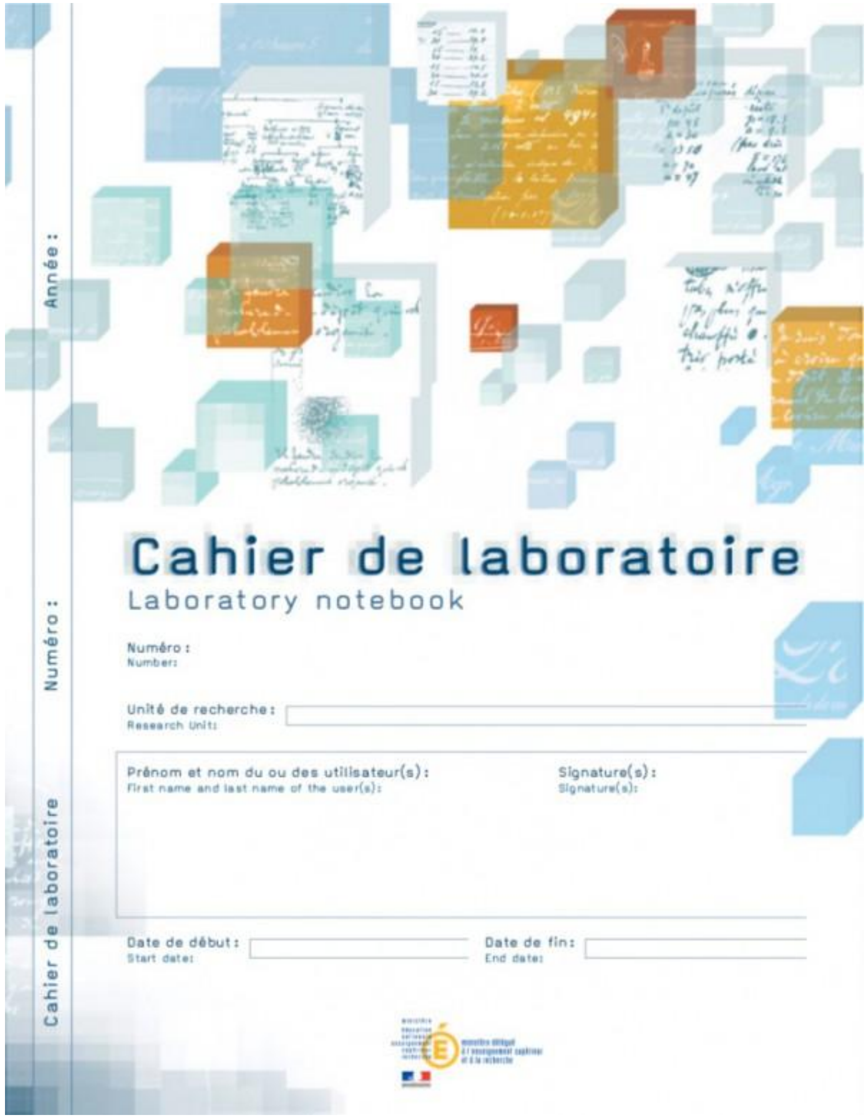
Prénom et nom du ou des utilisateur(s) :
First name and last name of the user(s):

Signature(s) :
Signature(s):

Date de début :
Start date:

Date de fin :
End date:

What is it for ?



Année :

Numéro :

Cahier de laboratoire

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Laboratory notebook

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Signature(s) :
Signature(s):

Date de début :
Start date:

Date de fin :
End date:

The laboratory notebook allows :

- day-to-day recording of the details of the work
- to report on the progress and scientific experimentation, from the idea to the conclusion
- to keep knowledge in a lab

Also very useful for drafting a patent or for proving anteriority.

What is it for ?

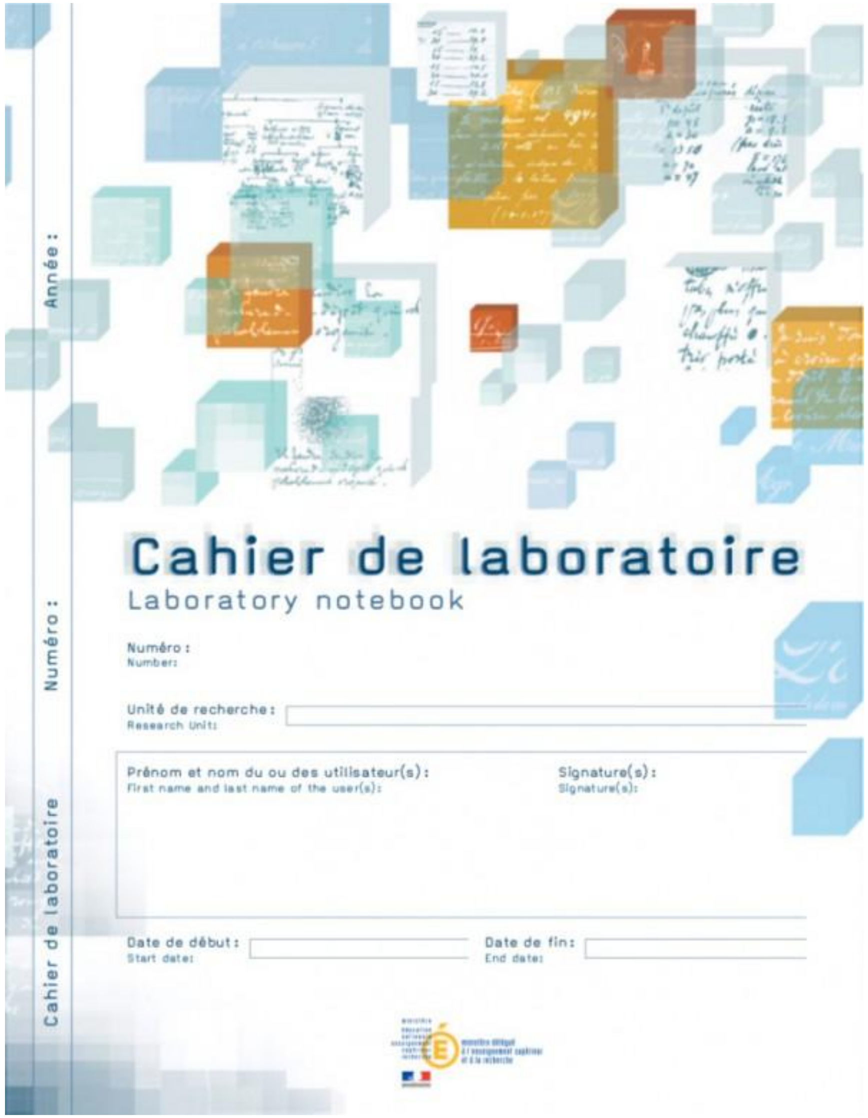
A legal tool :

- Each notebook and the pages are numbered.
- On the cover page, we find on each notebook the mentions of the owner of the results.
- Each page has two parts at the bottom intended to be dated and signed: two signatures = two people, user and third party (witness),
  - ideally a third party not involved in the research work but capable of understanding it

https://www.curie.asso.fr/-Cahier-de-laboratoire-national-.html

https://slideplayer.fr/slide/3817405/

What is it for ?



Année :

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Signature(s):

Date de début :
Start date:

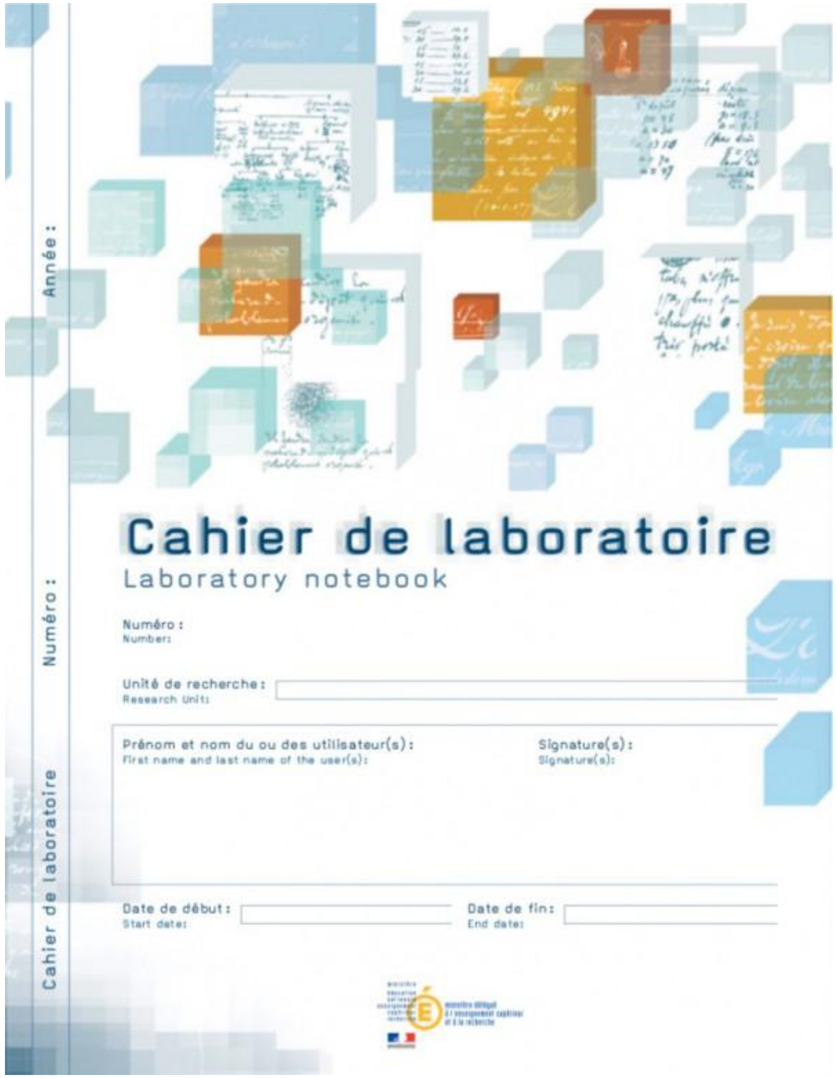
Date de fin :
End date:

For all those who carry out research work :

- researchers,
- engineers,
- technicians,
- doctoral students,
- trainees,
- etc.

And you ?

Are you using it ?



Année :

Numéro :

Cahier de laboratoire

Cahier de laboratoire

Laboratory notebook

Numéro :
Number:

Unité de recherche :
Research Unit:

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First name and last name of the user(s):

Signature(s) :
Signature(s):

Date de début :
Start date:

Date de fin :
End date:

Electronic Laboratory Notebooks (ELN)

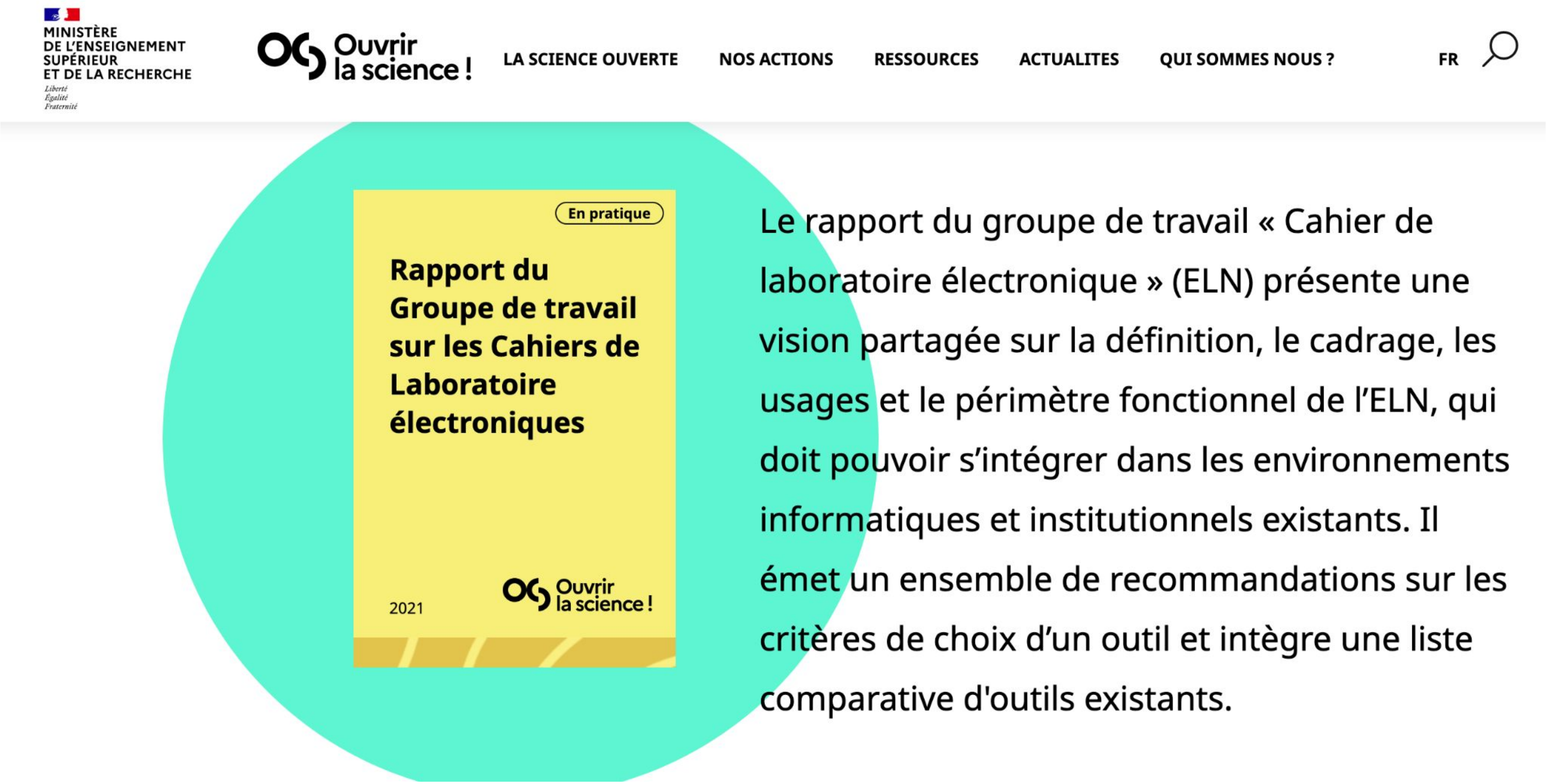
Modern LN since 2009 (C.U.R.I.E. Network)

But less and less adapted to recent evolutions of our work

- Increased data quantity
- Change in the nature of data
- Dematerialization
- Security

We need an electronic tool for individual traceability.

Electronic Laboratory Notebook



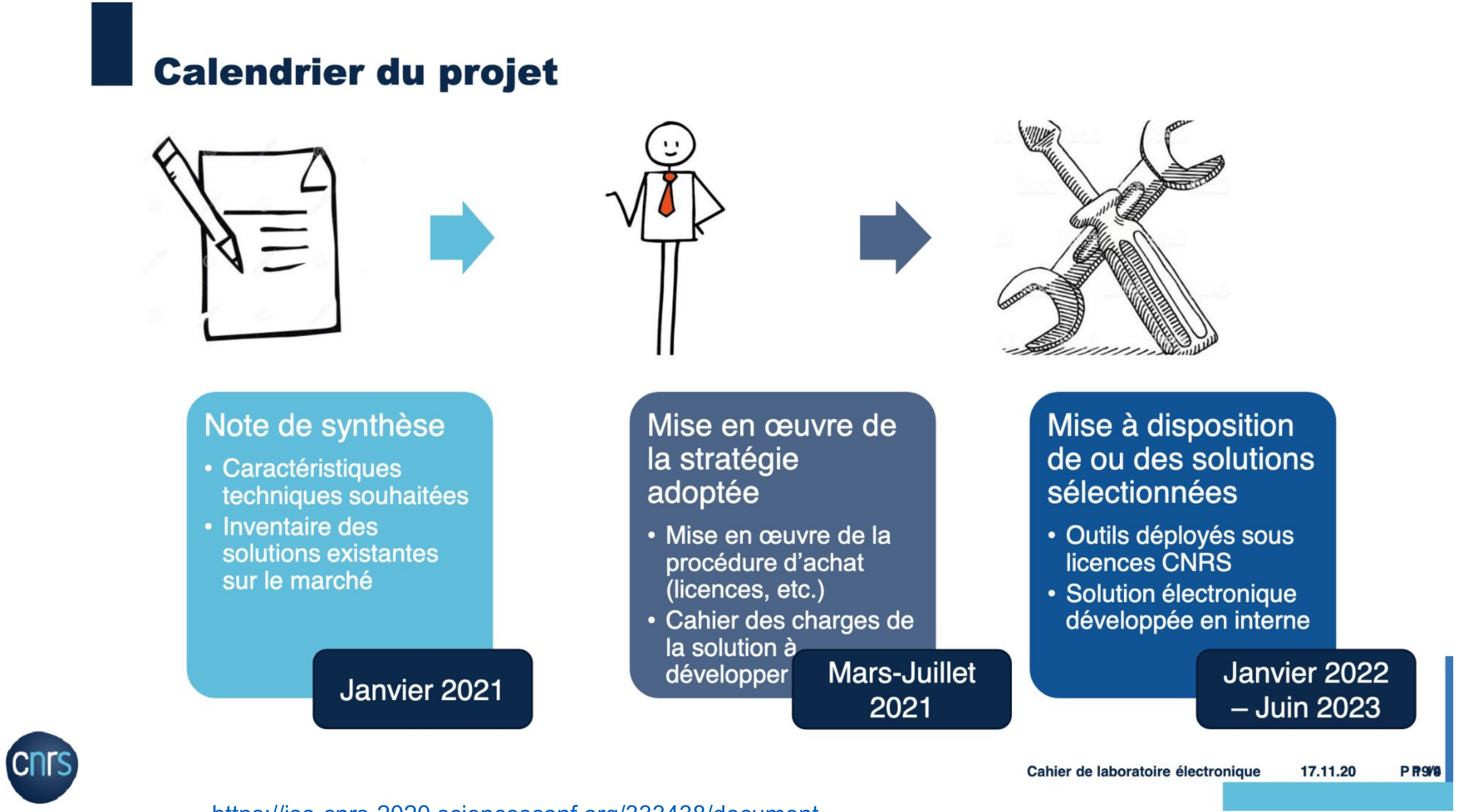
Rapport du Groupe de travail sur les Cahiers de Laboratoire électroniques

2021

Ouvrir la science !

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 Laboratory Notebook



Calendrier du projet

Note de synthèse
- Caractéristiques techniques souhaitées
- Inventaire des solutions existantes sur le marché

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-Juillet 2021

Mise à disposition de ou des solutions sélectionnées
- Outils déployés sous licences CNRS
- Solution électronique développée en interne

Janvier 2022 – Juin 2023

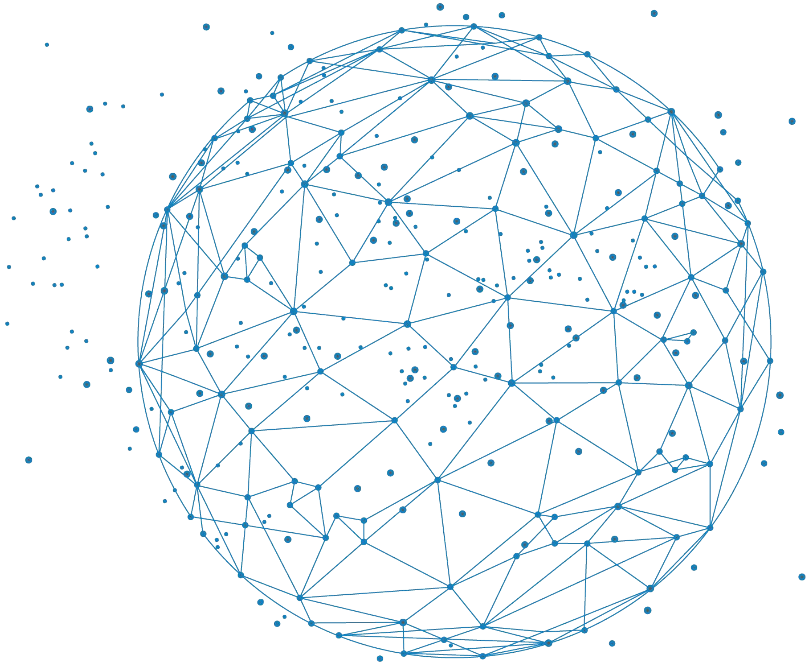
Cahier de laboratoire électronique 17.11.20 P R9/8

https://jso-cnrs-2020.sciencesconf.org/333438/document

This session

- Introduction to Laboratory Notebooks ✓
- Literate programming
- Markdown
- Notebooks for bioinformatics
  - R Notebooks (Rmarkdown)
  - Quarto
  - Jupyter(Lab)
- Practical session (JupyterLab)

Literate programming



Literate programming

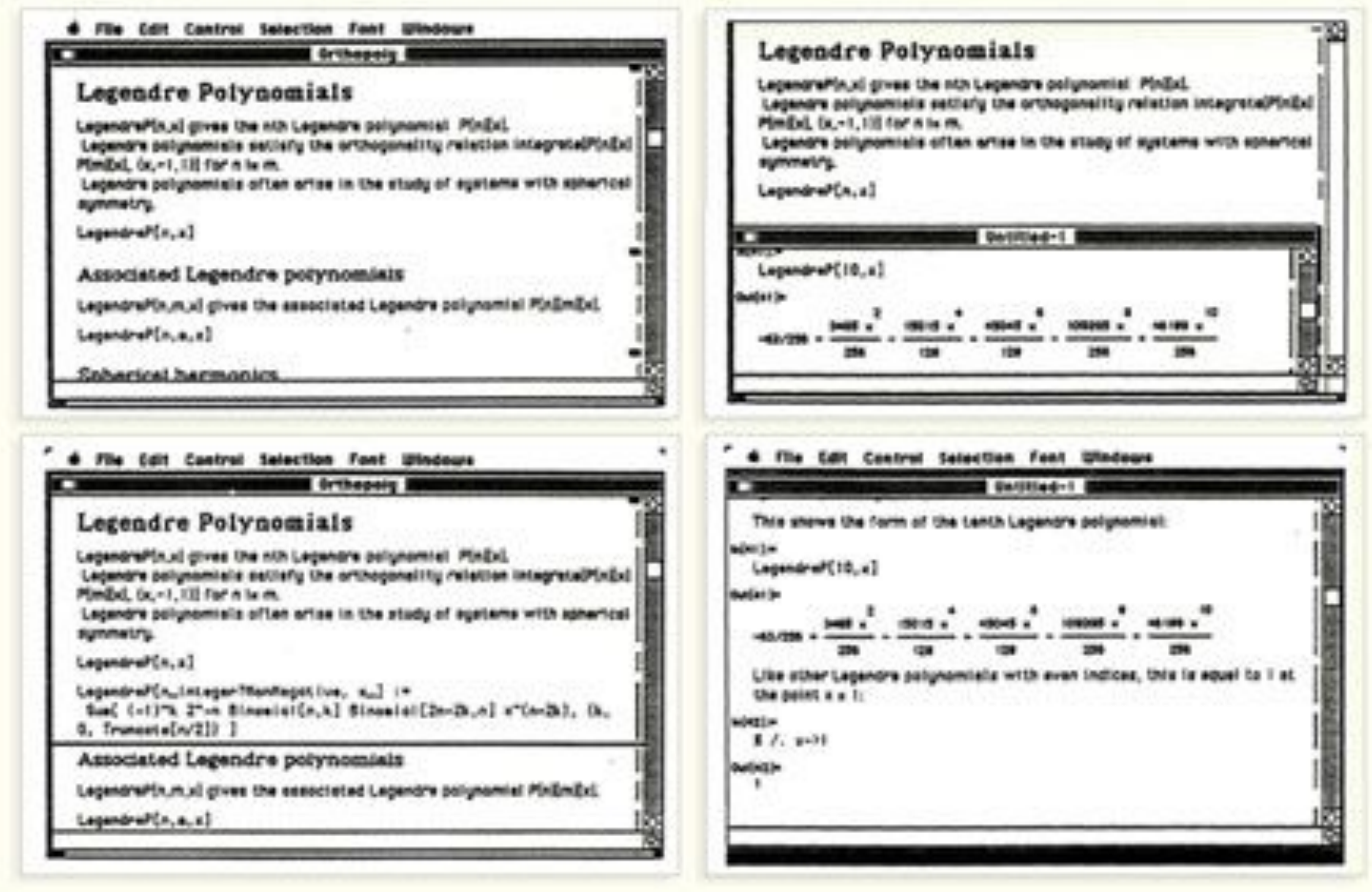
> Instead of imagining that our main task is to instruct a computer what to do, let us concentrate rather on explaining to human beings what we want a computer to do.
>
> — Donald E. Knuth, Literate Programming, 1984

Literate programming

A literate computing environment is one that allows users not only to execute commands interactively, but also to store in a literate document the results of these commands along with figures and free-form text.

- Millman KJ and Perez F (2014)

And the concept was already in place in the 1980s



Legendre Polynomials

LegendreP[n,x] gives the nth Legendre polynomial P[n][x].
Legendre polynomials satisfy the orthogonality relation integrate[P[n][x] P[m][x], {x,-1,1}] for n != m.
Legendre polynomials often arise in the study of systems with spherical symmetry.

LegendreP[n,x]

Associated Legendre polynomials

LegendreP[n,m,x] gives the associated Legendre polynomial P[n][m][x].

LegendreP[n,m,x]

Spherical harmonics

Legendre Polynomials

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Legendre polynomials often arise in the study of systems with spherical symmetry.

LegendreP[n,x]

```
In[1]:=
  LegendreP[10,x]
Out[1]=
```

$$-63/256 + \frac{3465\ x^{2}}{256} - \frac{15015\ x^{4}}{128} + \frac{45045\ x^{6}}{128} - \frac{109395\ x^{8}}{256} + \frac{46189\ x^{10}}{256}$$

Legendre Polynomials

LegendreP[n,x] gives the nth Legendre polynomial P[n][x].
Legendre polynomials satisfy the orthogonality relation integrate[P[n][x] P[m][x], {x,-1,1}] for n != m.
Legendre polynomials often arise in the study of systems with spherical symmetry.

LegendreP[n,x]

```
LegendreP[n_Integer?NonNegative, x_] :=
 Sum[ (-1)^k 2^-n Binomial[n,k] Binomial[2n-2k,n] x^(n-2k), {k,
0, Truncate[n/2]} ]
```

Associated Legendre polynomials

LegendreP[n,m,x] gives the associated Legendre polynomial P[n][m][x].

LegendreP[n,m,x]

This shows the form of the tenth Legendre polynomial:

```
In[1]:=
  LegendreP[10,x]
Out[1]=
```

$$-63/256 + \frac{3465\ x^{2}}{256} - \frac{15015\ x^{4}}{128} + \frac{45045\ x^{6}}{128} - \frac{109395\ x^{8}}{256} + \frac{46189\ x^{10}}{256}$$

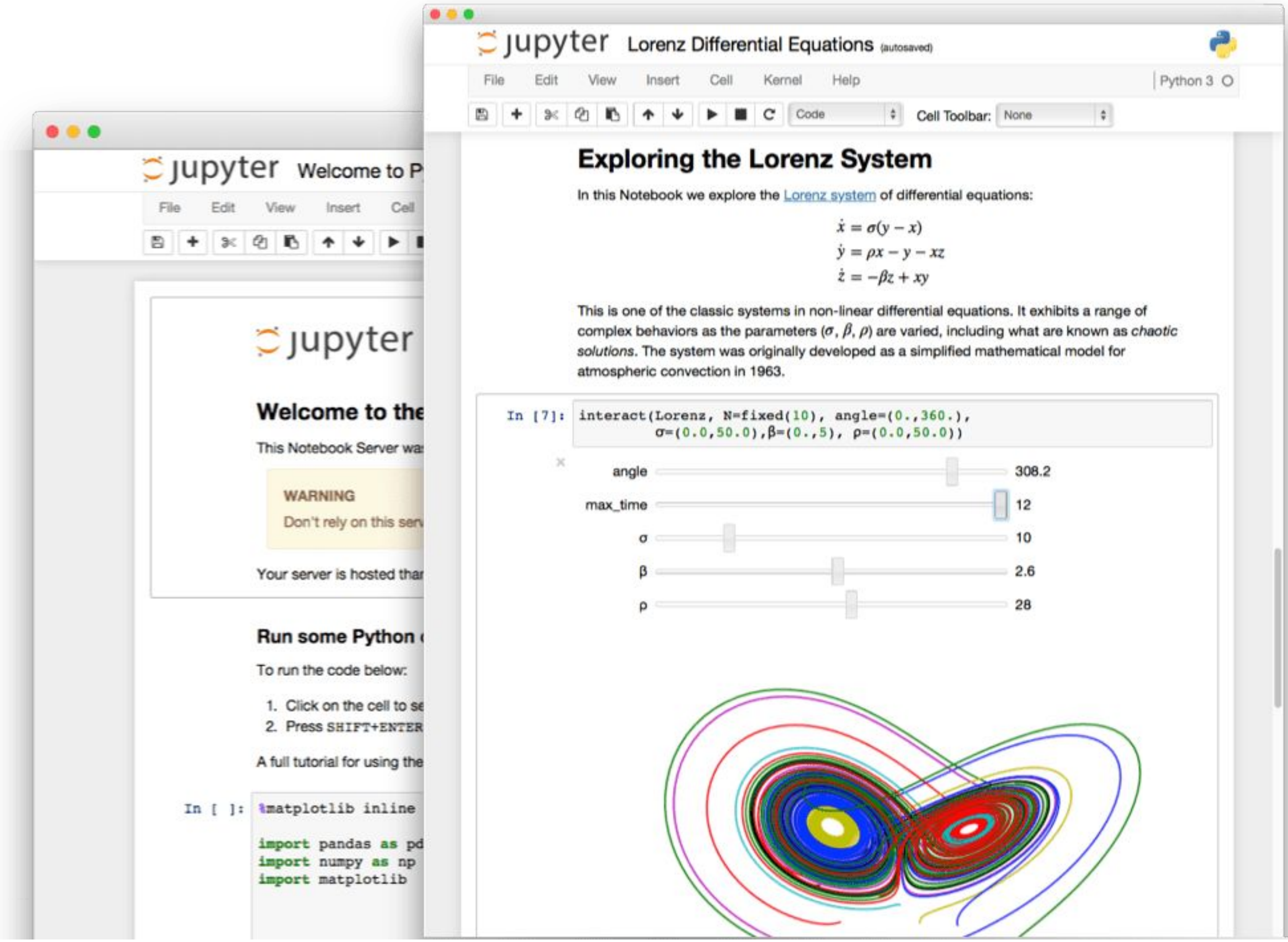
Like other Legendre polynomials with even indices, this is equal to 1 at the point x = 1:

```
In[2]:=
  % /. x->1
Out[2]=
  1
```

Wolfram Mathematica notebook (1987)

Literate programming

What does it look like ?



jupyter

Welcome to the

This Notebook Server was

WARNING

Don't rely on this serv

Your server is hosted thar

Run some Python

To run the code below:

1. Click on the cell to se
2. Press SHIFT+ENTER

A full tutorial for using the

```
In [ ]: %matplotlib inline

        import pandas as pd
        import numpy as np
        import matplotlib
```

Exploring the Lorenz System

In this Notebook we explore the Lorenz system of differential equations:

$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = \rho x - y - xz$$
$$\dot{z} = -\beta z + xy$$

This is one of the classic systems in non-linear differential equations. It exhibits a range of complex behaviors as the parameters (σ, β, ρ) are varied, including what are known as *chaotic solutions*. The system was originally developed as a simplified mathematical model for atmospheric convection in 1963.

```
In [7]: interact(Lorenz, N=fixed(10), angle=(0.,360.),
                 σ=(0.0,50.0),β=(0.,5), ρ=(0.0,50.0))
```

angle 308.2

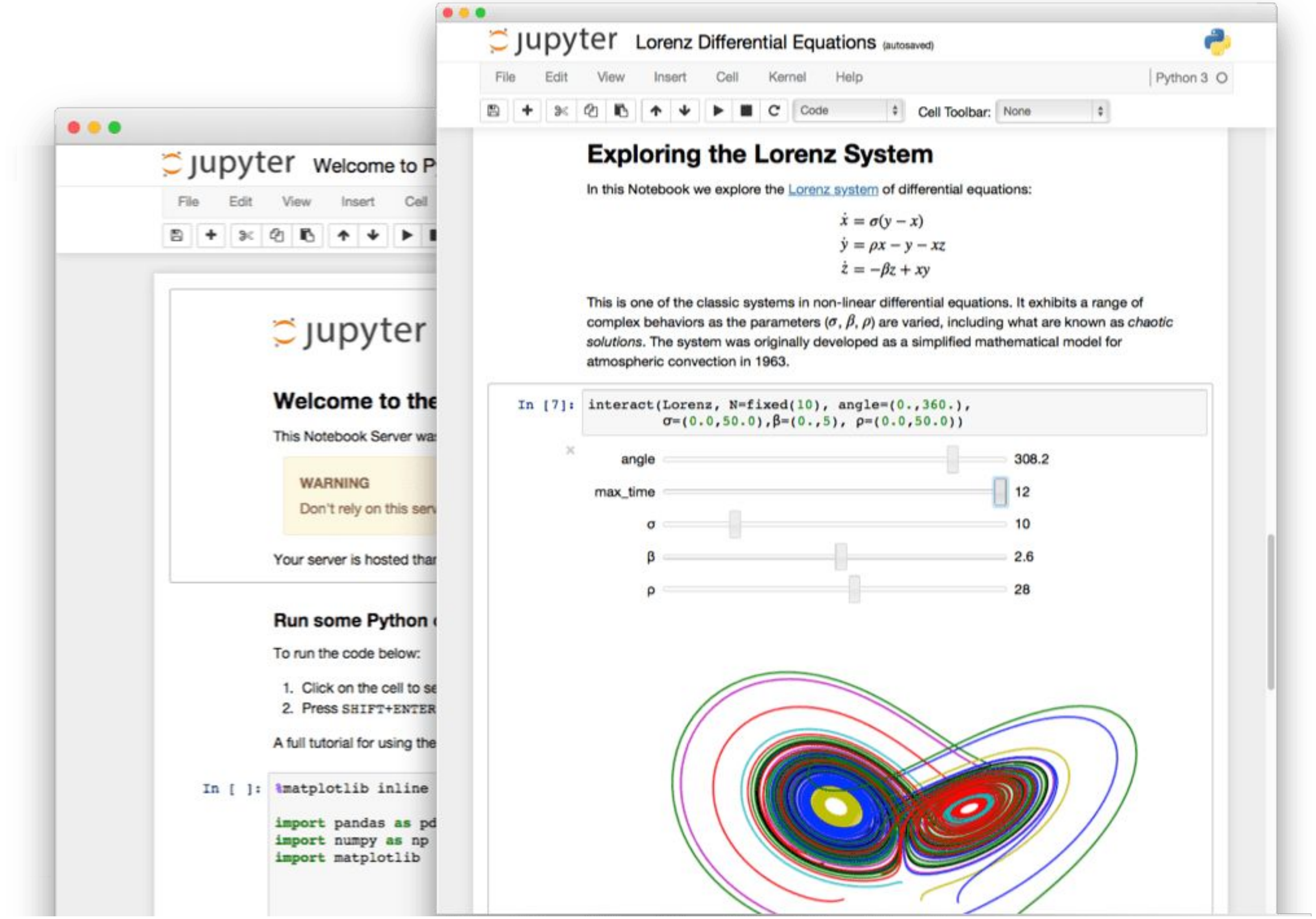
max_time 12

σ 10

β 2.6

ρ 28

Literate programming



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```

angle 308.2

max_time 12

σ 10

β 2.6

ρ 28

Interactive programming interface

allowing to combine both natural and computer languages.

In one file:

- Explanations
- Code
- Results
- Graphs and plots

Literate programming

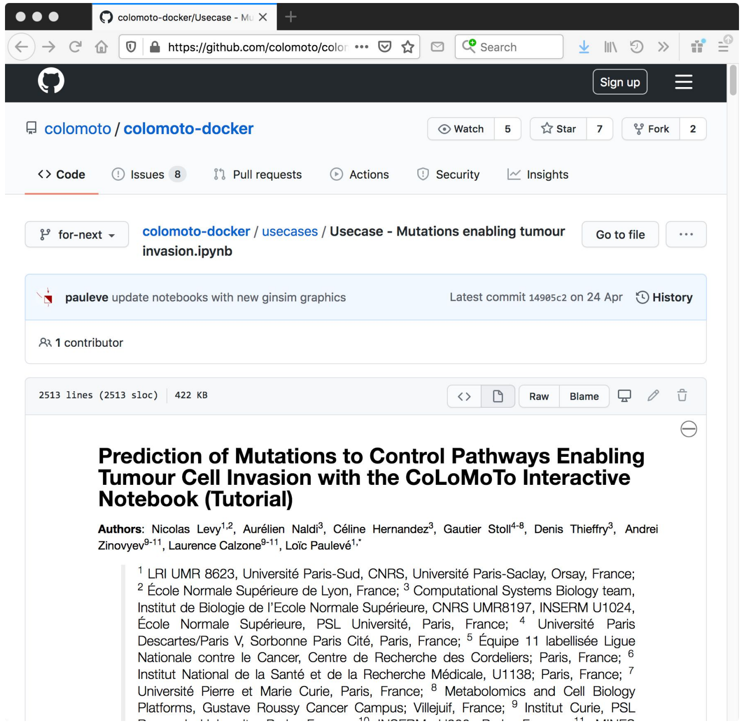
Why using literate programming frameworks ?

Use cases:

- Labbook
- Day to day analyses
- Analysis reports
- Writing scientific article

Example of an article entirely written using a notebook

File (on a repository)



colomoto / colomoto-docker

colomoto-docker / usecases / Usecase - Mutations enabling tumour invasion.ipynb

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

1 contributor

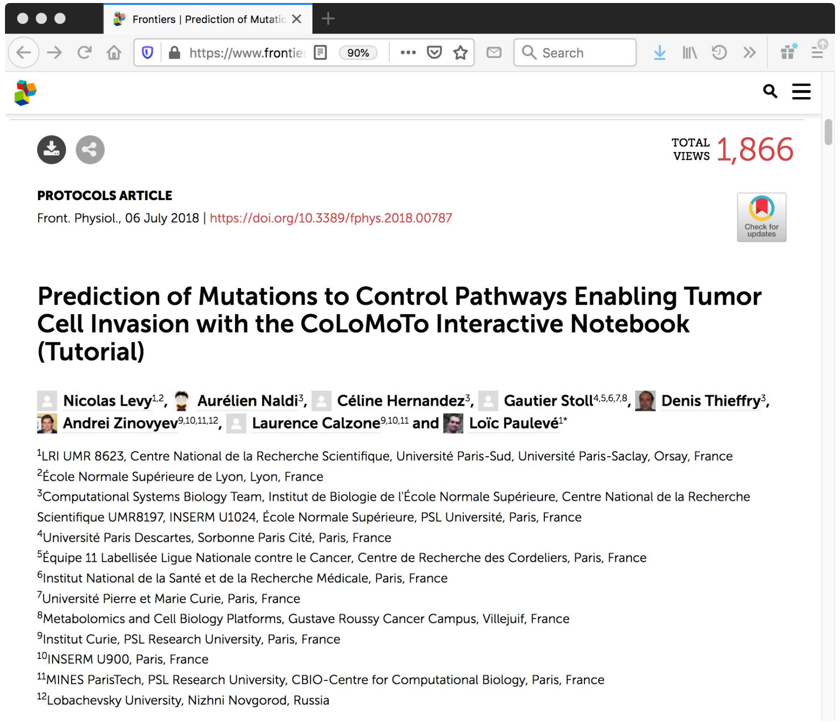
2513 lines (2513 sloc) | 422 KB

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

Authors: Nicolas Levy[1,2], Aurélien Naldi[3], Céline Hernandez[3], Gautier Stoll[4-8], Denis Thieffry[3], Andrei Zinovyev[9-11], Laurence Calzone[9-11], Loïc Paulevé[1,*]

> [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'Ecole 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 Curie, Paris, France; [8] Metabolomics and Cell Biology Platforms, Gustave Roussy Cancer Campus; Villejuif, France; [9] Institut Curie, PSL

Published article



PROTOCOLS ARTICLE

Front. Physiol., 06 July 2018 | https://doi.org/10.3389/fphys.2018.00787

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[1] LRI UMR 8623, Centre National de la Recherche Scientifique, Université Paris-Sud, Université Paris-Saclay, Orsay, France
[2] École Normale Supérieure de Lyon, Lyon, France
[3] Computational Systems Biology Team, Institut de Biologie de l'École Normale Supérieure, Centre National de la Recherche Scientifique UMR8197, INSERM U1024, École Normale Supérieure, PSL Université, Paris, France
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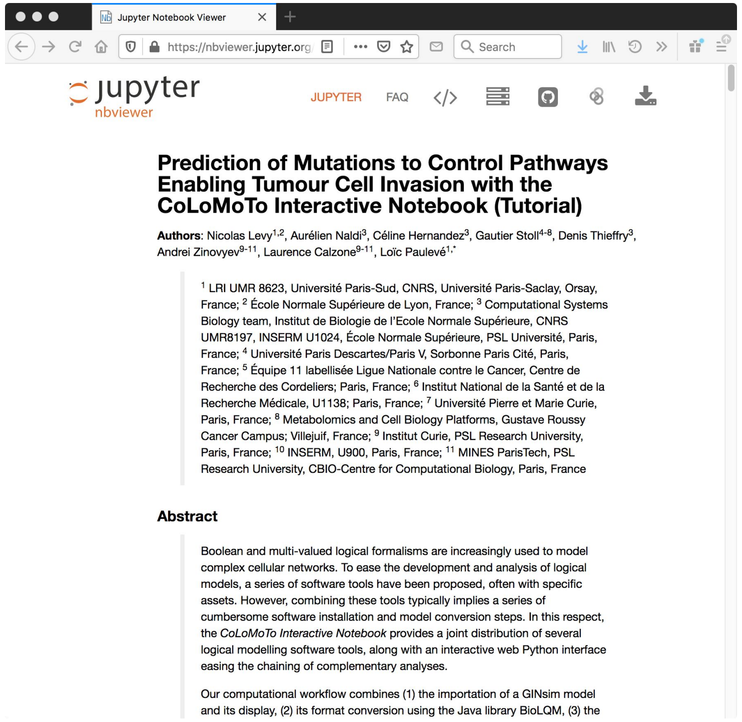
[10] INSERM U900, Paris, France
[11] MINES ParisTech, PSL Research University, CBIO-Centre for Computational Biology, Paris, France
[12] Lobachevsky University, Nizhni Novgorod, Russia

Executable file



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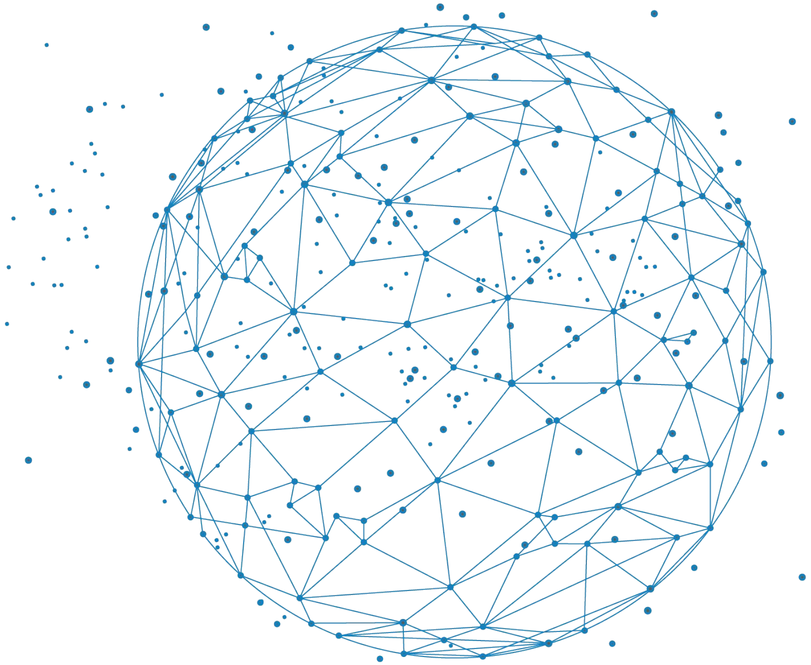
Abstract

> 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

DOI:10.3389/fphys.2018.00787

Markup / Markdown



Markup

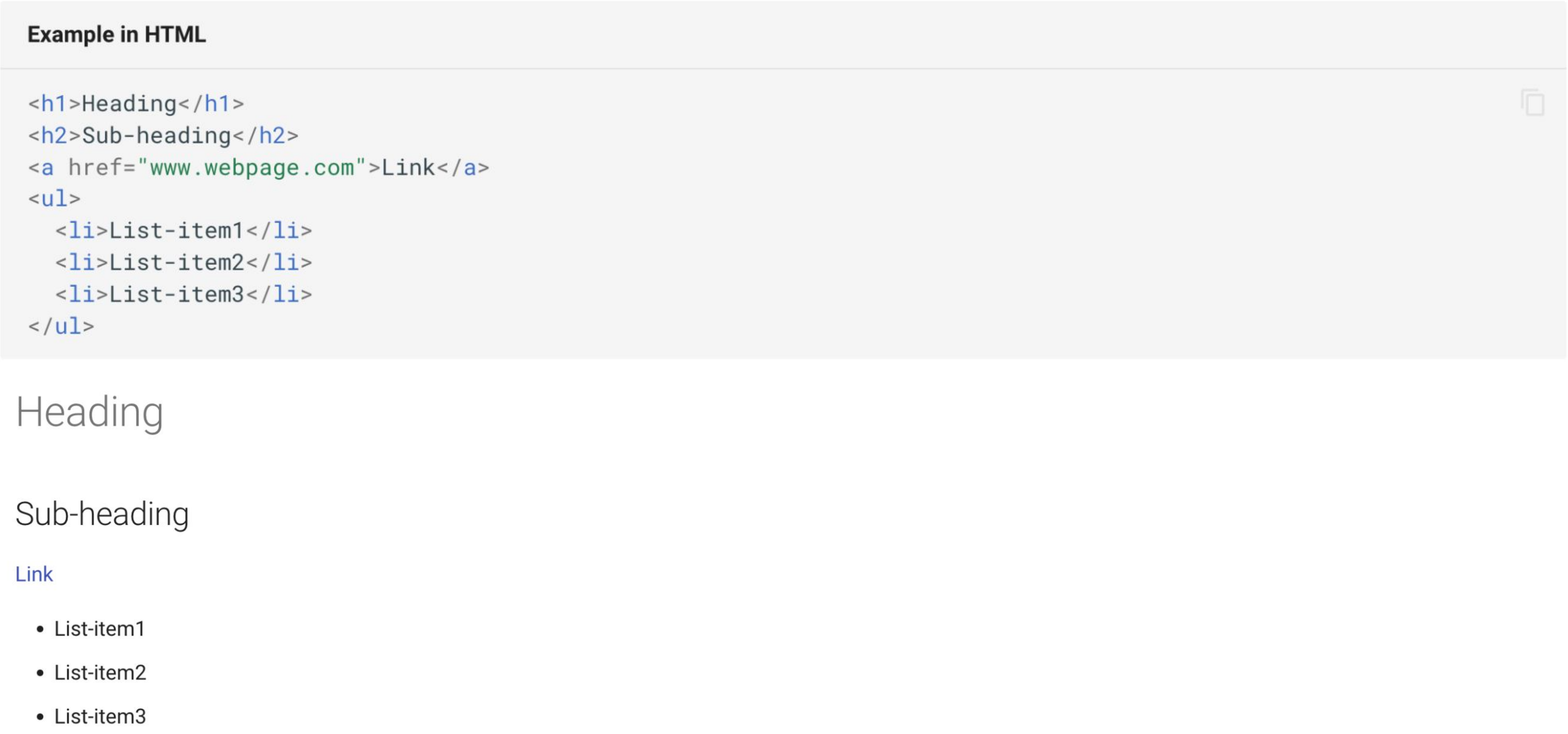
Definition

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

Three different types and usage

- Presentational (used by traditional word-processing systems)
  - Markup is invisible
- Procedural, provides instructions to process the text (e.g. TeX, PostScript)
  - Markup is visible and can be directly manipulated by the author.
- Descriptive, to label documents parts (e.g. LaTeX, HTML, XML...)
  - Emphasizes the document structure.

Example



Example in HTML

```
<h1>Heading</h1>
<h2>Sub-heading</h2>
<a href="www.webpage.com">Link</a>
<ul>
  <li>List-item1</li>
  <li>List-item2</li>
  <li>List-item3</li>
</ul>
```

Heading

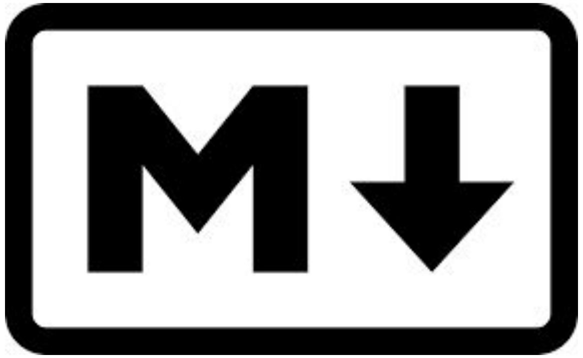
Sub-heading

Link

- List-item1
- List-item2
- List-item3

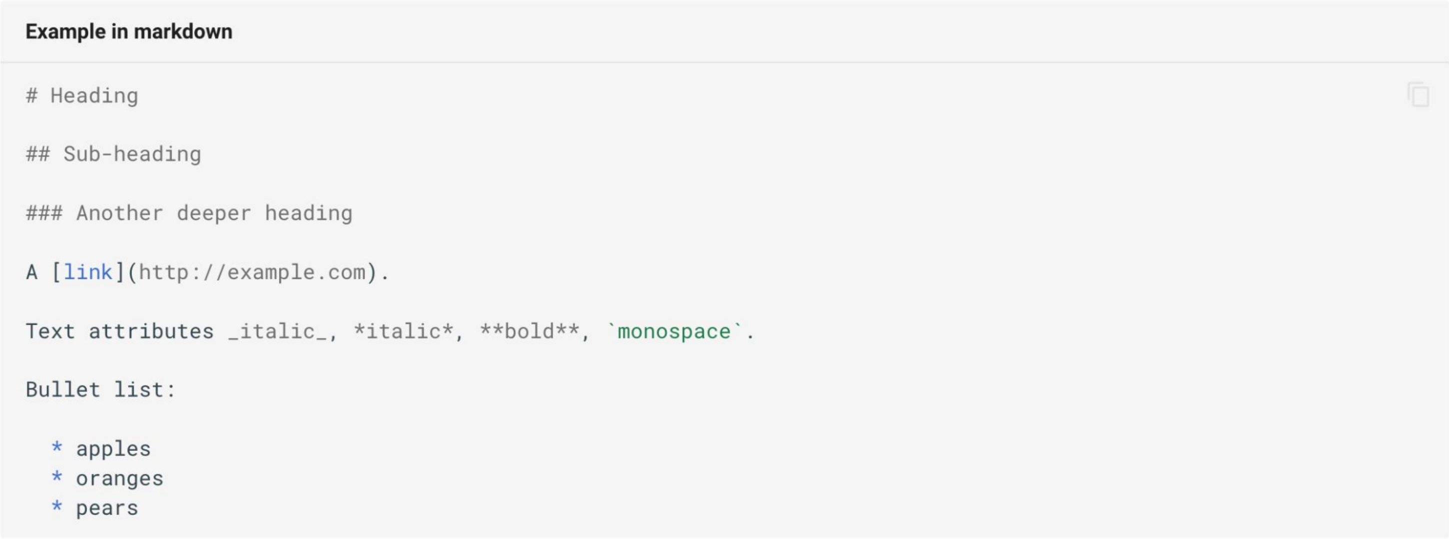
Markdown

Markdown is a Lightweight markup language



Designed to be :

- easy to write using any generic text editor (plain-text-formatting syntax)
- easy to read in its raw form



Example in markdown

```
# Heading

## Sub-heading

### Another deeper heading

A [link](http://example.com).

Text attributes _italic_, *italic*, **bold**, `monospace`.

Bullet list:

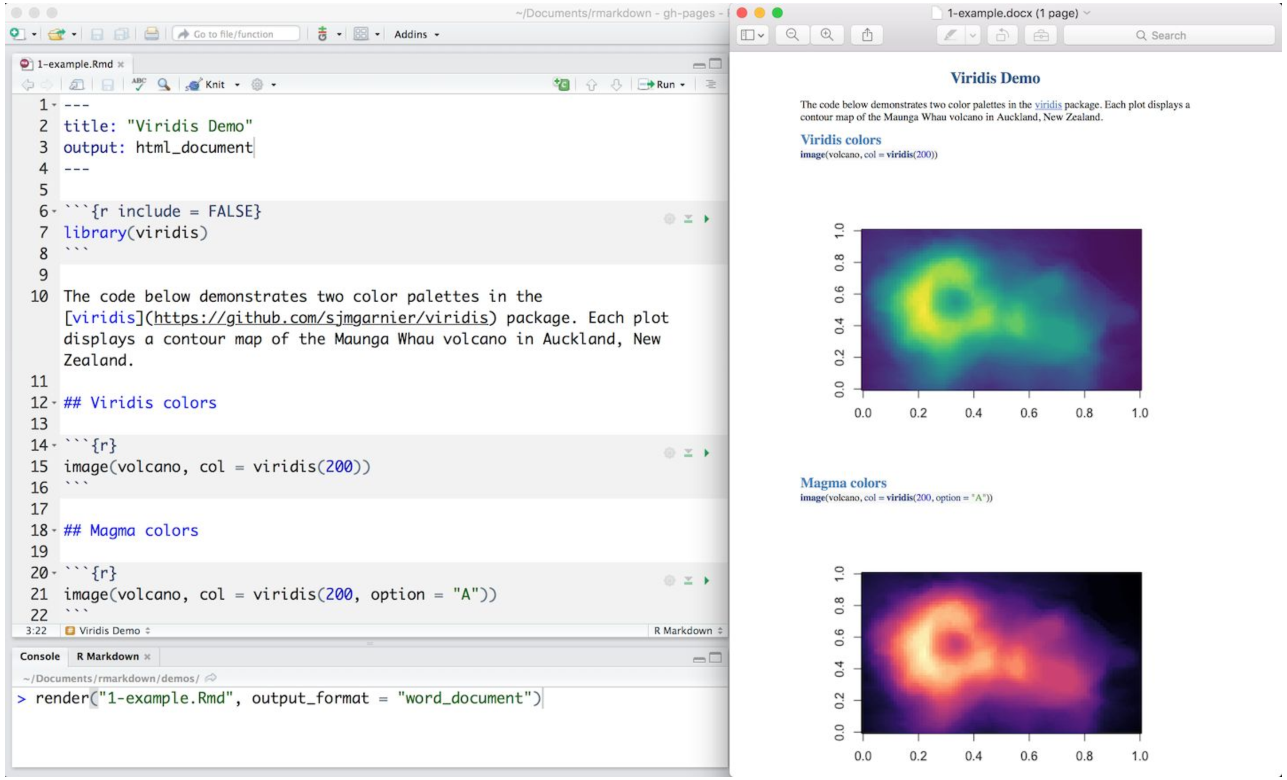
  * apples
  * oranges
  * pears
```

From GitHub’s help page
https://docs.github.com/en/get-started/writing-on-github/getting-started-with-writing-and-formatting-on-github/basic-writing-and-formatting-syntax

Markdown

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.



~~~
---
title: "Viridis Demo"
output: html_document
---

```{r include = FALSE}
library(viridis)
~~~

The code below demonstrates two color palettes in the [viridis](https://github.com/sjmgarnier/viridis) package. Each plot displays a contour map of the Maunga Whau volcano in Auckland, New Zealand.

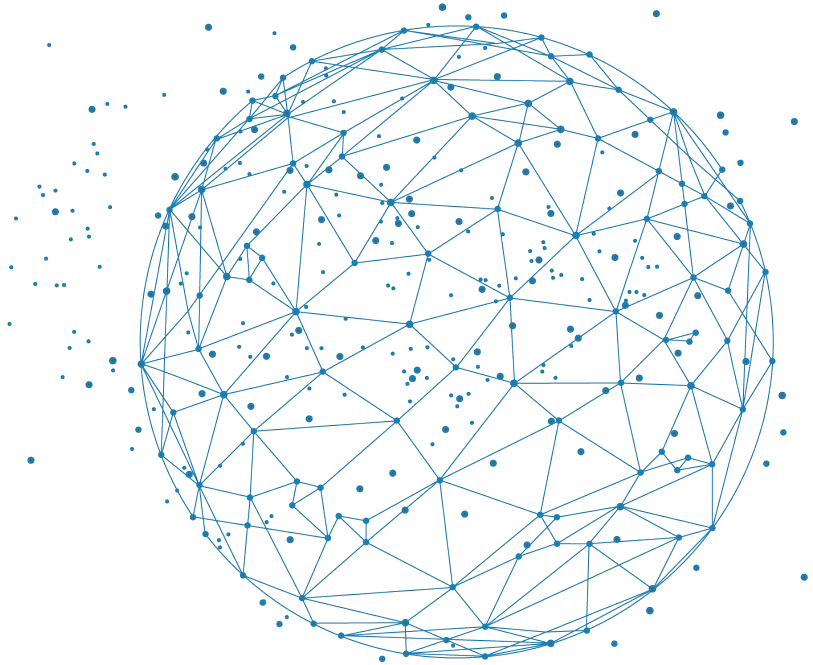
Viridis colors

```{r}
image(volcano, col = viridis(200))
```

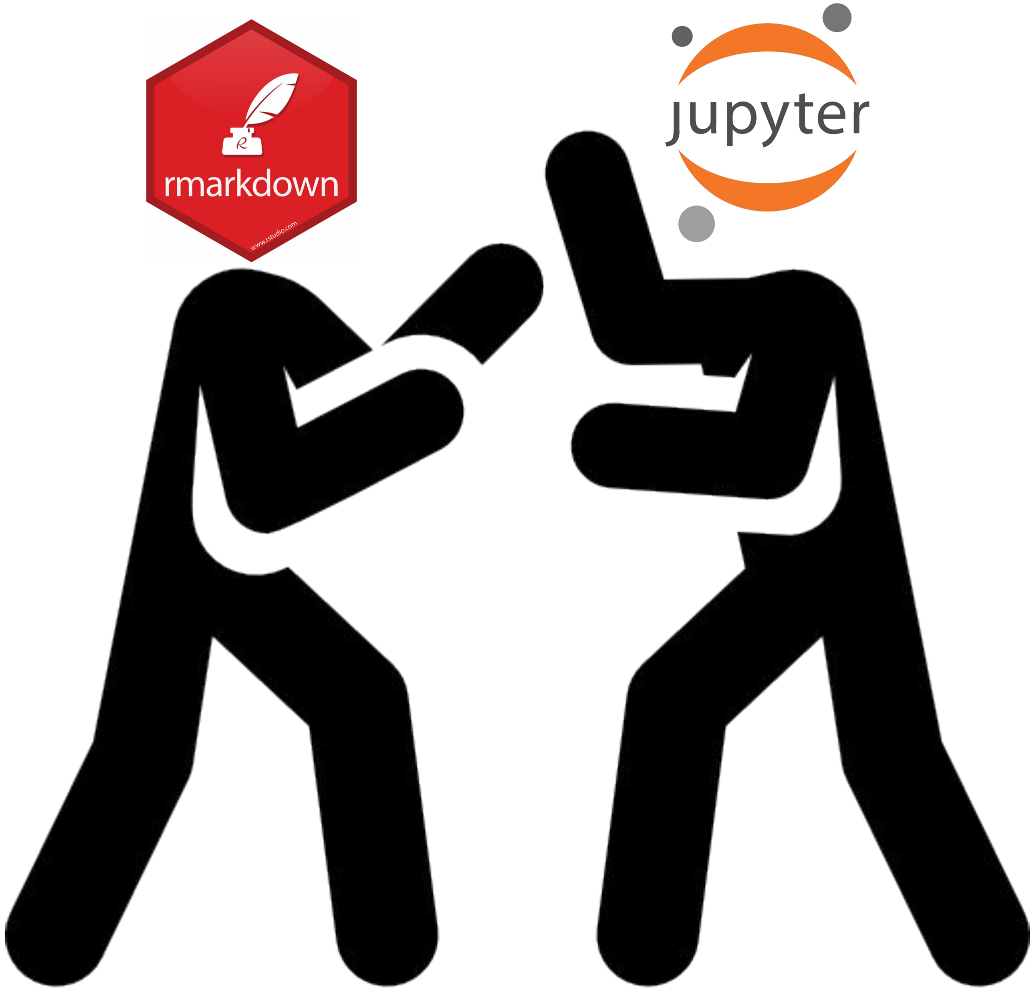
Magma colors

```{r}
image(volcano, col = viridis(200, option = "A"))
```
```

```
> render("1-example.Rmd", output_format = "word_document")
```

Viridis Demo

The code below demonstrates two color palettes in the viridis package. Each plot displays a contour map of the Maunga Whau volcano in Auckland, New Zealand.

Viridis colors

image(volcano, col = viridis(200))

Magma colors

image(volcano, col = viridis(200, option = "A"))
```

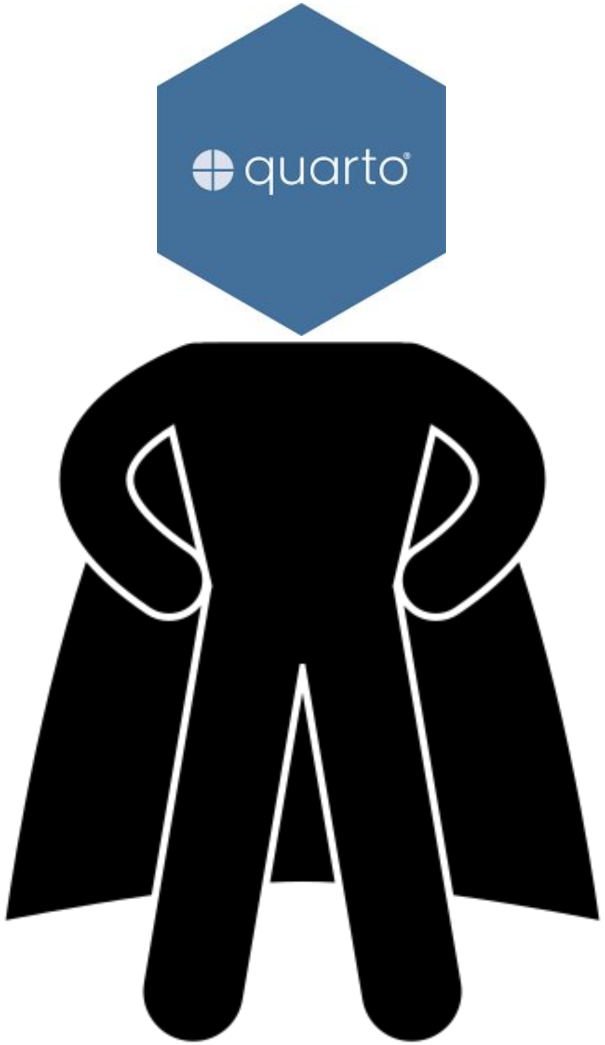
# Notebooks for bioinformatics



# Notebooks for bioinformatics

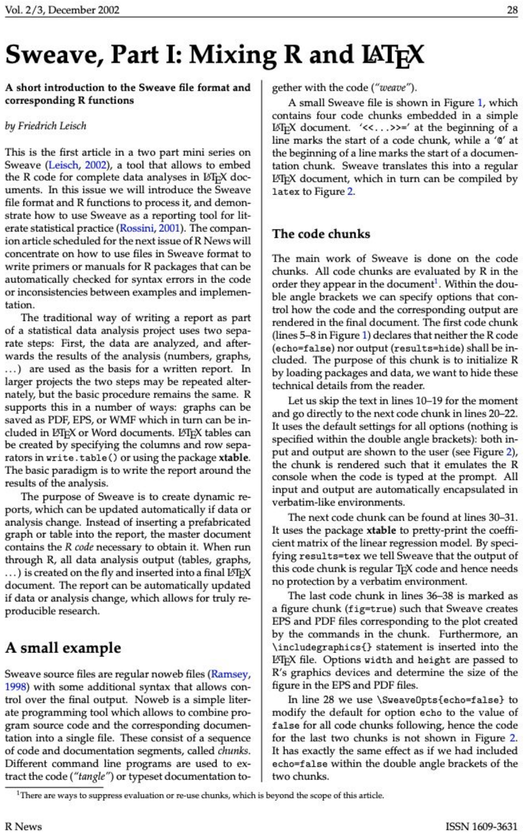


# A replacement?



# R Notebooks : Sweave (2002)

At the beginning, there was nothing. Then came Sweave.



## Sweave, Part I: Mixing R and LATEX

**A short introduction to the Sweave file format and corresponding R functions**

*by Friedrich Leisch*

This is the first article in a two part mini series on Sweave (Leisch, 2002), a tool that allows to embed the R code for complete data analyses in LATEX documents. In this issue we will introduce the Sweave file format and R functions to process it, and demonstrate how to use Sweave as a reporting tool for literate statistical practice (Rossini, 2001). The companion article scheduled for the next issue of R News will concentrate on how to use files in Sweave format to write primers or manuals for R packages that can be automatically checked for syntax errors in the code or inconsistencies between examples and implementation.

The traditional way of writing a report as part of a statistical data analysis project uses two separate steps: First, the data are analyzed, and afterwards the results of the analysis (numbers, graphs, ...) are used as the basis for a written report. In larger projects the two steps may be repeated alternately, but the basic procedure remains the same. R supports this in a number of ways: graphs can be saved as PDF, EPS, or WMF which in turn can be included in LATEX or Word documents. LATEX tables can be created by specifying the columns and row separators in `write.table()` or using the package **xtable**. The basic paradigm is to write the report around the results of the analysis.

The purpose of Sweave is to create dynamic reports, which can be updated automatically if data or analysis change. Instead of inserting a prefabricated graph or table into the report, the master document contains the *R code* necessary to obtain it. When run through R, all data analysis output (tables, graphs, ...) is created on the fly and inserted into a final LATEX document. The report can be automatically updated if data or analysis change, which allows for truly reproducible research.

### A small example

Sweave source files are regular noweb files (Ramsey, 1998) with some additional syntax that allows control over the final output. Noweb is a simple literate programming tool which allows to combine program source code and the corresponding documentation into a single file. These consist of a sequence of code and documentation segments, called *chunks*. Different command line programs are used to extract the code (*"tangle"*) or typeset documentation together with the code (*"weave"*).

A small Sweave file is shown in Figure 1, which contains four code chunks embedded in a simple LATEX document. '`<<...>>=`' at the beginning of a line marks the start of a code chunk, while a '`@`' at the beginning of a line marks the start of a documentation chunk. Sweave translates this into a regular LATEX document, which in turn can be compiled by `latex` to Figure 2.

### The code chunks

The main work of Sweave is done on the code chunks. All code chunks are evaluated by R in the order they appear in the document[1]. Within the double angle brackets we can specify options that control how the code and the corresponding output are rendered in the final document. The first code chunk (lines 5–8 in Figure 1) declares that neither the R code (`echo=false`) nor output (`results=hide`) shall be included. The purpose of this chunk is to initialize R by loading packages and data, we want to hide these technical details from the reader.

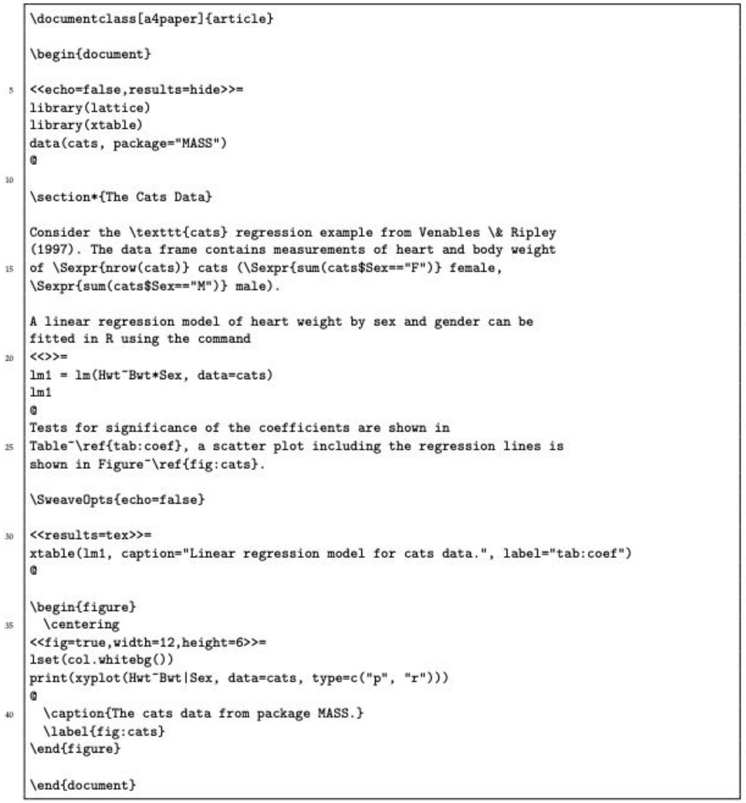
Let us skip the text in lines 10–19 for the moment and go directly to the next code chunk in lines 20–22. It uses the default settings for all options (nothing is specified within the double angle brackets): both input and output are shown to the user (see Figure 2), the chunk is rendered such that it emulates the R console when the code is typed at the prompt. All input and output are automatically encapsulated in verbatim-like environments.

The next code chunk can be found at lines 30–31. It uses the package **xtable** to pretty-print the coefficient matrix of the linear regression model. By specifying `results=tex` we tell Sweave that the output of this code chunk is regular TEX code and hence needs no protection by a verbatim environment.

The last code chunk in lines 36–38 is marked as a figure chunk (`fig=true`) such that Sweave creates EPS and PDF files corresponding to the plot created by the commands in the chunk. Furthermore, an `\includegraphics{}` statement is inserted into the LATEX file. Options `width` and `height` are passed to R's graphics devices and determine the size of the figure in the EPS and PDF files.

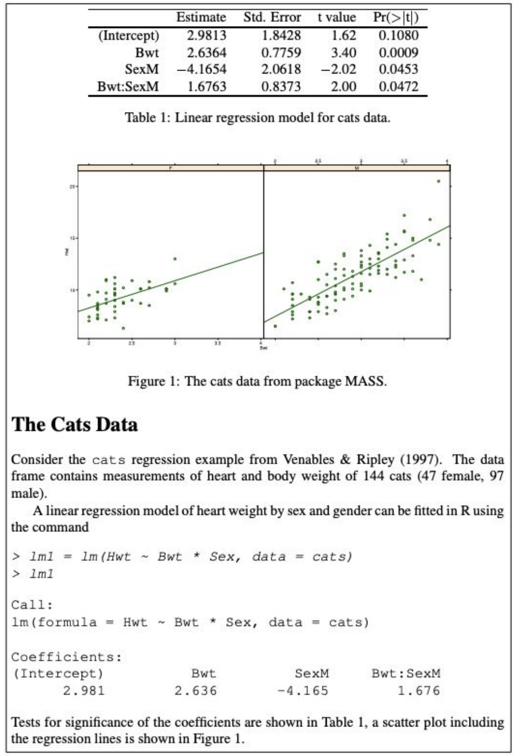
In line 28 we use `\SweaveOpts{echo=false}` to modify the default for option `echo` to the value of `false` for all code chunks following, hence the code for the last two chunks is not shown in Figure 2. It has exactly the same effect as if we had included `echo=false` within the double angle brackets of the two chunks.

[1] There are ways to suppress evaluation or re-use chunks, which is beyond the scope of this article.



```
   \documentclass[a4paper]{article}

   \begin{document}

 5 <<echo=false,results=hide>>=
   library(lattice)
   library(xtable)
   data(cats, package="MASS")
   @
10
   \section*{The Cats Data}

   Consider the \texttt{cats} regression example from Venables \& Ripley
   (1997). The data frame contains measurements of heart and body weight
15 of \Sexpr{nrow(cats)} cats (\Sexpr{sum(cats$Sex=="F")} female,
   \Sexpr{sum(cats$Sex=="M")} male).

   A linear regression model of heart weight by sex and gender can be
   fitted in R using the command
20 <<>>=
   lm1 = lm(Hwt~Bwt*Sex, data=cats)
   lm1
   @
   Tests for significance of the coefficients are shown in
25 Table~\ref{tab:coef}, a scatter plot including the regression lines is
   shown in Figure~\ref{fig:cats}.

   \SweaveOpts{echo=false}

30 <<results=tex>>=
   xtable(lm1, caption="Linear regression model for cats data.", label="tab:coef")
   @

   \begin{figure}
35   \centering
   <<fig=true,width=12,height=6>>=
   lset(col.whitebg())
   print(xyplot(Hwt~Bwt|Sex, data=cats, type=c("p", "r")))
   @
40   \caption{The cats data from package MASS.}
     \label{fig:cats}
   \end{figure}

   \end{document}
```

Figure 1: A minimal Sweave file: `example.Snw`.



	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	2.9813	1.8428	1.62	0.1080
Bwt	2.6364	0.7759	3.40	0.0009
SexM	−4.1654	2.0618	−2.02	0.0453
Bwt:SexM	1.6763	0.8373	2.00	0.0472

Table 1: Linear regression model for cats data.

Figure 1: The cats data from package MASS.

The Cats Data

Consider the `cats` regression example from Venables & Ripley (1997). The data frame contains measurements of heart and body weight of 144 cats (47 female, 97 male).

A linear regression model of heart weight by sex and gender can be fitted in R using the command

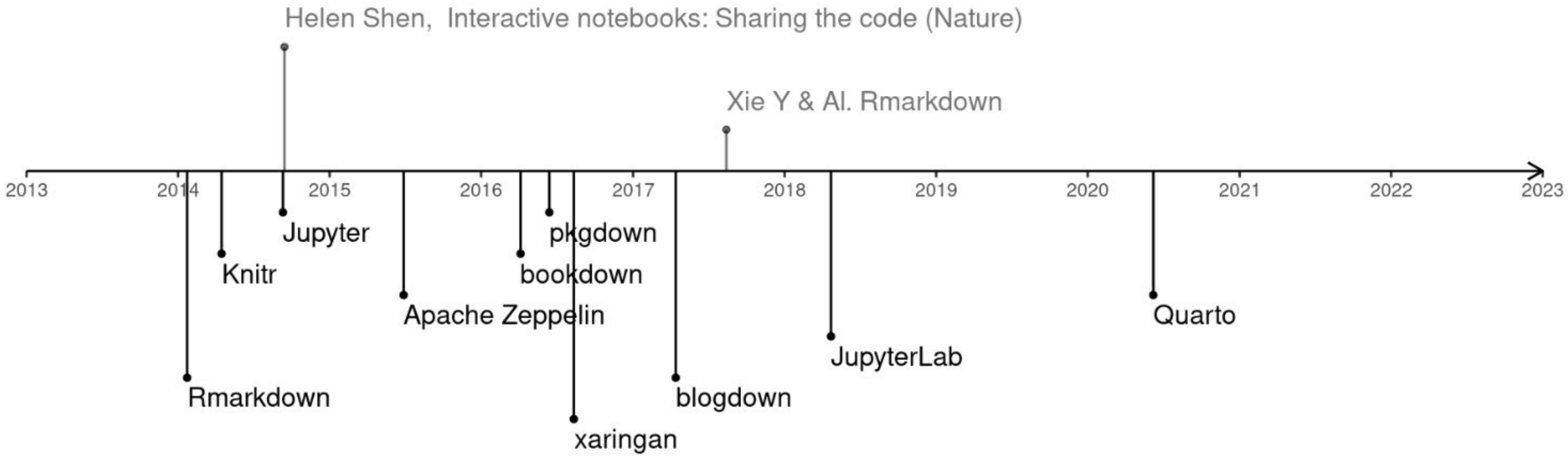
```
> lm1 = lm(Hwt ~ Bwt * Sex, data = cats)
> lm1

Call:
lm(formula = Hwt ~ Bwt * Sex, data = cats)

Coefficients:
(Intercept)          Bwt         SexM     Bwt:SexM
      2.981        2.636       -4.165        1.676
```

Tests for significance of the coefficients are shown in Table 1, a scatter plot including the regression lines is shown in Figure 1.

Figure 2: The final document is created by running `latex` on the intermediate file 'example.tex' created by `Sweave("example.Snw")`.

And people saw that the path would be long...

Appearance of packages allowing the creation of notebooks



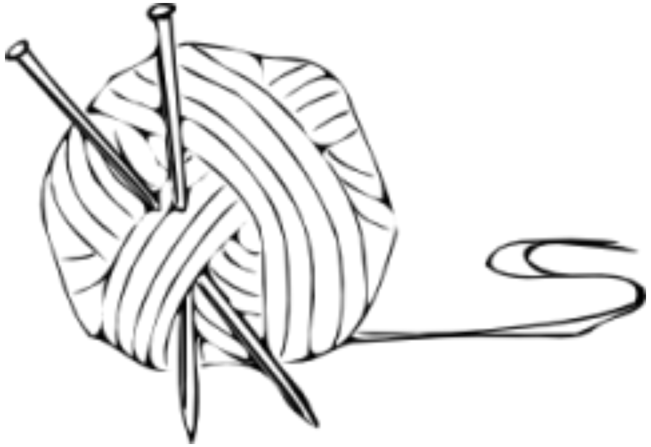
https://camembr.quarto.pub/hello-quarto/#/les-packages

R solutions

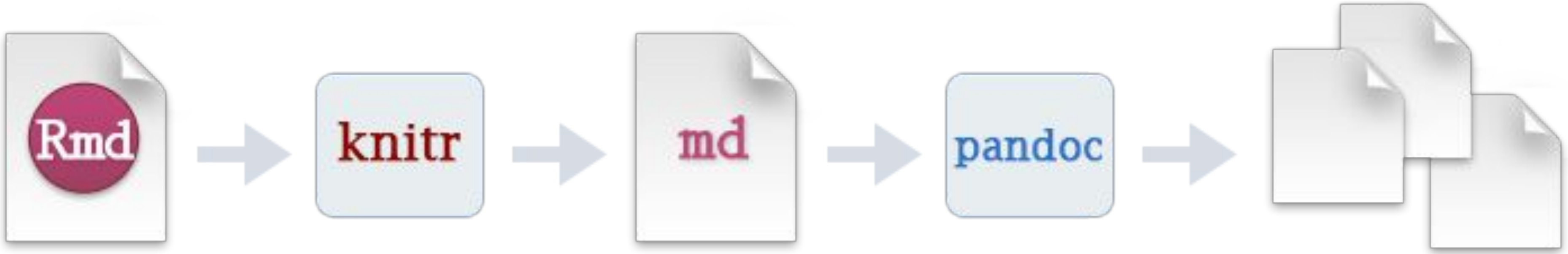
R Notebooks : knitR (2011)

”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”

https://yihui.org/knitr/



R Notebooks : RMarkdown (2012)

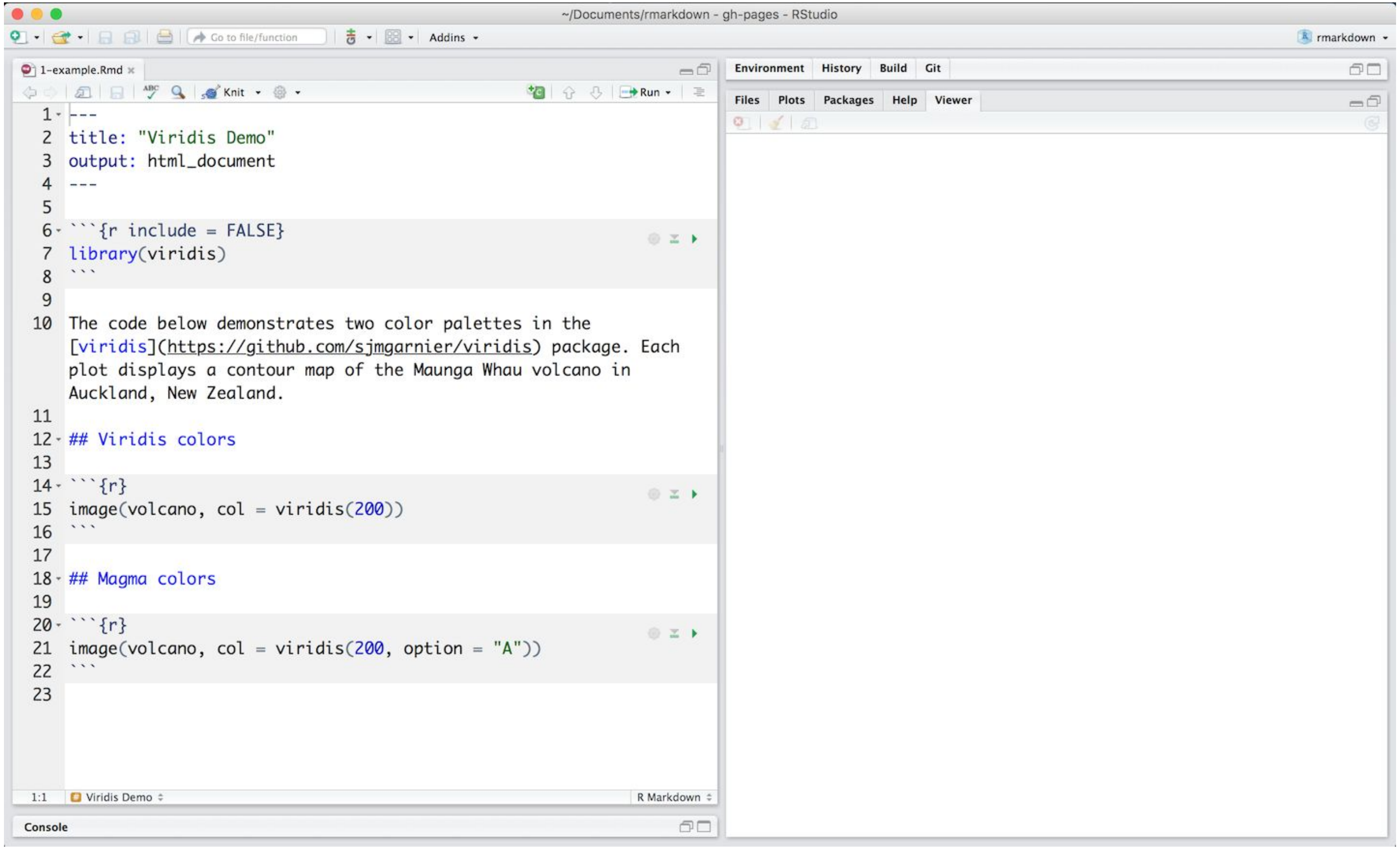


”When you run render, R Markdown feeds the .Rmd file to knitr, which executes all of the code chunks and creates a new markdown (.md) document which includes the code and its output.

The markdown file generated by knitR is then processed by pandoc which is responsible for creating the finished format.”

https://rmarkdown.rstudio.com

R Notebooks : RMarkdown (2012)



~~~
---
title: "Viridis Demo"
output: html_document
---

```{r include = FALSE}
library(viridis)
~~~

The code below demonstrates two color palettes in the
[viridis](https://github.com/sjmgarnier/viridis) package. Each
plot displays a contour map of the Maunga Whau volcano in
Auckland, New Zealand.

Viridis colors

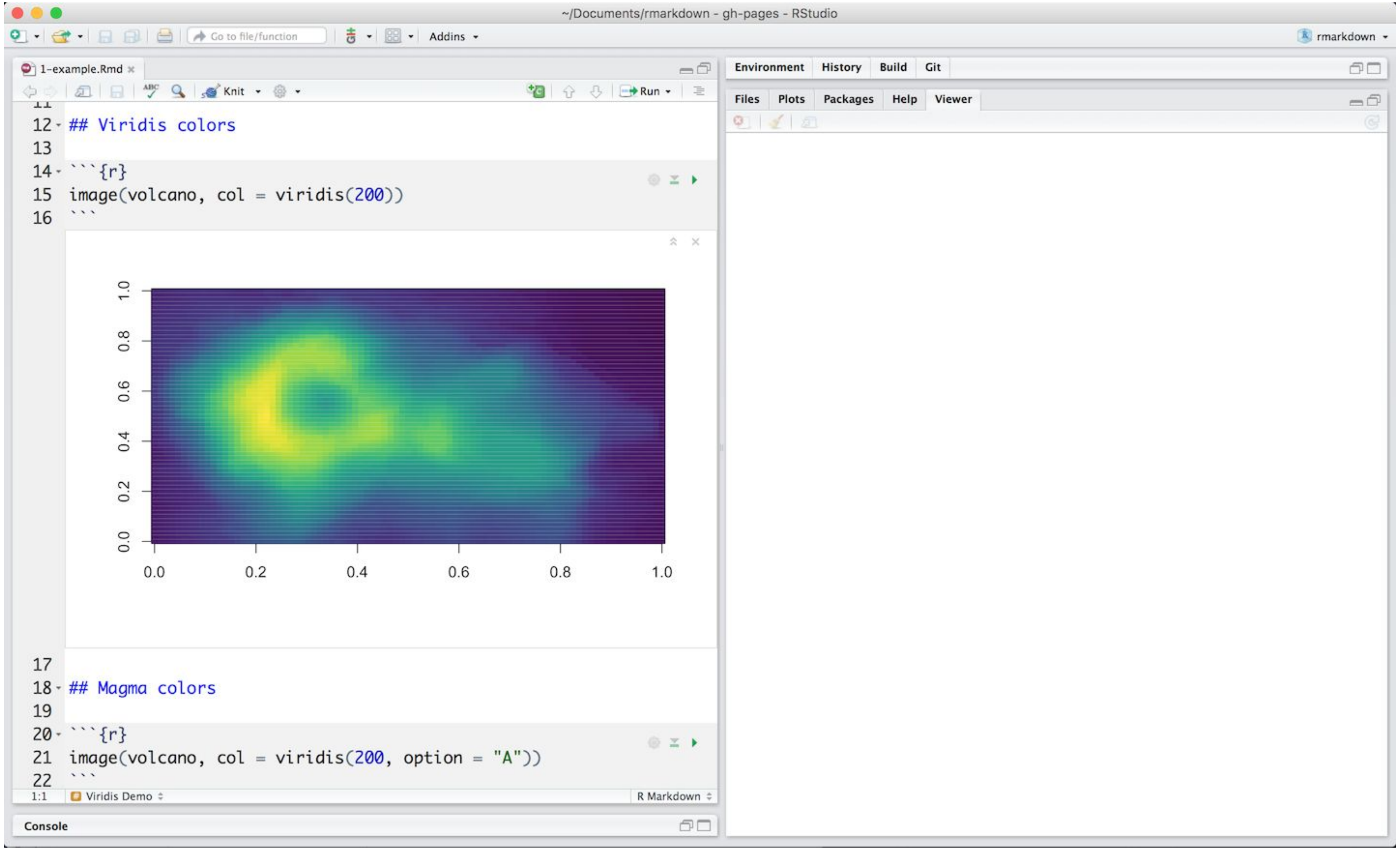
```{r}
image(volcano, col = viridis(200))
```

Magma colors

```{r}
image(volcano, col = viridis(200, option = "A"))
```

```
```

R Notebooks : RMarkdown (2012)

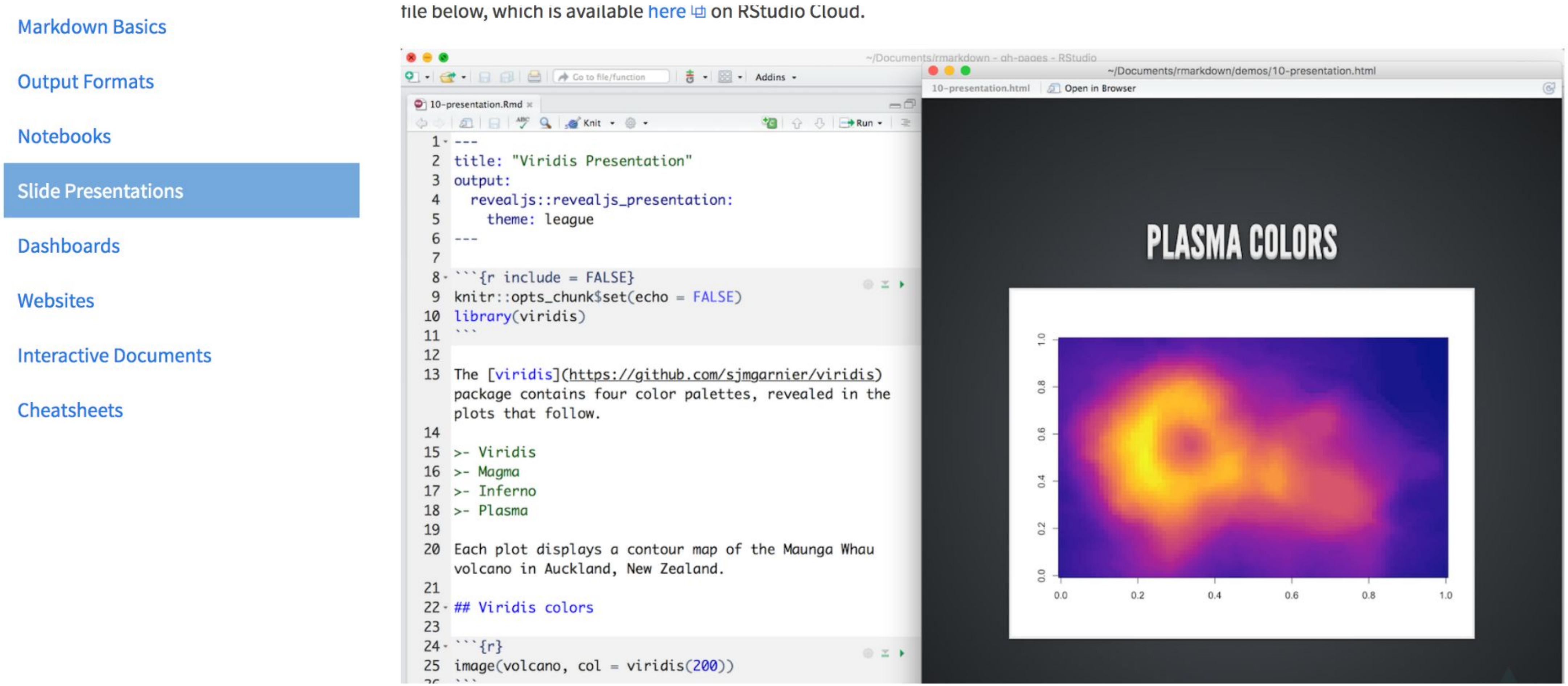


~~~
## Viridis colors

```{r}
image(volcano, col = viridis(200))
~~~

Magma colors

```{r}
image(volcano, col = viridis(200, option = "A"))
```
```
```

R Notebooks and more…



- Markdown Basics
- Output Formats
- Notebooks
- Slide Presentations
- Dashboards
- Websites
- Interactive Documents
- Cheatsheets

file below, which is available here on RStudio Cloud.

~~~
---
title: "Viridis Presentation"
output:
  revealjs::revealjs_presentation:
    theme: league
---

```{r include = FALSE}
knitr::opts_chunk$set(echo = FALSE)
library(viridis)
~~~

The [viridis](https://github.com/sjmgarnier/viridis)
package contains four color palettes, revealed in the
plots that follow.

>- Viridis
>- Magma
>- Inferno
>- Plasma

Each plot displays a contour map of the Maunga Whau
volcano in Auckland, New Zealand.

Viridis colors

```{r}
image(volcano, col = viridis(200))
```
```
```

Jupyter

Jupyter

A bit of history...

2011 : IPython (interactive Python shell) with notebook functionalities

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

”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)

https://jupyter.org/

Jupyter

What is it exactly ?

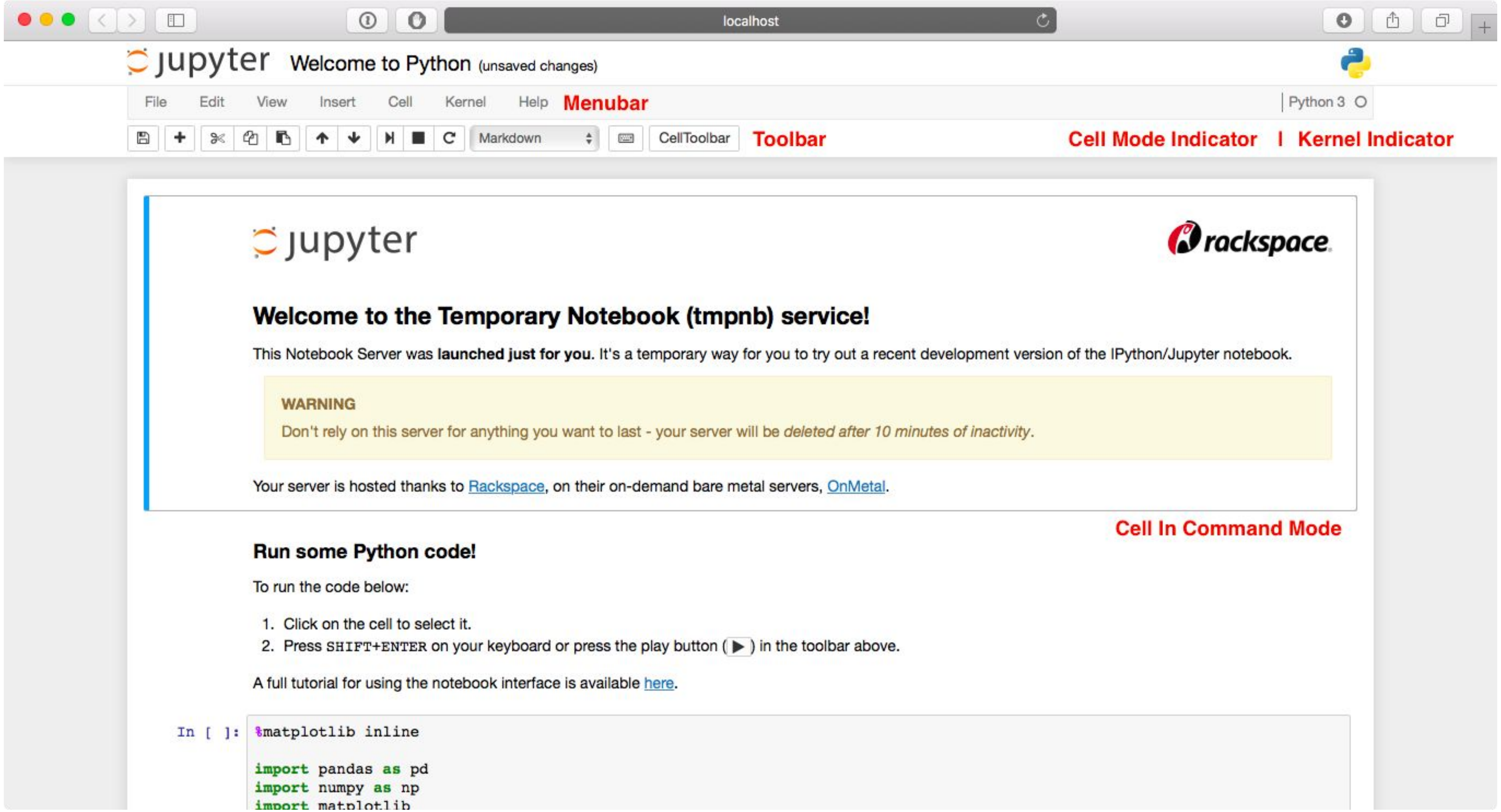
Web-based interactive computational environment.

Web-based : client/server

Interactive : notebook system

Computational environment : console, many kernels available...

Jupyter : Notebook editor



localhost
jupyter Welcome to Python (unsaved changes)
File Edit View Insert Cell Kernel Help
Menubar
Python 3 ○
Markdown
CellToolbar
Toolbar
Cell Mode Indicator | Kernel Indicator
Cell In Command Mode
rackspace

jupyter

Welcome to the Temporary Notebook (tmpnb) service!

This Notebook Server was **launched just for you**. It's a temporary way for you to try out a recent development version of the IPython/Jupyter notebook.

WARNING

Don't rely on this server for anything you want to last - your server will be *deleted after 10 minutes of inactivity*.

Your server is hosted thanks to Rackspace, on their on-demand bare metal servers, OnMetal.

Run some Python code!

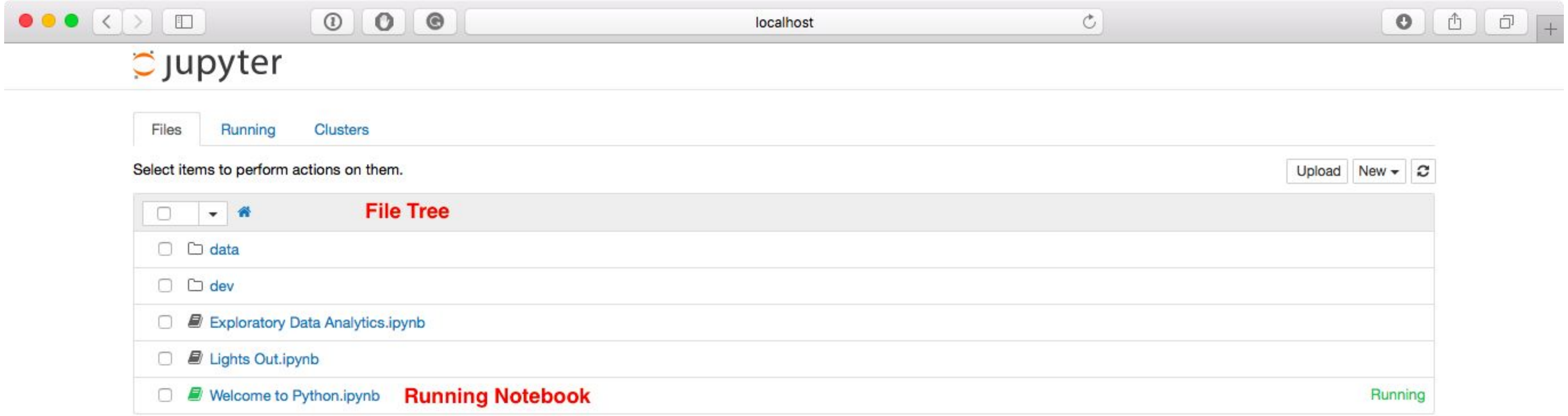
To run the code below:

1. Click on the cell to select it.
2. Press `SHIFT+ENTER` on your keyboard or press the play button (▶) in the toolbar above.

A full tutorial for using the notebook interface is available here.

```
In [ ]: %matplotlib inline

        import pandas as pd
        import numpy as np
        import matplotlib
```

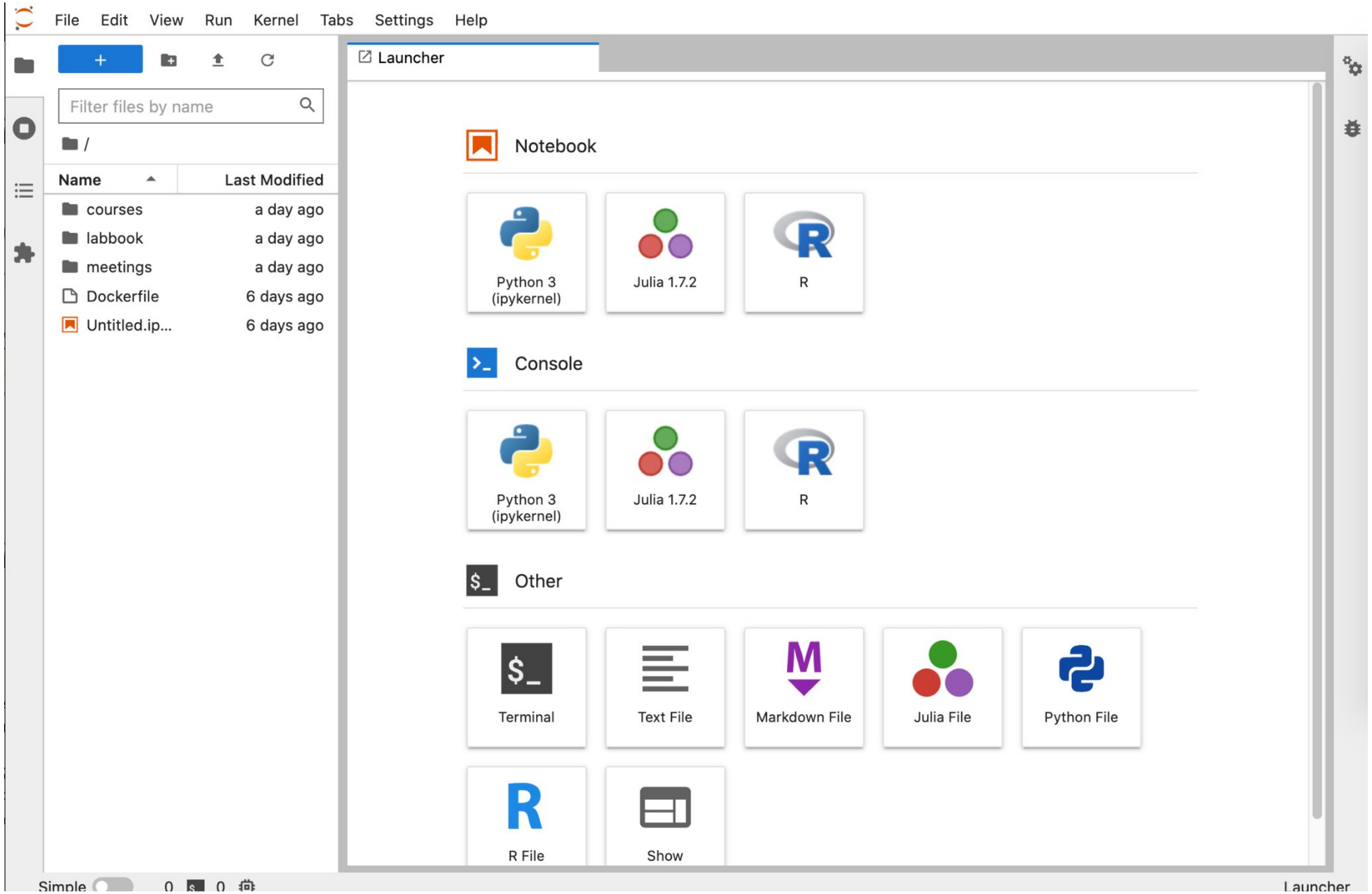
Jupyter : Dashboard (Project Jupyter only)



Select items to perform actions on them.

- data
- dev
- Exploratory Data Analytics.ipynb
- Lights Out.ipynb
- Welcome to Python.ipynb

JupyterLab : Dashboard



Name	Last Modified
courses	a day ago
labbook	a day ago
meetings	a day ago
Dockerfile	6 days ago
Untitled.ip...	6 days ago

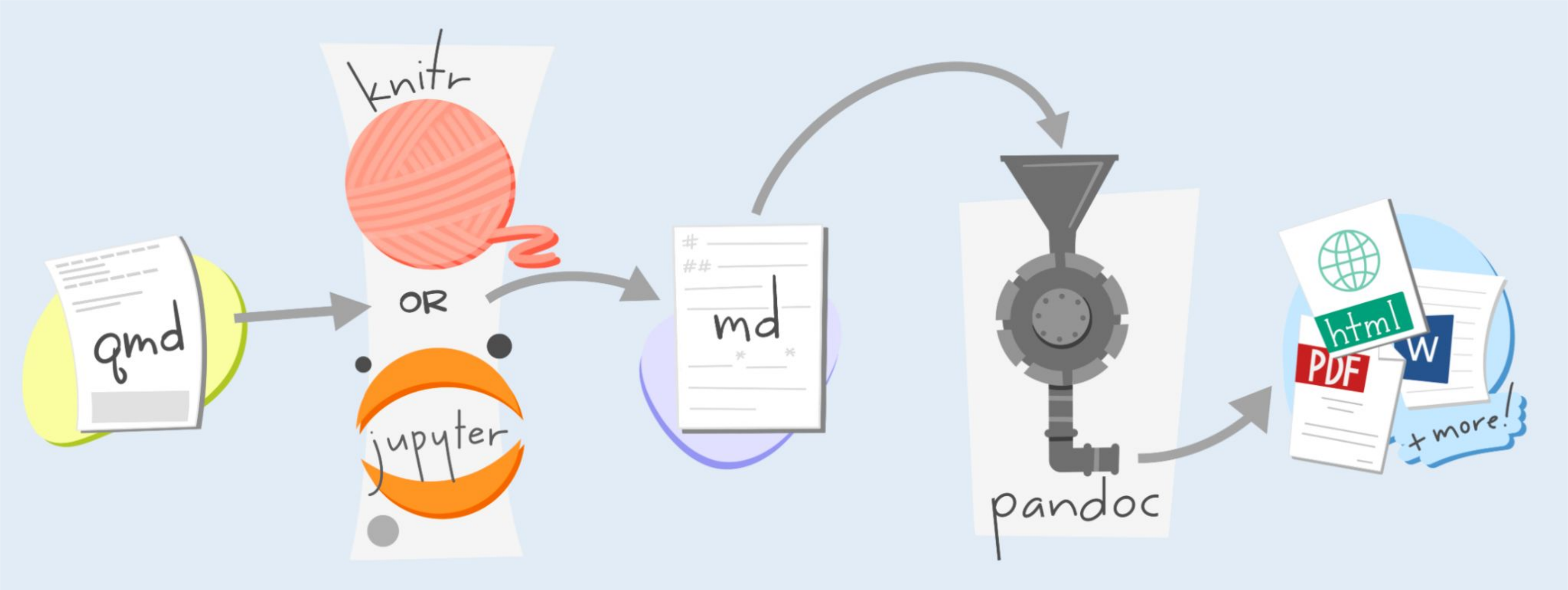
Quarto

Quarto

Quarto is an open-source scientific and technical publishing system where authors :

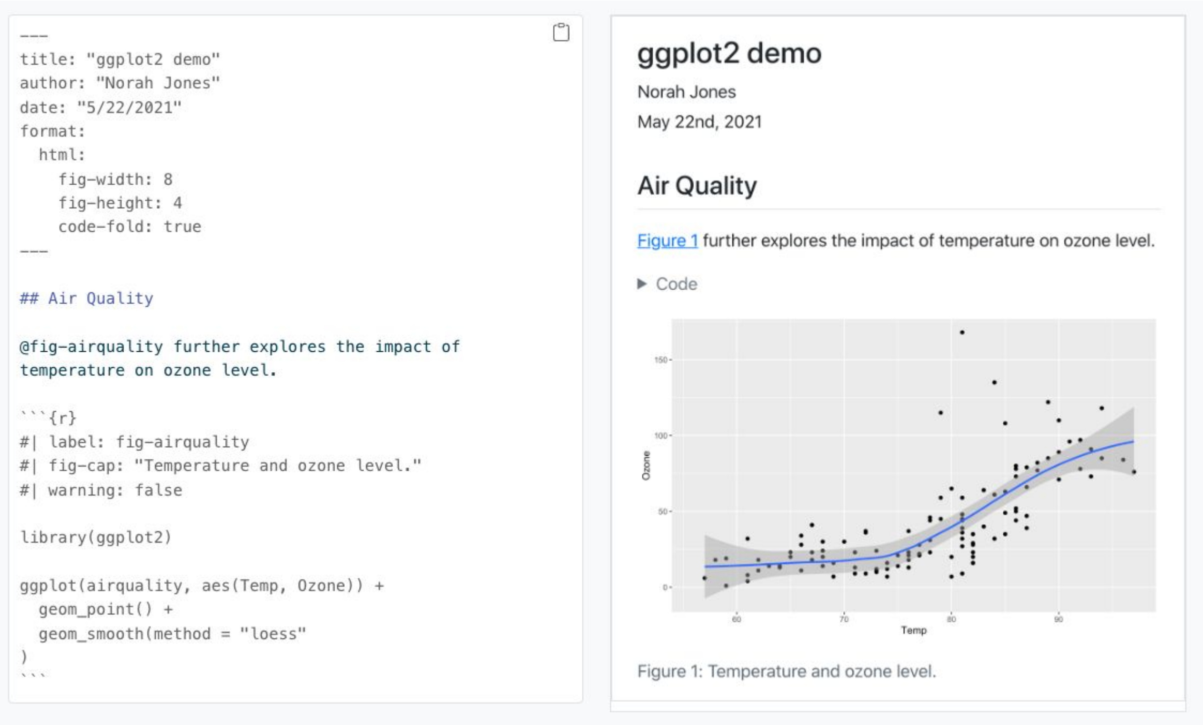
- Can use Jupyter notebooks or with plain text markdown in your favorite editor.
- Create dynamic content with Python, R, Julia, and Observable.
- Publish reproducible, production quality articles, presentations, websites, blogs, and books in HTML, PDF, MS Word, ePub, and more.
- Share results in a lot of publishing systems like GitHub.

Quarto



Examples

With R



~~~
---
title: "ggplot2 demo"
author: "Norah Jones"
date: "5/22/2021"
format:
  html:
    fig-width: 8
    fig-height: 4
    code-fold: true
---

## Air Quality

@fig-airquality further explores the impact of
temperature on ozone level.

```{r}
#| label: fig-airquality
#| fig-cap: "Temperature and ozone level."
#| warning: false

library(ggplot2)

ggplot(airquality, aes(Temp, Ozone)) +
  geom_point() +
  geom_smooth(method = "loess"
)
```
~~~

ggplot2 demo

Norah Jones

May 22nd, 2021

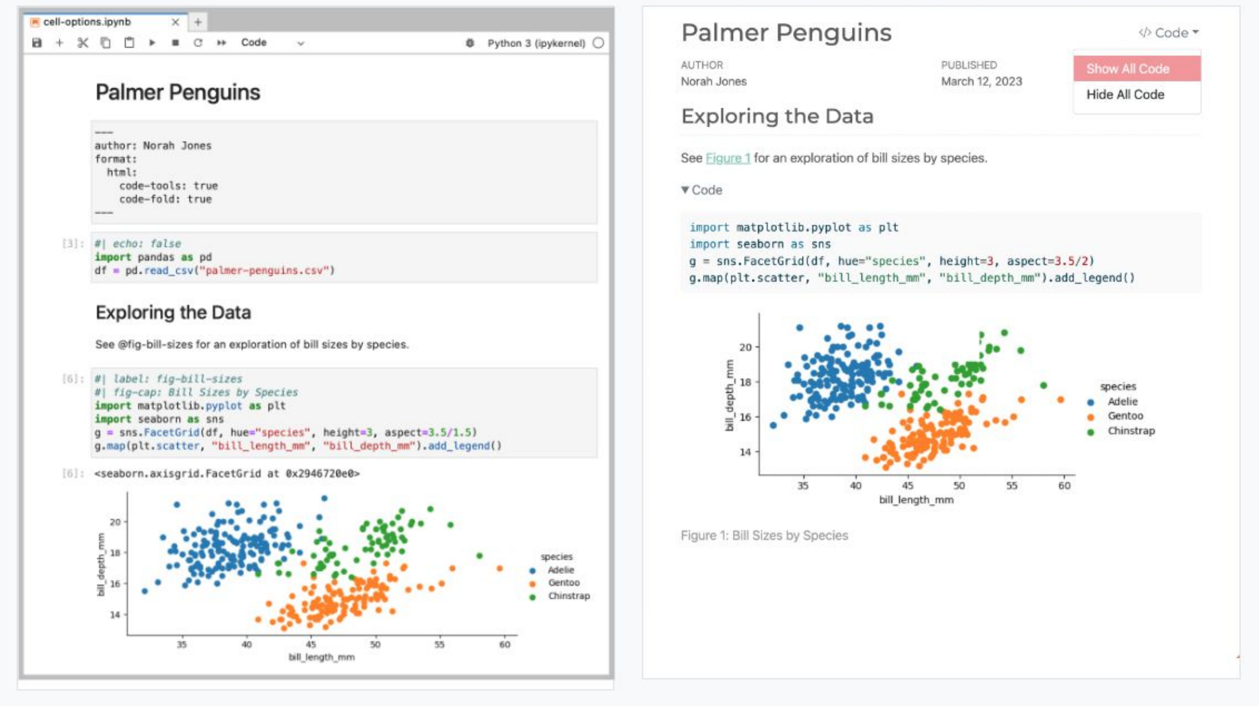
Air Quality

Figure 1 further explores the impact of temperature on ozone level.

▶ Code

Figure 1: Temperature and ozone level.

With Jupyter



Palmer Penguins

```
---
author: Norah Jones
format:
  html:
    code-tools: true
    code-fold: true
---
```

```
[3]: #| echo: false
     import pandas as pd
     df = pd.read_csv("palmer-penguins.csv")
```

Exploring the Data

See @fig-bill-sizes for an exploration of bill sizes by species.

```
[6]: #| label: fig-bill-sizes
     #| fig-cap: Bill Sizes by Species
     import matplotlib.pyplot as plt
     import seaborn as sns
     g = sns.FacetGrid(df, hue="species", height=3, aspect=3.5/1.5)
     g.map(plt.scatter, "bill_length_mm", "bill_depth_mm").add_legend()

[6]: <seaborn.axisgrid.FacetGrid at 0x2946720e0>
```

Palmer Penguins

AUTHOR
Norah Jones

PUBLISHED
March 12, 2023

Exploring the Data

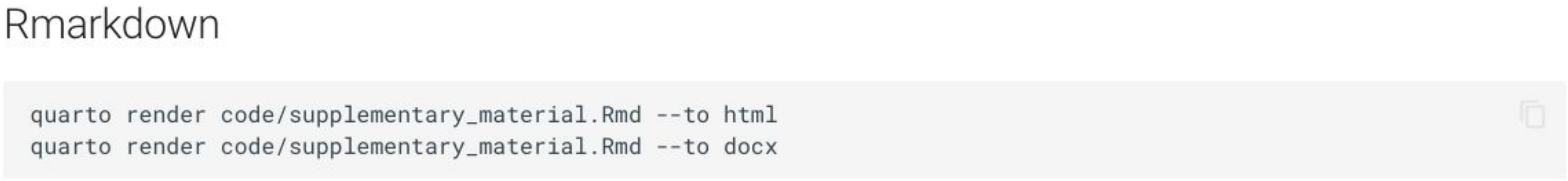
See Figure 1 for an exploration of bill sizes by species.

▼ Code

```
import matplotlib.pyplot as plt
import seaborn as sns
g = sns.FacetGrid(df, hue="species", height=3, aspect=3.5/2)
g.map(plt.scatter, "bill_length_mm", "bill_depth_mm").add_legend()
```

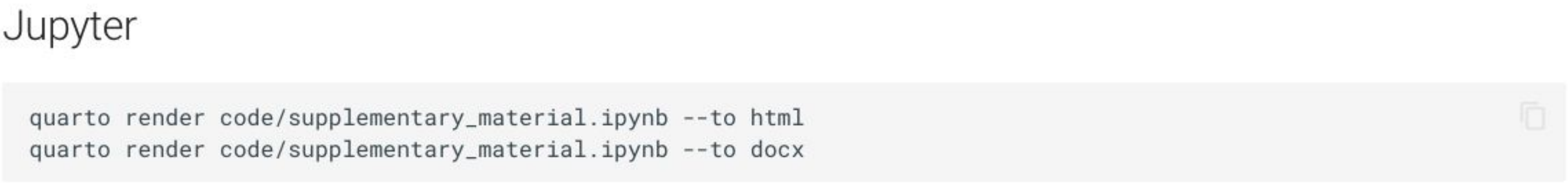
Figure 1: Bill Sizes by Species

Really simple?



Rmarkdown

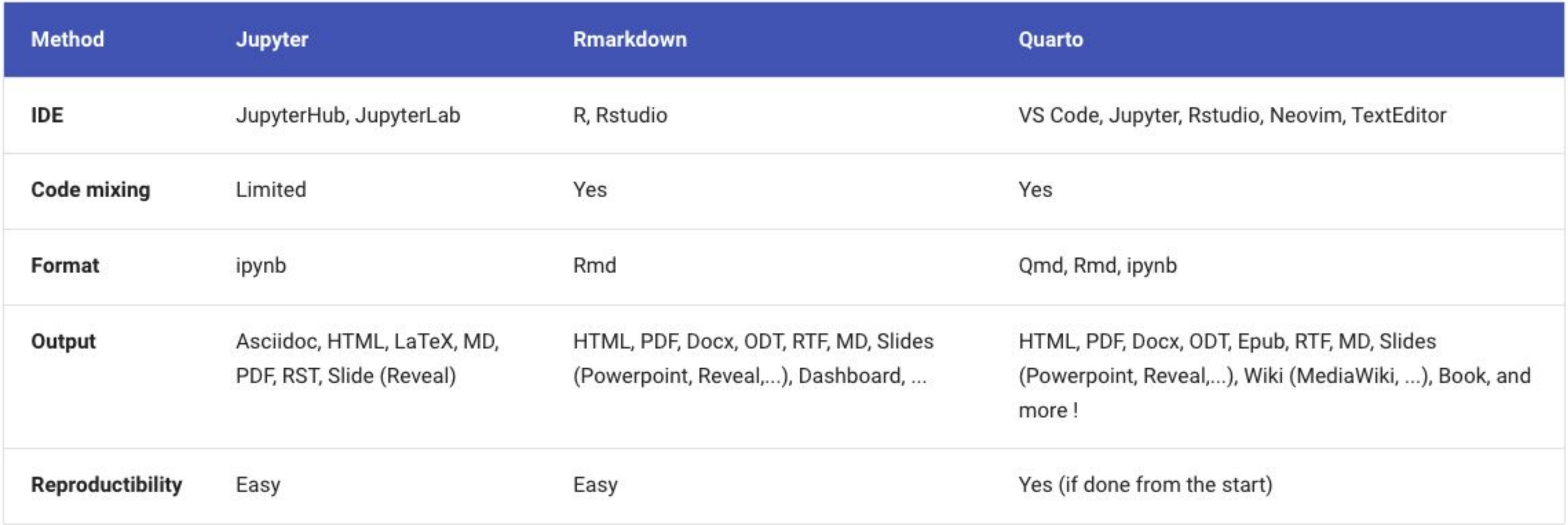
```
quarto render code/supplementary_material.Rmd --to html
quarto render code/supplementary_material.Rmd --to docx
```



Jupyter

```
quarto render code/supplementary_material.ipynb --to html
quarto render code/supplementary_material.ipynb --to docx
```

Comparaison



Method	Jupyter	Rmarkdown	Quarto
IDE	JupyterHub, JupyterLab	R, Rstudio	VS Code, Jupyter, Rstudio, Neovim, TextEditor
Code mixing	Limited	Yes	Yes
Format	ipynb	Rmd	Qmd, Rmd, ipynb
Output	Asciidoc, HTML, LaTeX, MD, PDF, RST, Slide (Reveal)	HTML, PDF, Docx, ODT, RTF, MD, Slides (Powerpoint, Reveal,...), Dashboard, ...	HTML, PDF, Docx, ODT, Epub, RTF, MD, Slides (Powerpoint, Reveal,...), Wiki (MediaWiki, ...), Book, and more !
Reproductibility	Easy	Easy	Yes (if done from the start)

And now we try?