FAIR_bioinfo for bioinformaticians

Introduction to the tools of reproducibility in bioinformatics

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à compléter

Sept. 2020

Literate programming

Introduction

What is literate programming ?

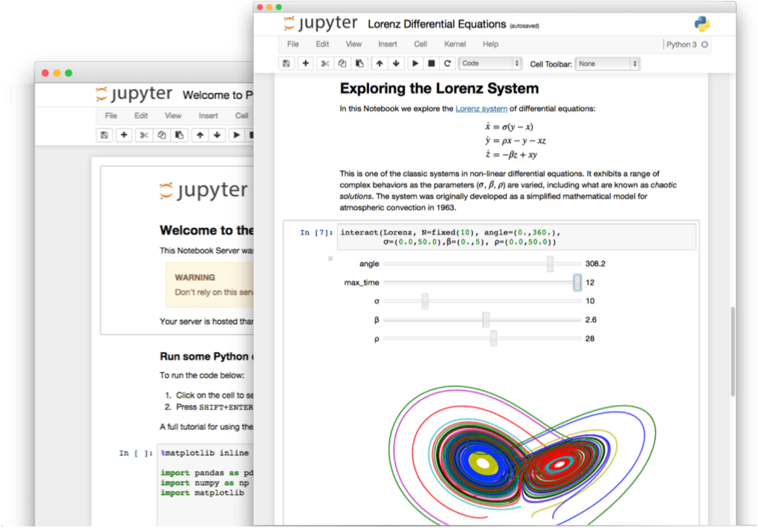
Definition

"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."

Wikipedia, 18/08/2020 (https://en.wikipedia.org/wiki/Literate_programming#Workflow)

Introduction

What does it look like ?



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Run some Python

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A full tutorial for using the

```
In [ ]: %matplotlib inline

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

jupyter Lorenz Differential Equations (autosaved)
File Edit View Insert Cell Kernel Help
Python 3
Code
Cell Toolbar: None

Exploring the Lorenz System

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

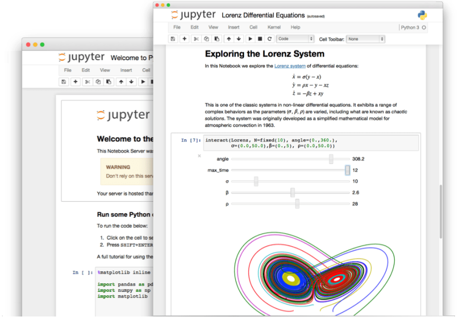
$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = \rho x - y - xz$$
$$\dot{z} = -\beta z + xy$$

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
```

Introduction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Interactive programming interface allowing to combine both natural and computer languages.

In one file:

- Explanations
- Code
- Results
- Graphs and plots

Introduction

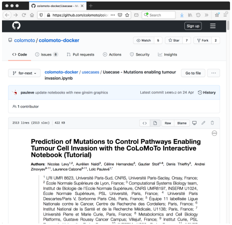
Why using literate programming frameworks ?

Use cases:

- Day to day analyses
- Analysis reports
- Writing scientific articles

Example of an article entirely written using a notebook

File (on a repository)



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

pauleve update notebooks with new ginsim graphics Latest commit 1498c2 on 24 Apr History

1 contributor

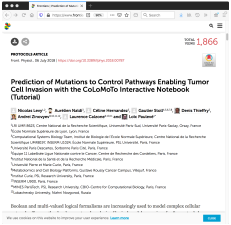
2513 lines (2513 sloc) 422 KB

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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[11]MINES ParisTech, PSL Research University, CBIO-Centre for Computational Biology, Paris, France
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Boolean and multi-valued logical formalisms are increasingly used to model complex cellular

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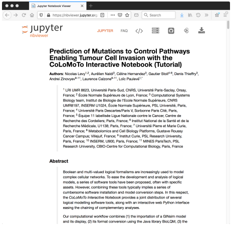
Executable file



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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

Literate programming

This session :

- Markdown
- Rmarkdown and RStudio
- Jupyter

Markup and markdown

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.

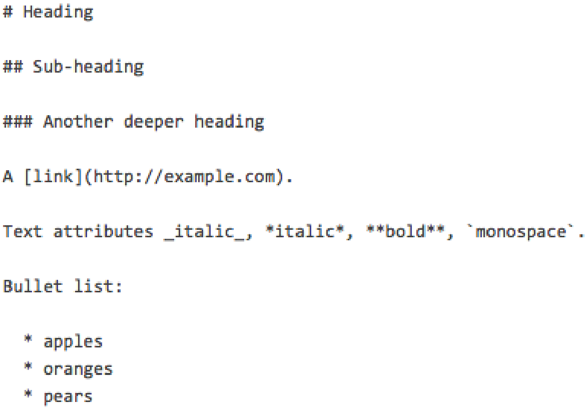
Markdown language

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

Markdown language

You've probably see it already on GitHub (README), Wikipedia...

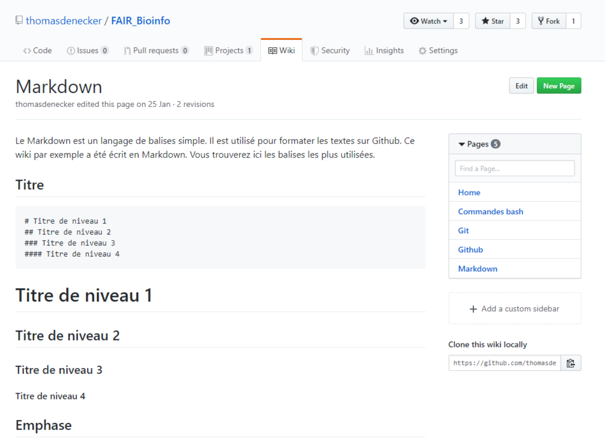


```
# Heading

## Sub-heading

### Another deeper heading

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

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

Bullet list:

  * apples
  * oranges
  * pears
```

Github guides : https://guides.github.com/features/mastering-markdown/

Markdown language

Une page de wiki est disponible sur FAIR_bioinfo
https://github.com/thomasdenecker/FAIR_Bioinfo/wiki/Markdown



Markdown

thomasdenecker edited this page on 25 Jan · 2 revisions

Le Markdown est un langage de balises simple. Il est utilisé pour formater les textes sur Github. Ce wiki par exemple a été écrit en Markdown. Vous trouverez ici les balises les plus utilisées.

Titre

```
# Titre de niveau 1
## Titre de niveau 2
### Titre de niveau 3
#### Titre de niveau 4
```

Titre de niveau 1

Titre de niveau 2

Titre de niveau 3

Titre de niveau 4

Emphase