

# Development and calibration of tumor models

Ernesto A. B. F. Lima  
Emanuelle A. Paixão



MINISTÉRIO DA  
CIÊNCIA, TECNOLOGIA  
E INOVAÇÕES



# Working with Python

- Introduction to Python
- Solving Ordinary Differential Equations

# Python advantages and disadvantages

## Disadvantages

- Slow speed (interpreted and dynamically-typed language)
- Not memory efficient
- Runtime errors

## Advantages

- Easy to read, learn, write, and debug
- Dynamically typed
- Free and open-source
- Vast libraries support
- Portability

A web-based, interactive computing tool for capturing the whole computation process: developing, documenting, and executing code, as well as communicating the results.

# Jupyter Notebook

jupyter example Last Checkpoint: a few seconds ago (autosaved)



Logout

File Edit View Insert Cell Kernel Help

Trusted

Python 3



In [ ]:

# Jupyter Notebook

jupyter example Last Checkpoint: 2 minutes ago (autosaved)



Logout

Trusted

Python 3

File Edit View Insert Cell Kernel Help



- Code
- Code
- Markdown
- Raw NBConvert
- Heading



In [ ]:



Logout

File Edit View Insert Cell Kernel Help

Trusted | Python 3



## # Day 02 ## Python

```
\begin{equation}
\frac{\partial \phi}{\partial t} = x\phi
\end{equation}
```

In [ ]: var=2

In [ ]: print(var)  
var=3

In [ ]: print(var)  
var=4

In [ ]:

jupyter example Last Checkpoint: 24 minutes ago (unsaved changes)



Logout

File Edit View Insert Cell Kernel Help

Trusted

Python 3



## Day 02

### Python

$$\frac{\partial \phi}{\partial t} = x\phi$$

In [1]: `var=2`

In [2]: `print(var)`  
`var=3`

2

In [3]: `print(var)`  
`var=4`

3

In [ ]:

# Jupyter Notebook

jupyter example Last Checkpoint: 24 minutes ago (unsaved changes)



Logout

File Edit View Insert Cell Kernel Help

Trusted

Python 3



## Day 02

### Python

$$\frac{\partial \phi}{\partial t} = x\phi$$

In [1]: `var=2`

In [ ]: `print(var)`  
`var=3`

In [2]: `print(var)`  
`var=4`

2

In [ ]:

jupyter example Last Checkpoint: 24 minutes ago (unsaved changes)



Logout

File Edit View Insert Cell Kernel Help

Trusted

Python 3



## Day 02

### Python

$$\frac{\partial \phi}{\partial t} = x\phi$$

In [1]: `var=2`

In [3]: `print(var)`  
`var=3`

4

In [2]: `print(var)`  
`var=4`

2

In [ ]:

# Jupyter Notebook - Binder

A screenshot of a Jupyter Notebook interface. The top navigation bar includes File, Edit, View, Run, Kernel, Tabs, Settings, and Help. The tabs show Launcher, part2\_python.ipynb, and Untitled.ipynb, with Untitled.ipynb currently active. The toolbar below the tabs includes icons for file operations like New, Open, Save, and Print, along with links for Download, GitHub, and Binder, and a Code dropdown menu. The main workspace shows a single code cell starting with '[ ]:'.

Python 3 (ipykernel)

Simple  0  2  Python 3 (ipykernel) | Idle Mem: 218.83 / 2048.00 MB Mode: Command  Ln 1, Col 1 Untitled.ipynb

# Jupyter Notebook - Binder ( $\approx$ 10 min)

The screenshot shows a Jupyter Notebook interface with the following details:

- File Bar:** File, Edit, View, Run, Kernel, Tabs, Settings, Help.
- Launcher:** Shows the current notebook tab: part2\_python.ipynb.
- File Explorer:** Displays a list of files in the current directory:
  - part2\_pyth... (selected, an hour ago)
  - part3\_calib... (2 hours ago)
  - README.... (2 hours ago)
  - requireme... (2 hours ago)
- Code Editor:** Shows code cells and their outputs.
  - [1]:

```
# Here I am printing
print(5)
print(1+1)
```

Output:  
5  
2
  - Section Header:** Variables
  - [2]:

```
variable = 2.3
Five = 5
message = "This is a string"
print (variable)
print (Five + Five)
print(variable,message,Five)
```

Output:  
2.3  
10  
2.3 This is a string 5
  - [3]:

```
print("Message:", message)
print("{0} is an int and {1} is a float".format(Five,variable))
print("{1} is a float and {0} is an int".format(Five,variable))
```
  - [4]:

```
print("hello" + " world")
print("number" * 5)
```
- Bottom Status Bar:** Simple, 0 5 0, No Kernel | Unknown, Mem: 98.76 / 2048.00 MB, Mode: Command, Ln 1, Col 1, part2\_python.ipynb.

# Jupyter Notebook - Binder ( $\approx$ 10 min)

The screenshot shows a Jupyter Notebook interface within a browser window. The top navigation bar includes File, Edit, View, Run, Kernel, Tabs, Settings, and Help. A sidebar on the left contains a file tree with items like 'part2\_python.ipynb' (selected), 'part3\_calib...', 'README...', and 'requireme...'. The main area displays a code cell [1] with the following Python code:

```
[1]: # Here I am printing
      print(5)
      print(1+1)
```

The output of this cell is:

```
5
2
```

## Variables

When declaring a variable, capitalization is important!

The next code cell [2] demonstrates this:

```
[2]: variable = 2.3
      Five = 5
      message = "This is a string"
      print(variable)
      print(Five + Five)
      print(variable,message,Five)
```

The output of this cell is:

```
2.3
10
2.3 This is a string 5
```

The final code cell [1] shows an attempt to mix variable types in a print statement:

```
[1]: print("Message:", message)
      print("{0} is an int and {1} is a float".format(Five,variable))
      print("{1} is a float and {0} is an int".format(Five,variable))
```

This results in a **NameError**:

```
NameError Traceback (most recent call last)
<ipython-input-1-92ed82c22121> in <module>
```

The bottom status bar indicates the kernel is 'Python 3 (ipykernel)', memory usage is 'Mem: 158.77 / 2048.00 MB', and the current mode is 'Command'.

# Jupyter Notebook - Binder ( $\approx 10$ min)

The screenshot shows a Jupyter Notebook interface with a 'Select Kernel' dialog box overlaid on the main workspace.

**File Edit View Run Kernel Tabs Settings Help**

**Launcher** part2\_python.ipynb GitHub Binder Code No Kernel

**Variables**

Select Kernel

Select kernel for: "part2\_python.ipynb"

Python 3 (ipykernel) Select

No Kernel

**Code Cells:**

```
[1]: # Here I am printing
      print(5)
      print(1+1)

      5
      2
```

```
[2]: variable = 2.3
      Five = 5
      message = "This is a string"
      print (variable)
      print (Five + variable)
      print(variable,message,Five)

      2.3
      10
      2.3 This is a string 5
```

```
[3]: print("Message:", message)
      print("{0} is an int and {1} is a float".format(Five,variable))
      print("{1} is a float and {0} is an int".format(Five,variable))

      Message: This is a string 5
      5 is an int and 10.0 is a float
      10.0 is a float and 5 is an int
```

```
[4]: print("hello" + "world")
      print("number" * 5)

      helloelloworld
      numbernumbernumbernumbernumber
```

Simple 0 0 No Kernel | Unknown Mem: 98.76 / 2048.00 MB Mode: Command Ln 1, Col 1 part2\_python.ipynb

# Jupyter Notebook - Binder

Search or jump to... Pull requests Issues Marketplace Explore

Ernesto-Lima / ISMCO2021 Public

Code Issues Pull requests Actions Projects Wiki Security Insights Settings

master 1 branch 0 tags Go to file Add file Code

Ernesto-Lima Update README.md 2845d48 1 hour ago 5 commits

File	Commit	Date
.gitignore	Initial commit	yesterday
README.md	Update README.md	1 hour ago
part2_python.ipynb	Adding the code	1 hour ago
part3_calibration.ipynb	Adding the code	1 hour ago
requirements.txt	Adding requirements	5 hours ago

About How can (experimental) data go on tumor growth models?

Readme

Releases No releases published Create a new release

Packages No packages published Publish your first package

Languages Jupyter Notebook 100.0%

ISMCO2021

## How can (experimental) data go on tumor growth models?

Our goal in this tutorial is to show an introduction about modeling in the context of cancer, addressing discrete, continuous, and hybrid models. Examples and interpretation of different types of functions are addressed for the description of tumor growth, mortality, and therapies, among other biological phenomena. We also aim to introduce the attendees to the Python programming language, methods of solving ordinary differential equation models, and model calibration via Bayesian methods. The attendees will have hands-on experience on ordinary differential equation solvers and model calibration.

### Intended Audience

Any person interested in the development and calibration of tumor models, or people already familiar with tumor models that are interested in learning how to calibrate these models.

Show all

README.md

**Objectives**

- Provide an overview on the development of tumor growth models.
- Provide an introduction to Python and how to solve ordinary differential equations.
- Provide hands-on training on how to calibrate tumor growth models.

**Duration**

Full-day course.

**Activities**

- Development of tumor growth models (theory): an introduction to discrete, continuous, and hybrid models. Our goal is to familiarize the participants with the biological motivation for using different models of tumor growth.
- Introduction to Python + Development of tumor growth models (hands-on): show basic concepts of Python (variables, read/write files, loops, ...) and how to solve ordinary differential equation models and visualize the results.
- Calibration of tumor growth models (theory and hands-on): an introduction to concepts related to Bayesian calibration. We will present a brief introduction to model calibration and the Bayesian theory. In the hands-on part, the attendees will generate *in silico* data using the model implemented in (2) and calibrate the model parameters using the emcee Python library.

**Organizers**

Ernesto Lima, The University of Texas at Austin, USA

Emanuelle Paixao, National Laboratory of Scientific Computing (LNCC), Brazil

 [launch binder](#)

README.md

No pre-requisites are required to follow this tutorial. We will give an introduction to Python such as everyone can follow the exercises.

**Objectives**

- Provide an overview on the development of tumor growth models.
- Provide an introduction to Python and how to solve ordinary differential equations.
- Provide hands-on training on how to calibrate tumor growth models.

**Duration**

Full-day course.

**Activities**

- Developing tumor growth models in Python
- Introduction to Python and ODEs
- Calibration of tumor growth models

is to familiarize attendees with the Python ecosystem for scientific computing.

Introduction to discrete, continuous, and hybrid models. Our goal is to introduce basic concepts of Python and its libraries for solving ordinary differential equation models and visualize the results.

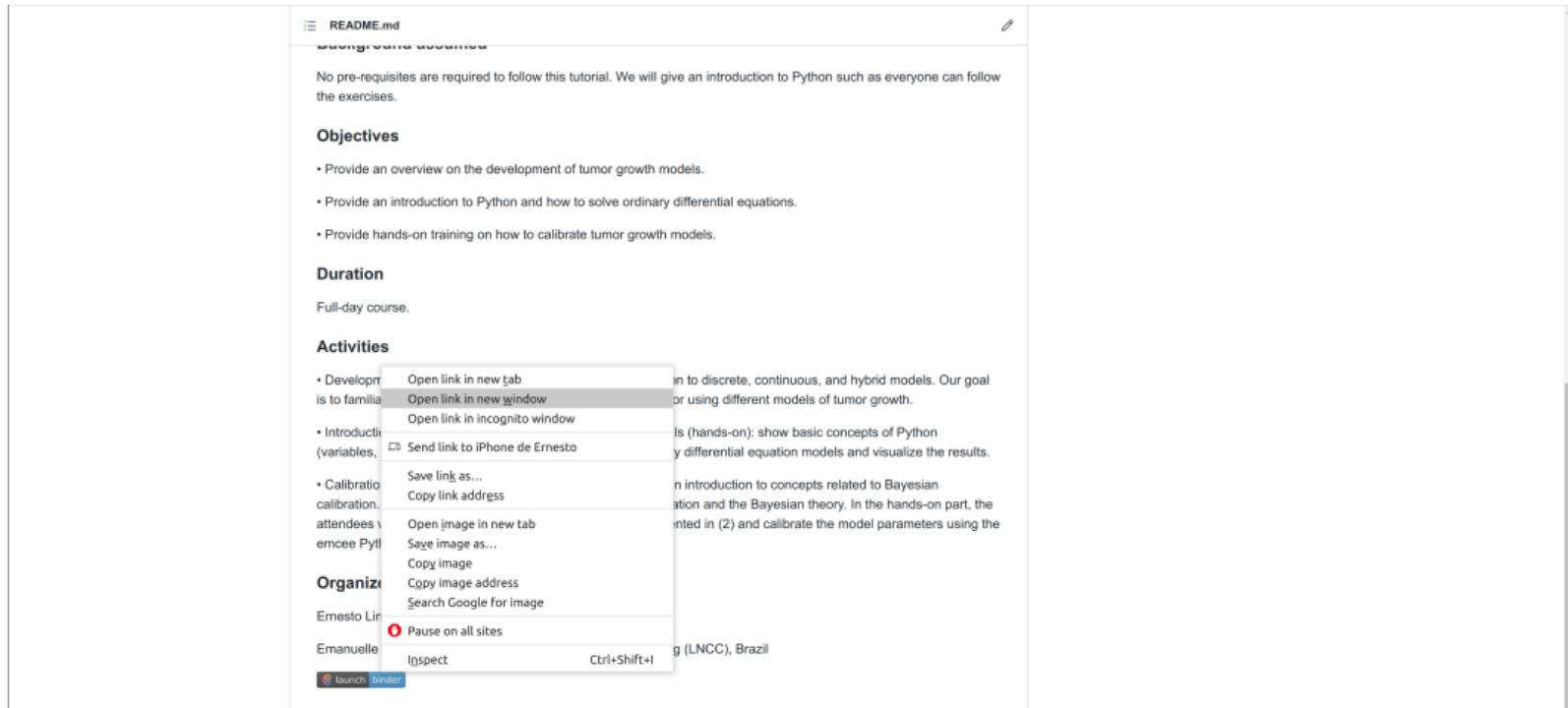
Send link to iPhone de Ernesto Linhares

Save link as...  
Copy link address  
Open image in new tab  
Save image as...  
Copy image  
Copy image address  
Search Google for image

Organized by Ernesto Linhares and Emanuelle Góes (LNCC), Brazil

● Pause on all sites

Launch binder



# Jupyter Notebook - Binder

Thanks to Google Cloud, OVH, GESIS Notebooks and the Turing Institute for supporting us! 🎉



Starting repository: Ernesto-Lima/ISMCO2021/HEAD

New to Binder? Check out the [Binder Documentation](#) for more information

Build logs

[view raw](#) [show](#)

Here's a non-interactive preview on nbviewer while we start a server for you. Your binder will open automatically when it is ready.



JUPYTER

FAQ



ISMCO2021

Name

◀◀ Ernesto-Lima's repositories

▶▶ part2\_python.ipynb

▶▶ part3\_calibration.ipynb

▶▶ .gitignore

▶▶ README.md

▶▶ requirements.txt

# Jupyter Notebook - Binder

File Edit View Run Kernel Tabs Settings Help

+ Filter files by name

Name / Last Modified

- part2\_pyth... an hour ago
- part3\_calib... an hour ago
- README.... an hour ago
- requireme... an hour ago

Launcher

Notebook

Python 3 (ipykernel)

Console

Python 3 (ipykernel)

Other

Terminal

Text File

Markdown File

Python File

Show Contextual Help

Simple 0 0 Mem: 98.77 / 2048.00 MB

Launcher

# Jupyter Notebook - Binder

File Edit View Run Kernel Tabs Settings Help

+ Filter files by name

Name / Last Modified

- part2\_pyth...
- part3\_calib...
- README....
- requireme...

Open With

- Open
- Open in New Browser Tab

Rename F2  
Delete  
Cut Ctrl+X  
Copy Ctrl+C  
Duplicate Ctrl+D  
Download

Shut Down Kernel

Copy Download Link  
Copy Path  
Copy Shareable Link

New Folder  
New File  
New Markdown File  
Paste Ctrl+V

Shift+Right Click for Browser Menu

Simple 0 5 0 Mem: 98.77 / 2048.00 MB

Launcher

Launcher

Notebook

Text File

Markdown File

Python File

Show Contextual Help

Simple 0 5 0 Mem: 98.77 / 2048.00 MB

Launcher

Shift+Right Click for Browser Menu

Simple 0 5 0 Mem: 98.77 / 2048.00 MB

Launcher

Shift+Right Click for Browser Menu

The image shows a Jupyter Notebook interface with the following components:

- File Browser:** On the left, there's a sidebar with a file tree. A file named "part2\_python.ipynb" is currently selected. Other files visible include "part3\_calib...", "README....", and "requireme...".
- Code Editor:** The main workspace displays the following text:

```
Part 02

Introduction to
Python and
ODE Solver

A web-based, interactive
computing tool for
capturing the whole
computation process:
developing, documenting,
and executing code, as
well as communicating the
results.

• Ctrl-Enter: run cell in-
place
• Shift-Enter: run cell
• Alt-Enter: run cell,
insert below

Indentation matters!
```
- Preview Area:** To the right of the code editor, there's a preview pane showing the rendered content of the notebook, which includes the title "Part 02" and the introduction text.
- Bottom Status Bar:** The status bar at the bottom provides information about the kernel, memory usage, and current mode.
- Bottom Navigation:** At the very bottom, there are navigation icons for back, forward, search, and other notebook operations.



The image shows a Jupyter Notebook interface running on a Binder instance. On the left, there's a dark sidebar featuring a portrait of a man (Ernesto Lima) and a small footer with his name. The main area is a notebook titled "part2\_python.ipynb". The first cell contains the title "Part 02" and a subtitle "Introduction to Python and ODE Solver". It also includes a brief description of what Jupyter is and some keyboard shortcuts for running cells. Below that, it says "Indentation matters!" and "Capitalization is important!". The bottom cell shows a code snippet that prints the number 5 and 2.

File Edit View Run Kernel Tabs Settings Help

Launcher part2\_python.ipynb

Part 02

## Introduction to Python and ODE Solver

A web-based, interactive computing tool for capturing the whole computation process: developing, documenting, and executing code, as well as communicating the results.

- Ctrl-Enter: run cell in-place
- Shift-Enter: run cell
- Alt-Enter: run cell, insert below

Indentation matters!

Capitalization is important!

```
[1]: 
```

```
[1]: # Here I am printing
      print(5)
      print(1+1)
```

```
5
2
```

Simple 0 s. 1 Python 3 (ipy... Mem: 159.80 / ... Mode: ... Ln ... part2\_py...

# Jupyter Notebook - Binder

The screenshot shows a Jupyter Notebook interface with the following details:

- Toolbar:** File, Edit, View, Run, Kernel, Tabs, Settings, Help.
- Tab Bar:** Launcher (selected), part2\_python.ipynb, Download, GitHub, Binder, Code, Python 3 (ipykernel).
- Section Headers:** Part 02, Introduction to Python and ODE Solver.
- Description:** A web-based, interactive computing tool for capturing the whole computation process: developing, documenting, and executing code, as well as communicating the results.
- Code and Output:**
  - Code cell [1]:

```
# Here I am printing
print(5)
print(1+1)
```
  - Output:

```
5
2
```
- Section Header:** Variables.
- Bottom Status Bar:** Simple, 0, Python 3 (ipykernel) | Idle, Mem: 218.24 / 2048.00 MB, Mode: Command, Ln 1, Col 1, part2\_python.ipynb, part2\_python.ipynb, Show all, x.

# Jupyter Notebook - Binder

File Edit View Run Kernel Tabs Settings Help

+ Filter files by name

Name Last Modified

- part2\_pyth... 5 minutes ago
- part3\_calib... an hour ago
- README.... an hour ago
- requireme... an hour ago
- Untitled.ip... a minute ago

Launcher

Notebook

Python 3 (ipykernel)

Console

Python 3 (ipykernel)

Other

Terminal Text File Markdown File Python File Show Contextual

Simple 0 Mem: 218.02 / 2048.00 MB Launcher

Show all x

part2\_pyth...ipynb

# Jupyter Notebook - Binder

File Edit View Run Kernel Tabs Settings Help

+ Filter files by name

Name / Last Modified

- part2\_pyth... seconds ago
- part3\_calib... an hour ago
- README.... an hour ago
- requireme... an hour ago
- Untitled.ip... 3 minutes ago

Launcher

Notebook

Python 3 (ipykernel)

Overwrite file?  
"part2\_python.ipynb" already exists, overwrite?

Cancel Overwrite

Console

Python 3 (ipykernel)

Other

Terminal Text File Markdown File Python File Show Contextual

Simple 0 Mem: 218.16 / 2048.00 MB Launcher

part2\_pyth...ipynb Show all

<https://github.com/Ernesto-Lima/ISMCO2021>