

# Data Visualization 201

Advanced concepts  
using OpenSource software



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# Introduction



A picture speaks a thousand words

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*Napoléon 1er*

# Outline



- ▶ Introduction : Why plotting ?
- ▶ Guidelines to plot **WELL**
- ▶ Tutorial: using matplotlib

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As scientists, we plot in order to:

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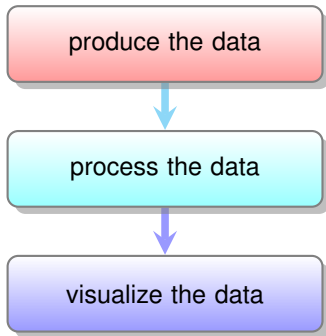
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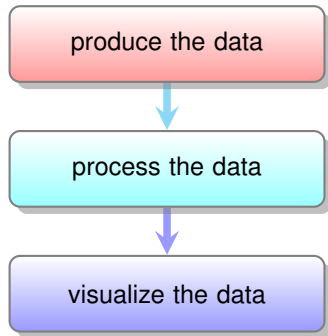
**Hence:** having good tools and work-flow is mandatory to be *efficient*



# Introduction : Why plotting ?



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- ▶ Produce the data
  - ▶ Experiment/ Simulation
  - ▶ Takes a lot of time
- ▶ process the data
  - ▶ use whatever tool you prefer (python, matlab, excel...)
  - ▶ stock and keep both the raw and the processed data
- ▶ Visualize
  - ▶ Use whatever tool you prefer
  - ▶ not necessary the same tool as for processing

# Introduction : Why plotting ?

My own tools



There is My own tools and work-flow:

- ▶ Produce data via simulation : takes **2-5 days** each
- ▶ store data in hierarchic format (**HDF5**, for management of extremely large and complex data collections).
- ▶ **Python** for processing
- ▶ **Matplotlib** (python library) for plotting
  - ▶ **homemade** library for systematic plots
  - ▶ generates **~25 plots and ~10 movies** automatically for each plots
  - ▶ dedicated **scripts** for presentation/paper/reports

# Guidelines to plot WELL



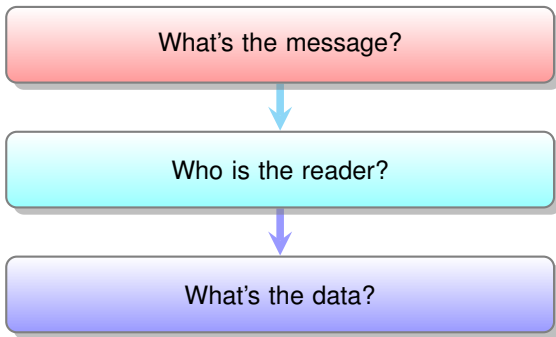
Plotting nice figures **is not magic**.

There is **some recipes** to help you.

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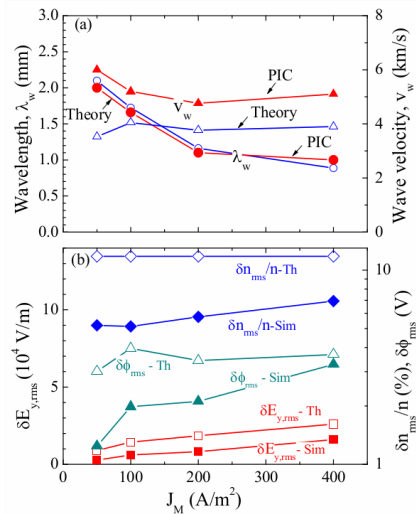
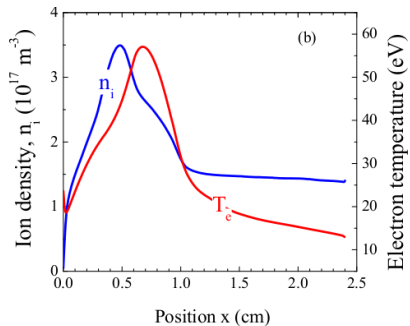
Questions to ask yourself before even starting:

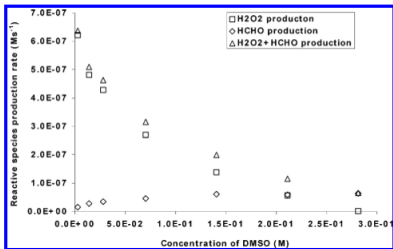


## Quiz time

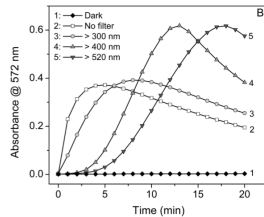


**Quiz time** : Which figure is the best ?



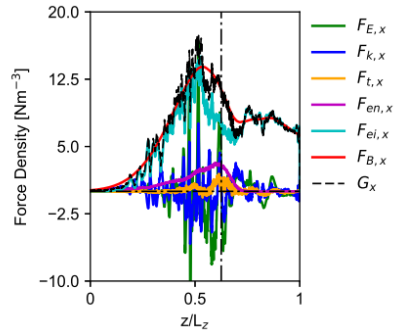
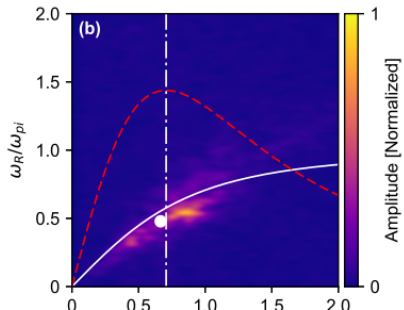
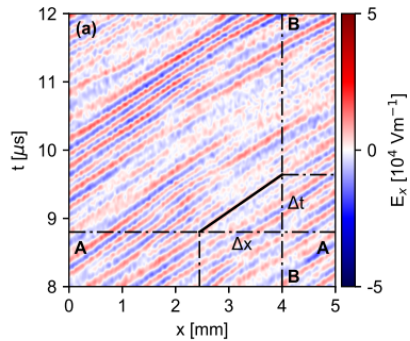


**Figure 8.** Production rate of stable molecular products from hydroxyl radical reactions as a function of DMSO concentration.

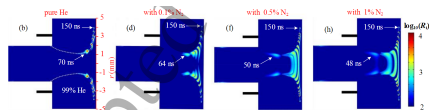
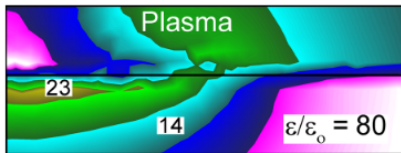
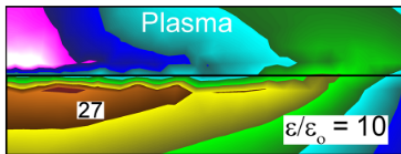
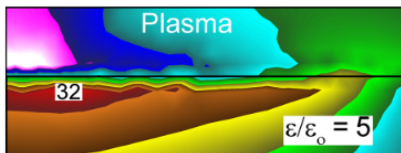
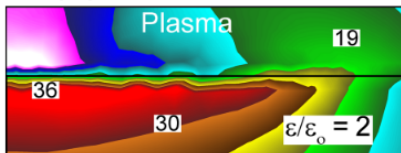


**Figure 1.** Photo-induced oxidation of Amplex Red with production of resorufin during irradiation as measured by UV-vis absorption. (A) Absorption spectra of 10 µM AR solution at pH 7.4 after irradiation (> 520 nm) for every minute from 0 to 18 min. The arrow indicates direction of the changes. (B) Plot of peak absorbance of RSF at 572 nm against irradiation time (1, dark; 2, no filter; 3, > 300 nm; 4, > 400 nm, and 5, > 520 nm). The fluence rate (from 250 to 850 nm) was 0, 0.392, 0.329, 0.322, and 0.271 W/cm<sup>2</sup> as measured with a SPR-4001 Spectroradiometer (Luzchem Research Inc., Ottawa Ontario, Canada).





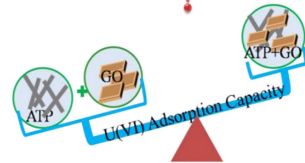
(b)  $|E|$  3 - 35 kV-cm<sup>-1</sup> 80 ns



## TOC



Two kinds of single adsorbents ? Heterogeneous aggregate



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Simple to understand

Enjoyable to look at

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*an **Enjoyable** figure will convey **more information** !*

## Some Rules, not absolute and not exhaustive:<sup>123</sup>

- ▶ 2-3 lines max if complex graph
- ▶ Think of the black-and-white prints
- ▶ Consistent representation
- ▶ Adapt to the Support Medium
- ▶ Be concise (save ink)
- ▶ Be efficient (script, optimize)
- ▶ Check of typos and consistency
- ▶ Do Not Trust the Defaults
- ▶ large font size
- ▶ Uses a good the font
- ▶ Use vectoriel format (\*.eps, \*.pdf, \*.svg)
- ▶ Use Color Effectively
- ▶ Label axis and use units

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<sup>1</sup>Ten Simple Rules for Better Figures,  
[journals.plos.org/ploscompbiol/article?id=10.1371/journal.pcbi.1003833](https://journals.plos.org/ploscompbiol/article?id=10.1371/journal.pcbi.1003833)

<sup>2</sup>Graphical Excellence in Scientific Presentations and Papers, [www3.nd.edu/~pkamat/pdf/graphs.pdf](http://www3.nd.edu/~pkamat/pdf/graphs.pdf)

<sup>3</sup>personal opinion and experience





Live example of matplotlib tips and tricks

Never do a live example

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*everyone*