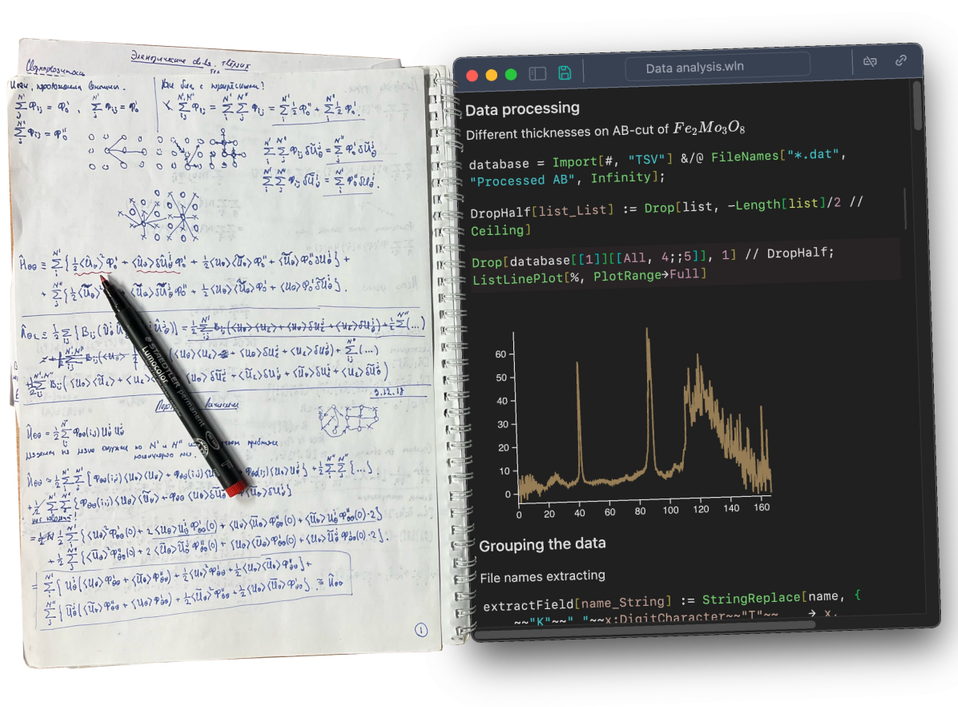
DPG 2024

Computational Notebook as a multitool for modern scientists

Kirill Vasin

To start the presentation Focus on a slide and press `f` key

Computational Notebook as a Modern Multitool for Scientists



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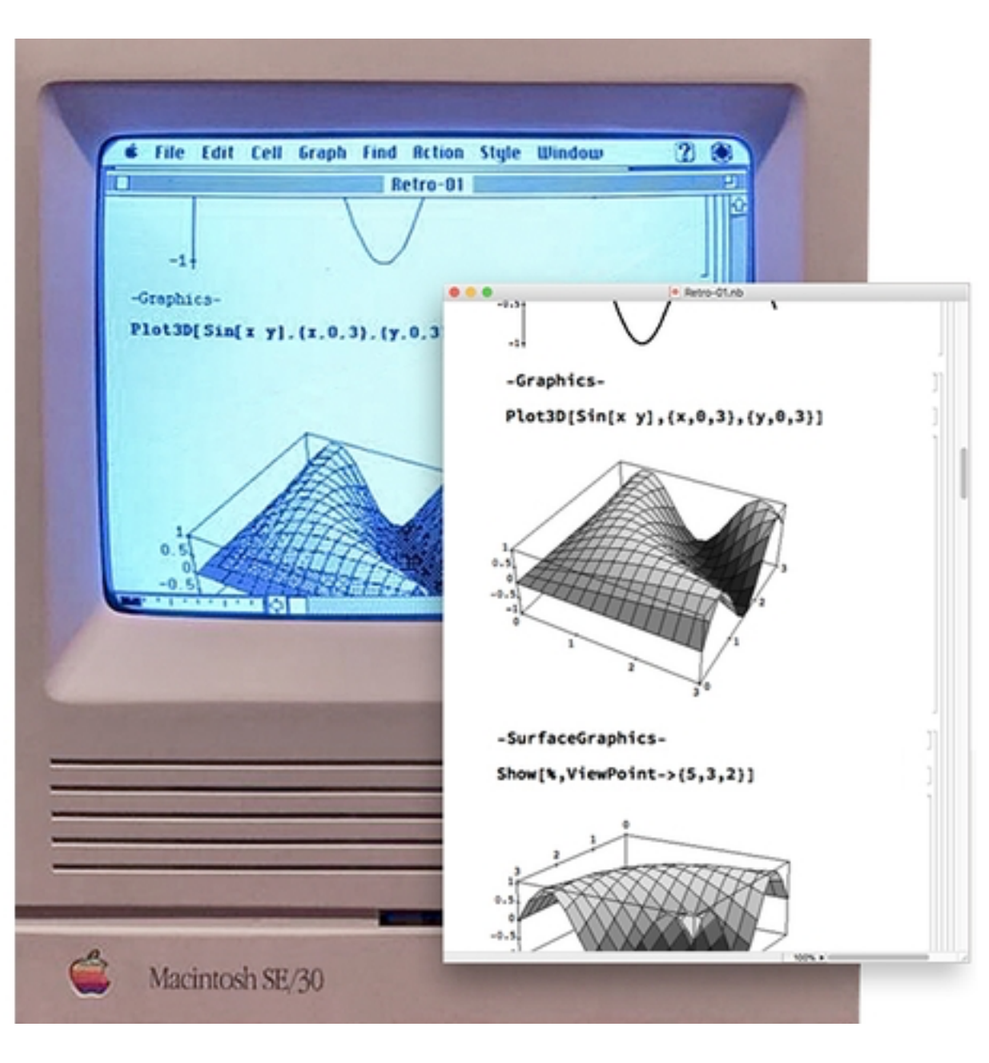
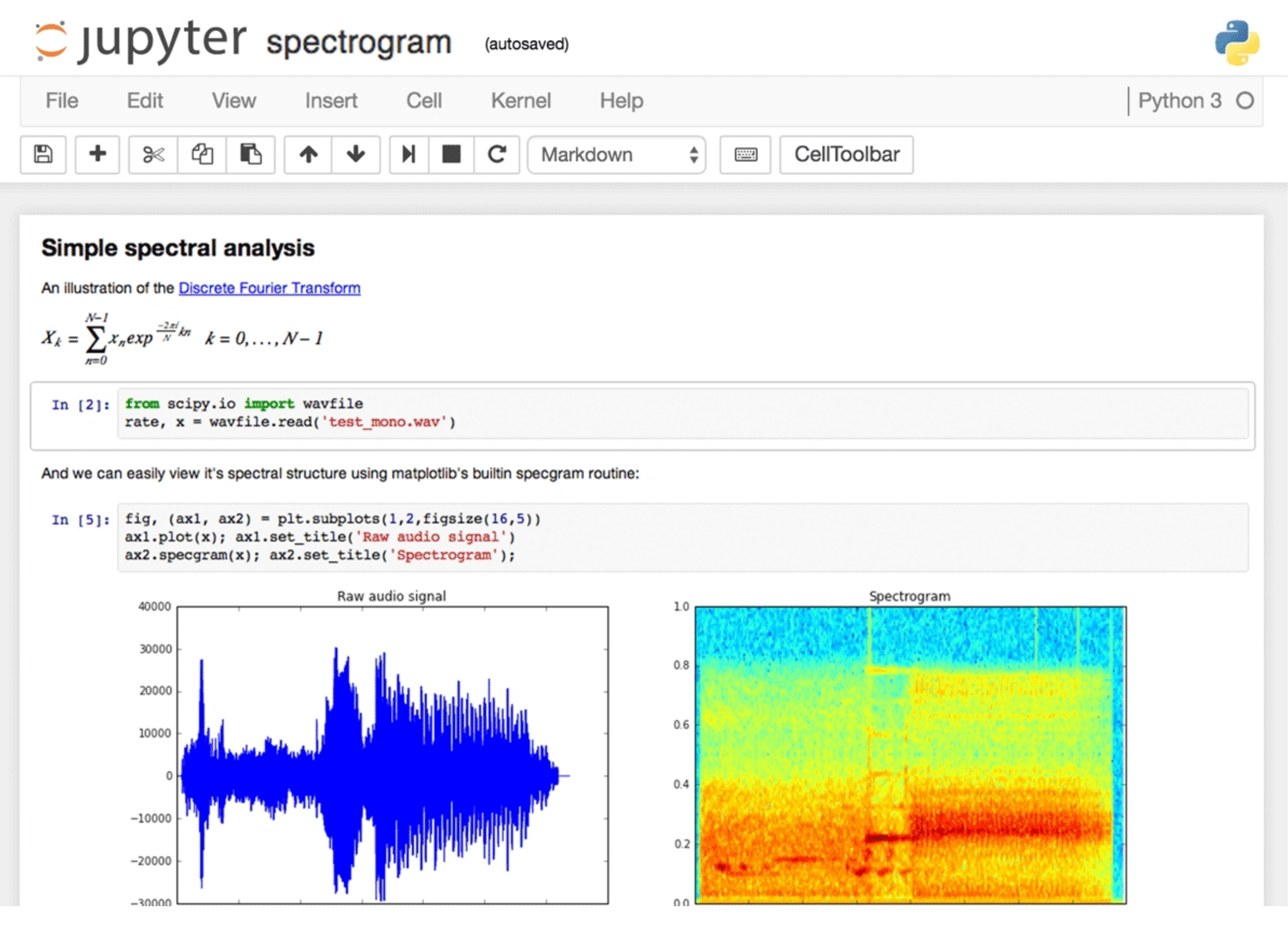
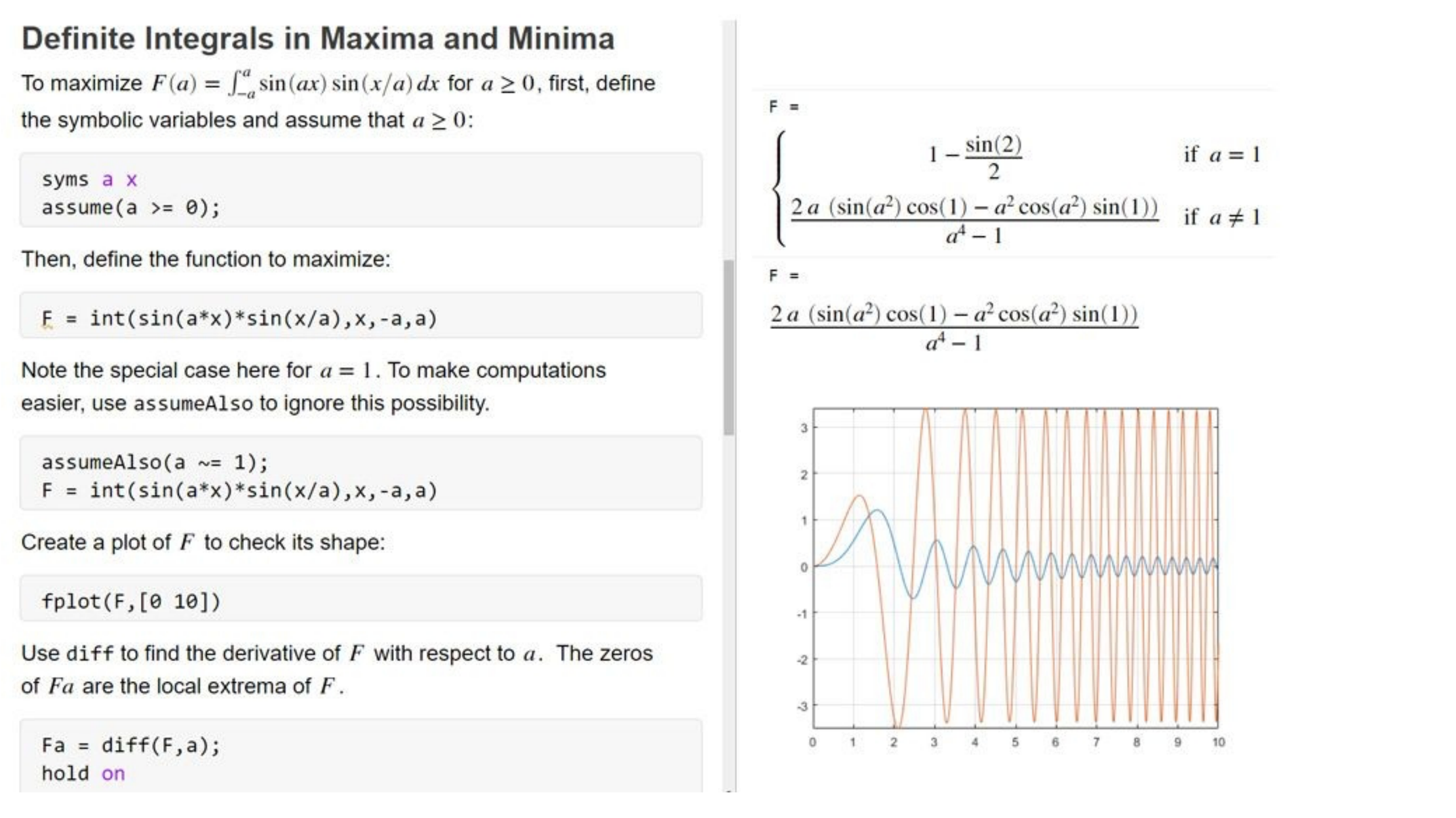




jupyter spectrogram (autosaved)
File Edit View Insert Cell Kernel Help
Python 3
Markdown
CellToolbar
Simple spectral analysis
An illustration of the Discrete Fourier Transform
In [2]: from scipy.io import wavfile
rate, x = wavfile.read('test_mono.wav')
And we can easily view it's spectral structure using matplotlib's builtin specgram routine:
In [5]: fig, (ax1, ax2) = plt.subplots(1,2,figsize(16,5))
ax1.plot(x); ax1.set_title('Raw audio signal')
ax2.specgram(x); ax2.set_title('Spectrogram');
Raw audio signal
Spectrogram



Definite Integrals in Maxima and Minima
the symbolic variables and assume that a ≥ 0:
syms a x
assume(a >= 0);
Then, define the function to maximize:
F = int(sin(a*x)*sin(x/a),x,-a,a)
Note the special case here for a = 1. To make computations easier, use assumeAlso to ignore this possibility.
assumeAlso(a ~= 1);
F = int(sin(a*x)*sin(x/a),x,-a,a)
Create a plot of F to check its shape:
fplot(F,[0 10])
Use diff to find the derivative of F with respect to a. The zeros of Fa are the local extrema of F.
Fa = diff(F,a);
hold on
F =

Why do we need something like this?

🍎

🔔 Portability problem #1

Sharing Data and Presentation

.opj, .opju Origin Pro

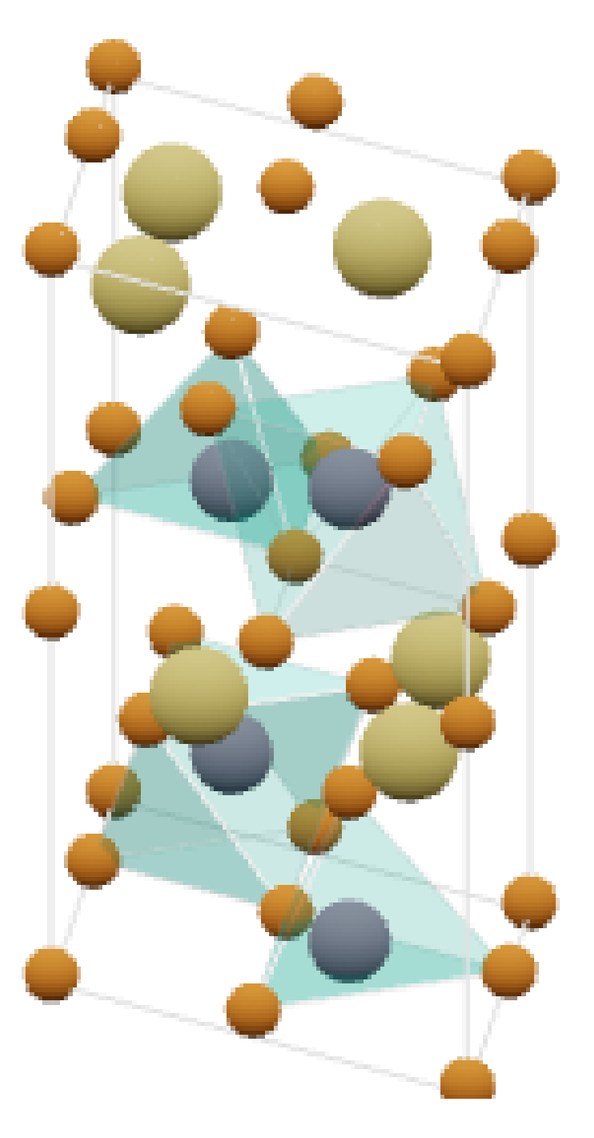
- non-human readable proprietary format
- requires *Origin Pro/Viewer*

What can we suggest instead?

1. Open-source
2. Text-based
3. Offline (no clouds, no internet-dependency)
4. Interactive and self-descriptive
5. No extra software installed (at least *for viewing*)

```
To     Friedrich Vormelker
From   Me
Topic  My beautiful data
--
Body
       Dear Friedrich,
       Just click this button
```

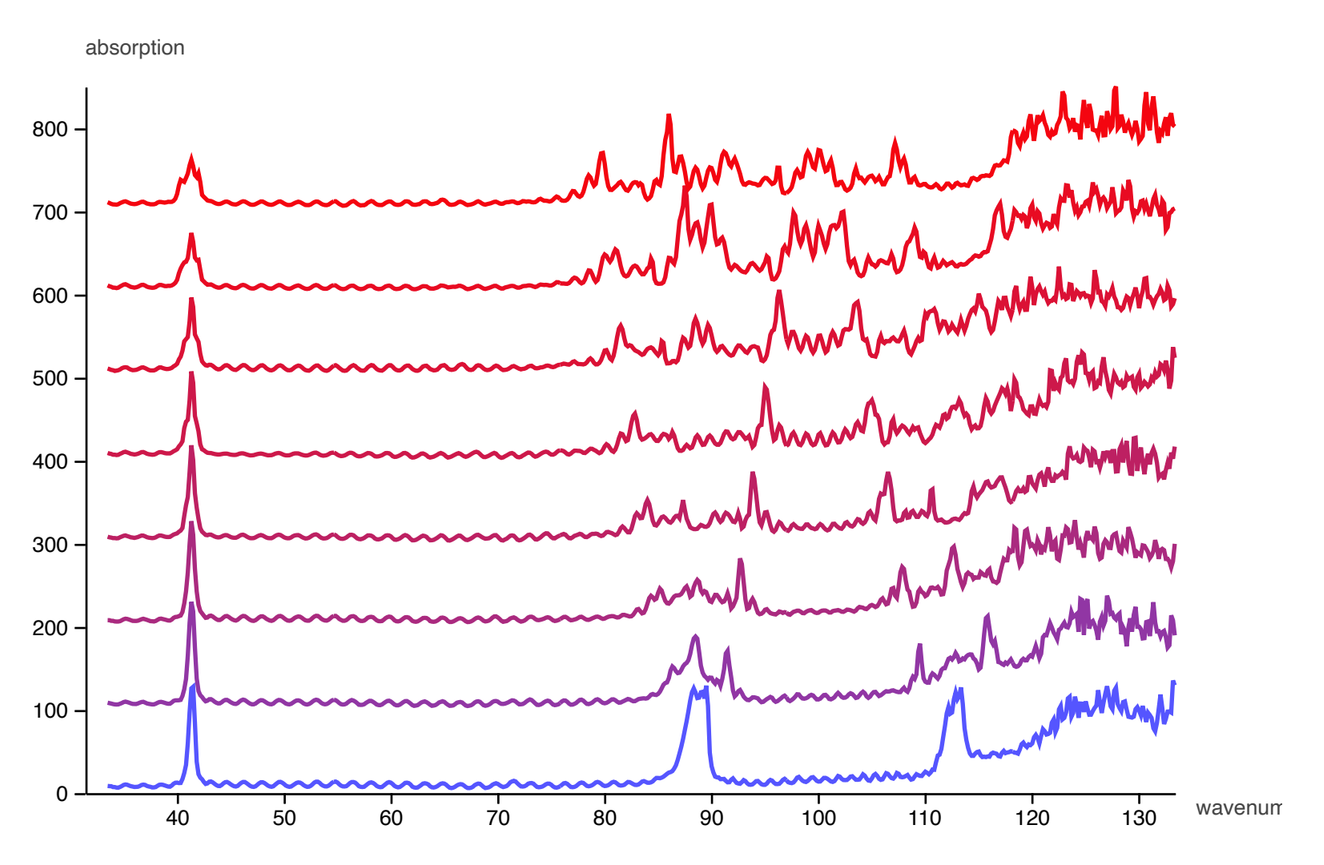
Open



no additional software installed

Report Title

Here is my beautiful data



Why not any other digital notebook on the market?

- Jupyter & Jupyter Lab
- Julia (Pluto)
- ~~Wolfram Mathematica~~ (closed source, slow, proprietary)

Equations are beautiful

$$\alpha = \frac{\omega_p^2}{(\omega_0^2 - \omega^2) - i\omega/\tau}$$

We can do better!

WLJS Notebook

An open-source notebook interface for Wolfram Language
Developed by scientists for scientists

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Resume presentation

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Introduction

Most of **you have probably heard about it, maybe as a digital notebook, but I will remind you of the concept.**
It is a sort of text document where you can write your notes, calculate something, plot graphs, produce data, model things, and so on.
It's been a long time since the first concept appeared, as with Wolfram Mathematica ages ago.
A Jupyter Notebook. Here, you see cells; they can contain just text, code, or pictures generated by code.

Traditional Way

Scientific work involves research and the exchange of knowledge.
However, there are some drawbacks to the usual methods people use:

- **OPJ files:** These are proprietary files used with Origin Pro, which is a Swiss army knife and a favorite tool among researchers. However, it's in a proprietary format and non-readable outside the Origin Pro ecosystem.
- **For presentations, we typically use PDFs and PPTs:** My main complaint is that they're static and limited, which shouldn't be the case in 2023. Usually, we export graphs to pictures and then import them into PowerPoint, arrange them, and so on. This process is quite lengthy, especially when you need to update something in your data.

The right direction, in my opinion, is Jupyter Notebooks. It's a computable notebook format that offers some solutions to the issues I mentioned, although it comes with other flaws I will discuss later.
What can we suggest instead?
Something that is:

- **Open-source**
- **...**

As simple as writing an email to your colleague,
and your colleague can simply open it as a file
without having anything installed on their PC,
and can see and do this...

Keeping it all interactive and having all **raw data inside**. This means that if my colleague wants, they could download some software to open the same file and edit it.
Or, if you could generate a report or create a presentation for your talk and manipulate the data representation live, like I am doing right now.

A long Path

If you think about it, it's actually a lengthy process when you prepare your figures or model the data and show the results. You have to export files, import them back, and so on.
I was thinking it would be great to integrate all of this. Because the basic principles of each individual program, its utility function, are simple and can be covered with some flexible language in a dynamic notebook environment.

Why Physicists don't like programming?

Equations are beautiful, but not in programming
Why not use Jupyter with Julia? Well, they all share a common flaw, and that's probably why physicists don't usually like programming.