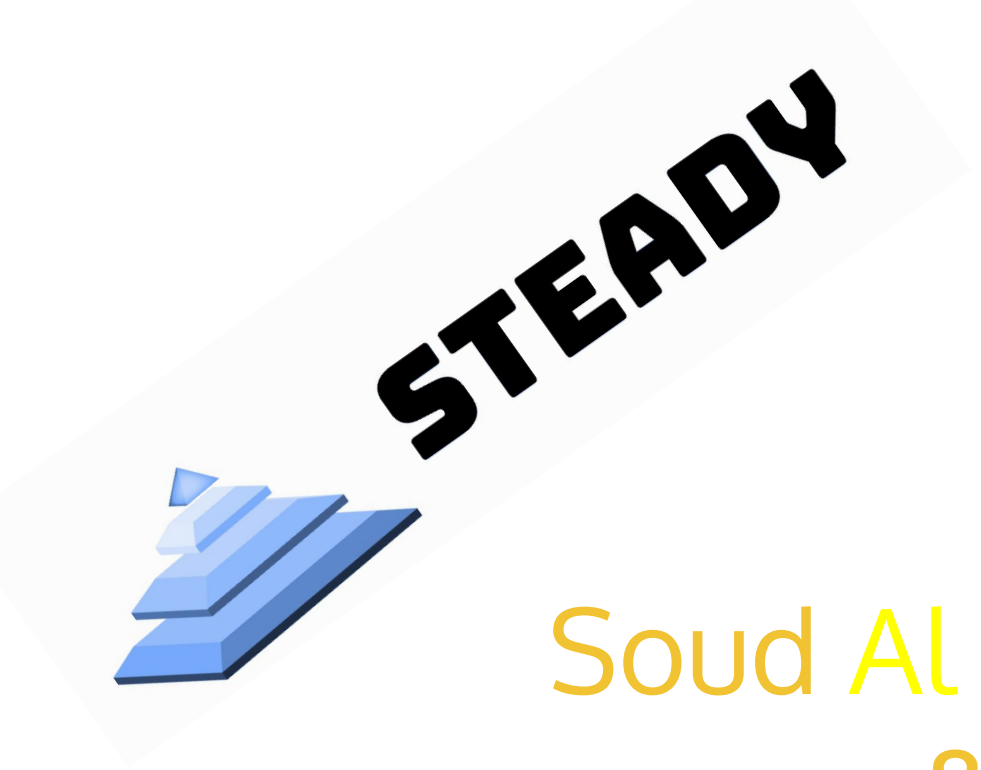
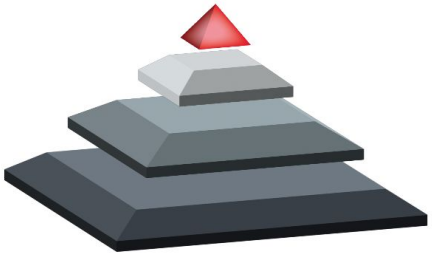


Visualization

Data

Soud Al Kharusi
&
Ahmad Mahmood

Data Visualization: The Why and How



STEADY

Soud Al Kharusi & Ahmad Mahmood & YOU


I want to play a game.

Blinking of Fluorescence Dyes as an Intracellular Biosensor: A k-Space Image Correlation Spectroscopy Approach

McGill UNIVERSITY

STEADY

Motivation

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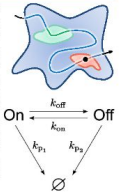

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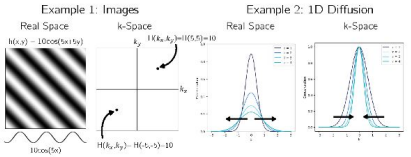

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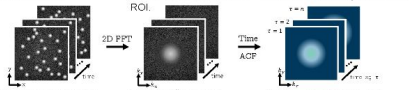

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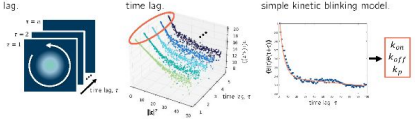

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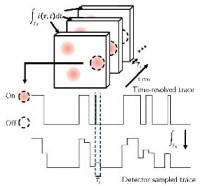

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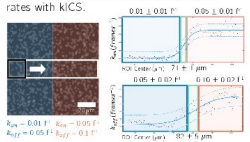

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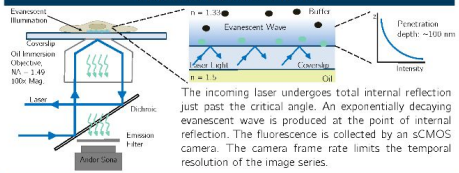

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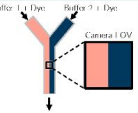

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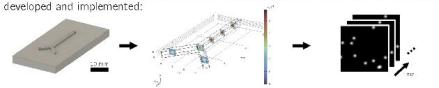

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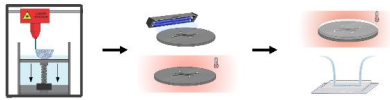

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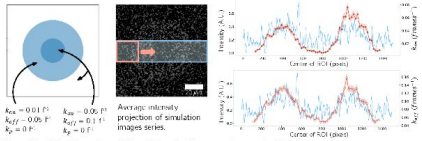

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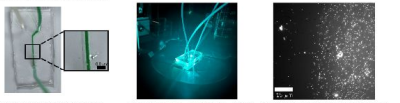

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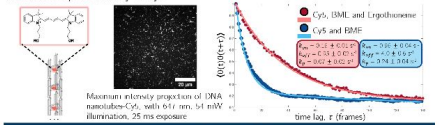
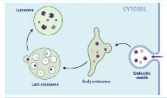


Future Directions



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Acknowledgements

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References

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Department of Chemistry[1], Department of Physics[2], McGill University, Montreal, Quebec, Canada.

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STEADY

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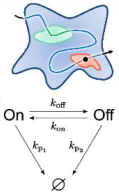

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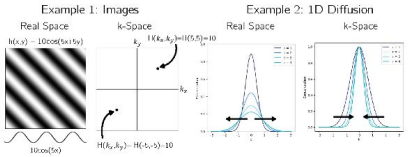

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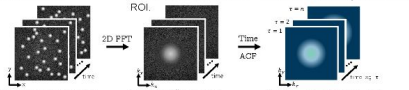

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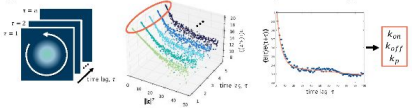

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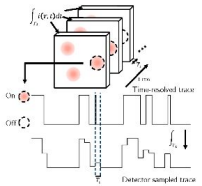

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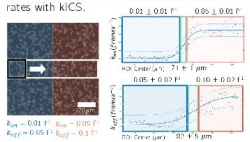

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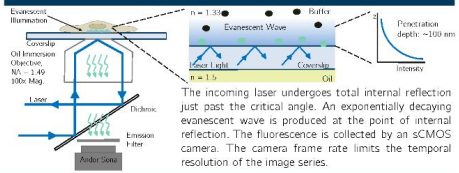

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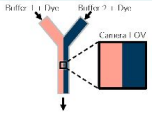

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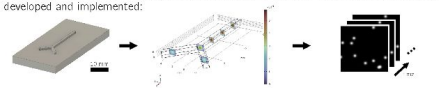

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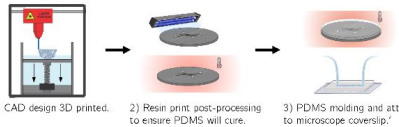

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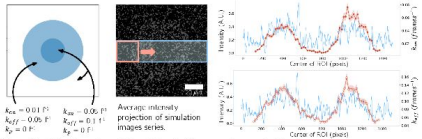

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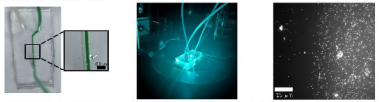

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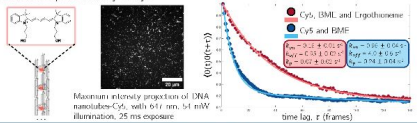
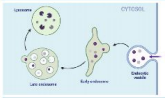


Maximum intensity projection of DNA nanotube-Cy5, with 647 nm, 54 mW illumination, 25 ms exposure

Future Directions



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Using GPUs to Design a Water Cherenkov Detector for a Neutrinoless Double Beta Decay Search in nEXO

scan for a digital copy

nEXO? 0νββ?? 🤔

nEXO is a proposed **neutrinoless double beta decay (0$\nu\beta\beta$) experiment** in ^{136}Xe [1].

0νββ is a **lepton number violating process.** An observation of such a process is an observation of **new physics from beyond the Standard Model.**

Cosmogenic Backgrounds

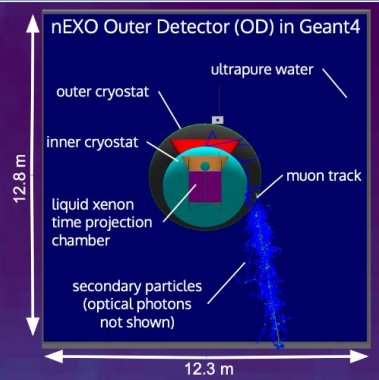
High-energy cosmogenic muons from the upper atmosphere travel deep underground and **induce backgrounds to experiments searching for rare events**, e.g. 0νββ.

The Outer Detector

nEXO's Outer Detector (OD), is being developed in part to **account for cosmogenic backgrounds by tagging the Cherenkov light of nearby muons** [2] as they pass through a cylindrical water tank.

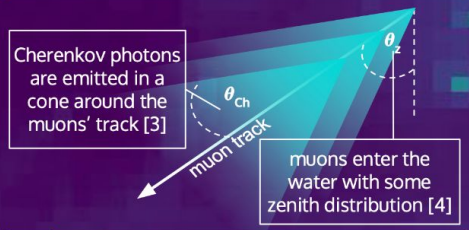
This study was conducted to determine the **optimal placement of photosensors (PMTs) to tag cosmogenic muons by their Cherenkov emission.**

1 Study Background Production with Conventional CPU-based Monte Carlo



CPU-based methods are computationally expensive (slow) for studying high energy particles while ray tracing many photons. GPU-based ray tracing is at least ~100x faster.

2 Break the Relevant Physics out of the Problem



3 Build the Physics into a GPU-based Ray-Tracing Program (Chroma) and Simulate the Photon Hit Patterns

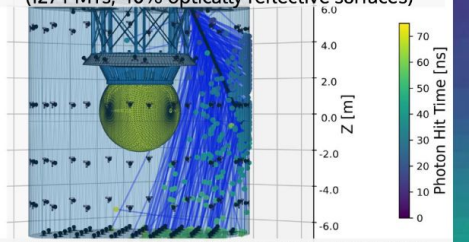
Component Name	OD Cylinder Wall	OD Floor	Outer Cryostat	OD Ceiling
% of incident light	52.9	39.7	6.8	0.6

The background of this poster is a **Cherenkov light map** of muons on the OD's cylindrical wall, unrolled.

4 Place PMTs in the Outer Detector According to the Light Map & Evaluate Muon Tag Efficiency

tag condition: 10 photons/PMT, 5 PMT coincidence within 25 ns

Example non-uniform PMT configuration
(127 PMTs, 40% optically reflective surfaces)



The **muon tagging efficiency** of the above PMT configuration is **84.4 ± 0.7 %.**
A uniform PMT distribution yields: **76.9 ± 0.8 %.**

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1. "nEXO: neutrinoless double…", J.Phys.G., 49.1 (2021): 015104
2. "PMT Response Simulation and…", L. Retty, CAP 2022 P#39
3. "Chroma Simulations of… ", E. Klemets, CAP 2022
4. "Cosmogenic Muon Background…", R. Ross, CAP 2022 P#40

STEADY

Using GPUs to Design a Water Cherenkov Detector for a Neutrinoless Double Beta Decay Search in nEXO

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nEXO? 0νββ?? 🤔

nEXO is a proposed **neutrinoless double beta decay (0$\nu\beta\beta$) experiment** in ^{136}Xe [1].

0νββ is a **lepton number violating process.** An observation of such a process is an observation of **new physics from beyond the Standard Model.**

Cosmogenic Backgrounds

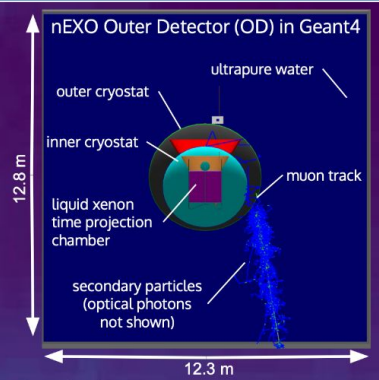
High-energy cosmogenic muons from the upper atmosphere travel deep underground and **induce backgrounds to experiments searching for rare events**, e.g. 0νββ.

The Outer Detector

nEXO's Outer Detector (OD), is being developed in part to **account for cosmogenic backgrounds by tagging the Cherenkov light of nearby muons** [2] as they pass through a cylindrical water tank.

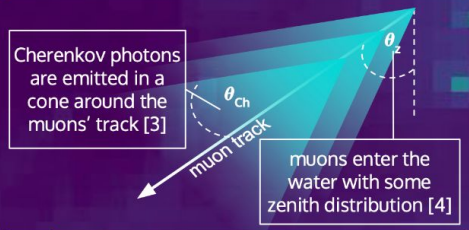
This study was conducted to determine the **optimal placement of photosensors (PMTs) to tag cosmogenic muons by their Cherenkov emission.**

1 Study Background Production with Conventional CPU-based Monte Carlo



CPU-based methods are computationally expensive (slow) for studying high energy particles while ray tracing many photons. GPU-based ray tracing is at least ~100x faster.

2 Break the Relevant Physics out of the Problem



3 Build the Physics into a GPU-based Ray-Tracing Program (Chroma) and Simulate the Photon Hit Patterns

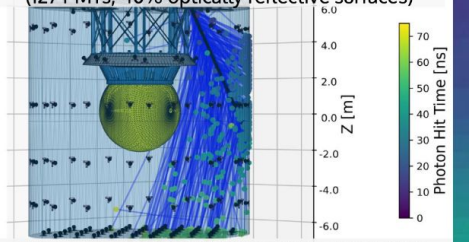
Component Name	OD Cylinder Wall	OD Floor	Outer Cryostat	OD Ceiling
% of incident light	52.9	39.7	6.8	0.6

The background of this poster is a **Cherenkov light map** of muons on the OD's cylindrical wall, unrolled.

4 Place PMTs in the Outer Detector According to the Light Map & Evaluate Muon Tag Efficiency

tag condition: 10 photons/PMT, 5 PMT coincidence within 25 ns

Example non-uniform PMT configuration
(127 PMTs, 40% optically reflective surfaces)



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Soud Al Kharusi, McGill University
(for the nEXO Collaboration)

contact: soud.alkharusi@mail.mcgill.ca

STEADY

Single-Electron Spectroscopy on Metalloenzymes

McGill University

STEADY

What are metalloenzymes?

Enzymes are **biological catalysts**, metalloenzymes have a **metal cofactor**.

Why are they important?
- Can be used in **sustainable energy generation** (ex. Hydrogen fuel)

What do we not yet understand?
- Enzymes have **large reorganization energies**
- **Electron transfer (ET) rates** are thus hard to predict

Goal:
Locate energy levels when a state is being oxidized or reduced
i.e., extracting magnitude of reorganization energy

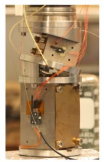
How can e-EFM be useful?

Electrostatic force microscopy can be used to detect charge states of quantum dots (QD) by **tunnelling electrons back and forth** between a QD and a back electrode.

The oscillating electrostatic force will result in **peaks in resonance frequency and damping** (dissipation) of the AFM cantilever.

Thus, at the single-molecule level, we can:
- Determine **QD density of states** (DOS)
- Measure single-electron **tunneling rates**
- Observe **transitions** between **quantized nuclear vibronic states** [1]

Single-electron spectroscopy (e-EFM) by AFM



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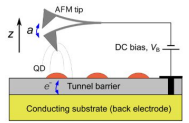

AFM tip used as a:
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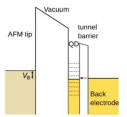
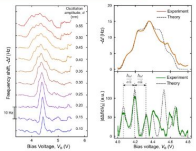
- Movable, scannable **gate**



Energy diagram of system



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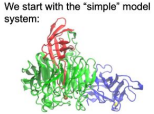
We start with the "simple" model system:



Galactose oxidase,
Single electron transfer site (Cu)

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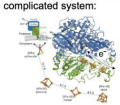

[NiFe]-hydrogenase,
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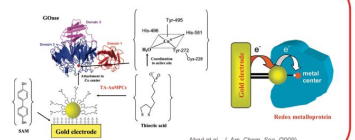
Metalloenzyme sample set-up



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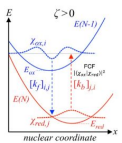
What quantum properties can be extracted from these metalloenzymes?

1. **Franck-Condon factors (FCF)** associated with redox transitions



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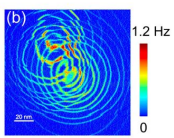
2. Map the **electronic coupling** between enzyme redox sites



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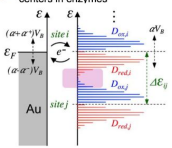

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- By probing single-electron transfers, e-EFM can be used to understand **redox energetics** and **electron transfer rates**
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Bullet points on this poster are [NiFe]-hydrogenase

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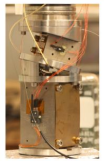

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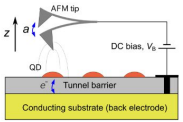

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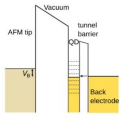

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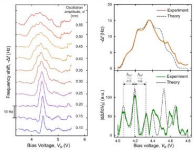

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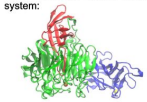

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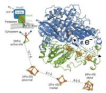

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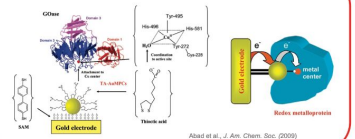

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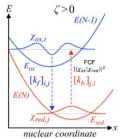

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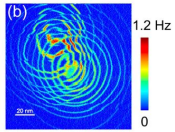

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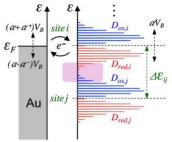

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Catherine Boisvert
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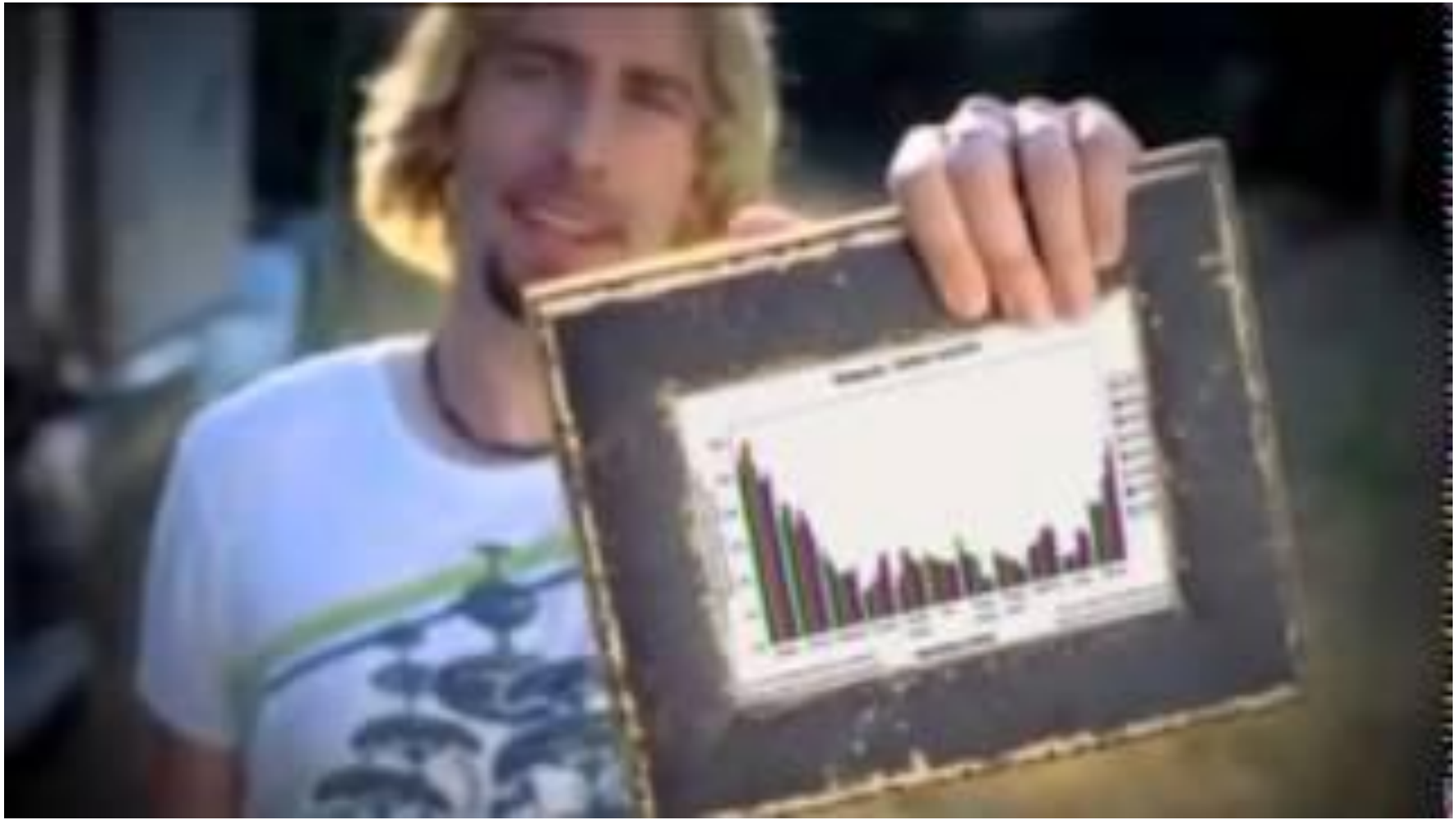
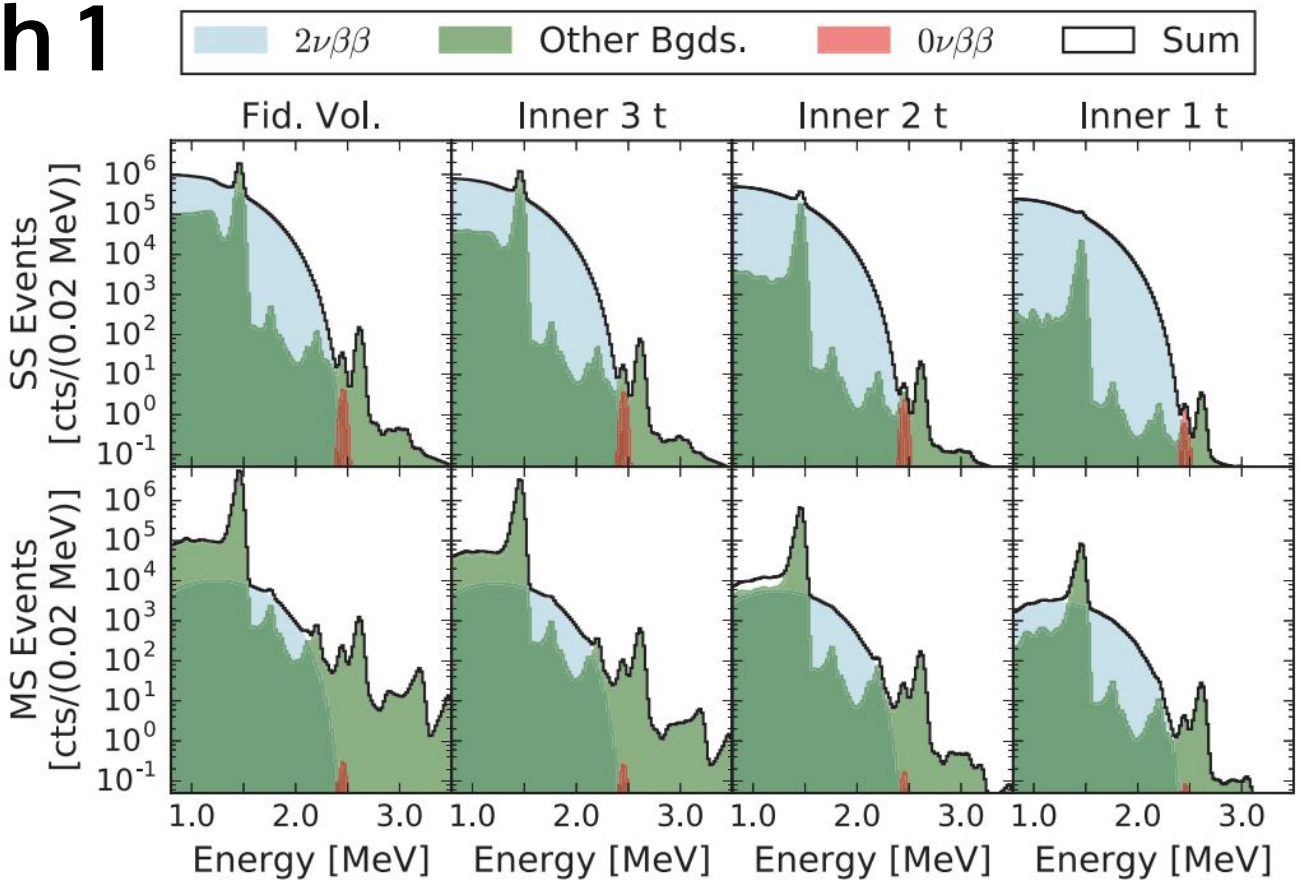
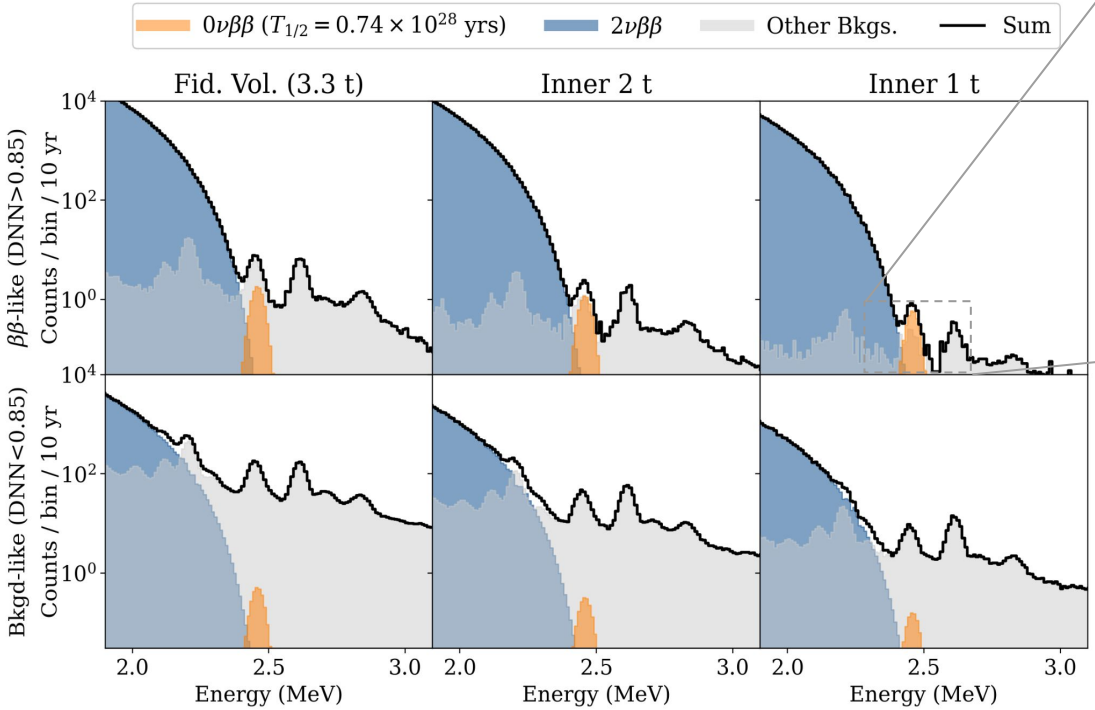


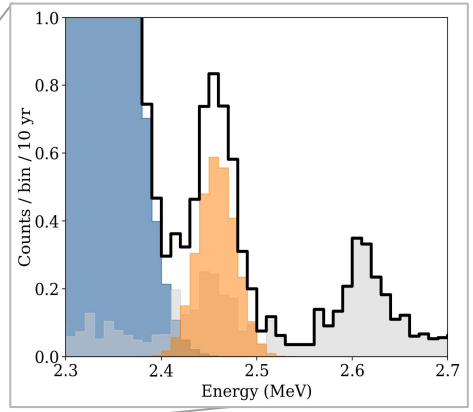
Graph 1



From: [Phys. Rev. C 97.065503]

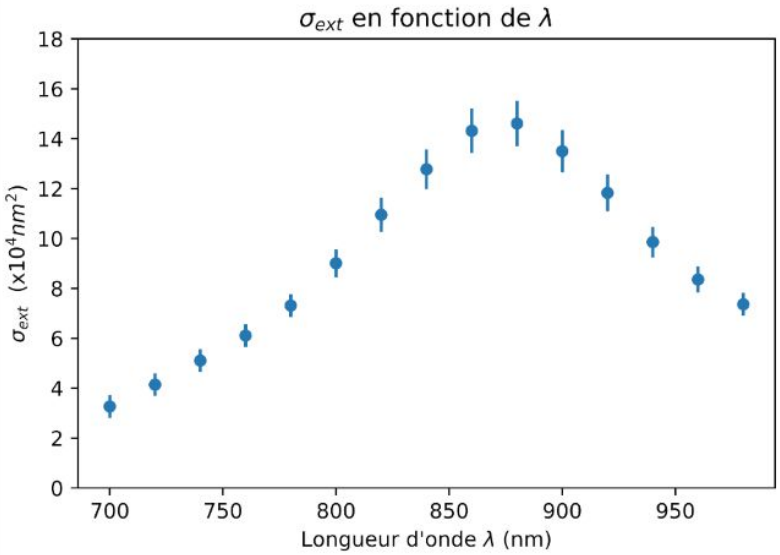
Graph 1.1 - Insets

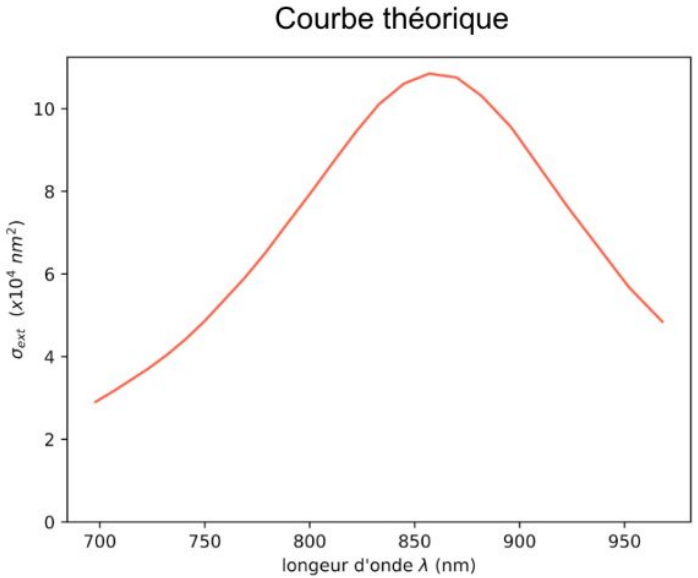




Graph 3

Spectre d'extinction optique (disque de 130 nm)





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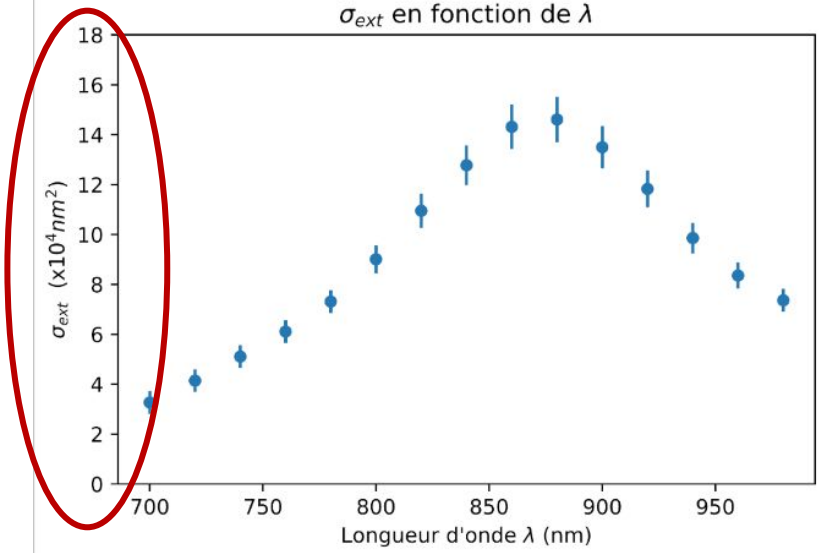

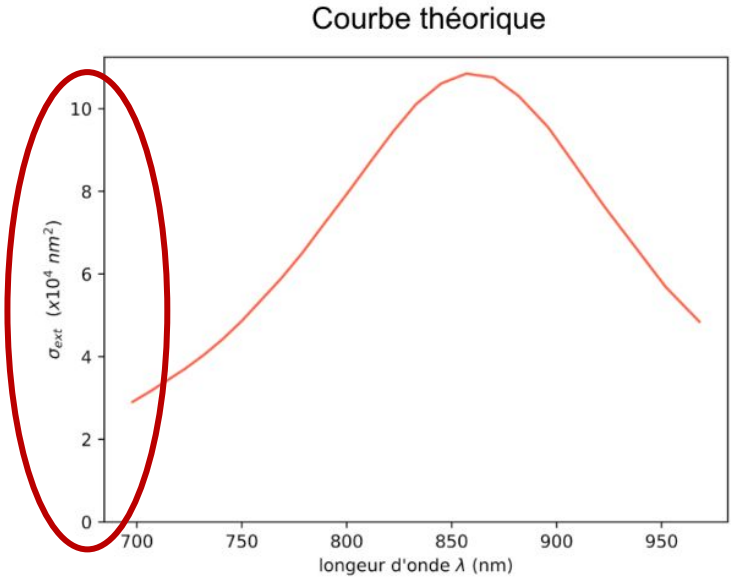

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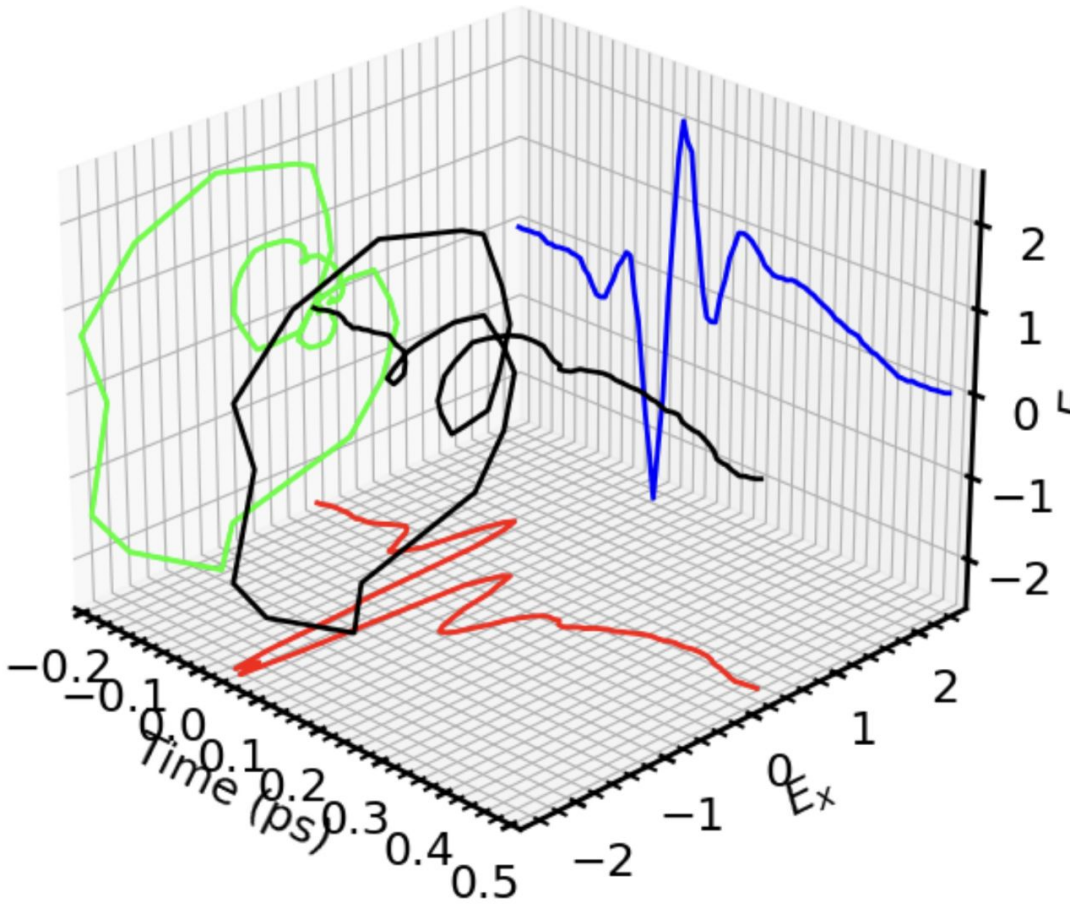
Graph 4



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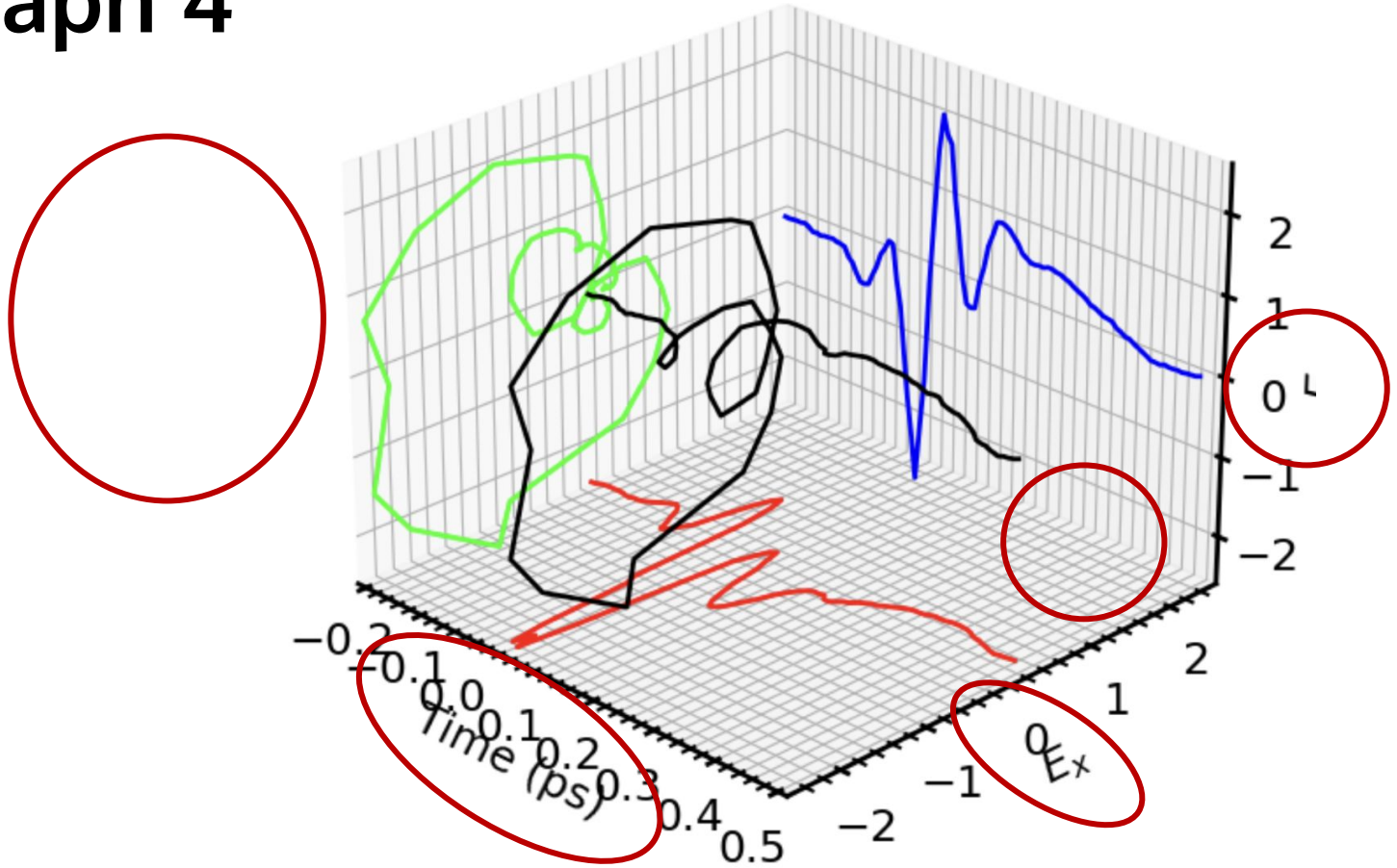
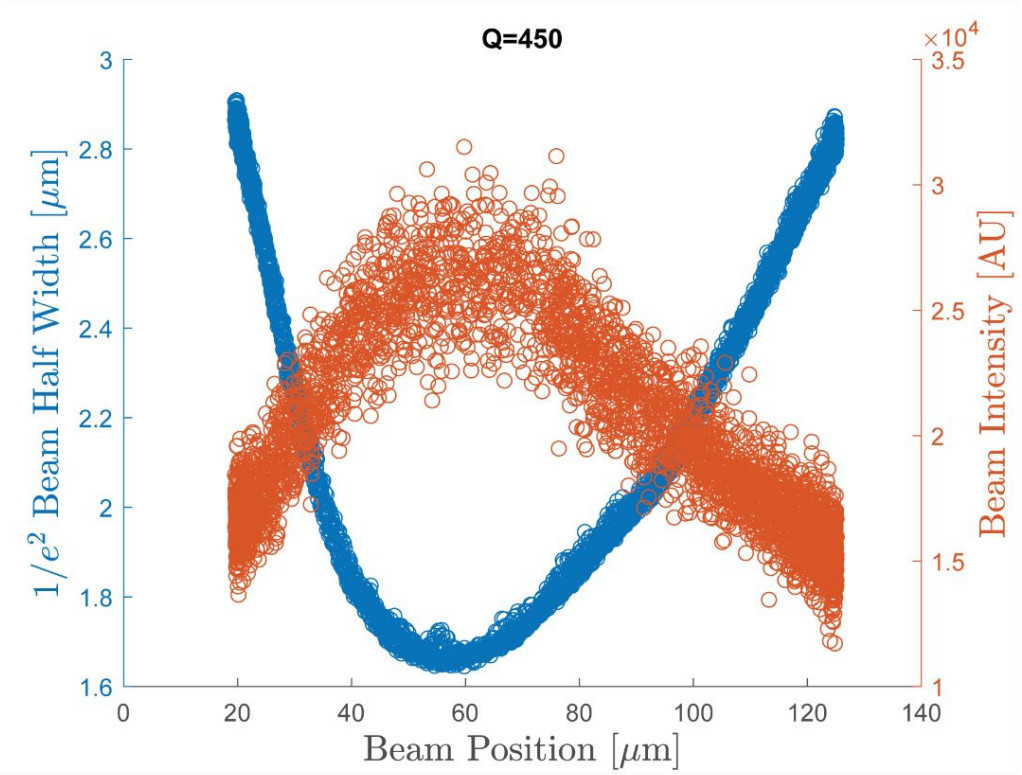


Graph 5


Q=450
$1/e^2$ Beam Half Width [μm]
Beam Intensity [AU]
$\times 10^4$
Beam Position [μm]
3
2.8
2.6
2.4
2.2
2
1.8
1.6
3.5
3
2.5
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1.5
1
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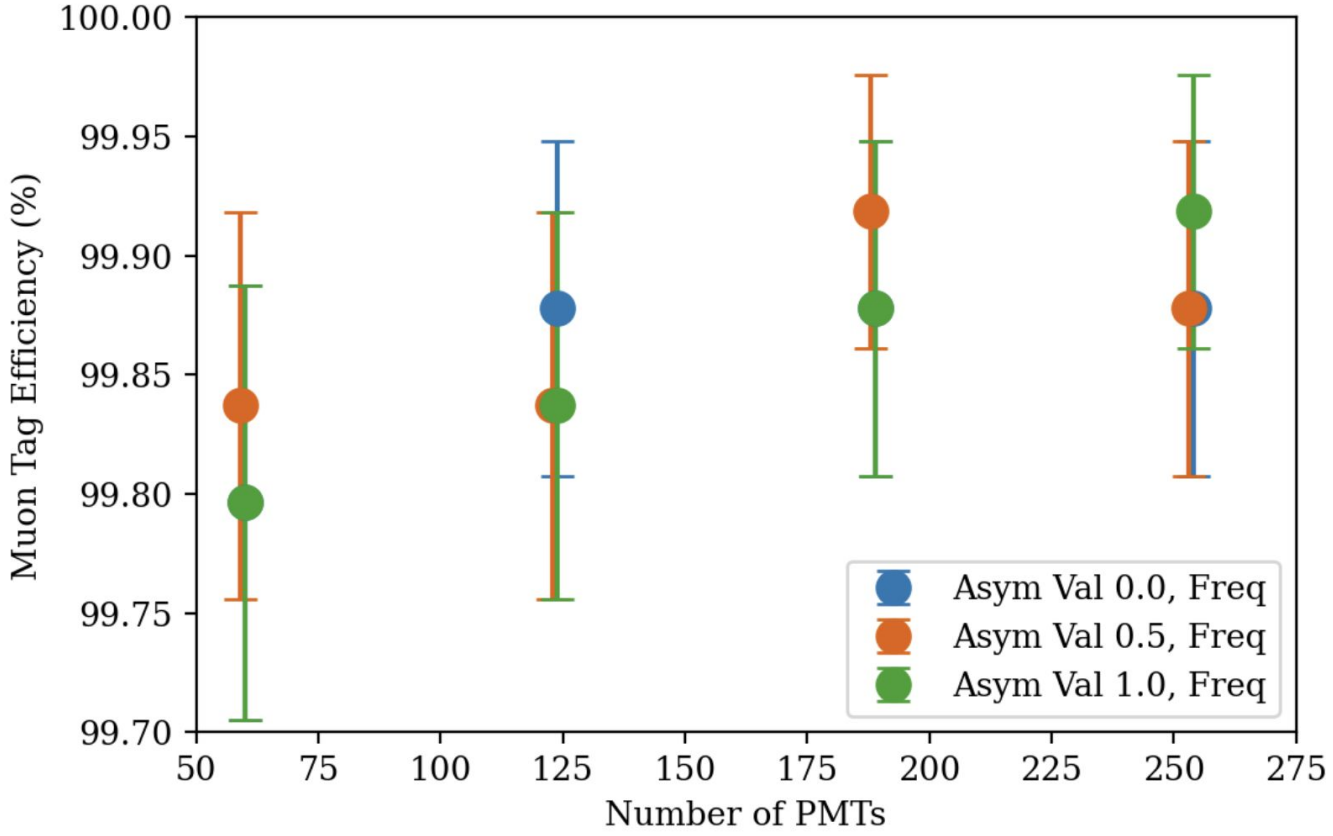
20
40
60
80
100
120
140

Graph 6


100.00
99.95
99.90
99.85
99.80
99.75
99.70
Muon Tag Efficiency (%)
50
75
100
125
150
175
200
225
250
275
Number of PMTs
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Asym Val 0.5, Freq
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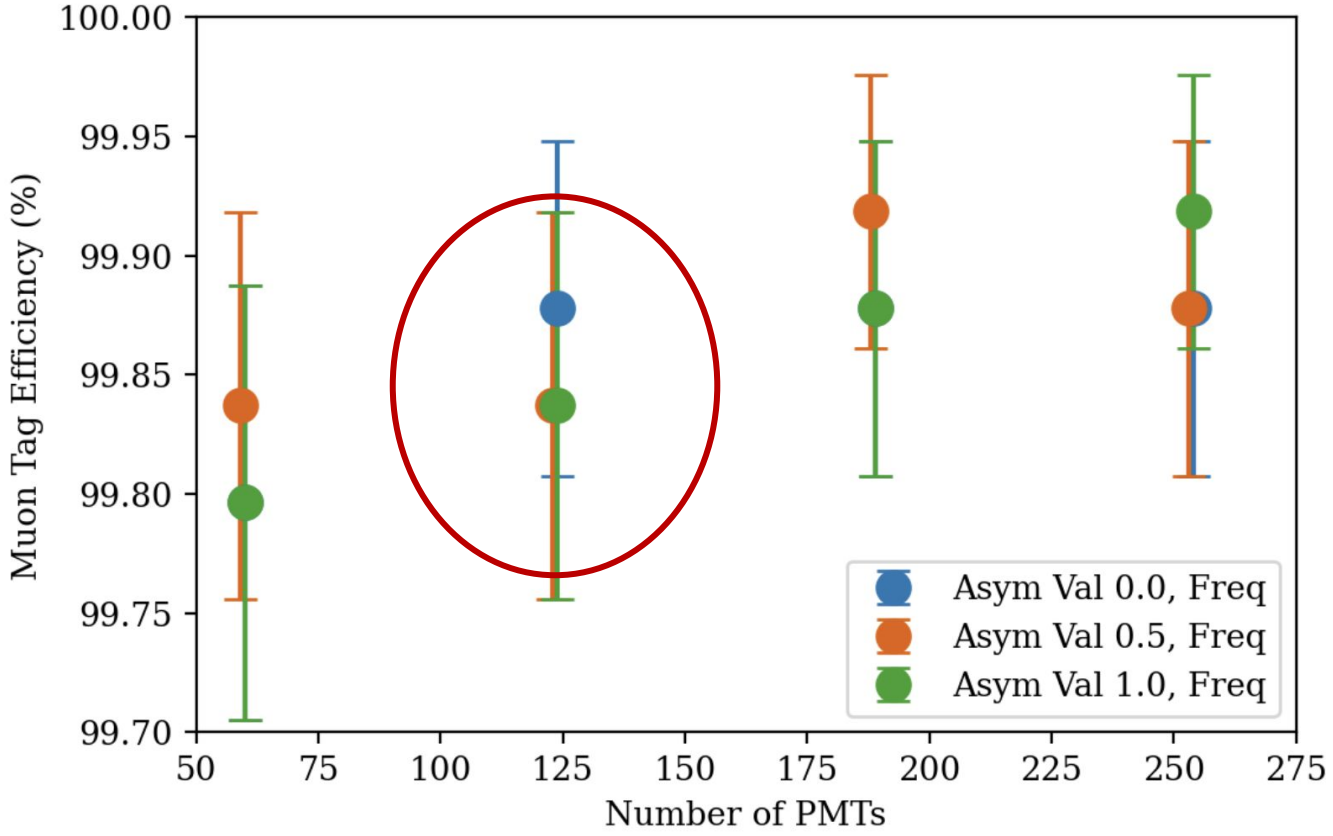
100.00
99.95
99.90
99.85
99.80
99.75
99.70
Muon Tag Efficiency (%)
50
75
100
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175
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275
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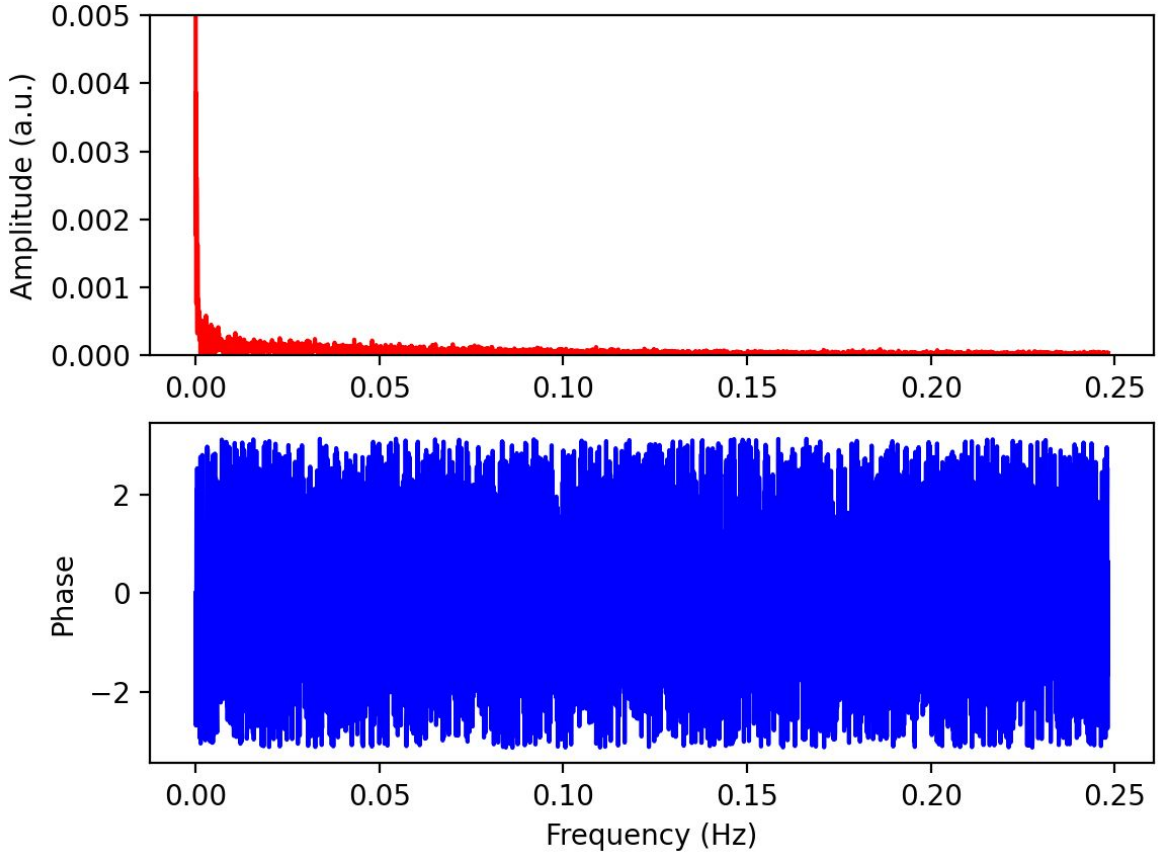
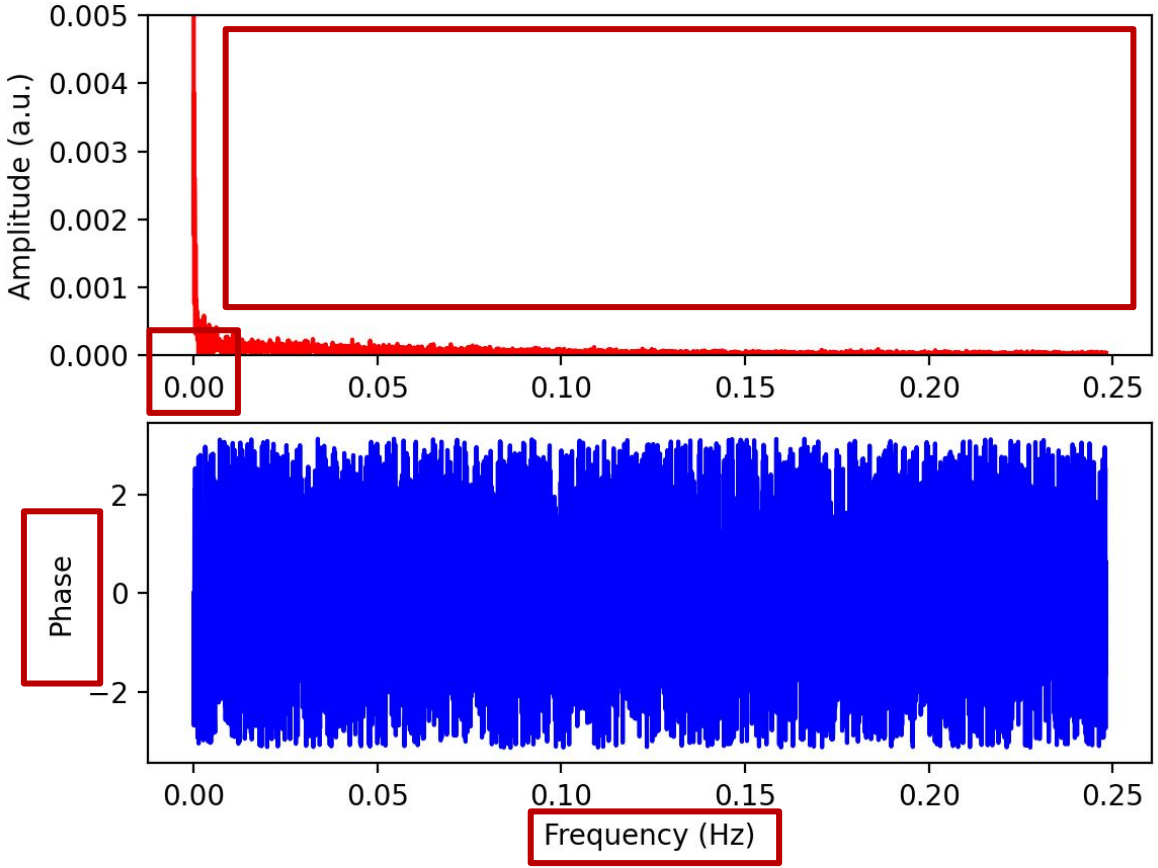
Asym Val 1.0, Freq

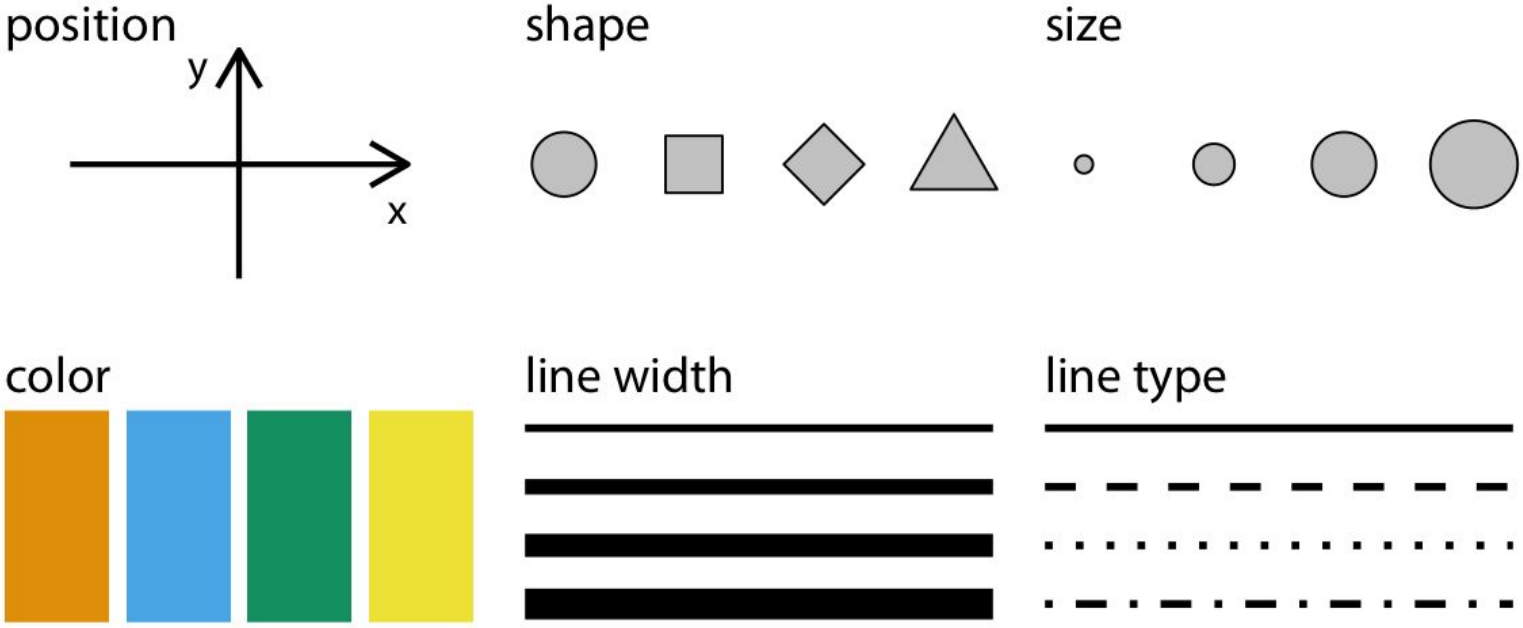
Graph 7


Amplitude (a.u.)
0.005
0.004
0.003
0.002
0.001
0.000
0.00
0.05
0.10
0.15
0.20
0.25
Phase
2
0
−2
0.00
0.05
0.10
0.15
0.20
0.25
Frequency (Hz)

Graph 7


Amplitude (a.u.)
0.005
0.004
0.003
0.002
0.001
0.000
0.00
0.05
0.10
0.15
0.20
0.25
Phase
2
0
−2
0.00
0.05
0.10
0.15
0.20
0.25
Frequency (Hz)

Data Viz 101



From: https://clauswilke.com/dataviz/aesthetic-mapping.html

Overview

- Common things to think about
- Types of plots, and when to use them
- Trendlines vs fits
- Visualizing Uncertainties
- Schematics
- Plots that are meant for: papers, posters, talks...
- Exercises

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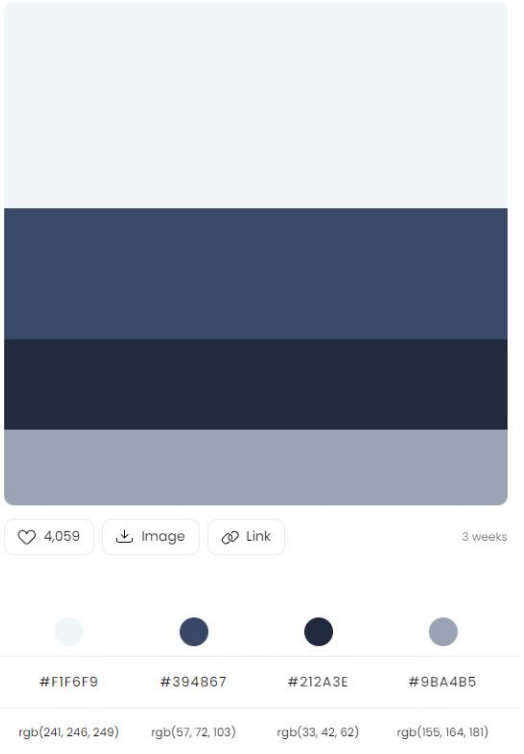
Colours

- Common colour blindness

  red green, blue/green, yellow/red

- Colour palettes: https://colorhunt.co/



Colours

- Common colour blindness
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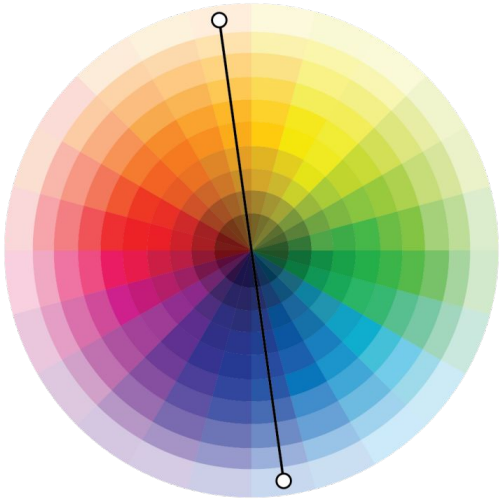
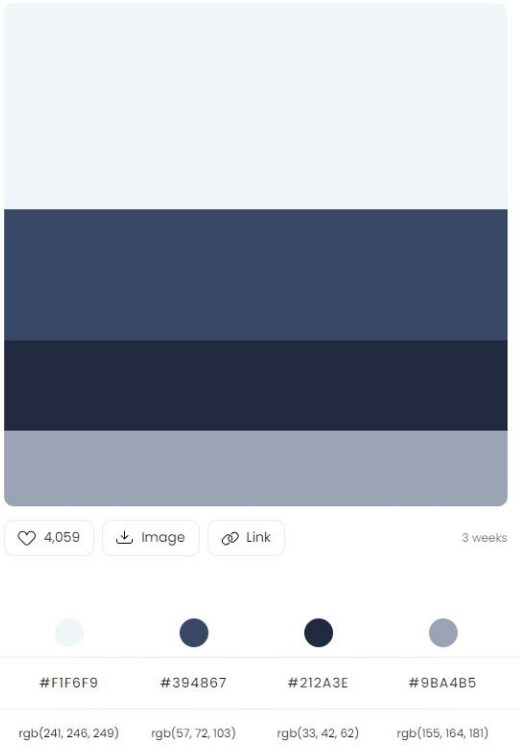
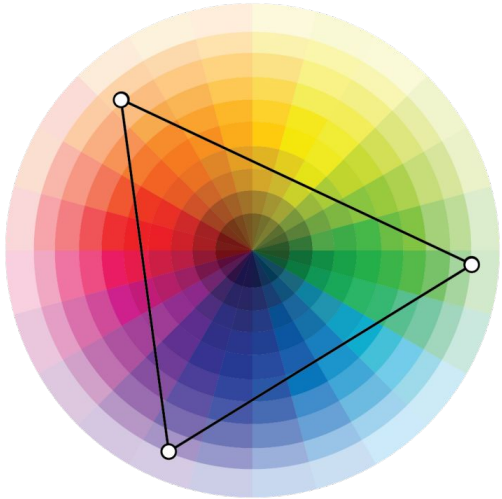


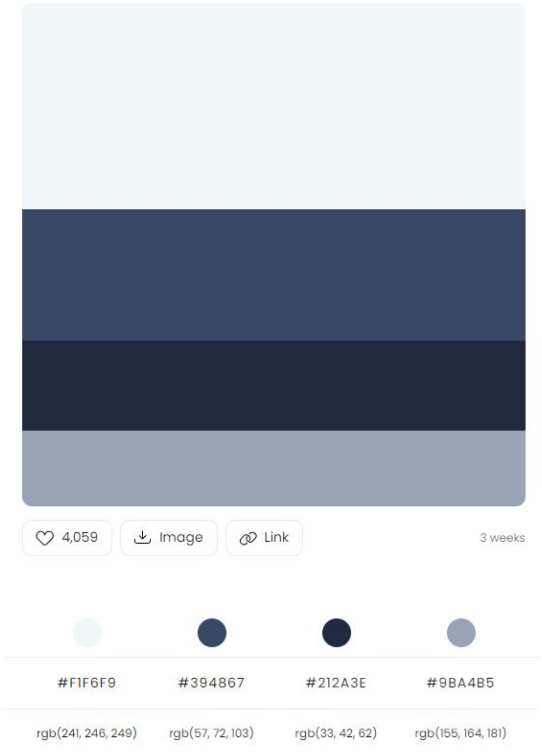


2 colours, relation?

Colours

- Common colour blindness
- Colour palettes: https://colorhunt.co/

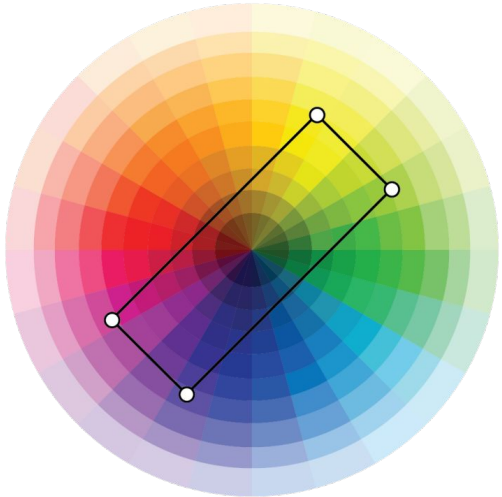


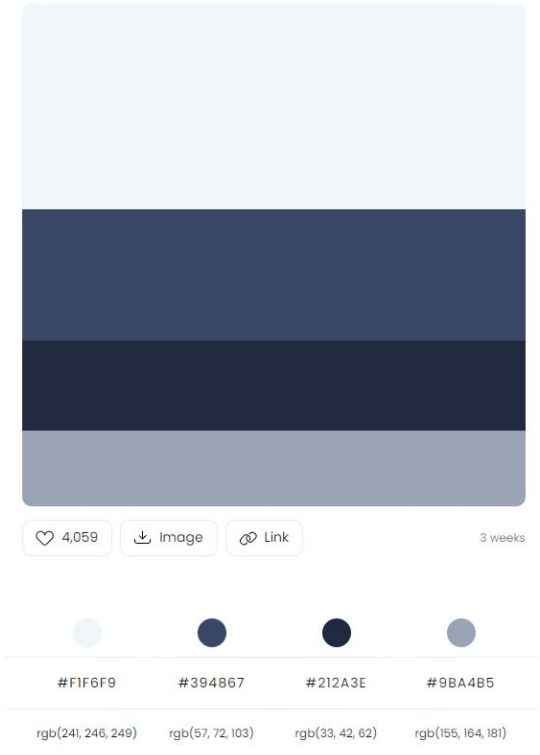


3 colours, relation?

Colours

- Common colour blindness
- Colour palettes: https://colorhunt.co/

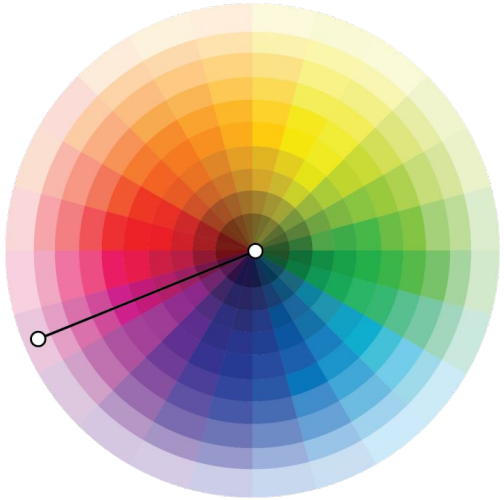


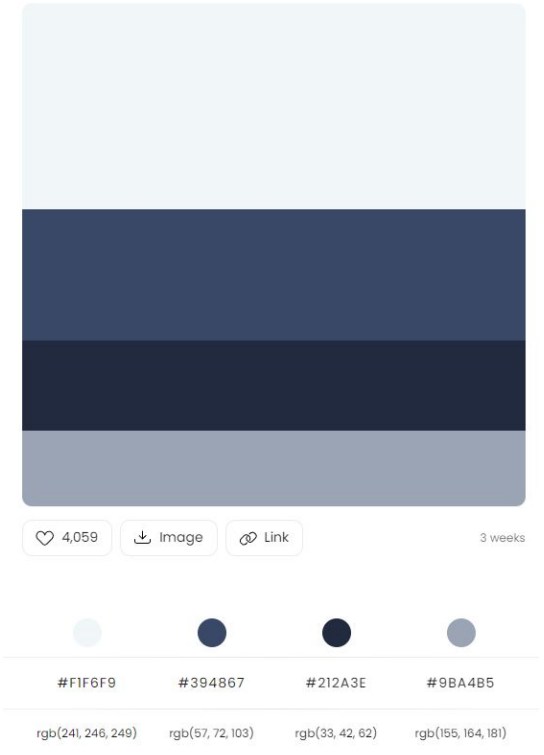


4 colours, relation?

Colours

- Common colour blindness
- Colour palettes: https://colorhunt.co/

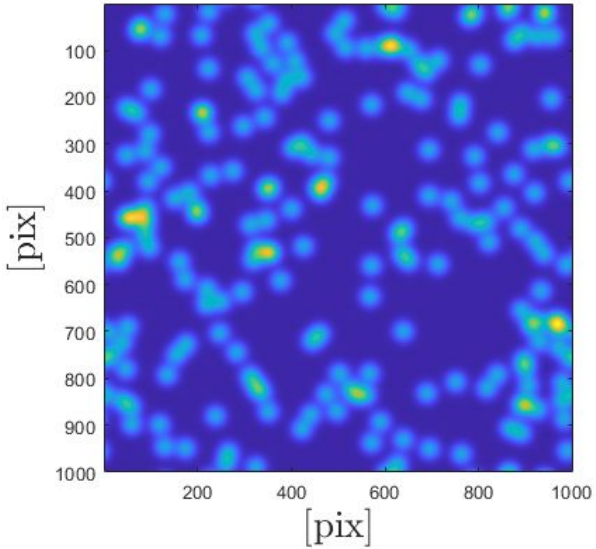


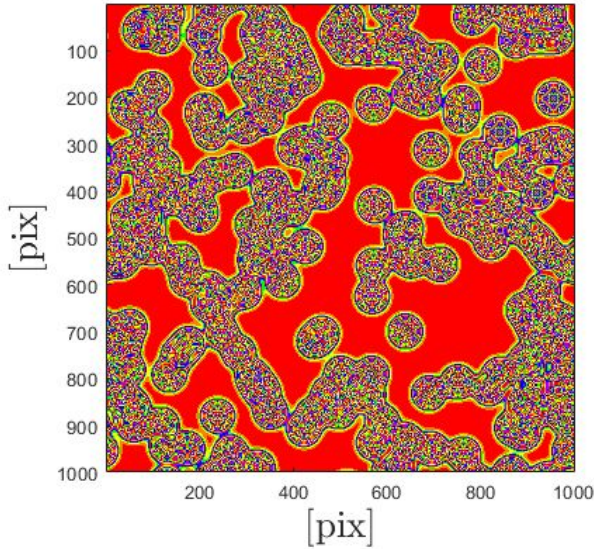


monochromatic, relation?

Colours 2

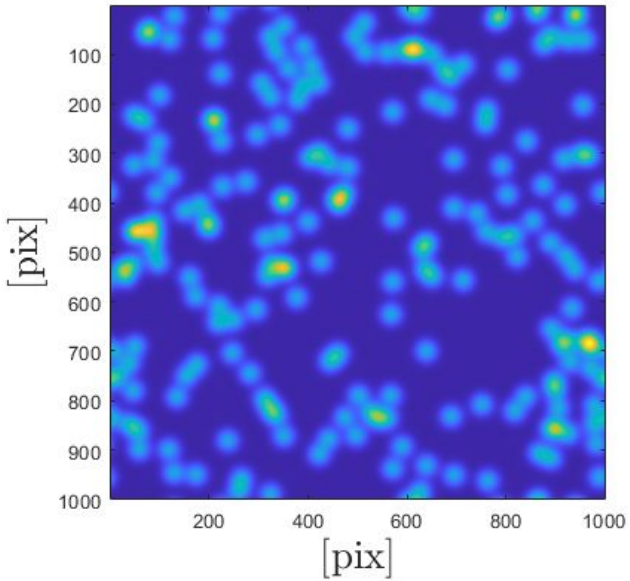
- Heatmap colour palettes
  - single **p**o**l**e vs linear & monochro**matic**

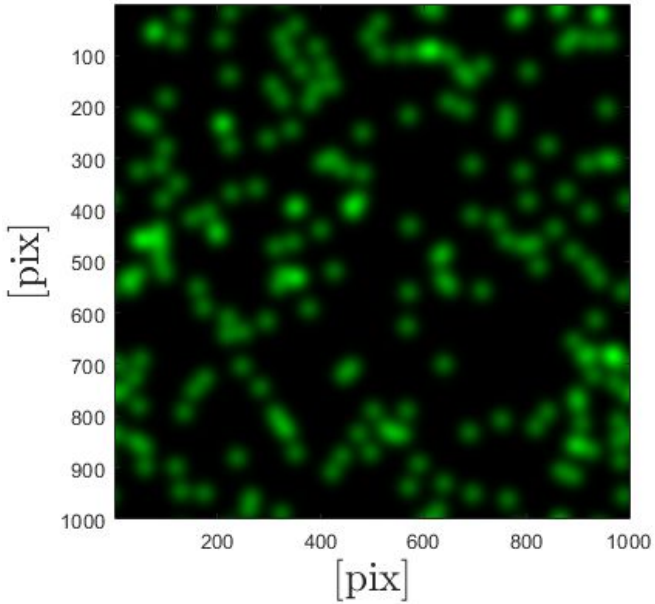




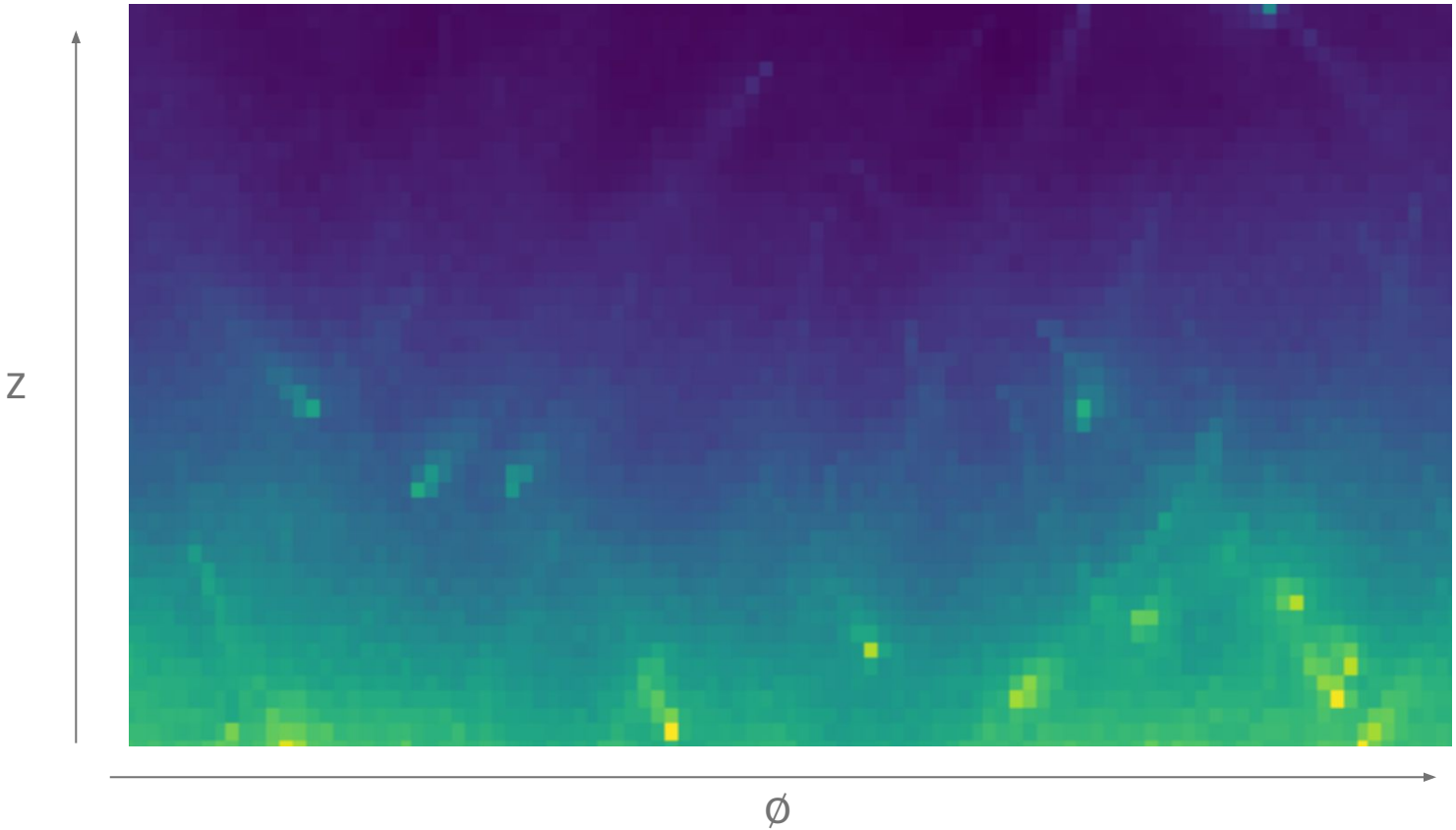
Colours 2

```
MyMap = [zeros(256,1),linspace(0,1,256)', zeros(256,1)]
```





Memorable Colour Scales



Photon hit patterns of Cherenkov **light from relativistic muons** on cylinder using the *viridis* colour scale

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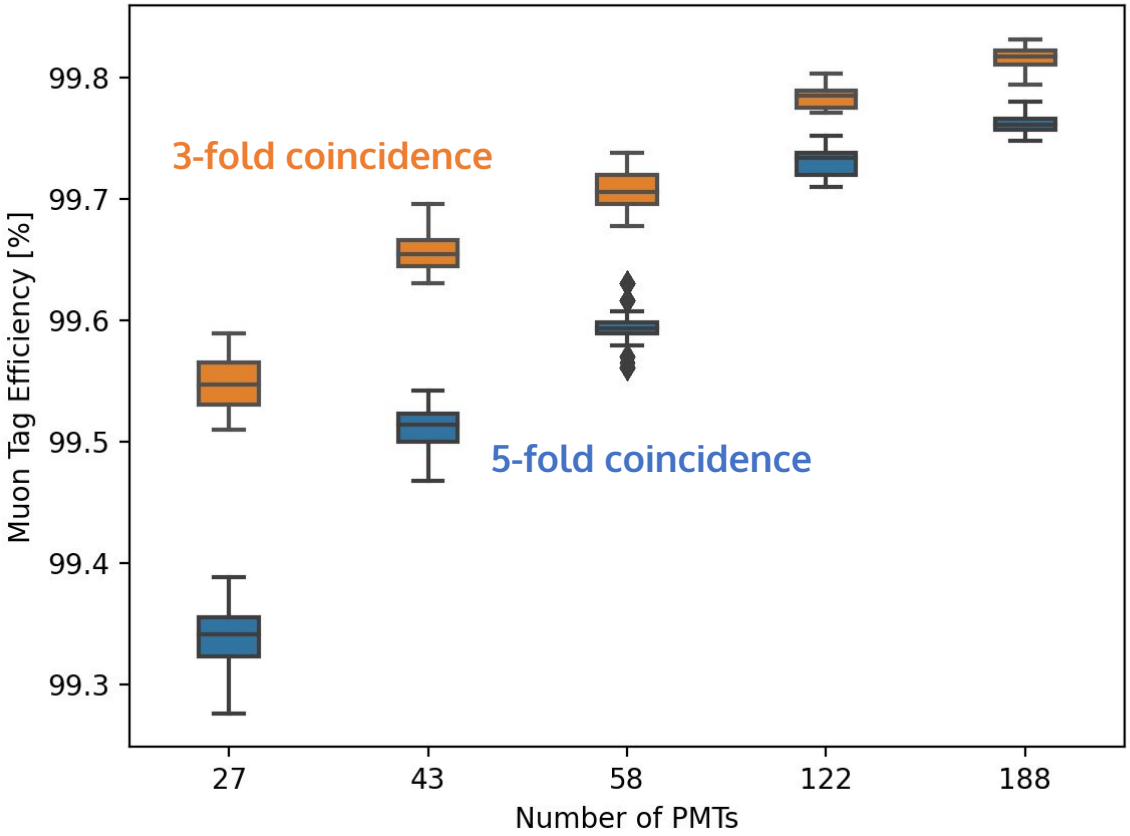
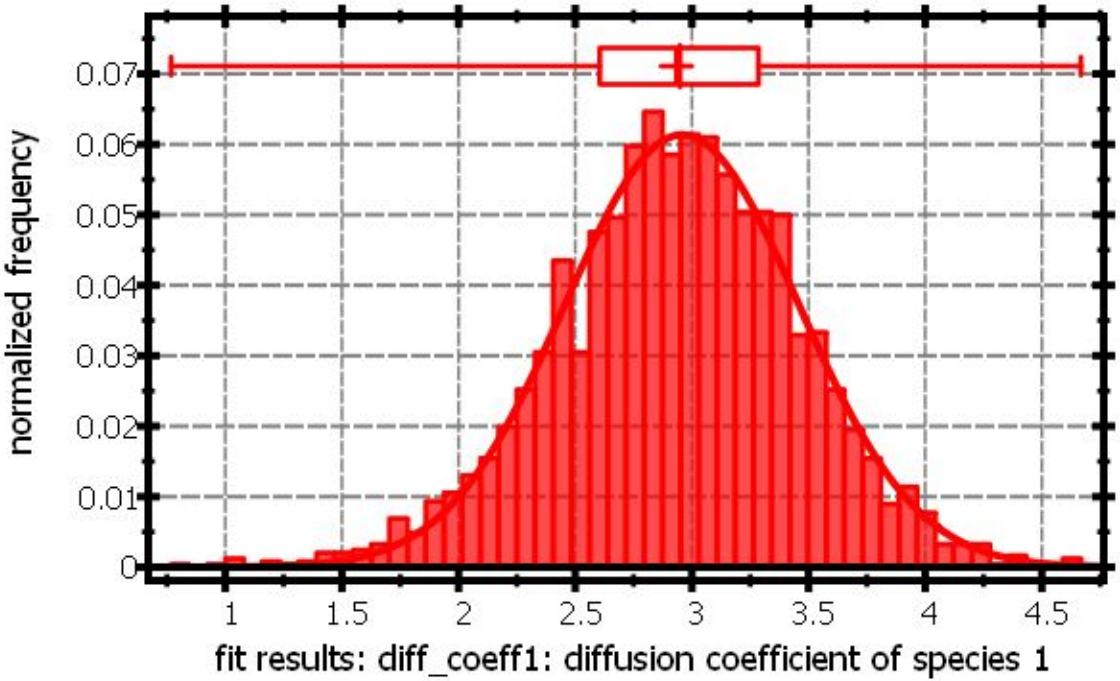
To Bar or Not to Bar

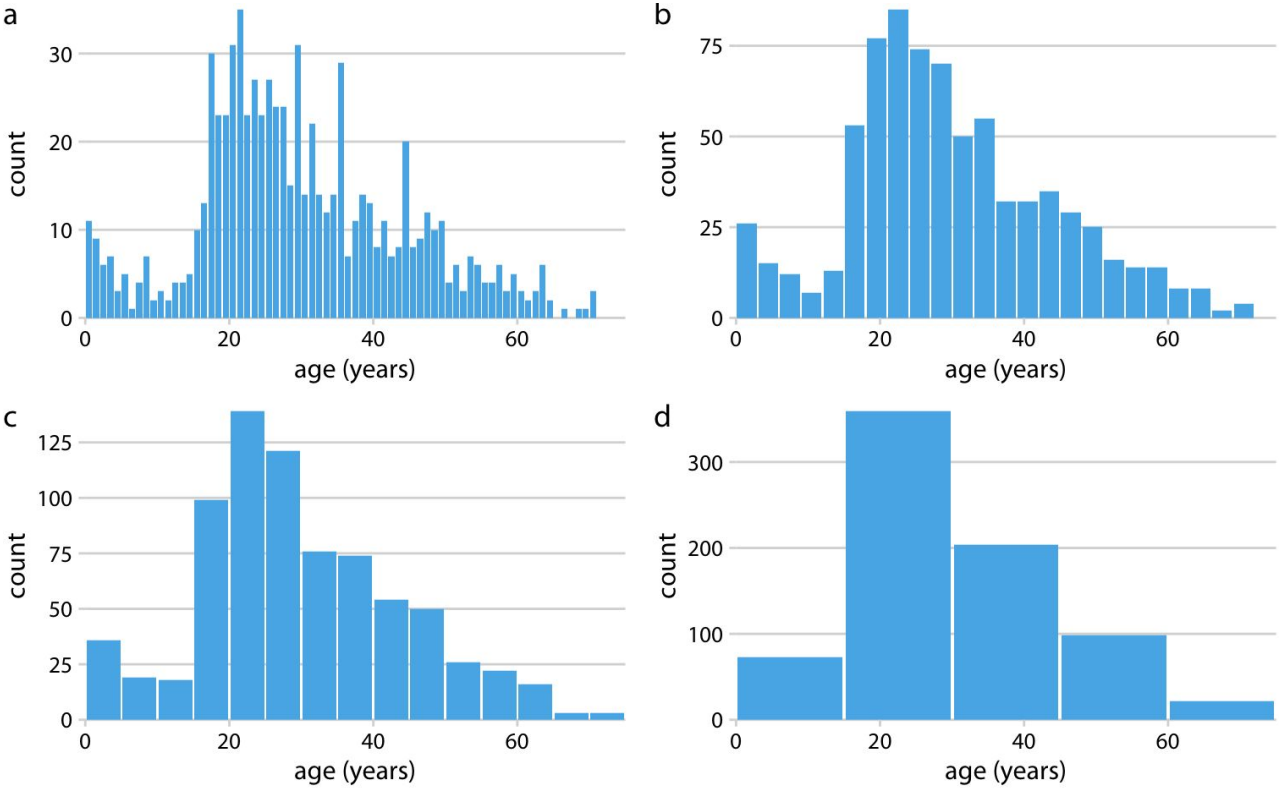


Distributions!

Histograms, Kernel Densities, Boxes, Violins *et al.*

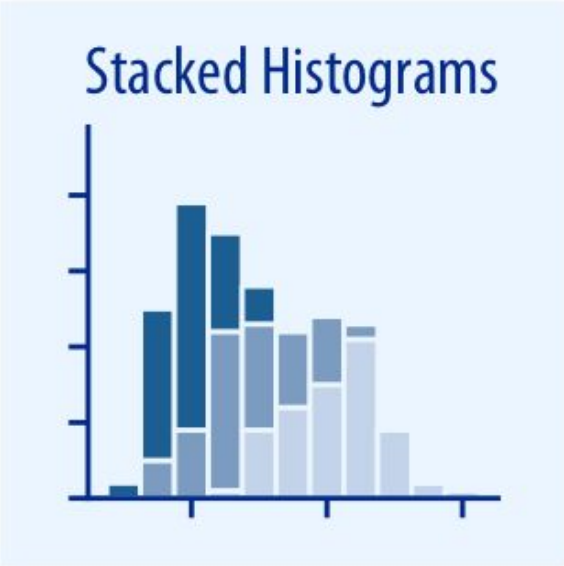


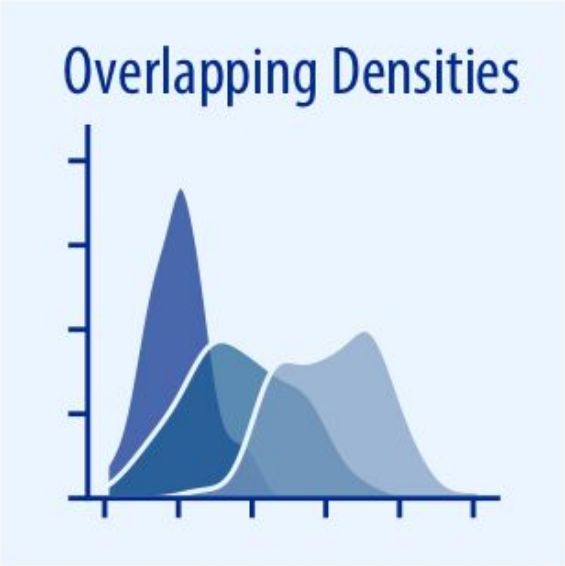
Histograms: Binning



From: https://clauswilke.com/dataviz/histograms-density-plots.html

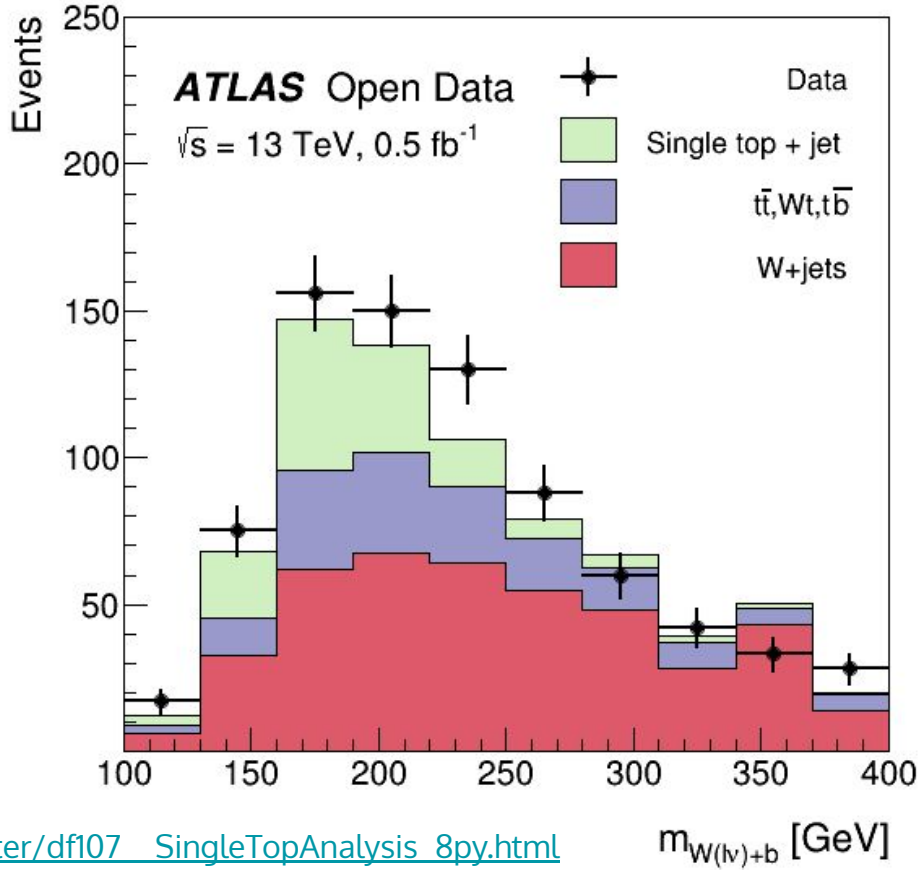
Histograms vs PDFs/Kernel Density





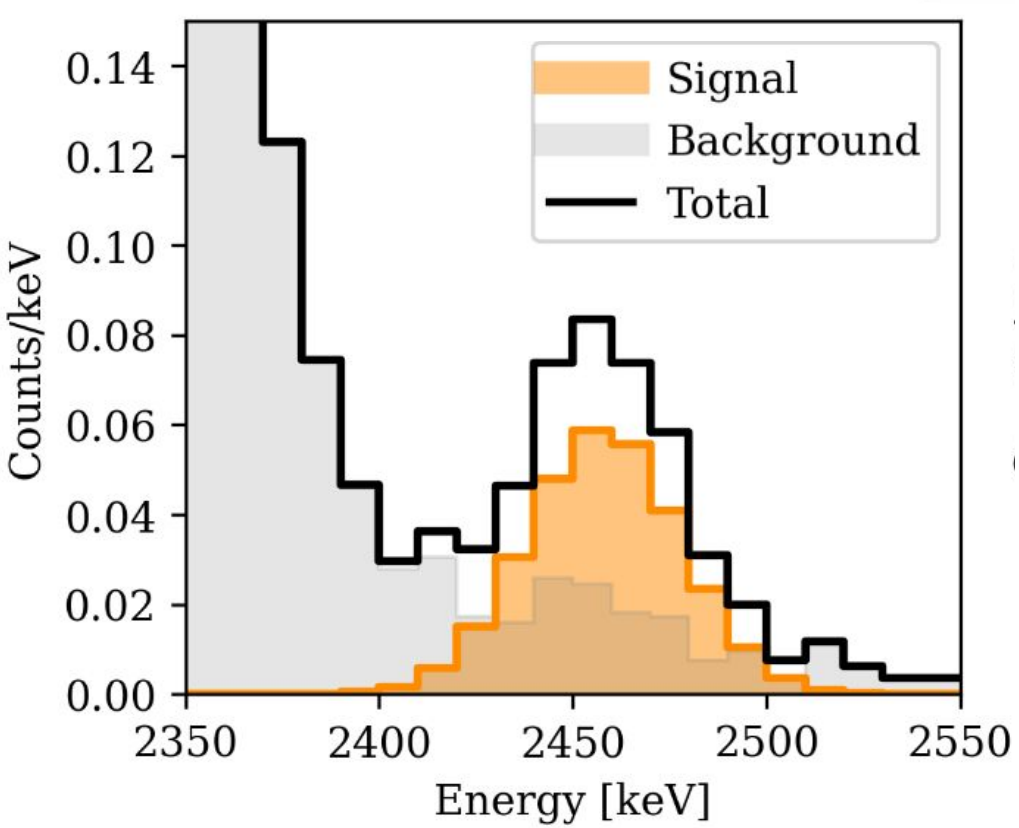
From: https://clauswilke.com/dataviz/histograms-density-plots.html

Stacked Histograms

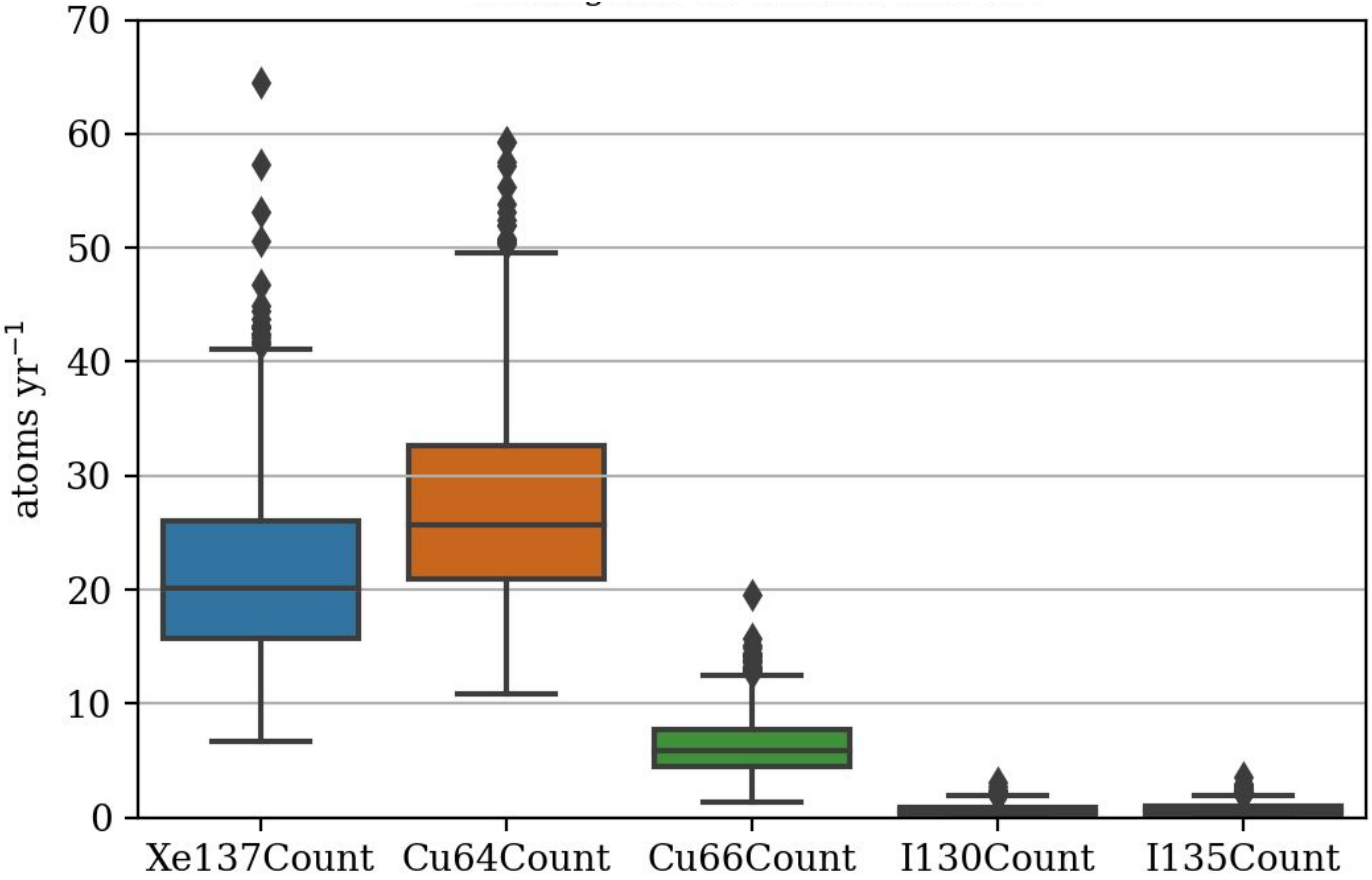


From: https://root.cern/doc/master/df107__SingleTopAnalysis_8py.html

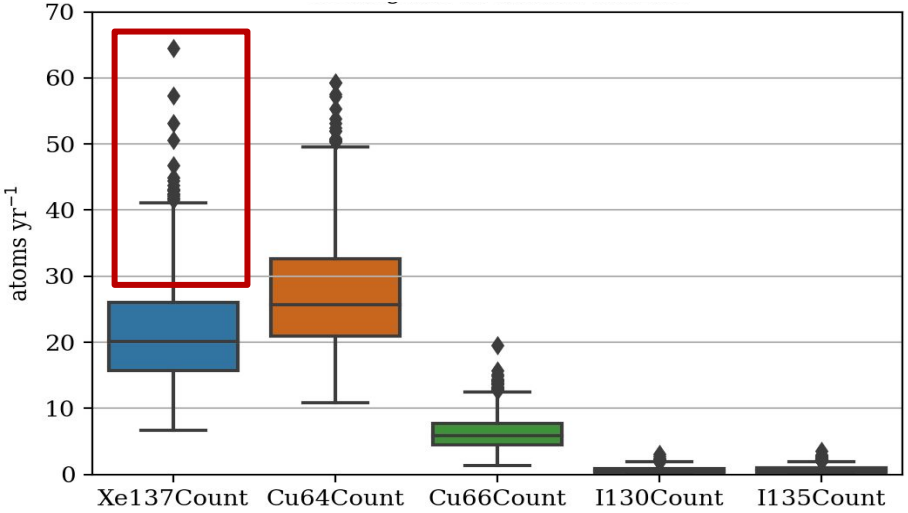
Overlaying Histograms/PDFs

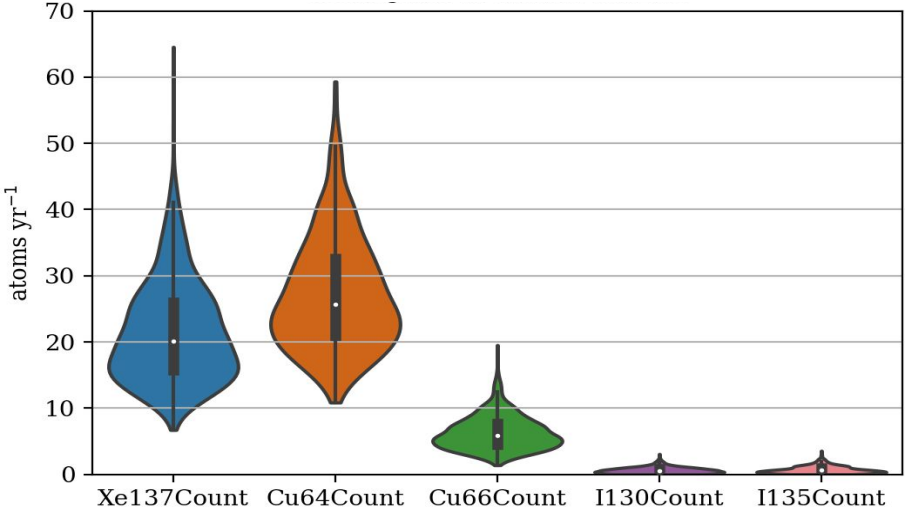


Box Plots

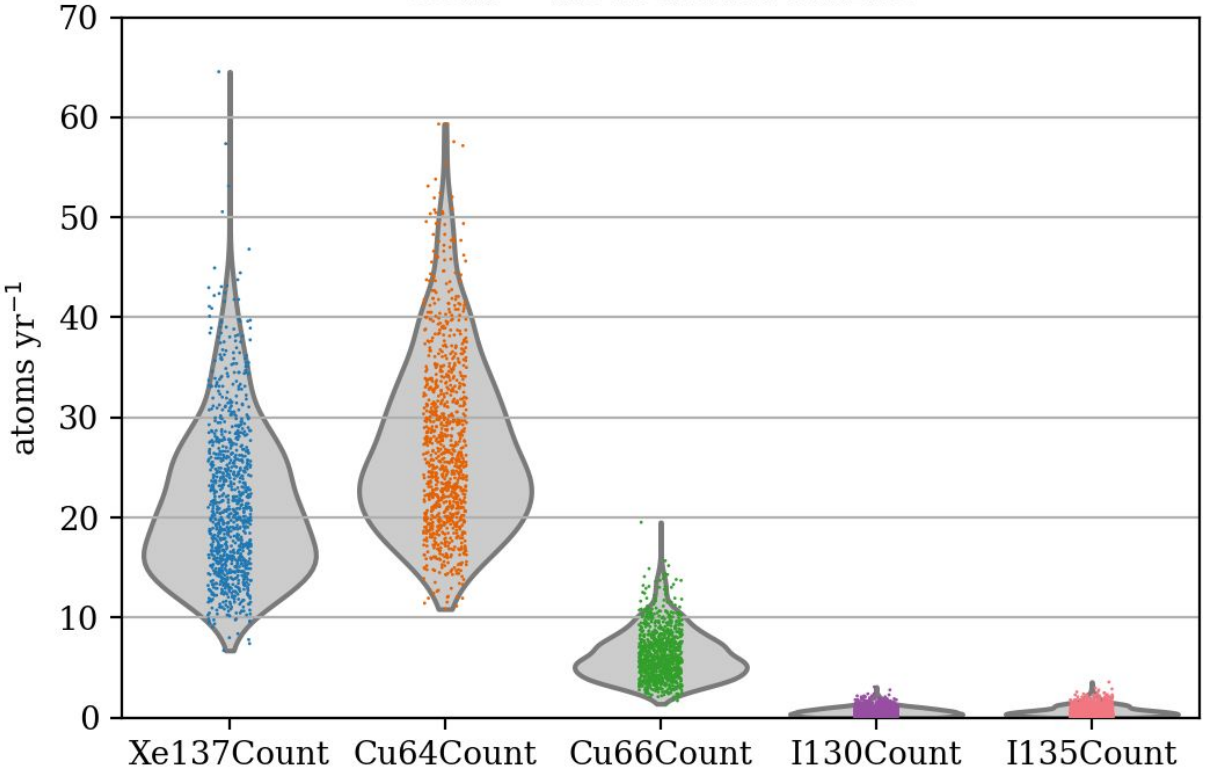

70
60
50
40
30
20
10
0
atoms yr^{-1}
Xe137Count
Cu64Count
Cu66Count
I130Count
I135Count

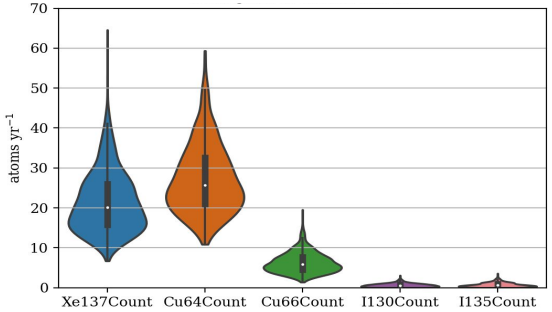
Box vs Violin Plot



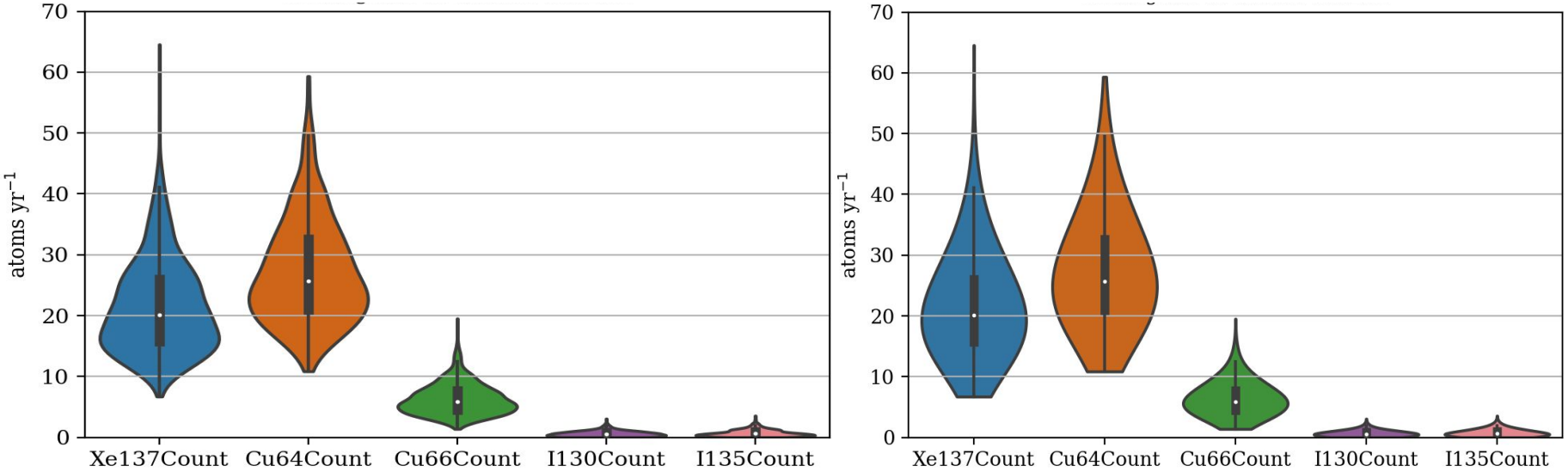


Violins with Strip Chart

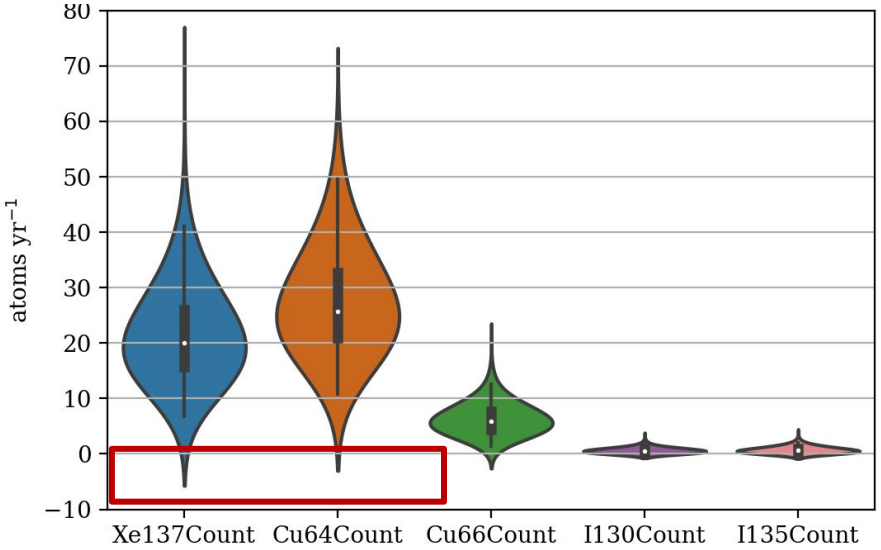


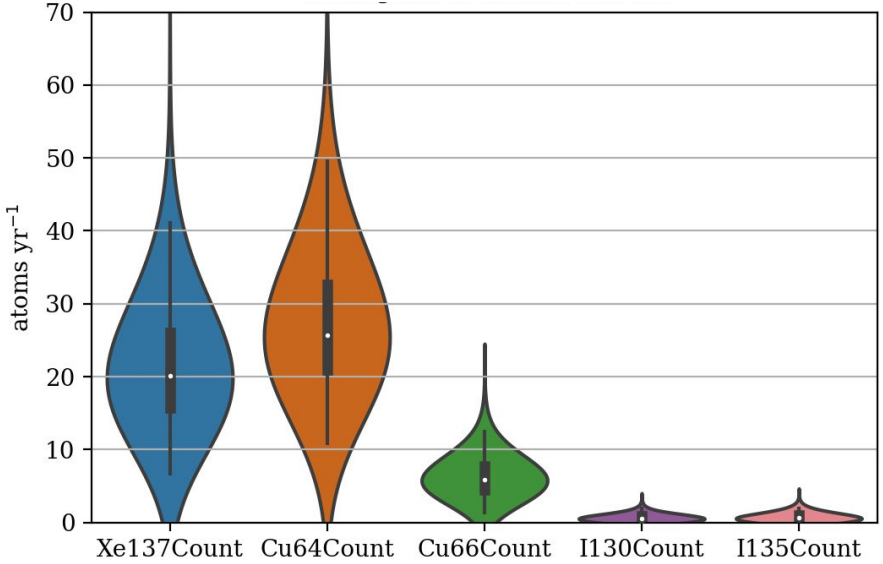


Smoothed Violin Plot



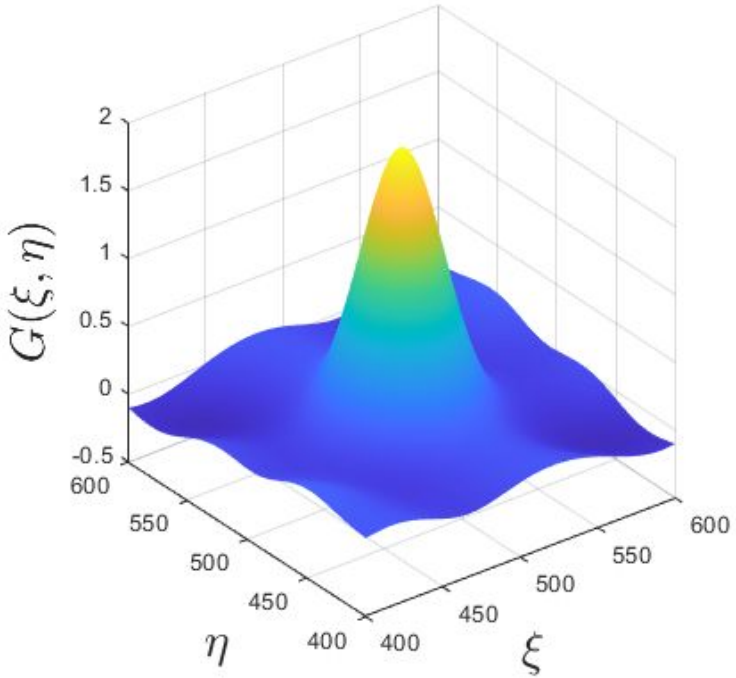
Smoothed Violin Plot

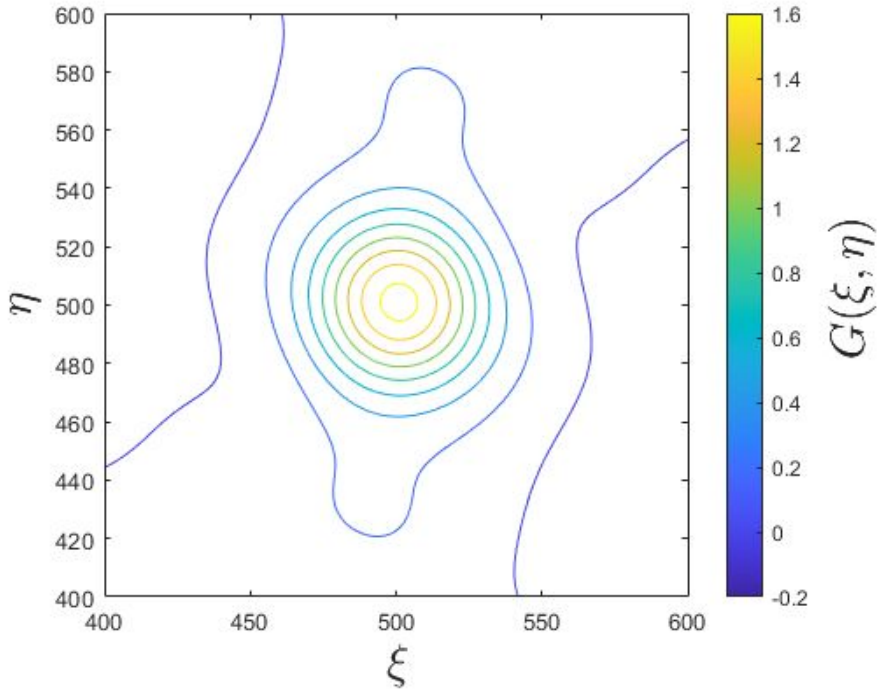




Changing “bandwidth” of kernel. I.e. number of σ to “smear by” can make things unphysical

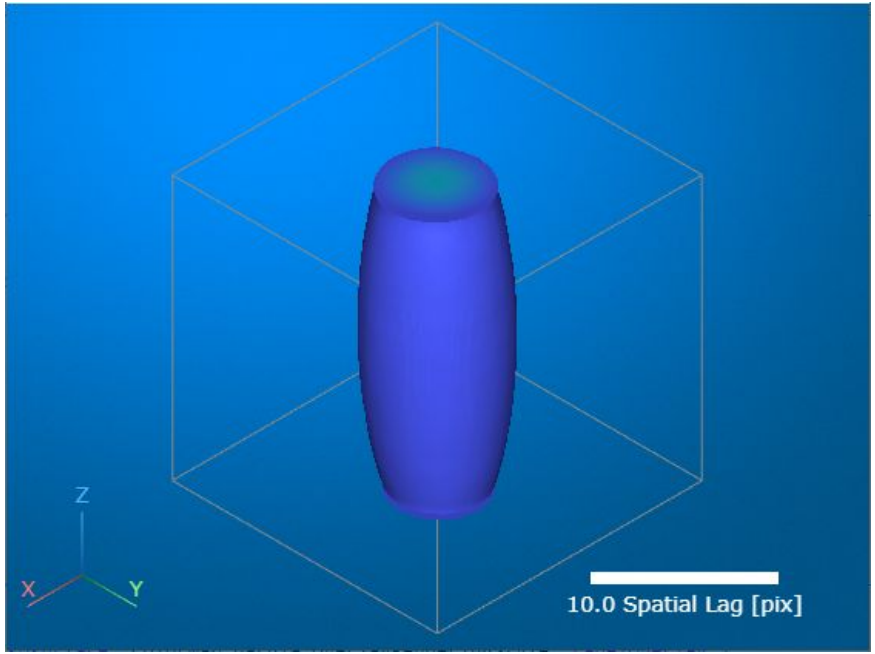
Surface vs Contour

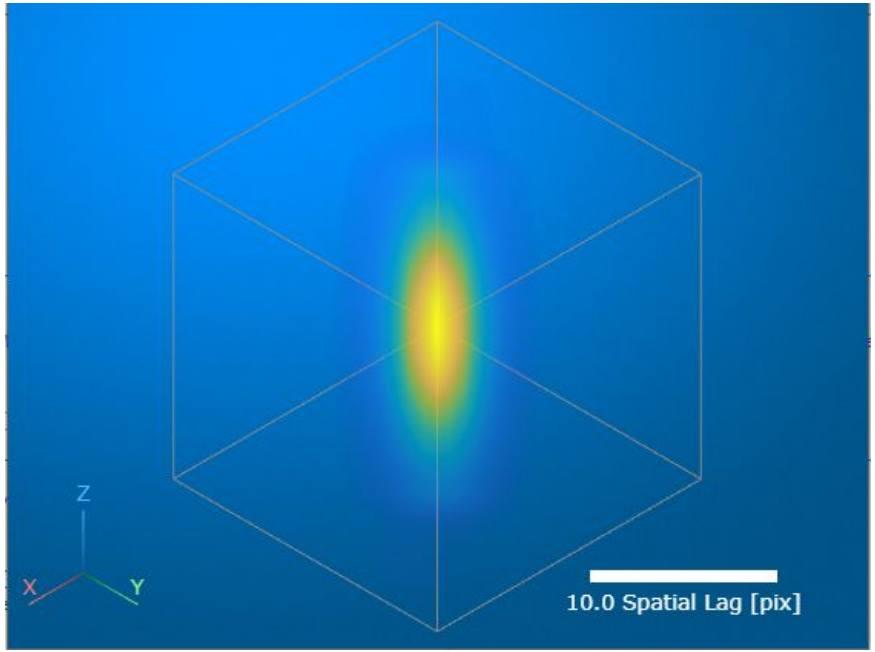




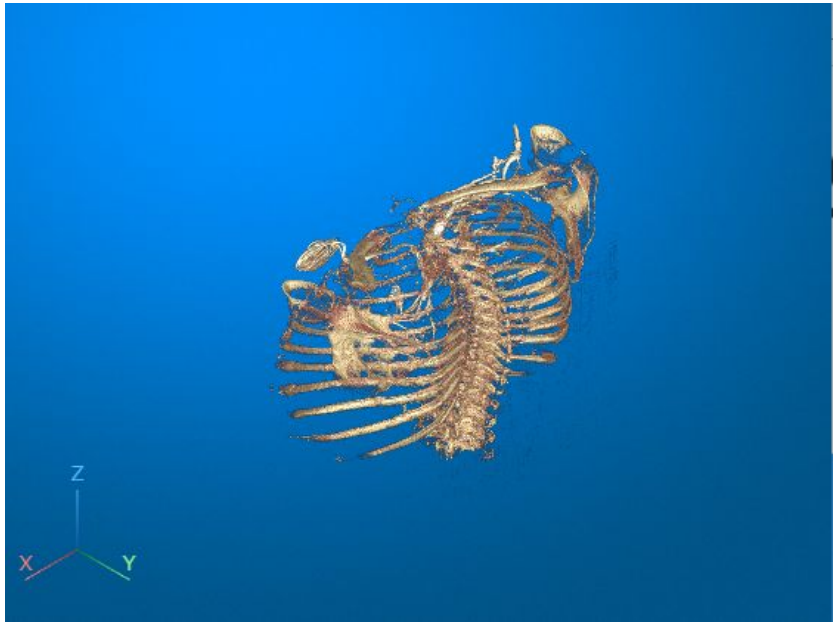
Surface vs Contour

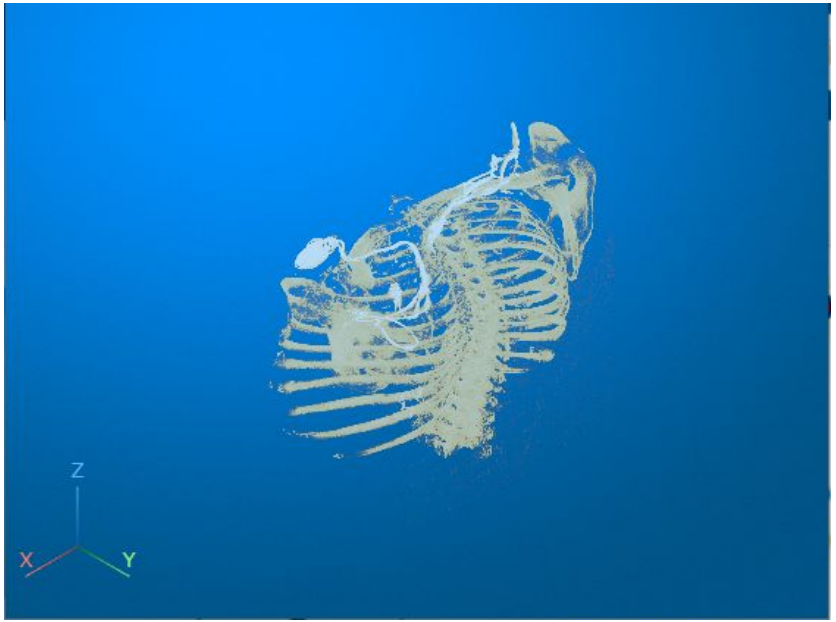
Isosurface vs Maximum Intensity





Isosurface vs Maximum Intensity





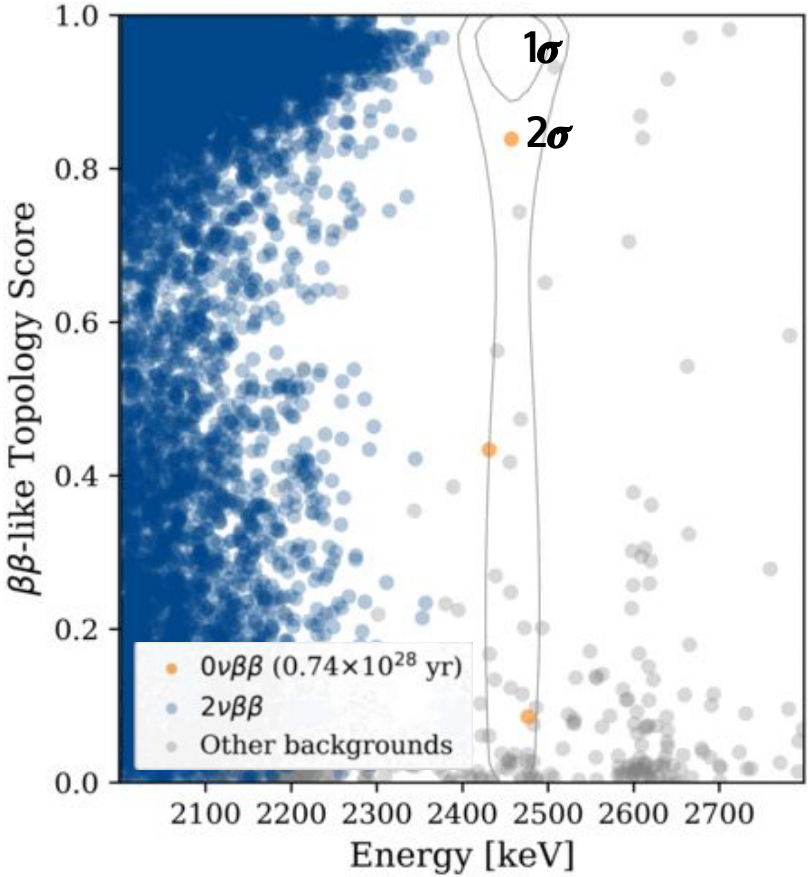
Contours

Contours can show

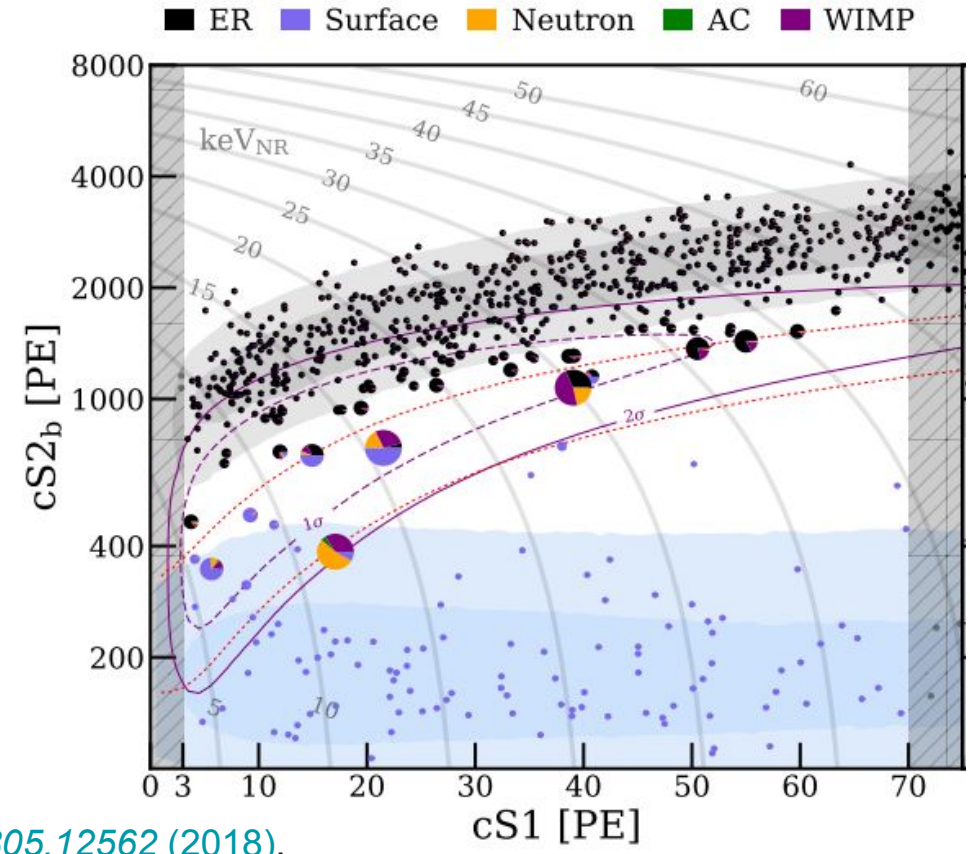
probability density contained within a region when used on scatter plots

or

isosurfaces (levels) of 3D surfaces



Multidimensional Scatter Plots



From XENON1T. arXiv:1805.12562 (2018).

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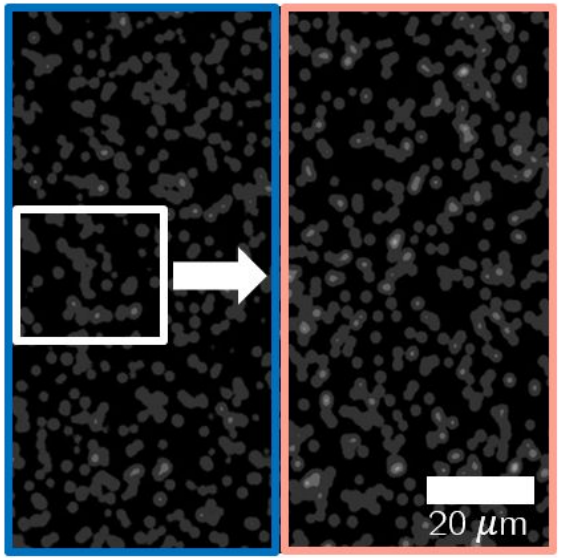
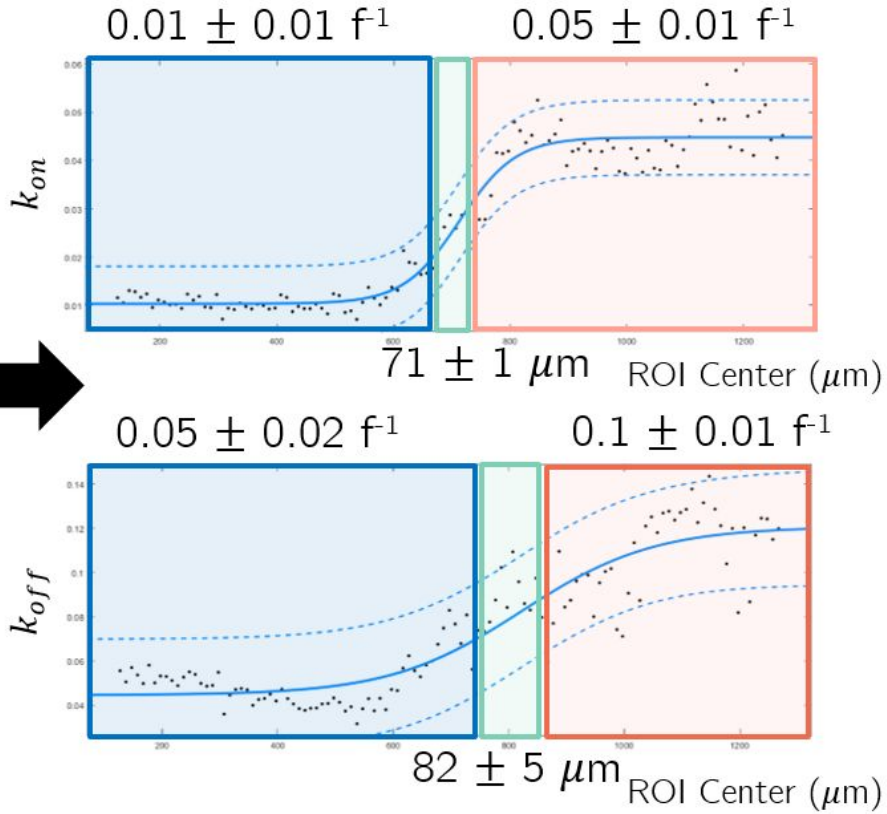
Trendlines vs Fits

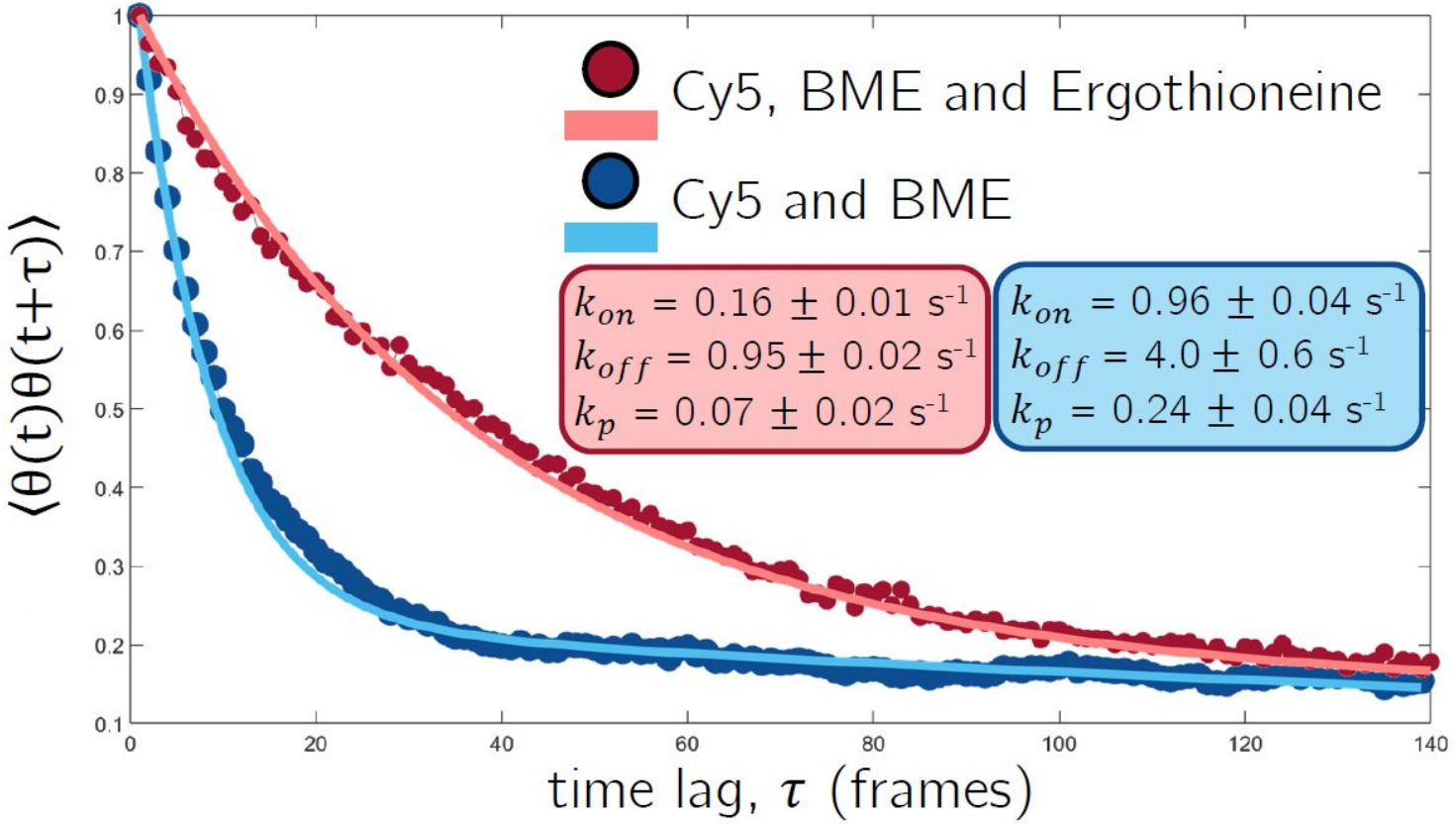


k_{on} = 0.01 f^{-1} k_{on} = 0.05 f^{-1}

k_{off} = 0.05 f^{-1} k_{off} = 0.1 f^{-1}



Trendlines vs Fits



Trendlines vs Fits: Summary

- When doing a fit, make sure to **show equations and fit results** somewhere!
- When needing a trendline to “guide the eye” either
  - Connect the dots by straight lines
  - Do some interpolation, e.g. cubic spline fit, but **state this!**
  - Consider showing the “confidence band” as a shaded region

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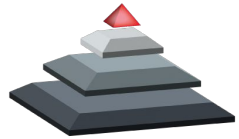
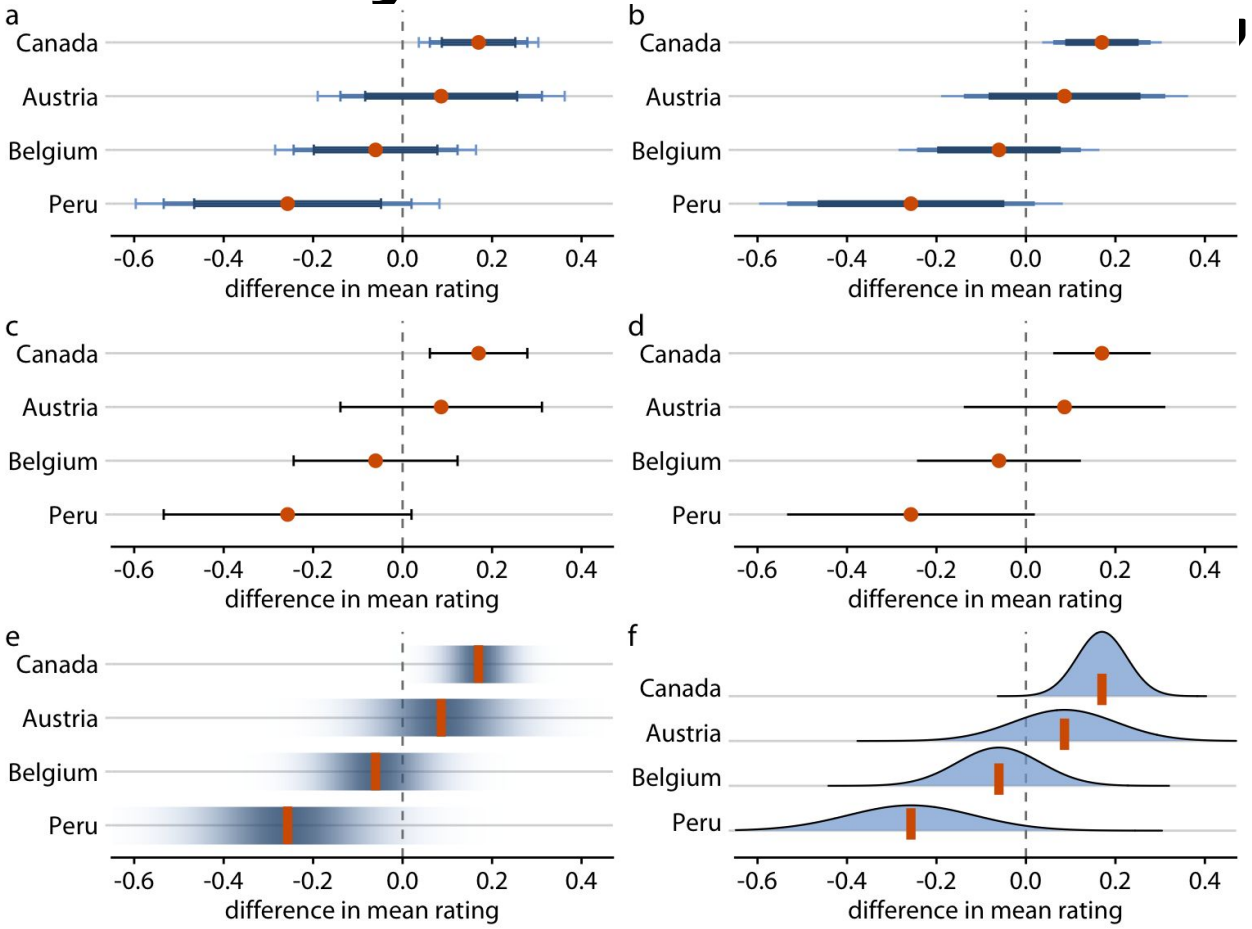
Visualizing Uncertainty

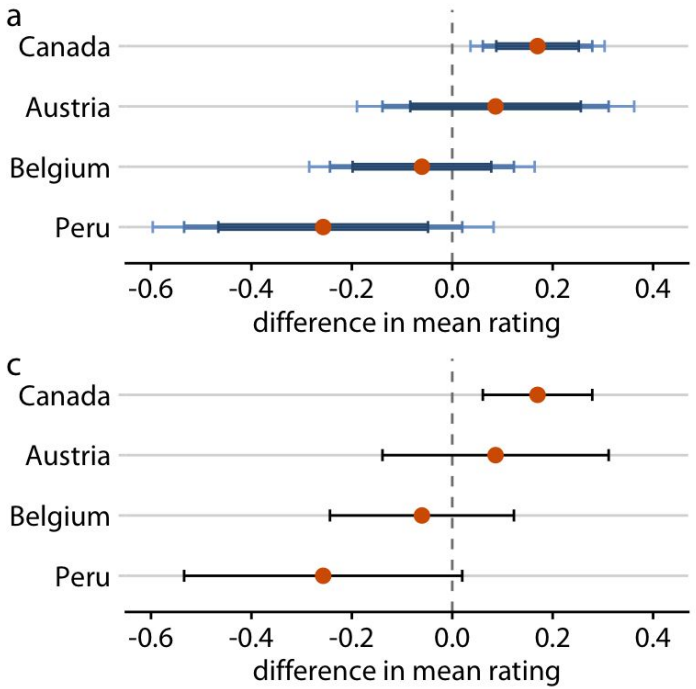




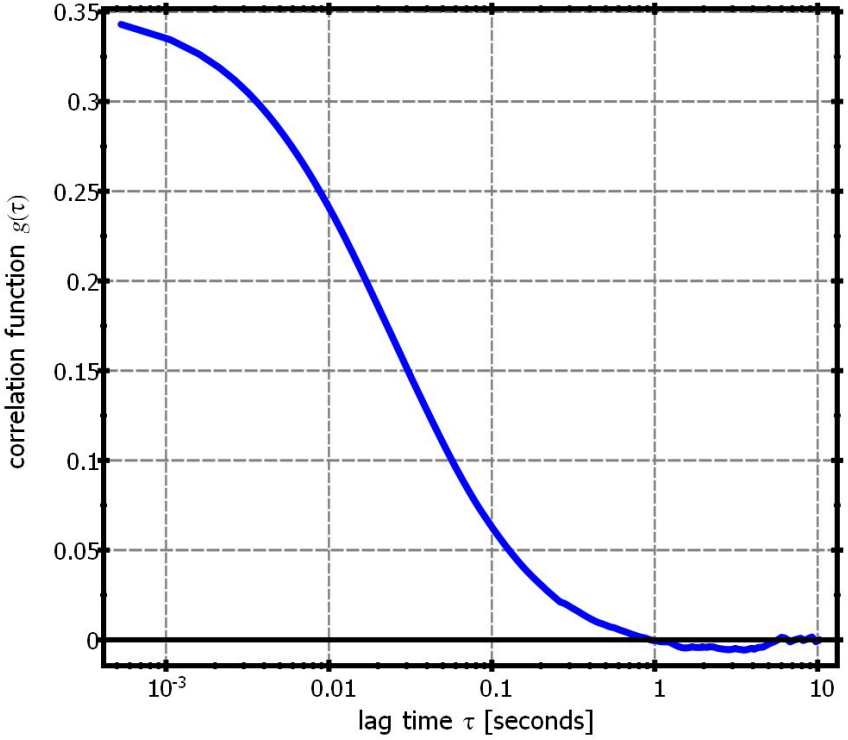
https://clauswilke.com/dataviz/visualizing-uncertainty.html#frequency-framing

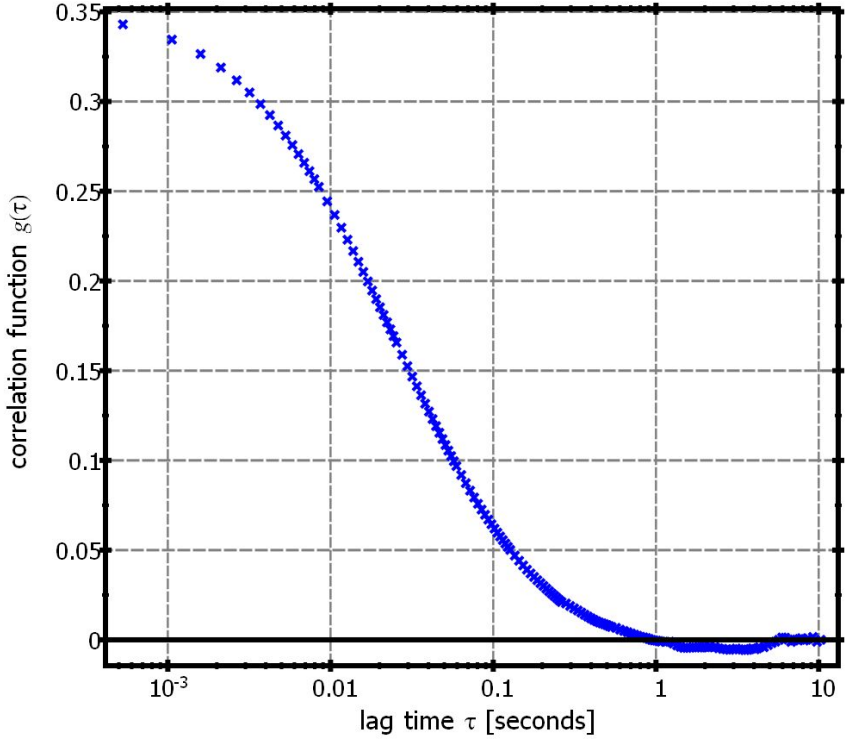
Visualizing Uncertainty

- When using error bars, you need to **state what they are!**

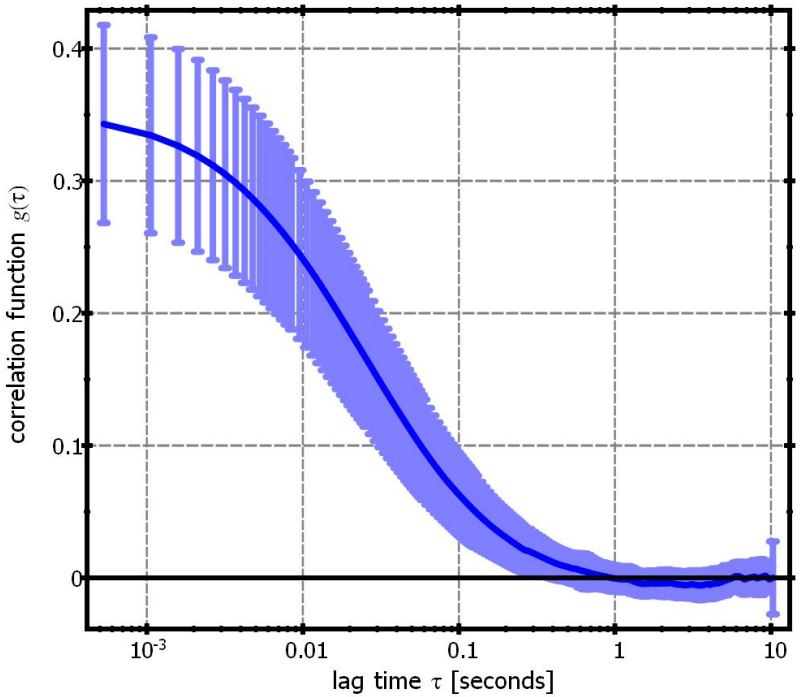


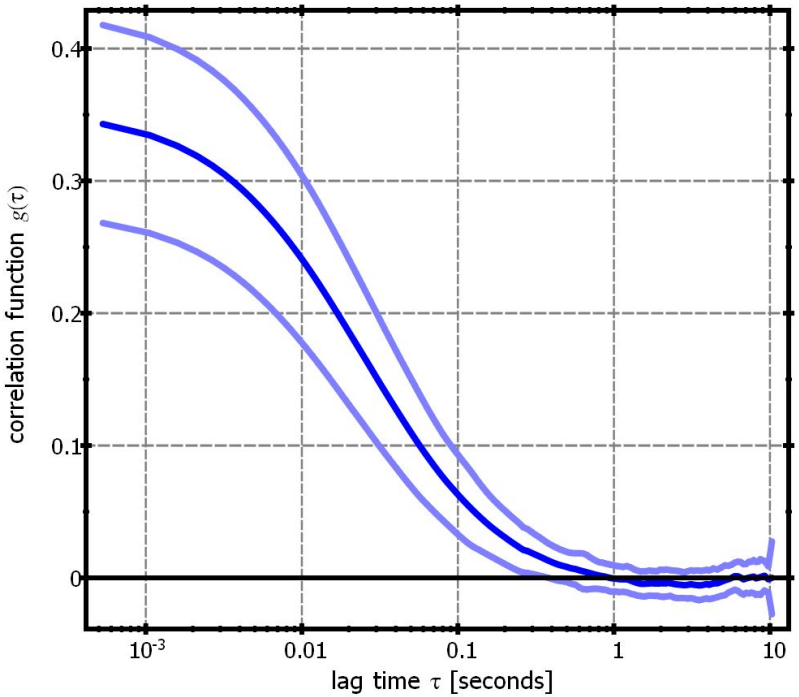
Visualizing Uncertainty



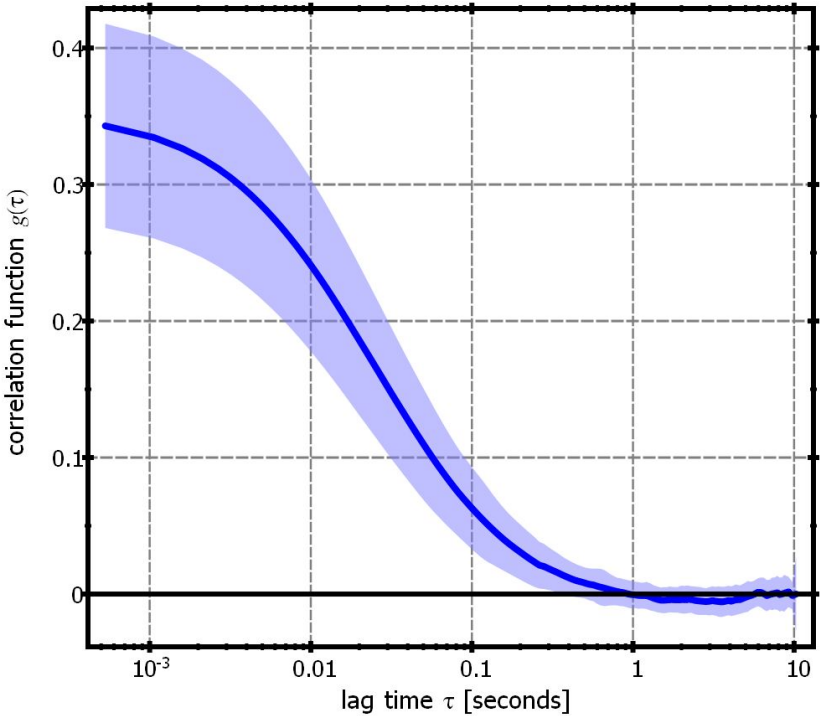


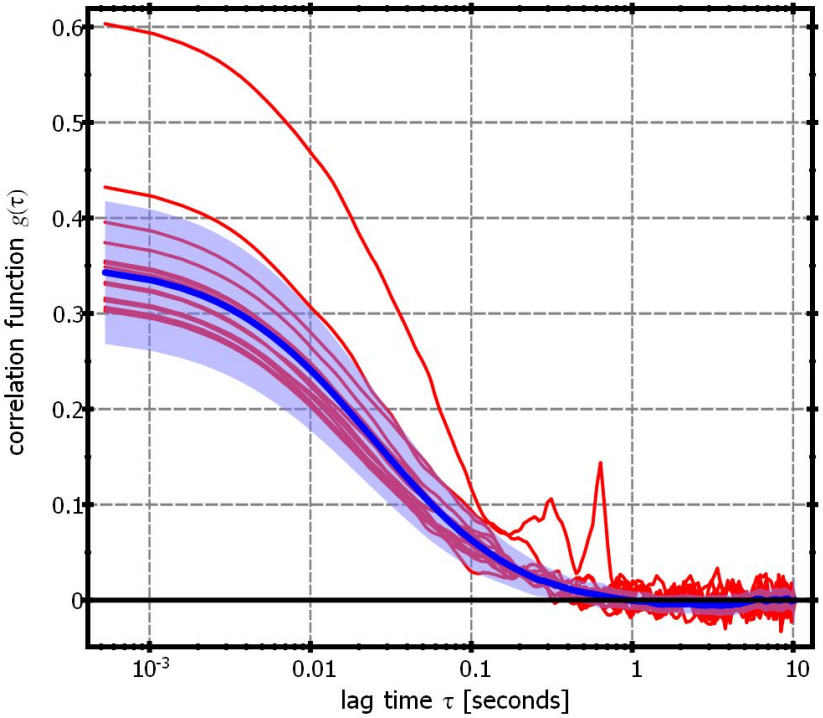
Visualizing Uncertainty



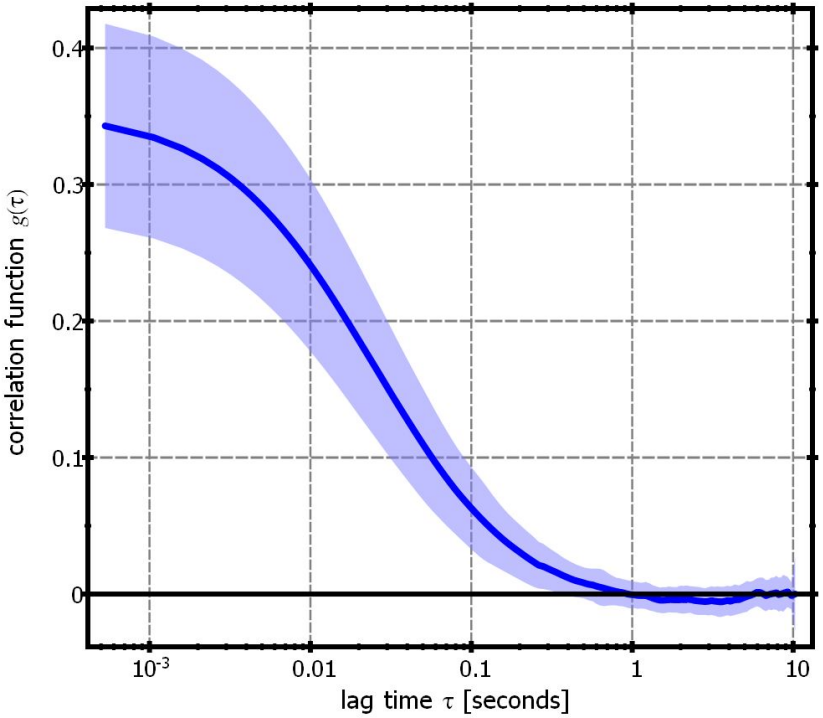


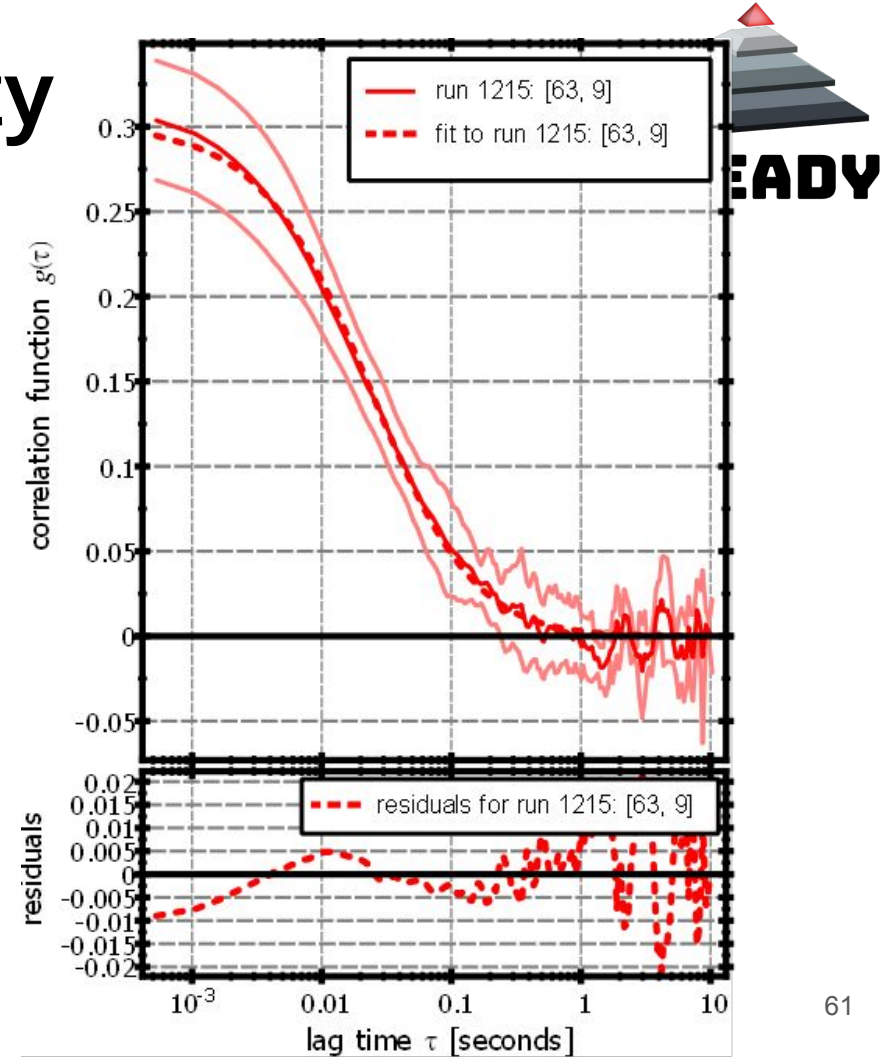
Visualizing Uncertainty





Visualizing Uncertainty

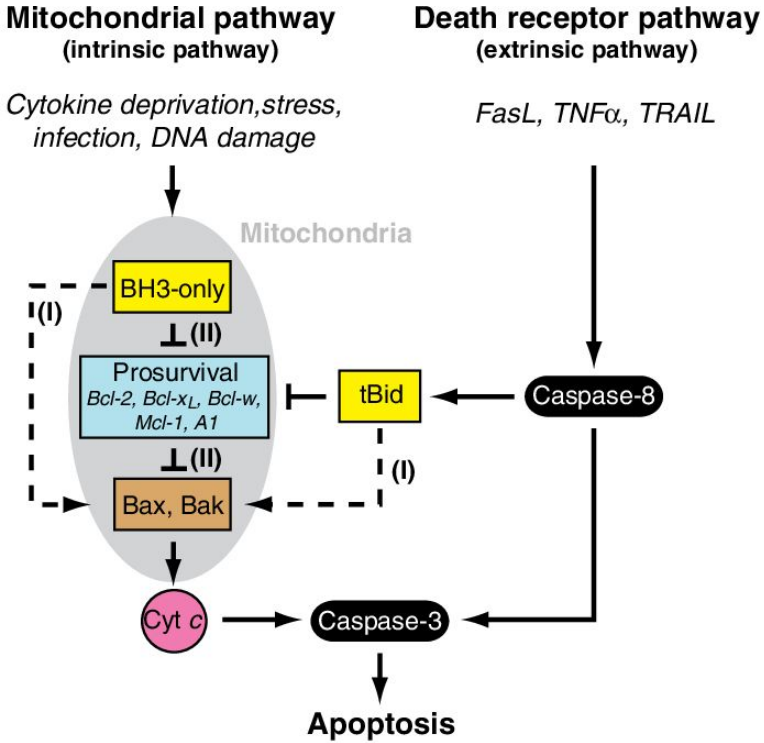




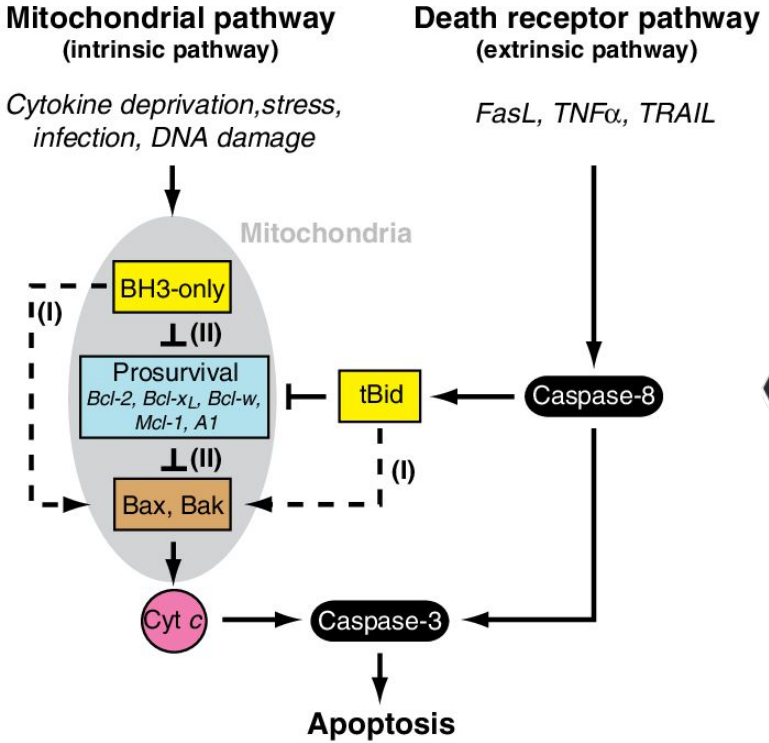
Overview

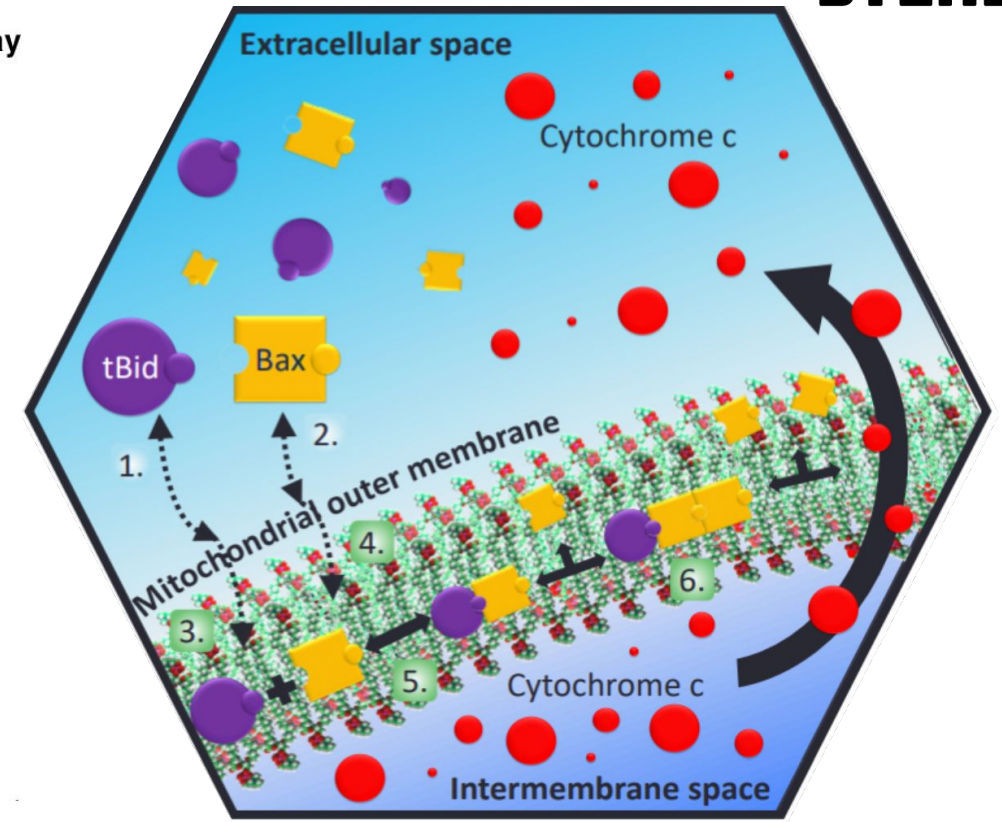
- Common things to think about
- Types of plots, and when to use them
- Trendlines vs fits
- Visualizing Uncertainties
- Schematics
- Plots that are meant for: papers, posters, talks...
- Exercises

Schematics: how to make them



Schematics: how to make them

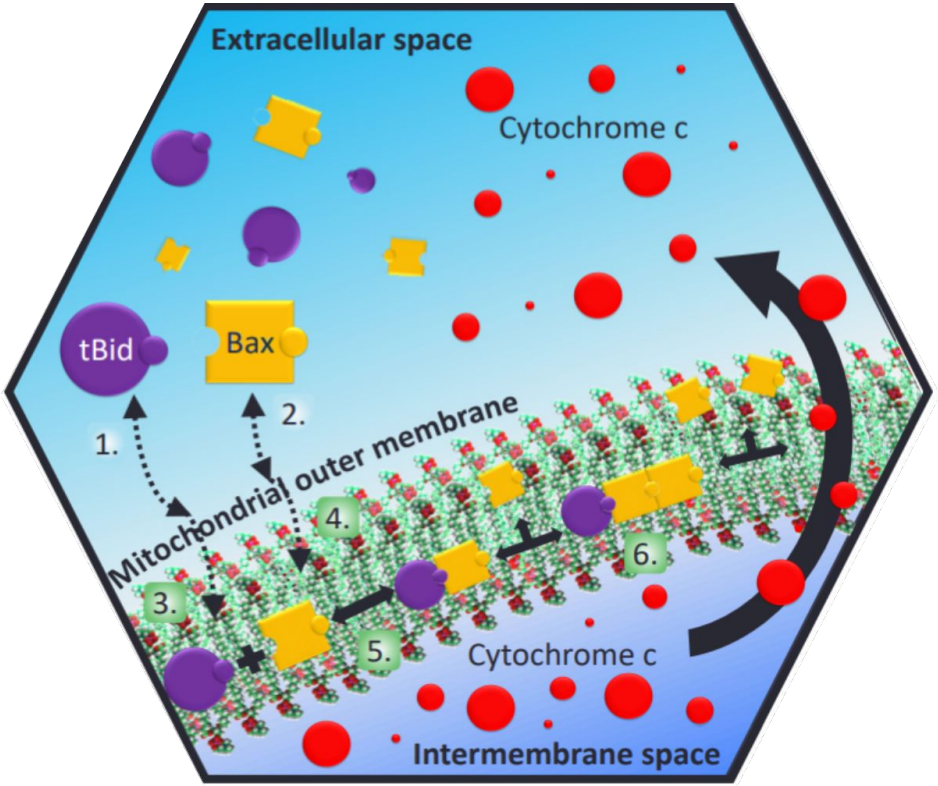




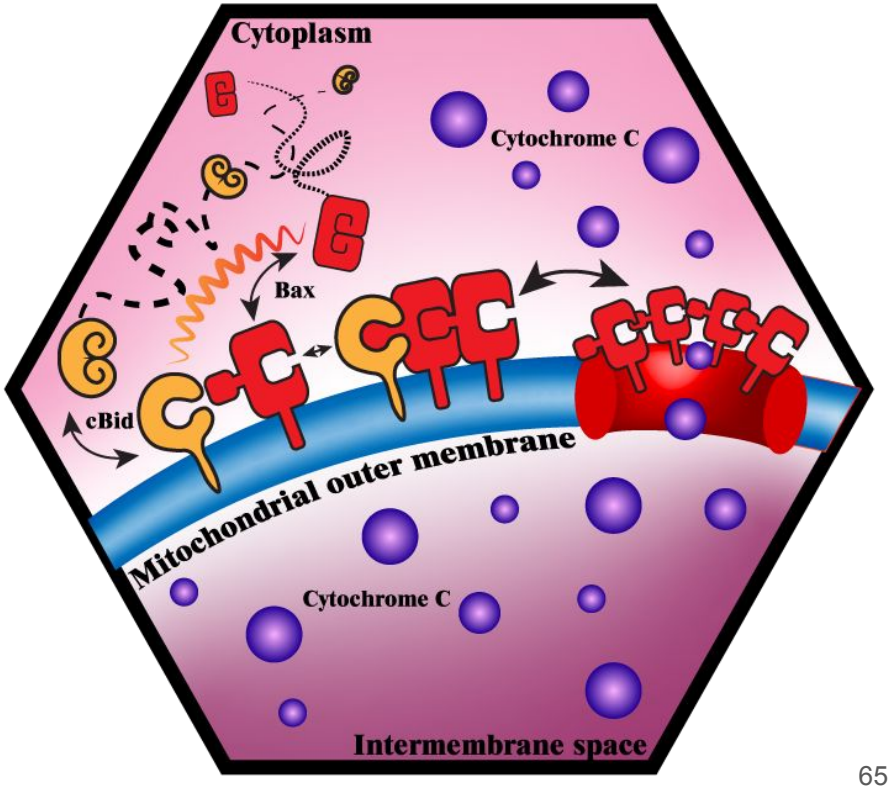
Schematics: how to make them

STEADY

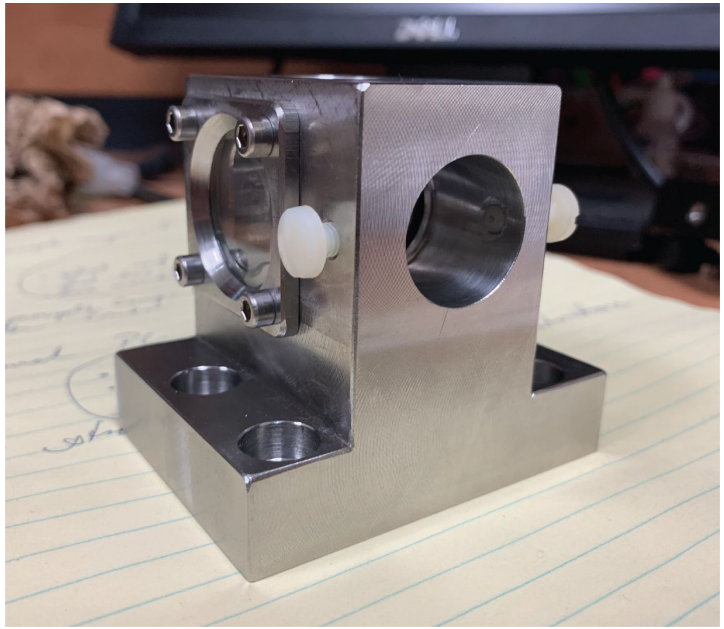
Powerpoint

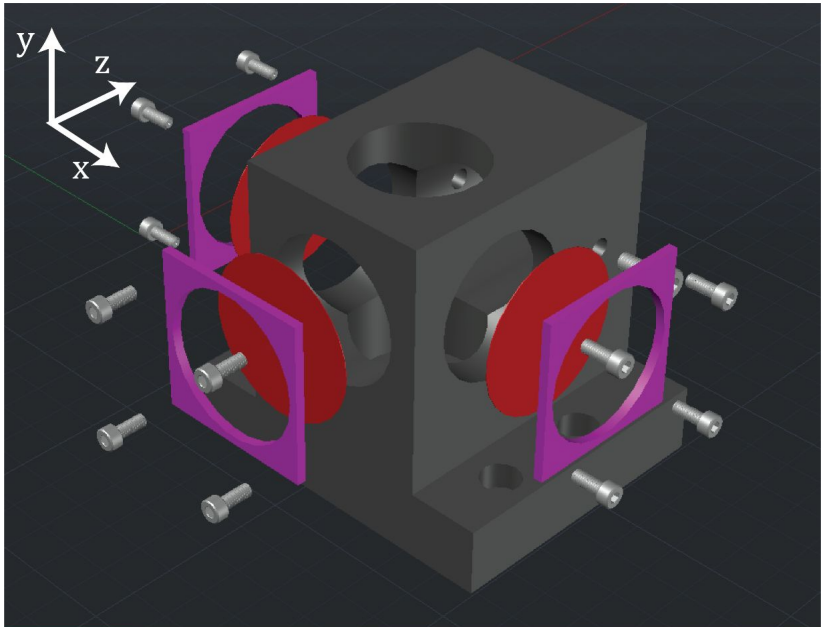


Adobe Illustrator

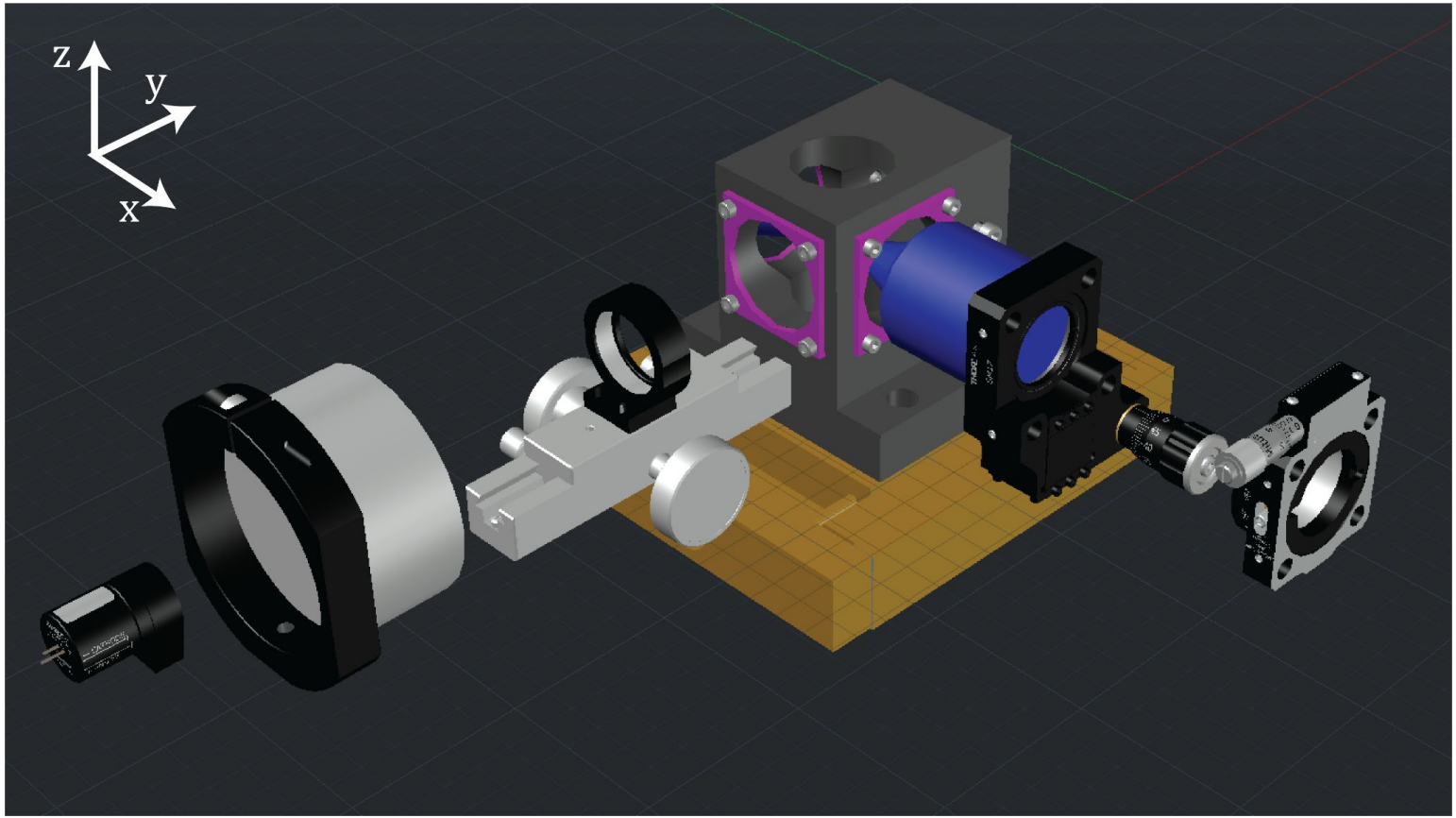


Schematics: AutoCAD





Schematics: CAD



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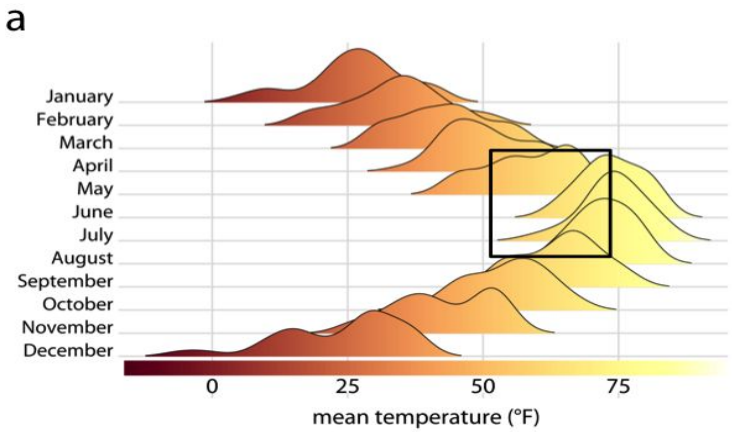
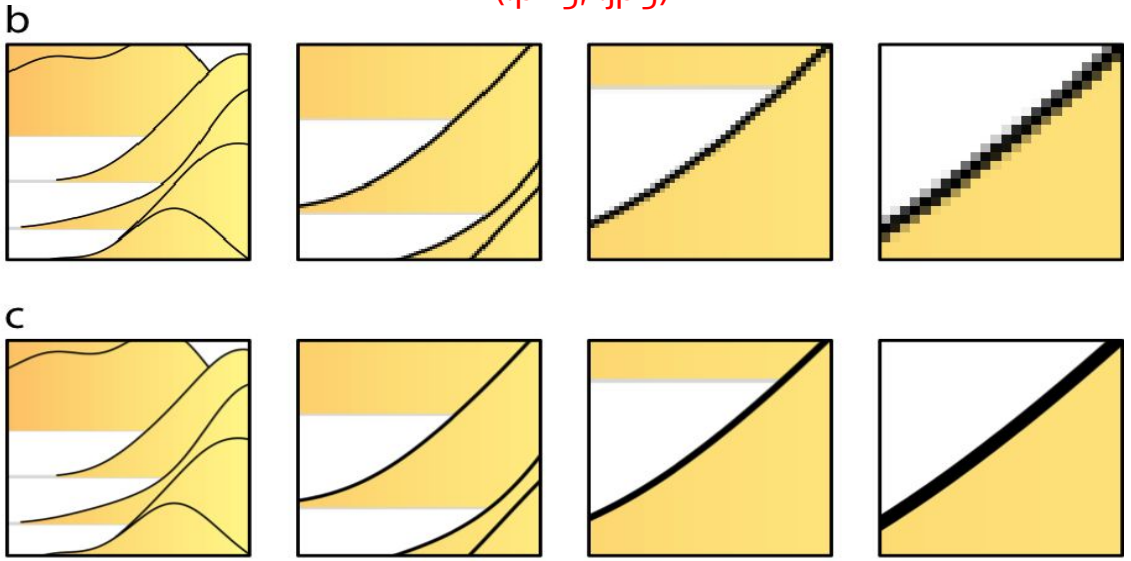
File Formats

Different formats are meant for different media



Bitmap formats
(.png, .jpg)



Vectorized formats
(.pdf, .svg, .eps)

From: https://clauswilke.com/dataviz/image-file-formats.html

File Formats

Different formats are meant for different media

Examples:

- .png are lightweight, good for online plots (load time)
- .pdf/.svg/.eps are vectorized (“infinite” zoom! 🧐)
- .jpg are generally not great, avoid except for compressed photographs
    - But, when *taking* photos (camera data) use .raw or .tif/.tiff file formats!

File Formats

General rule when making plots and saving them

save high-dpi (600+) .png files, **or** a pdf

convert and lower resolutions as needed and when necessary

Examples:

- .pdf/.eps for journals
- .svg for your website
- .png for slide presentations

Common Tripping Hazards

- Choose the **right type of plot**
  - What is it about your data that you are trying to get across?
- Choose your colours wisely
  - What is the **relationship** between the data products you are showing?
- Tick marks & axes labels
  - **always go bigger** than the default size
- Pick a plotting package you like, and get good at it ⟶ set custom defaults
  - e.g. matplotlib style files (.mplstyle)

Common Tripping Hazards 2

- Will the plot be printed out?
  - Are your **lines/points distinguishable** in **grayscale**?
- Choose the right file type for exporting
  - .pdf/.eps for papers, .png/.svg for web
- Always **specify what your “error bars” are**
  - Are they standard errors on mean? std, σ ? Or some confidence interval?
- **Don’t *overuse* Jupyter** Notebooks
  - Good for plotting, not good for coding...

Acknowledgements

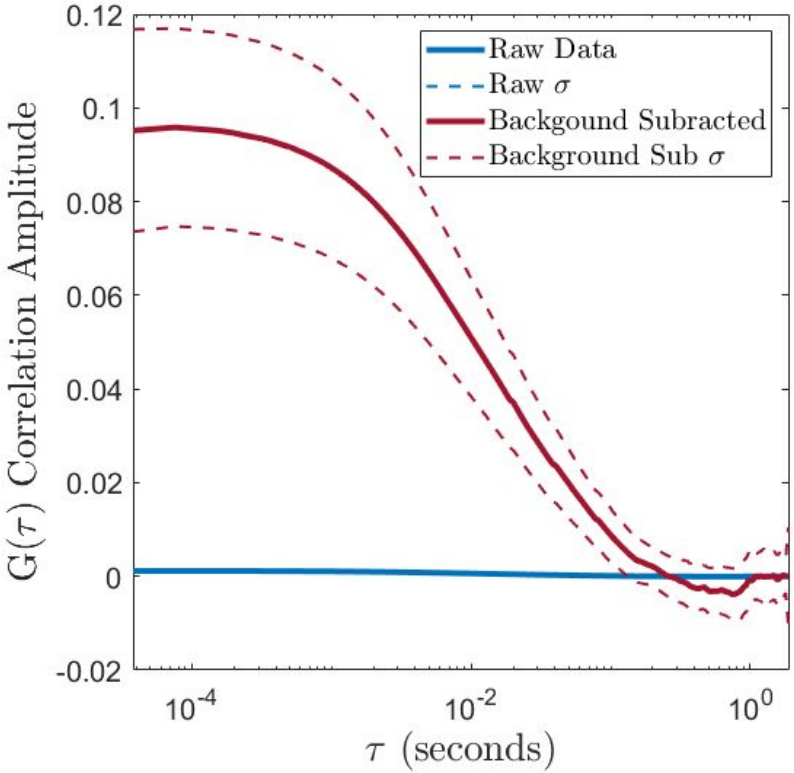
Thank you to everyone who contributed data and/or plots & posters to make this workshop happen!

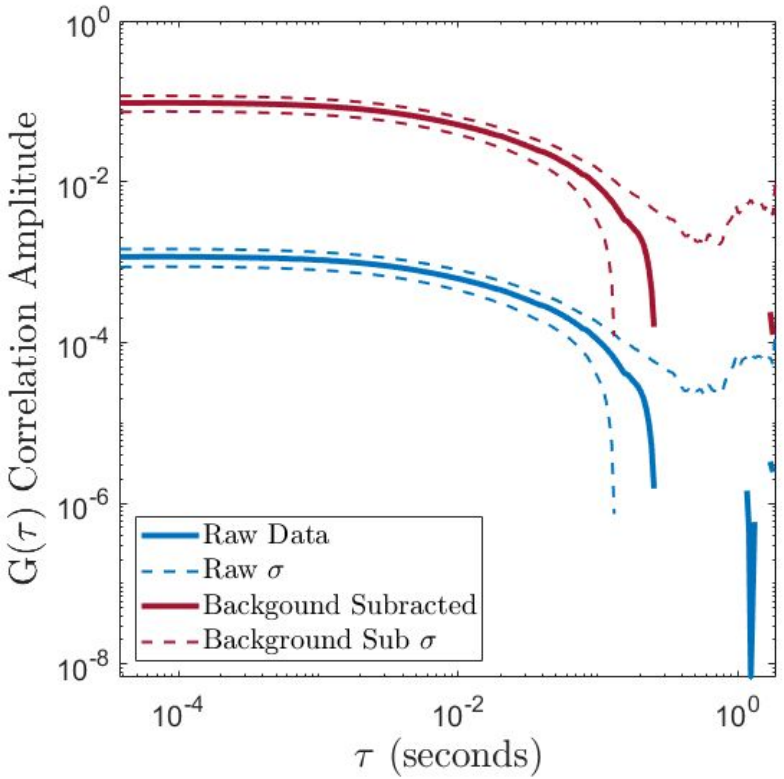
Catherine B., Rodrigo P., Adam C., Lauren P., Gaspard B.

Exercise

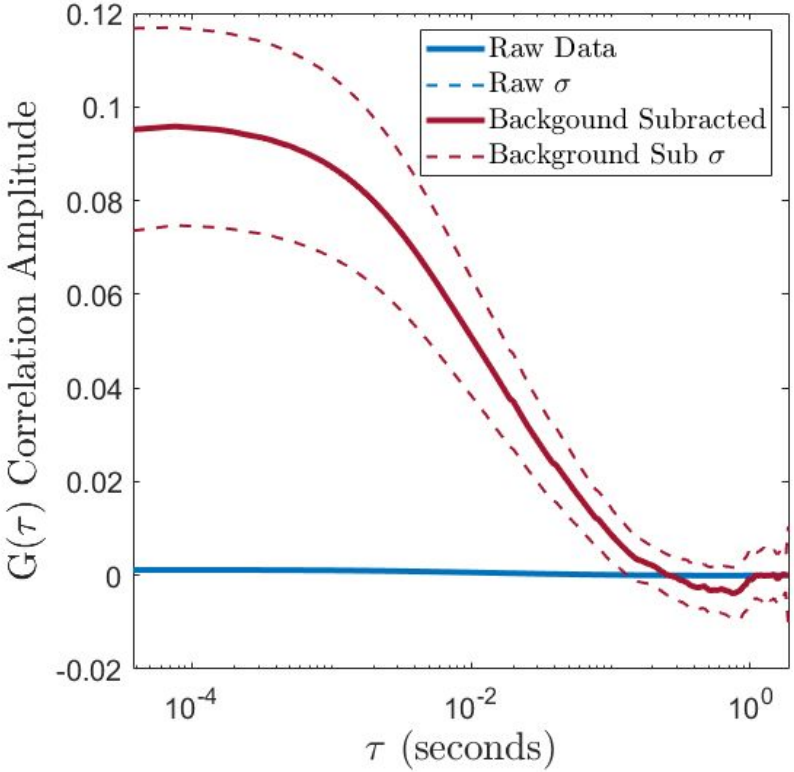
1. Open the onedrive link on Slack **#data-visualization** or the indico page
2. Download the **.csv** file
3. Try plotting the data
4. Upload your plots back to the onedrive!

Exercise


Raw Data
Raw σ
Backgound Subracted
Background Sub σ
G(τ) Correlation Amplitude
τ (seconds)
0.12
0.1
0.08
0.06
0.04
0.02
0
-0.02
10^-4
10^-2
10^0


Raw Data
Raw σ
Backgound Subracted
Background Sub σ
G(τ) Correlation Amplitude
τ (seconds)
10^0
10^-2
10^-4
10^-6
10^-8
10^-4
10^-2
10^0

Exercise


0.12
0.1
0.08
0.06
0.04
0.02
0
-0.02
G(τ) Correlation Amplitude
Raw Data
Raw σ
Backgound Subracted
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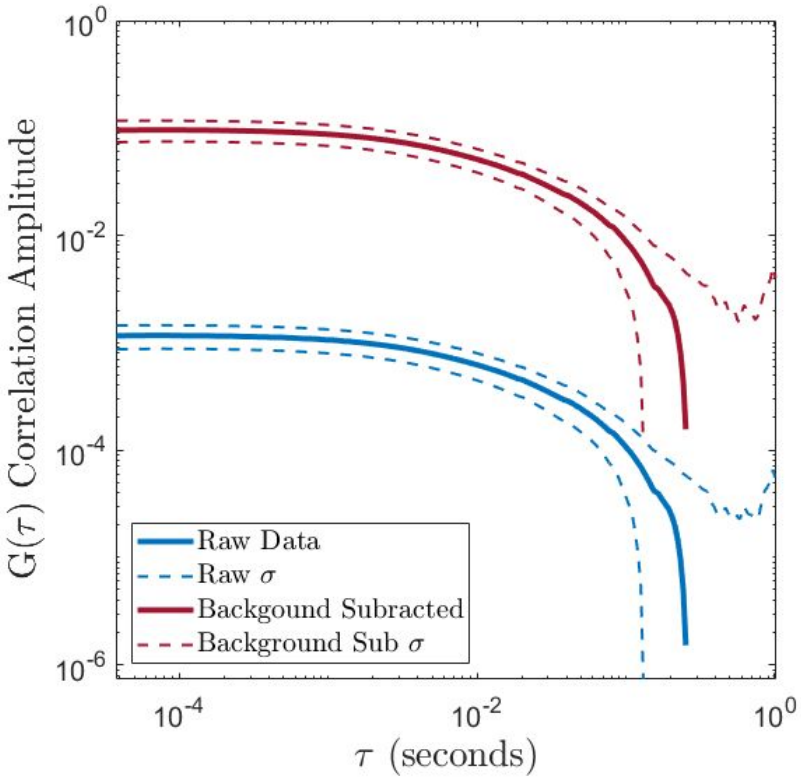
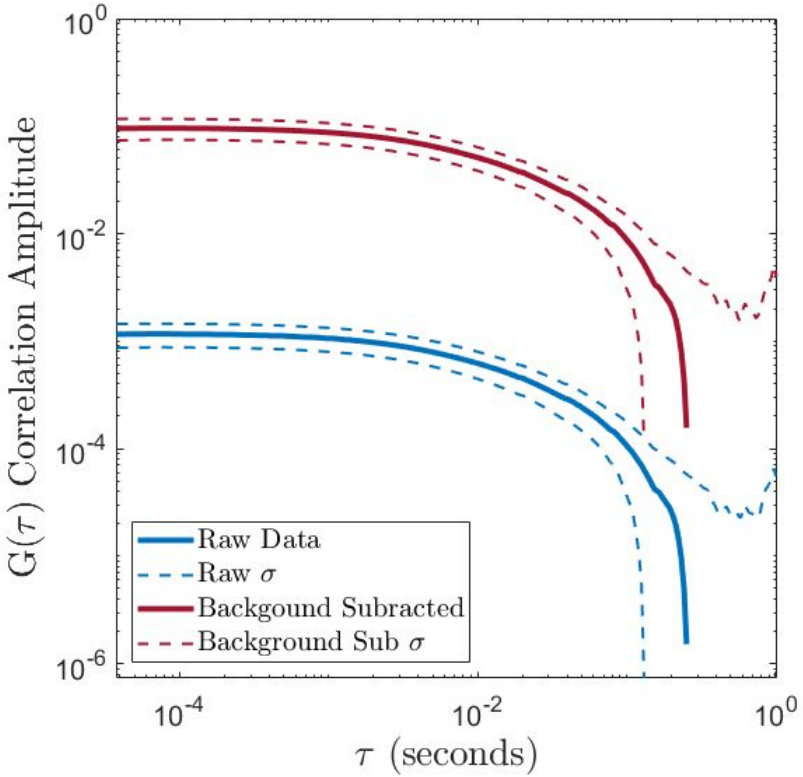
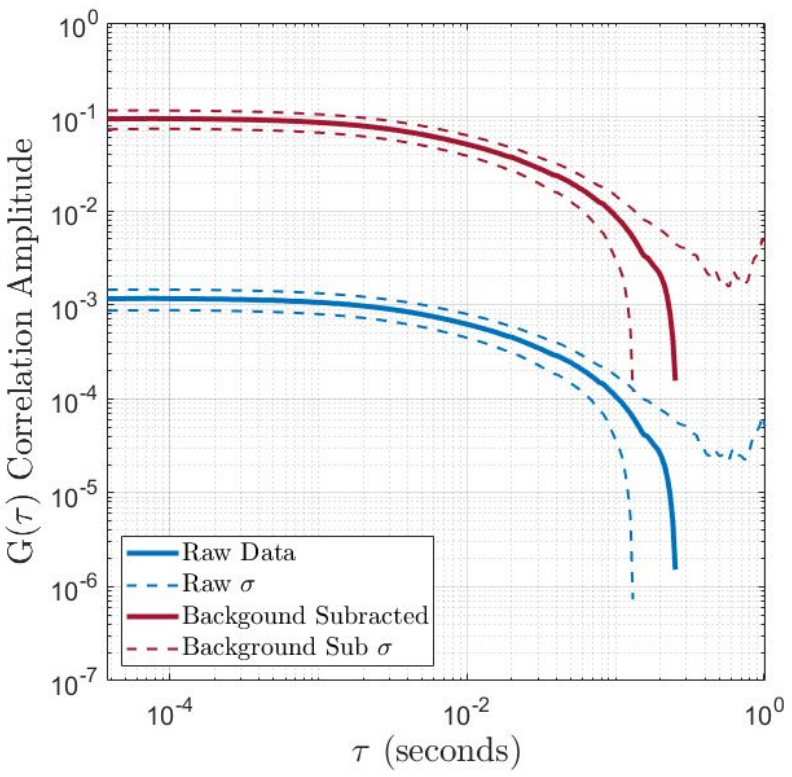
10^-4
10^-2
10^0
τ (seconds)


10^0
10^-2
10^-4
10^-6
G(τ) Correlation Amplitude
Raw Data
Raw σ
Backgound Subracted
Background Sub σ
10^-4
10^-2
10^0
τ (seconds)

Exercise


10^0
10^{-2}
10^{-4}
10^{-6}
G(τ) Correlation Amplitude
Raw Data
Raw σ
Backgound Subracted
Background Sub σ
10^{-4}
10^{-2}
10^0
τ (seconds)


10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
G(τ) Correlation Amplitude
Raw Data
Raw σ
Backgound Subracted
Background Sub σ
10^{-4}
10^{-2}
10^0
τ (seconds)

Some Resources

Data Visualization:

- Free crash-course book on data viz: https://clauswilke.com/dataviz/index.html

Posters:

- Audience should be able to get these items *without* you being present
  - Topic
  - Main method / workflow
  - Conclusion
- Check out #betterposter on YouTube

Fantastic Software Packages & Where to Find Them

STEADY

- **Python**: Matplotlib, seaborn
  - Consider editing your default .mplstyle file
- **Matlab**: (basically matplotlib)
- **Web pages**: plotly (javascript)