- A brief overview of the reflectometry technique
- Discussion of reflectometry analysis methodology
- Th

# Introduction to Reflectometry: With a Focus on Analysis

FASEM for Life Science — 2024/03/12


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♂ (he/him)

# Just a few housekeeping rules.

- between the accent and my speed of speech, I may be hard to understand — let me know.
- let's make this a dialogue; ask questions if you have them and I will ask you questions.
- unfortunately, I need to leave, to return to Bristol, straight after lunch, if you want to chat please drop me an email.

- A brief overview of the reflectometry technique
- Discussion of reflectometry analysis methodology
- Outline of some life science examples of reflectometry
- The opportunity to perform some reflectometry analysis using Python

# What is the difference between reflectometry and reflectivity?

- reflectometry: the technique used to measure reflectivity
- reflectivity: the quantity measured by reflectometry

Reflectometry is a surface sensitive analysis technique.

*"God made solids, but surfaces are the work of the devil",*

Wolfgang Pauli

# Reflectometry is a surface sensitive analysis technique.

- neutron or x-rays
- reflection geometry: angle of incidence = angle of reflection
- ratio of incidence to reflected intensity

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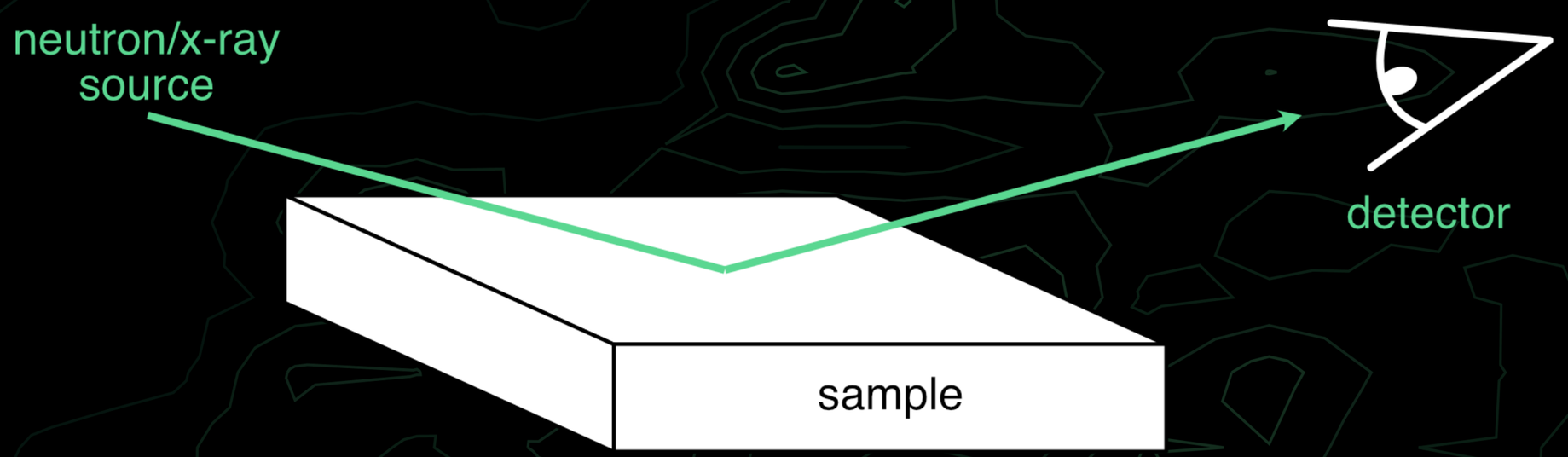

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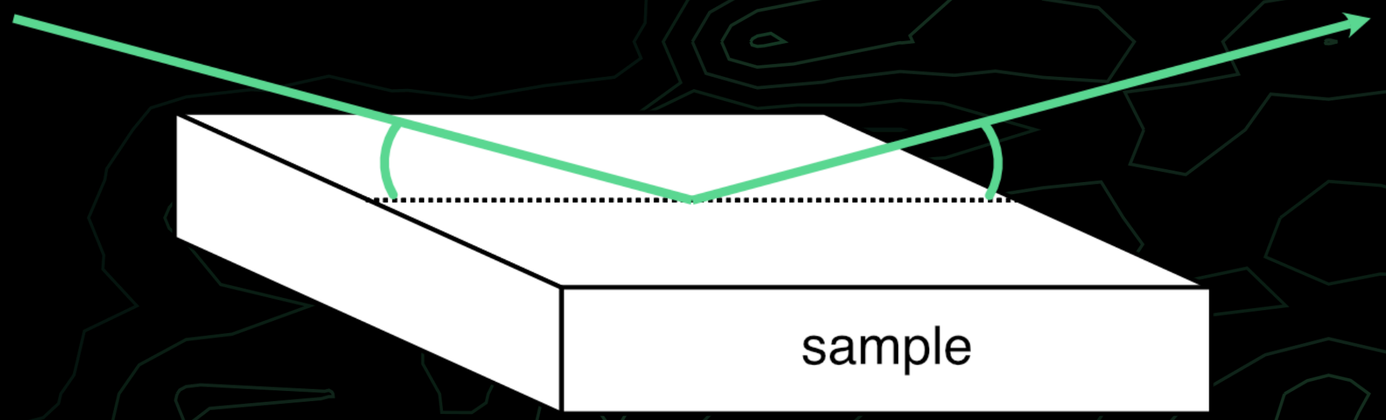
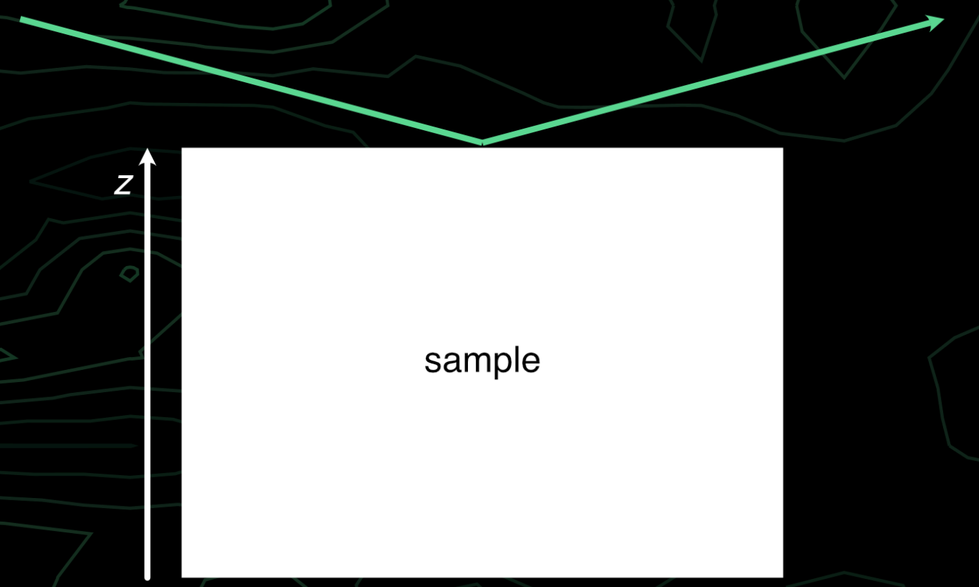



$$q = \frac{4\pi}{\lambda} \sin\theta$$

# Reflectometry measurements contain information about the material structure perpendicular to the interface.

- information about the scattering length density: $\boldsymbol{\rho} = \frac{\sum_{i=1}^{N} b_i}{V_m}$
  - $\rho$ is a material property
- we relate $\rho$ to our understanding of the system



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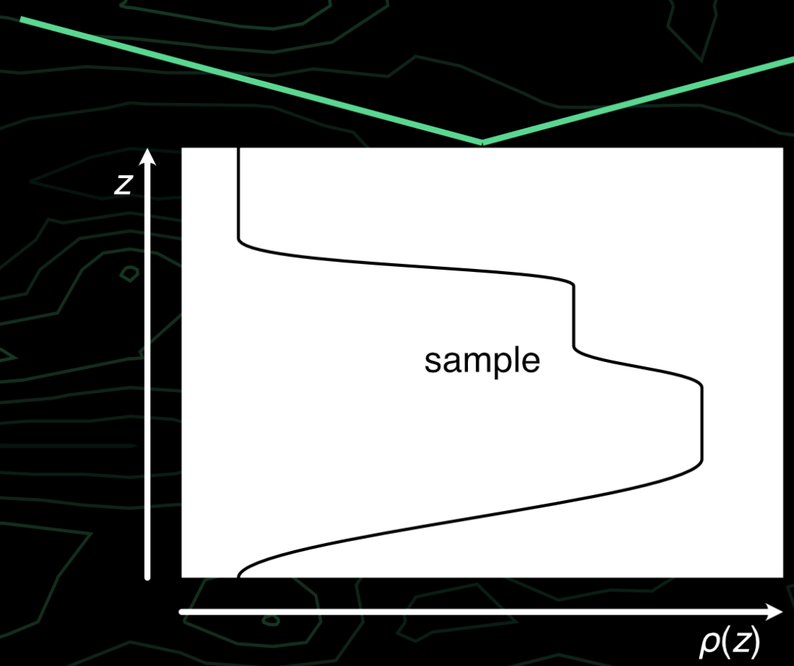

Under the Born approximation, the reflectometry profile can be estimated from a Fourier transform of the scattering length density profile.

- specifically, the Fourier transform of the derivative (or change) in the scattering length density:

$$R(q) \approx \frac{16\pi^2}{q^4} \left| \int_{-\infty}^{\infty} \frac{\mathrm{d}\rho}{\mathrm{d}z} \exp\left(izq\right) \, \mathrm{d}z \right|^2$$

Sivia, D. S. (2011). *Elementary Scattering Theory: For X-ray and Neutron Users*. Oxford University Press.

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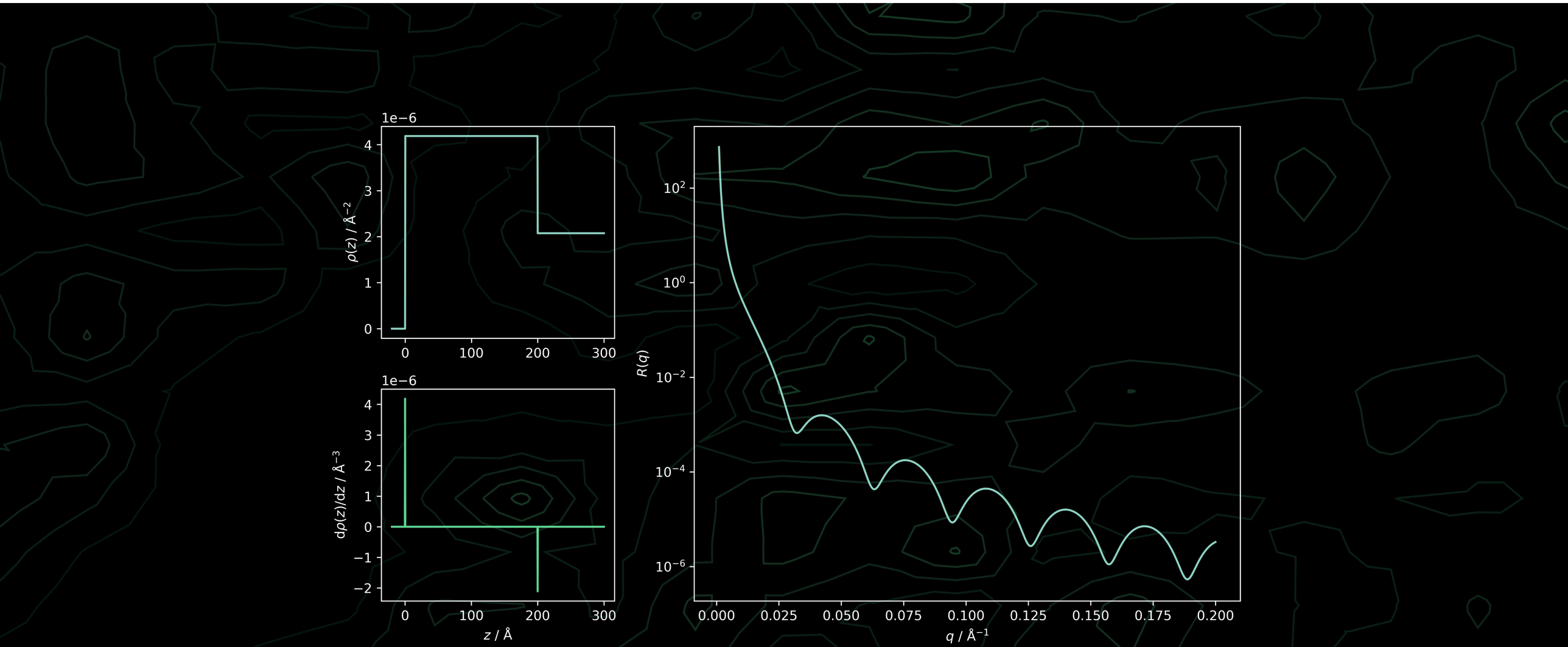

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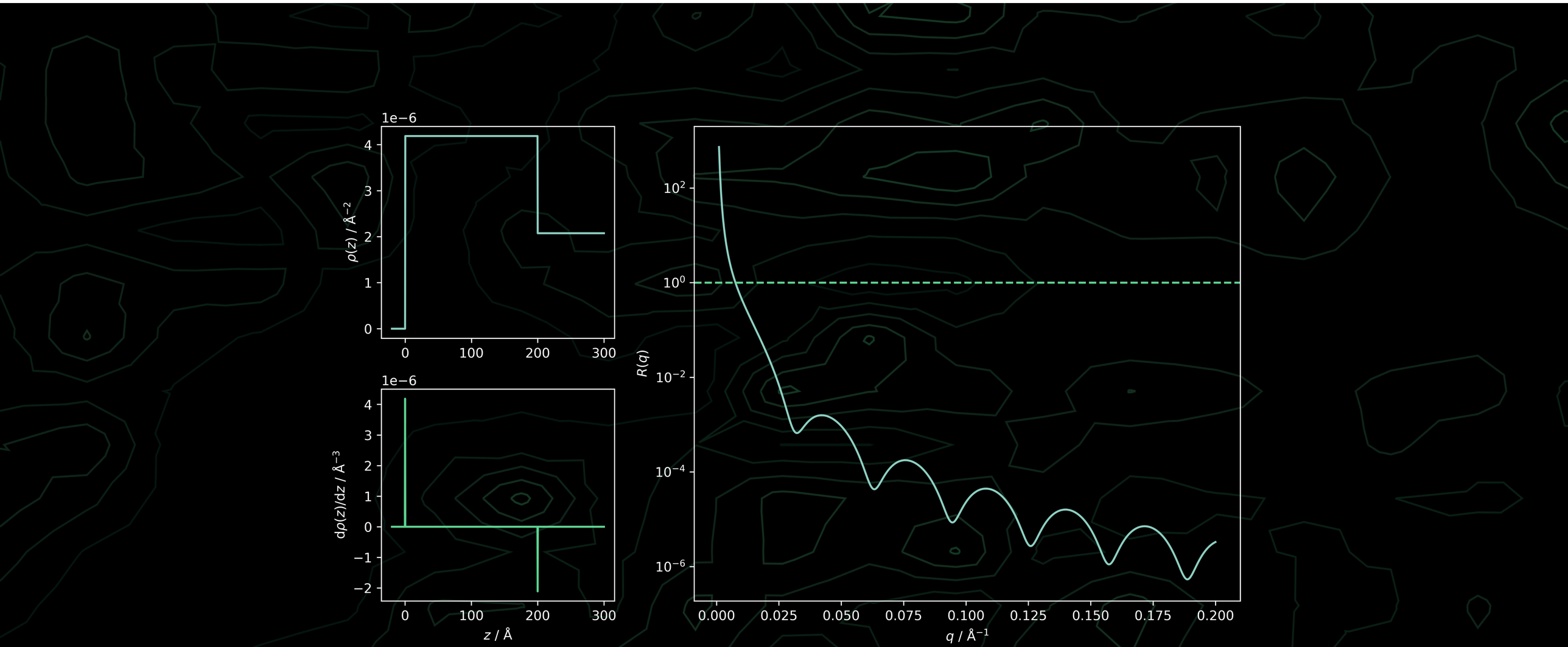
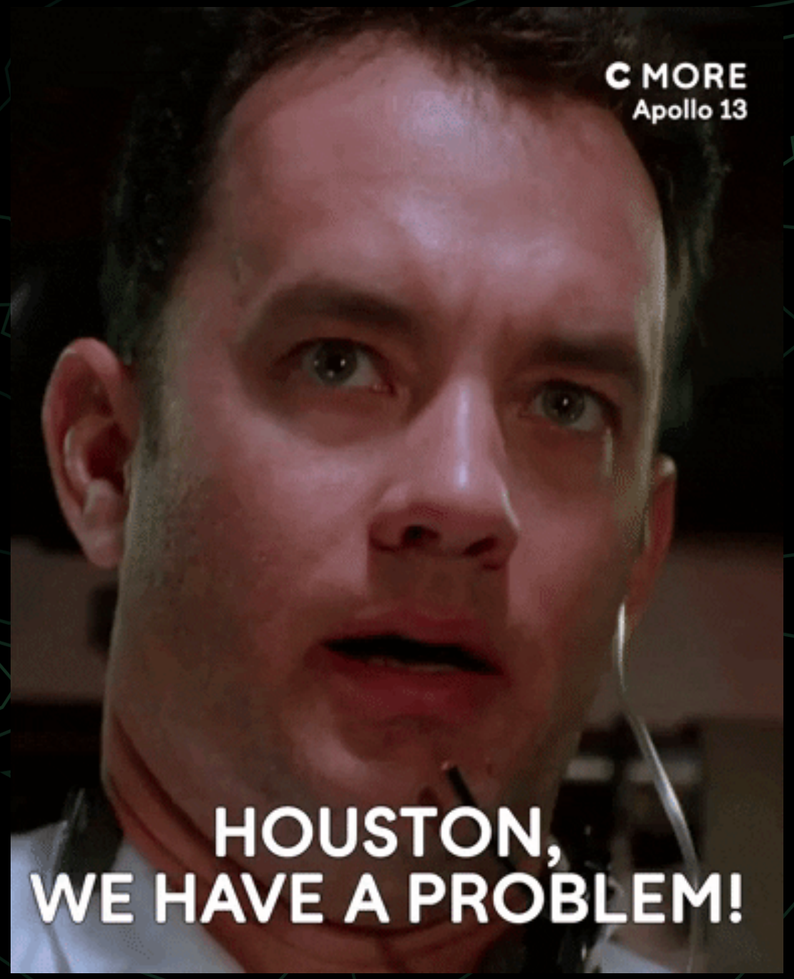
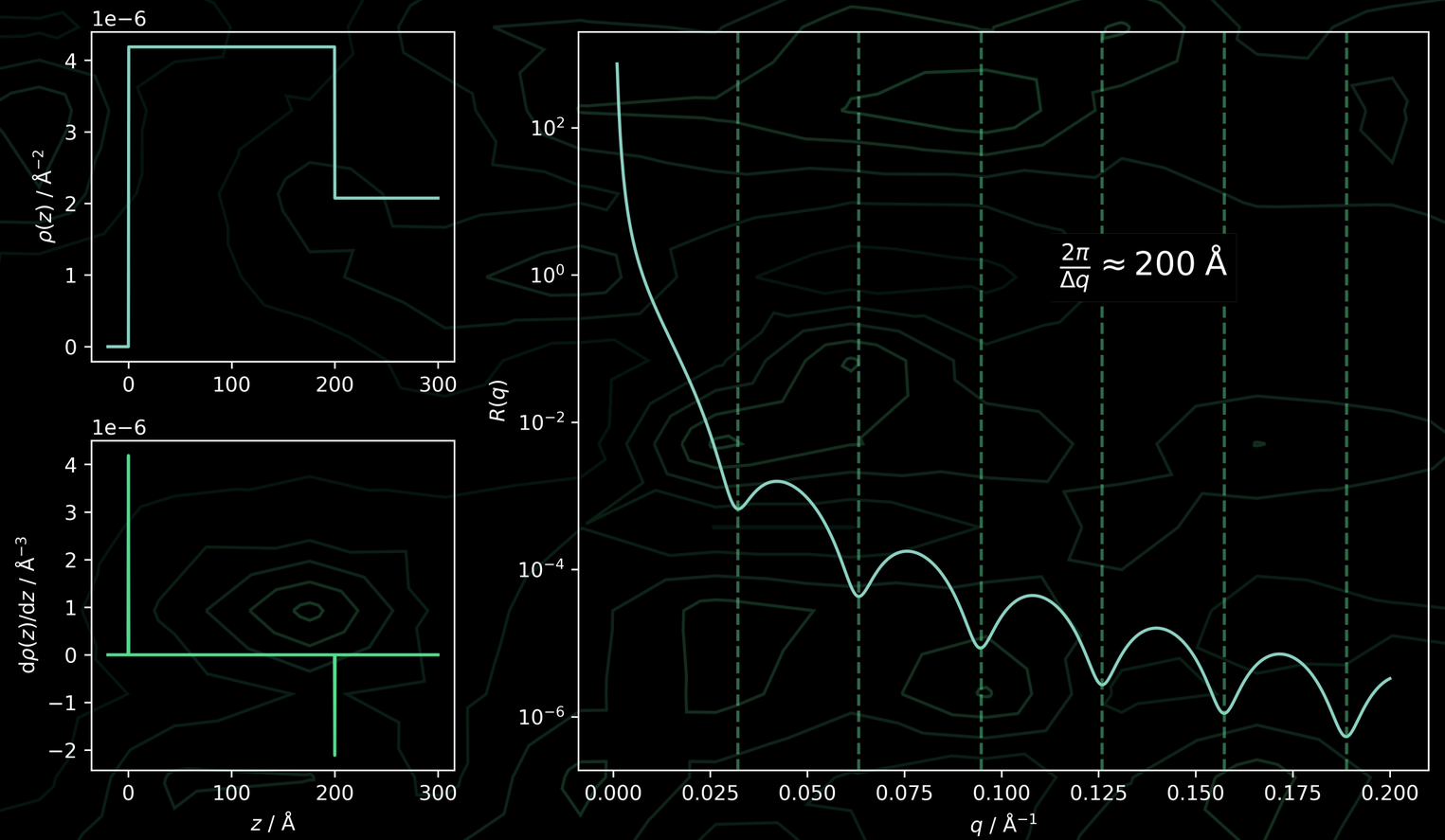


The Born approximation appears not to work for reflectometry.

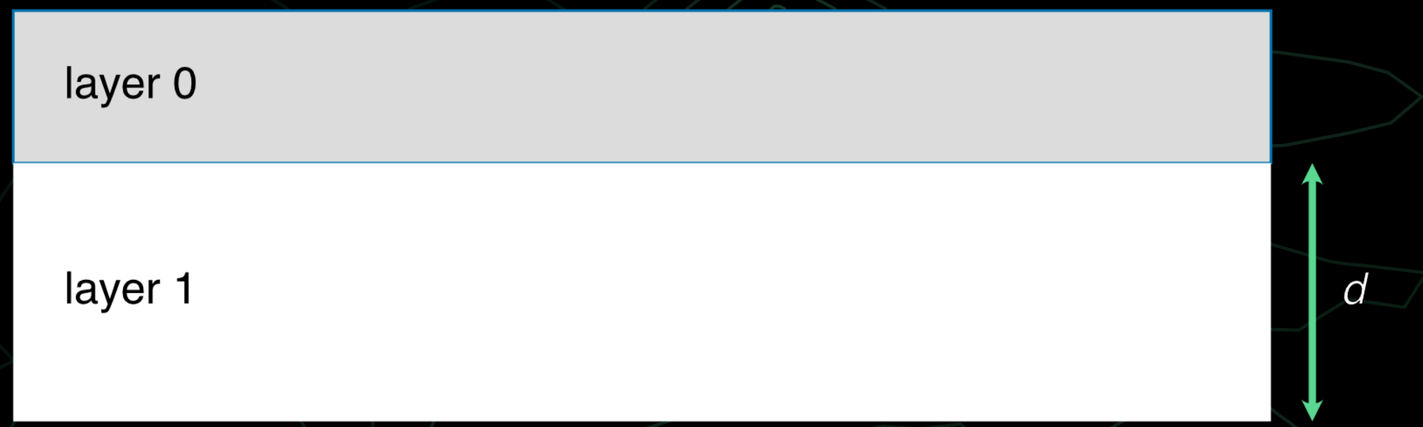


Before we leave the Born approximation behind, it is important to acknowledge all hope is not lost.



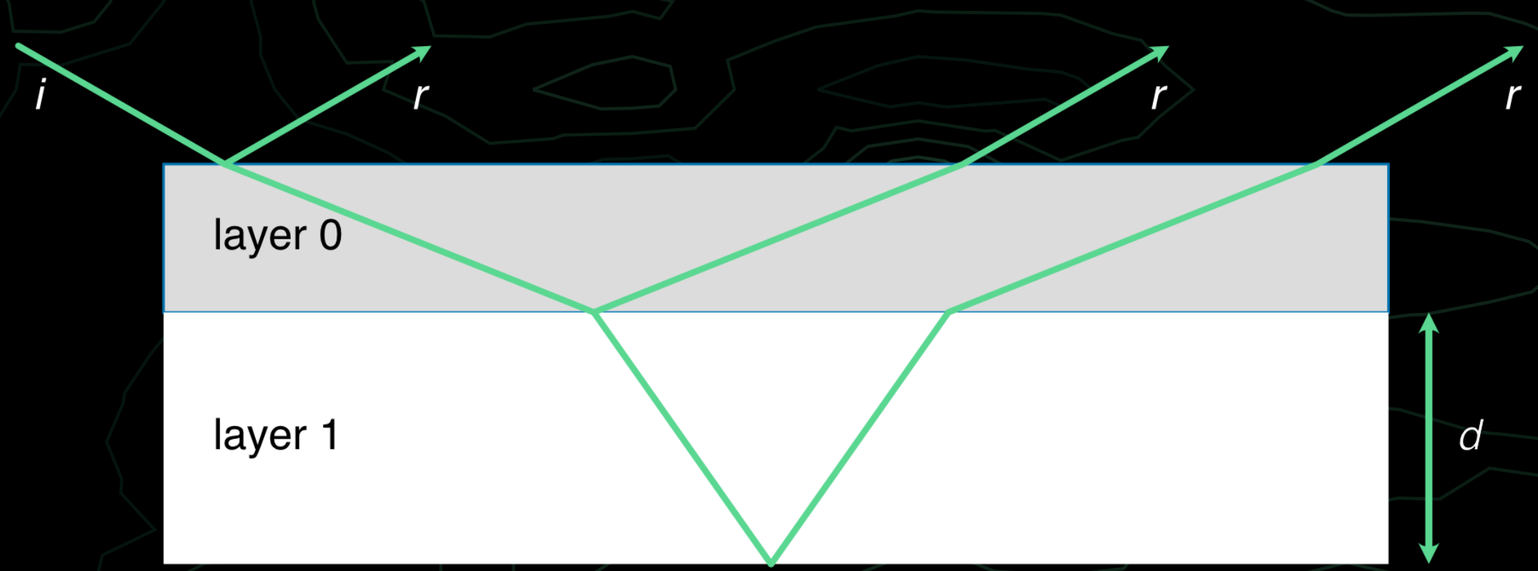
A different approach to understand reflectometry treats the system as a series of layers with optical properties.

- each layer has a given thickness, scattering length density, with a roughness parameter between each layer



A different approach to understand reflectometry treats the system as a series of layers with optical properties.

- optical matrix formalism computes the propagation of the neutron/x-ray waves through each material




*www.reflectometry.org/learn/3_reflectometry_slab_models/the_slab_model*

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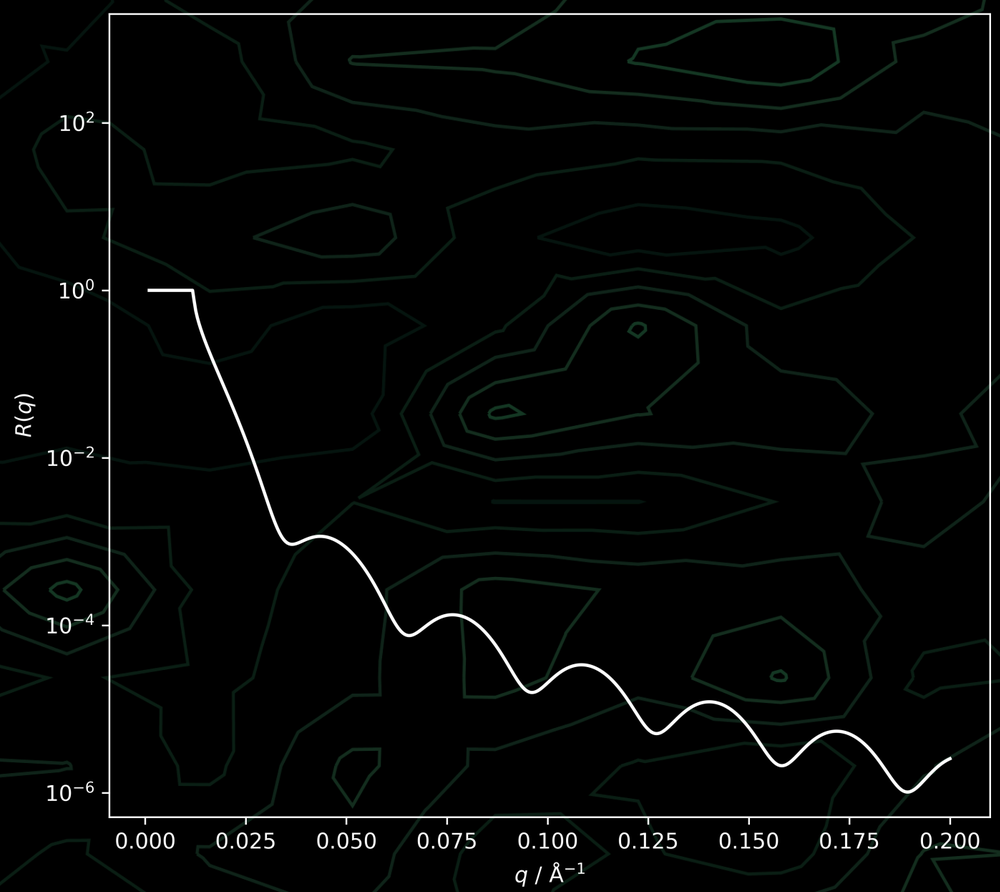
- this mathematical formalism calculates the accurate model reflectometry



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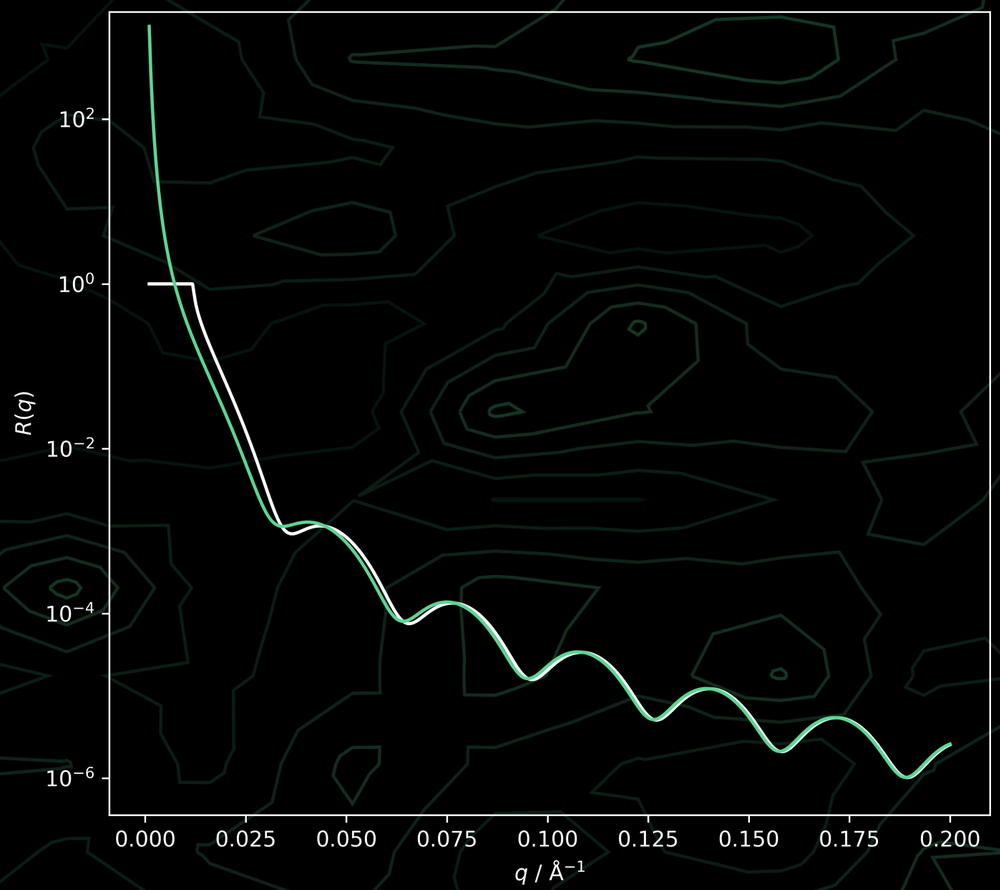
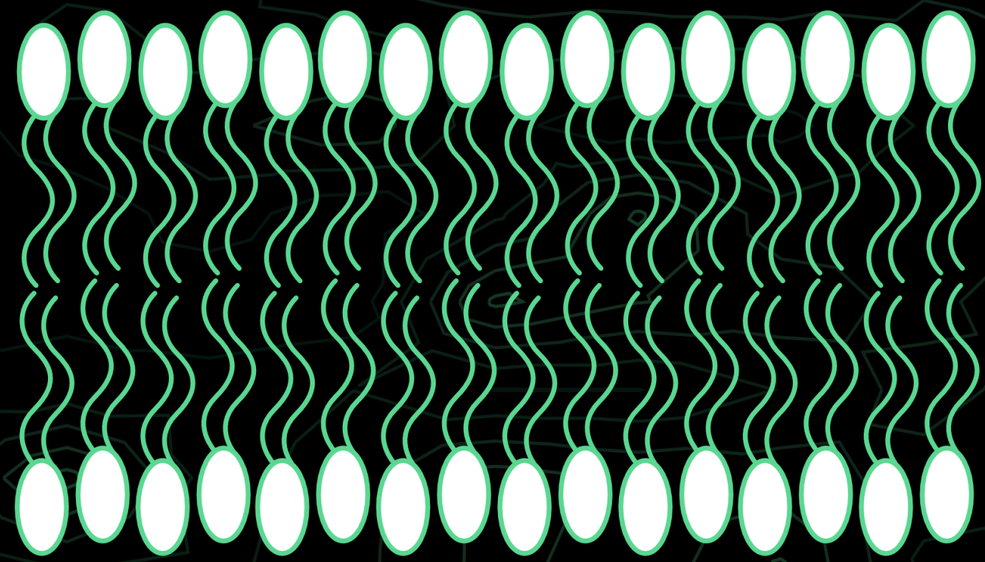


The difference between the Born approximation and the optical matrix formalism may be from the reflection geometry.

- perhaps mutliple scattering due to the long path length from shallow angles
    - though this is debated in the community

This means we must be able to describe our system as a series of distinct layers.



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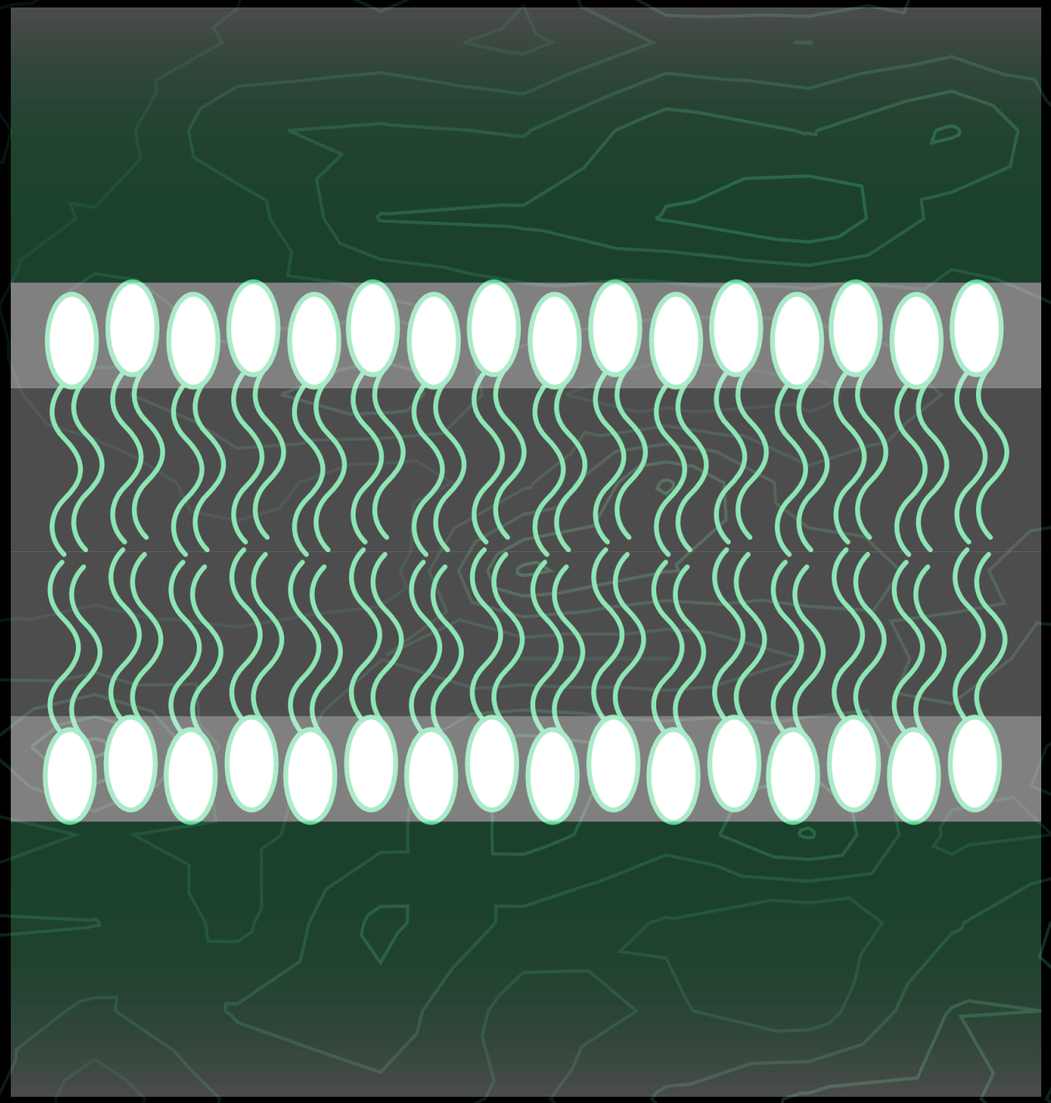
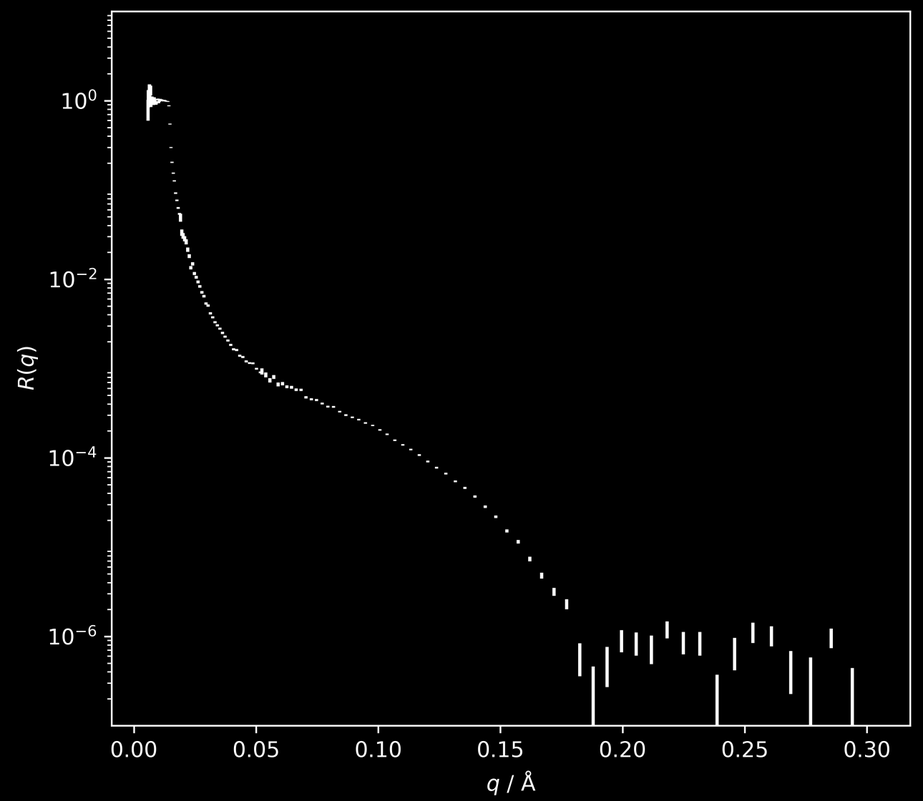


Once we have a model, it needs to be optimised with respect to the data.



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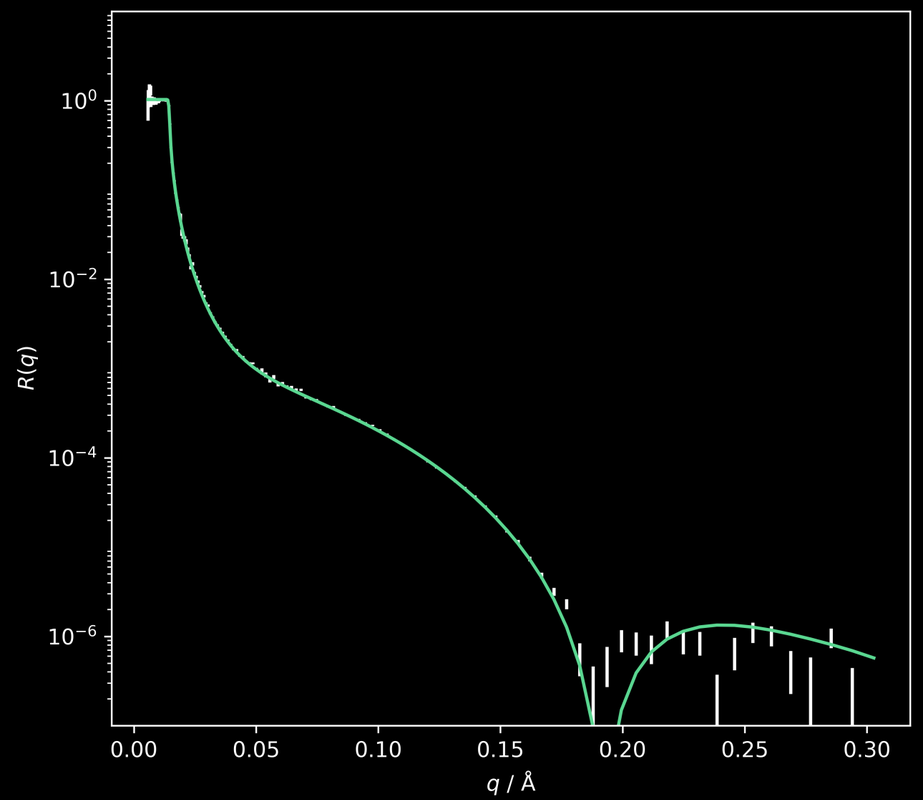

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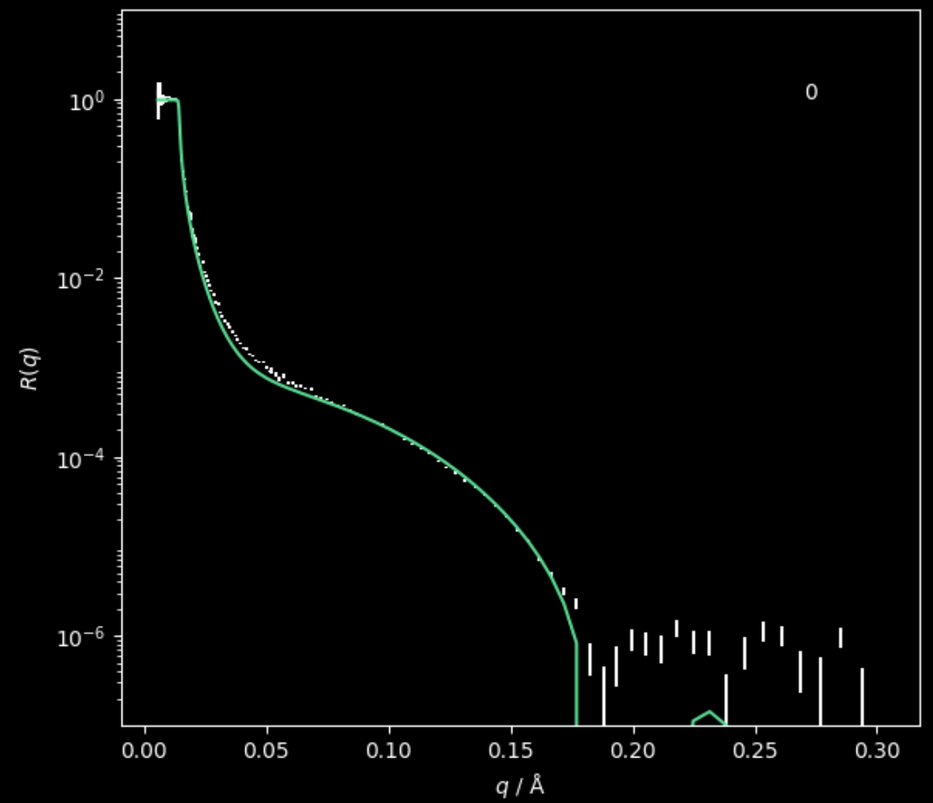
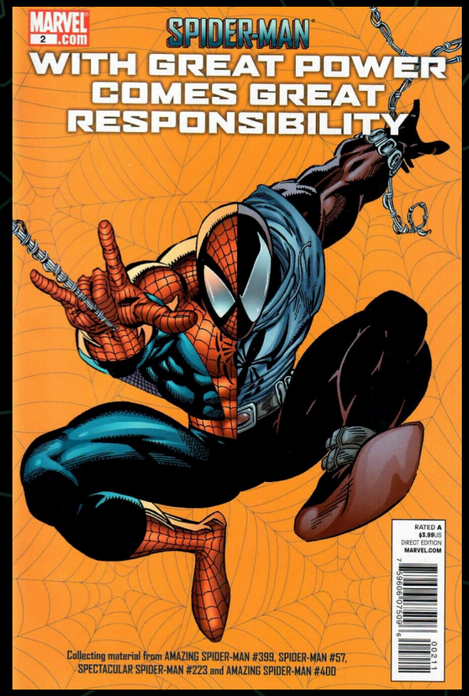


Optimisation is achieved through an optimisation algorithm that aims to maximise the agreement between the model and the data.

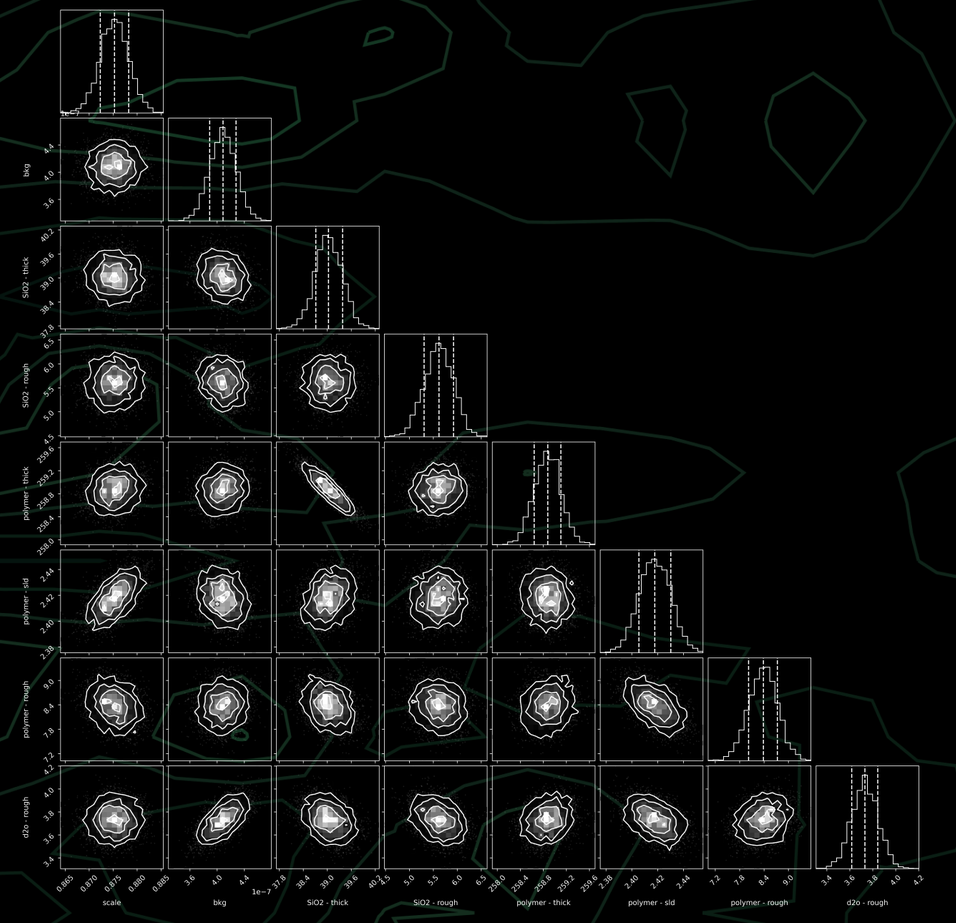
- this optimisation comes with great responsibility
- if you let a parameter vary, the algorithm will try and optimise its value
- popular algorithms: gradient descent methods, differential evolution, DREAM



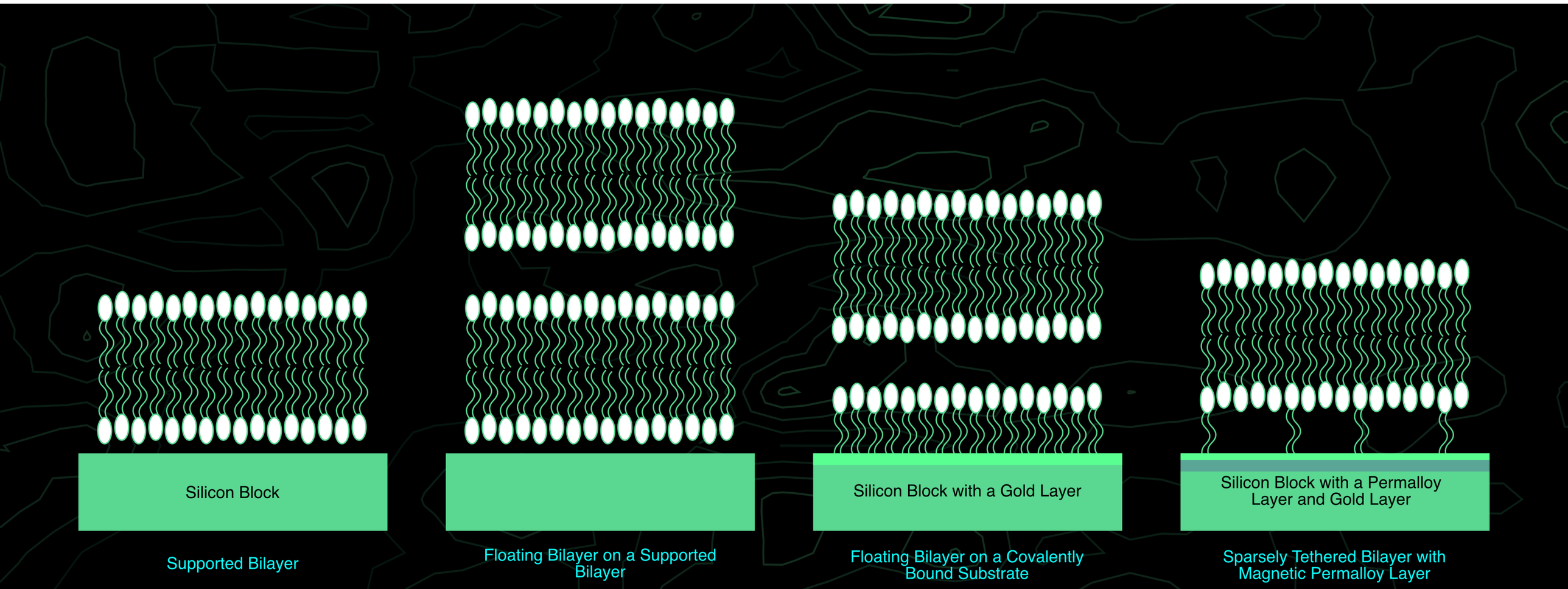

A. R. McCluskey, *et al. Mach. Learn.: Sci. Technol.*, **1**(3), 035002, 2020. DOI: 10.1088/2632-2153/ab94c4.

# Sampling the probability distribution is becoming a common approach in reflectometry analysis.

- reflectometry needs this, it is ill-posed
- gives a more complete picture of the parameter uncertainies and correlations
- this comes alongside the populatity of Bayesian modelling



In life sciences, reflectometry methods are particularly valuable for the study of biological, or near biological, membranes.




Foglia, F., *et al. Curr. Opin. Colloid Interface Sci.* **20**(4), 235, 2015. DOI: 10.1016/j.cocis.2015.08.001

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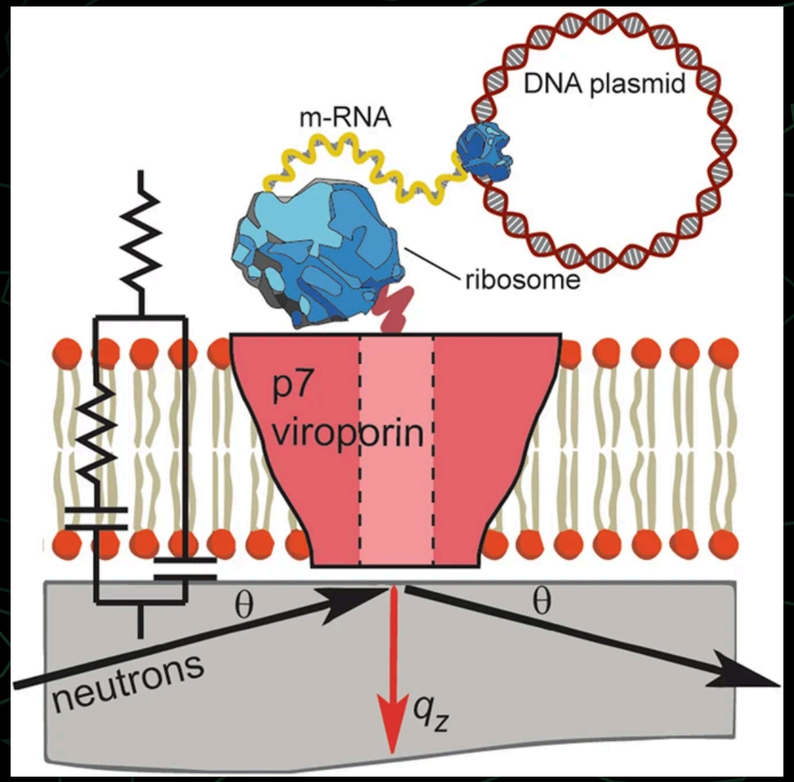


Soranzo, T., *et al. Sci Rep* **7**, 3399, 2017. DOI: 10.1038/s41598-017-03472-8

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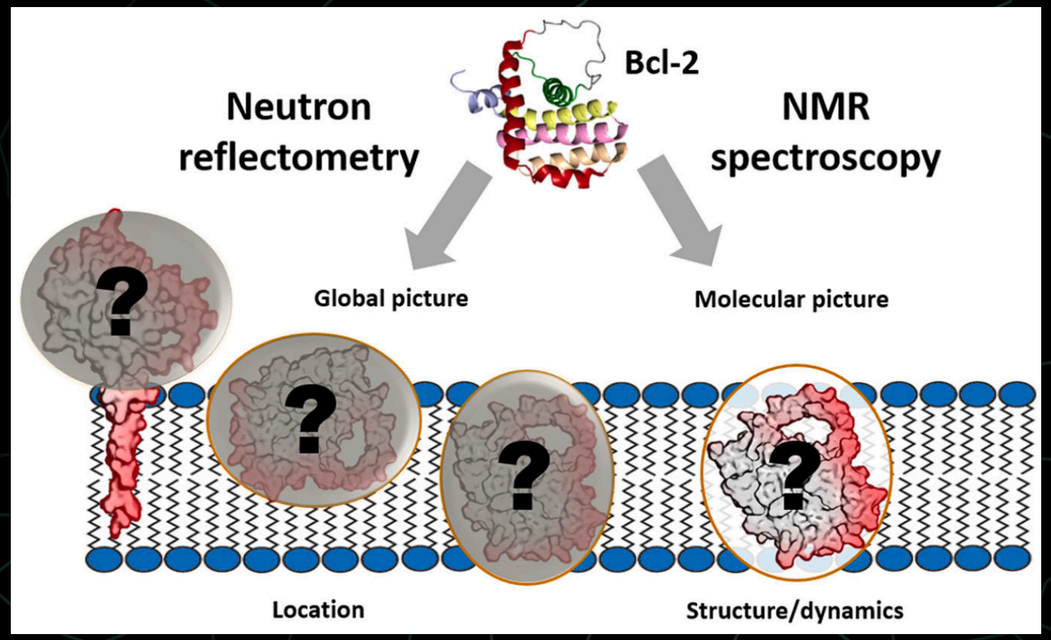


Mushtaq, A. U., *et al.*. *Commun Biol* **4**, 507, 2021. DOI: 10.1038/s42003-021-02032-1

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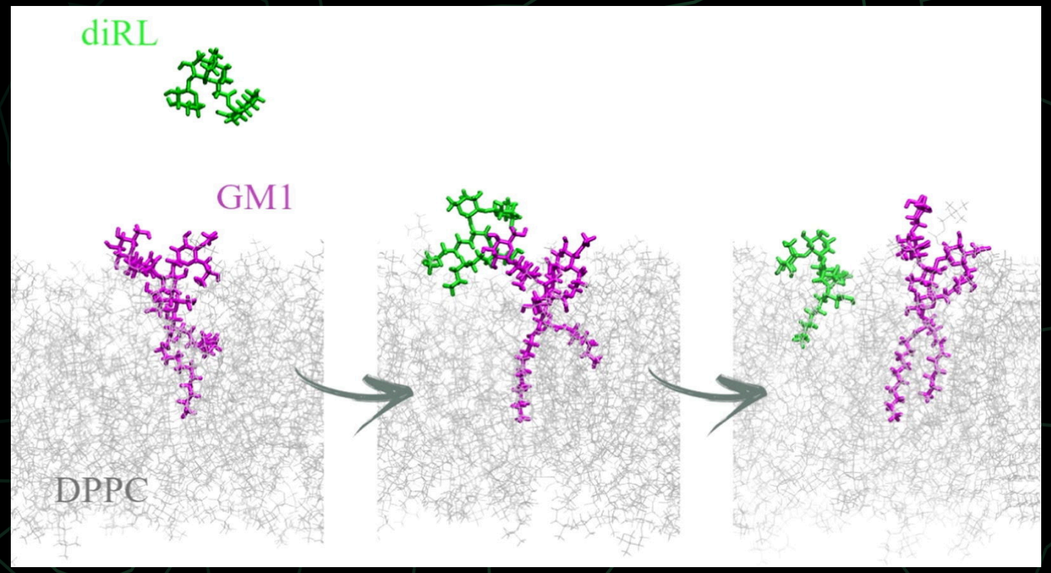


Rondelli, V., *et al.*. *J. Colloid Interface Sci.* **616**, 739, 2022. DOI: 10.1016/j.jcis.2022.02.120

Today we will be using Python and a Jupyter Notebook to analyse some reflectometry data.

- there are many Python packages to analyse reflectometry data: `refl1d`, `refnx`, **`anaklasis`**, BornAgain, **EasyReflectometry**, `genx`

- today we will use `refnx`, but the ideas you will learn are transferable

Today we will be using Python and a Jupyter Notebook to analyse some reflectometry data.

visit: https://github.com/arm61/fasem

click the "launch | binder" button

1. open and read/work through the `simple_fitting.ipynb` notebook, independently, use the "Run" button at the top to run code cells

2. together we will review the `simple_fitting.ipynb` notebook

3. work in pairs on the `bilayer_analysis.ipynb` notebook, completing the exercises where requested

ask questions!

thanks for listening!

questions?


- ORSO Reflectometry Tutorials: http://reflectometry.org/learn/
- Sivia, D. S. (2011). *Elementary Scattering Theory: For X-ray and Neutron Users*. Oxford University Press.
- Clifton, L.A., *et al*.. Lipid-Protein Interactions: Methods and Practices, **2003**, 201. 2019. DOI: 10.1007/978-1-4939-9512-7_11
- Gerelli, Y., *EPJ Web of Conference*, **236**, 04002, 2020. DOI: 10.1051/epjconf/202023604002



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