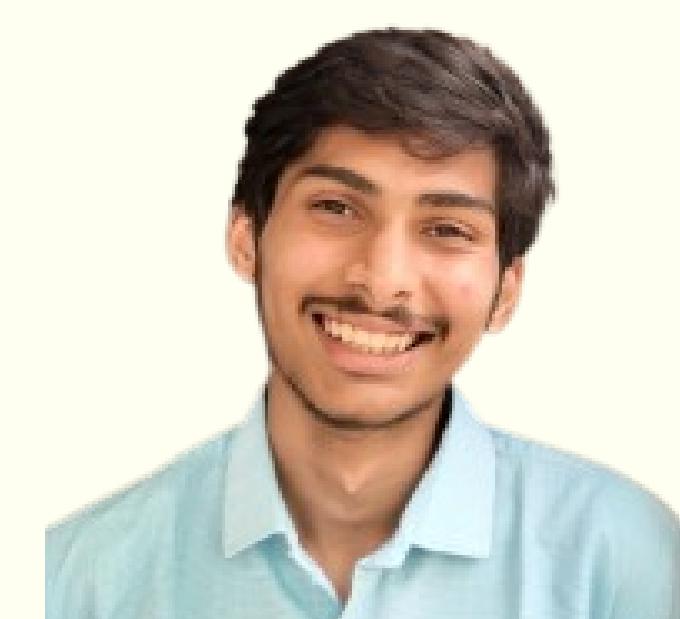


Simulating X-Ray Magnetic Scattering Using a Web App

Bellamkonda Sri Krishna Chaitanya¹, Rose Yemelyanova² & Alessandro Bombardi²



1. University of Warwick. University of Warwick, Coventry CV4 7AL, UK

2. Diamond Light Source Ltd, Harwell Science and Innovation Campus, Fermi Ave, Didcot OX11 0DE, UK

What is X-Ray Magnetic Scattering (XMS)?

- X-ray magnetic scattering is a technique that may be used to determine the **magnetic structure** of crystals, and requires the use of synchrotron beam.
- Magnetic structure refers to the **arrangement** of **magnetic moments** of the ions in a crystal. These moments originate from the **angular momentum** of the unpaired **electrons** of the atoms in the crystal structure.
- This technique utilises the **interaction** between the **x-rays** and **unpaired electrons** to determine the direction the moments. [1]

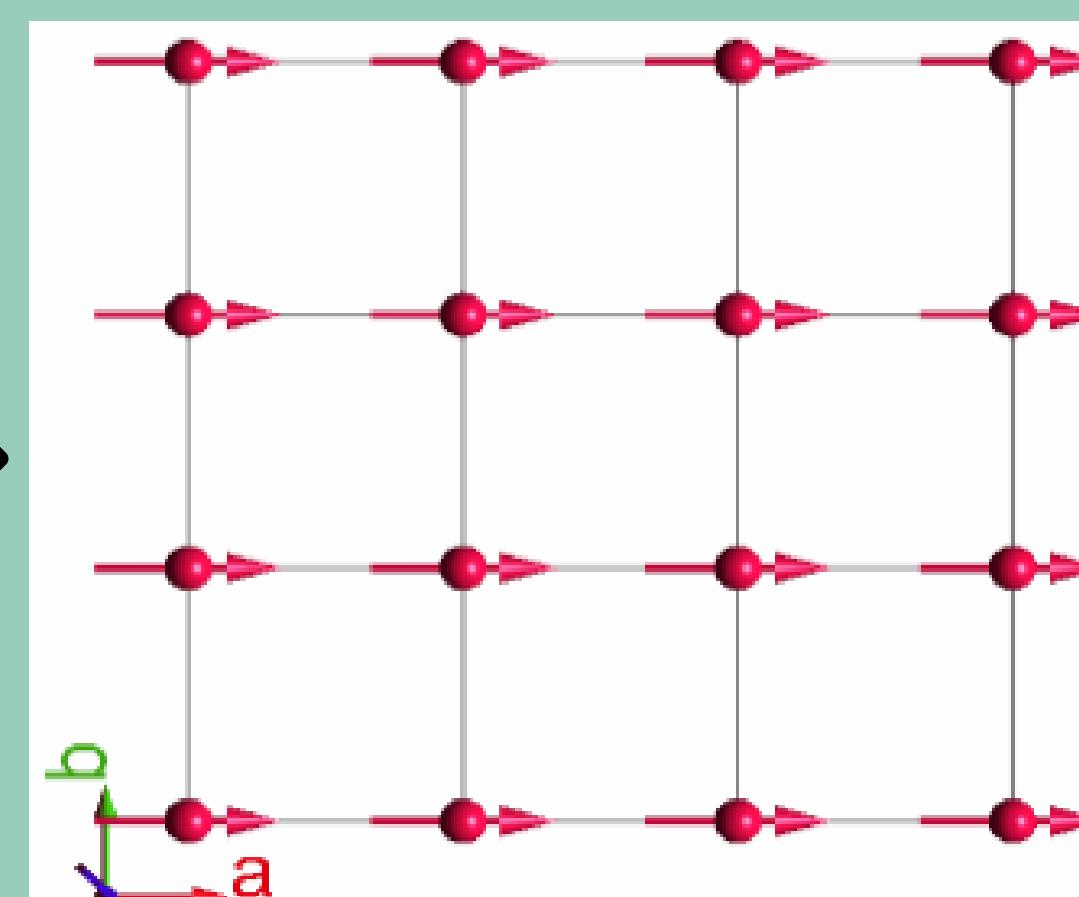


Fig 1: A simple ferromagnetic structure (for example Fe) with aligned magnetic moments.

Resonant Magnetic Scattering

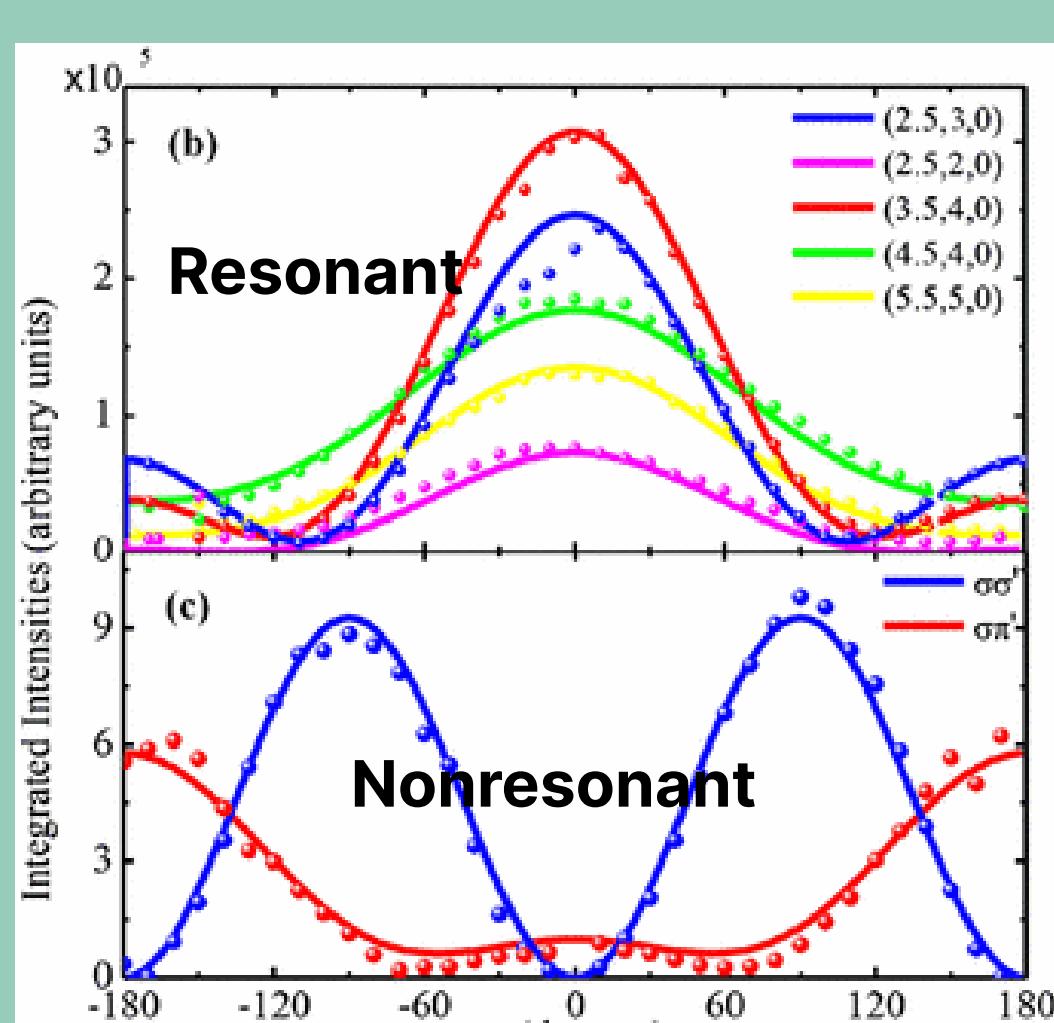


Fig 2: Intensity vs azimuth angle graph of Resonant and Nonresonant scattering in GdMn2O5 [2].

- For an arbitrary beam energy, **Nonresonant Magnetic Scattering (NRMS)** occurs.
- NRMS inherently produces weak scattering effects. However it is useful in **disentangling** the **orbital** from the **spin** contribution of the magnetisation.

Non
resonant

- If the energy of the incident X-ray beam is tuned to an **absorption edge** of the crystal; it leads to **resonant scattering**.
- This gives rise to scattering that is **several orders of magnitude** more **intense** than NRMS.
- It is helpful in obtaining **element specific** information, **polarisation dependence** and deducing the **magnetic order** of the crystals.

Resonant

Experimental Apparatus

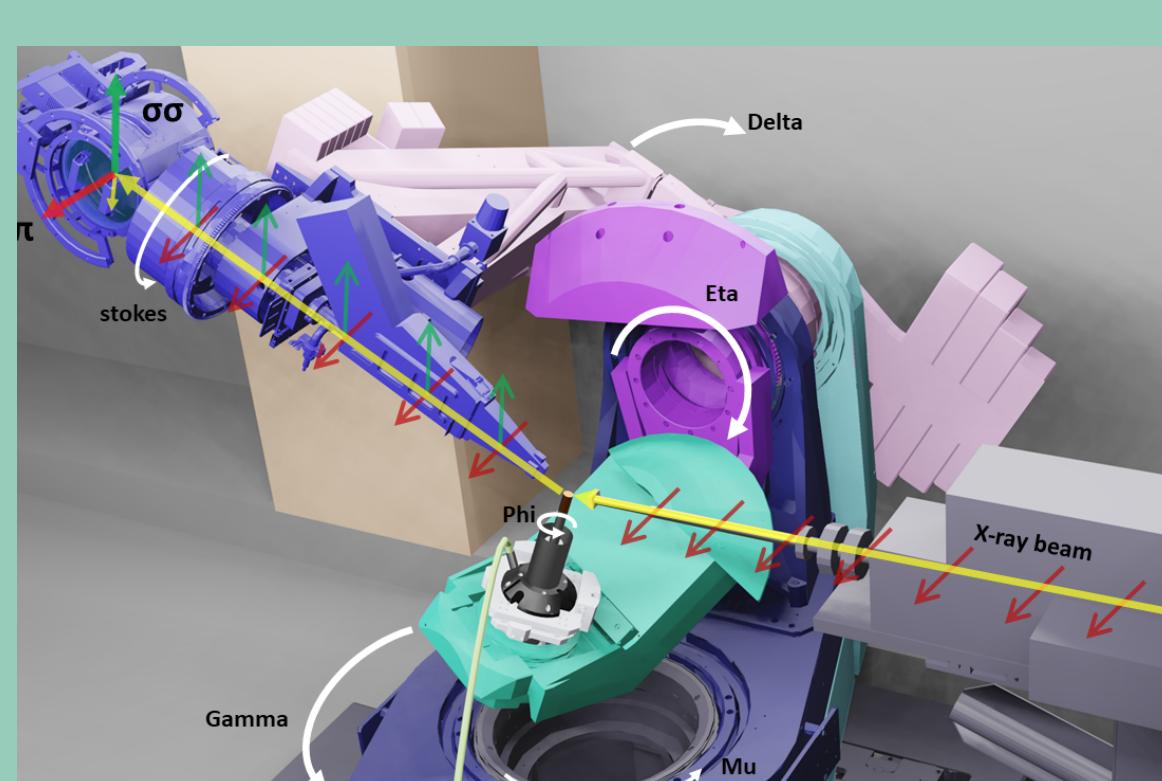


Fig 3: Typical experimental apparatus for x-ray magnetic scattering [3].

- Measuring the **intensity** of the scattered x-rays as the sample is **rotated** about a **magnetic reflection** can be used to provide information about the **direction** of **magnetic moments** in the crystal [1].

References

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The problem

- My project was built upon an initial software codebase to **simulate XMS** which was originally developed by **Alessandro Bombardi** in 2022.
- To build modern application for the simulation and allow for **future expansion**, a **refactoring** process on this codebase was performed while **retaining** its **core functionality**.
- However, a study reveals that **42%** of an average **developer's time** is spent on **technical debt** and **maintenance** issues. Roughly, the **opportunity cost** for maintaining **legacy code** comes to around **\$85 billion** dollars annually for tech companies [4].
- So, one of the main objectives of the project was to write **maintainable code**.

42%

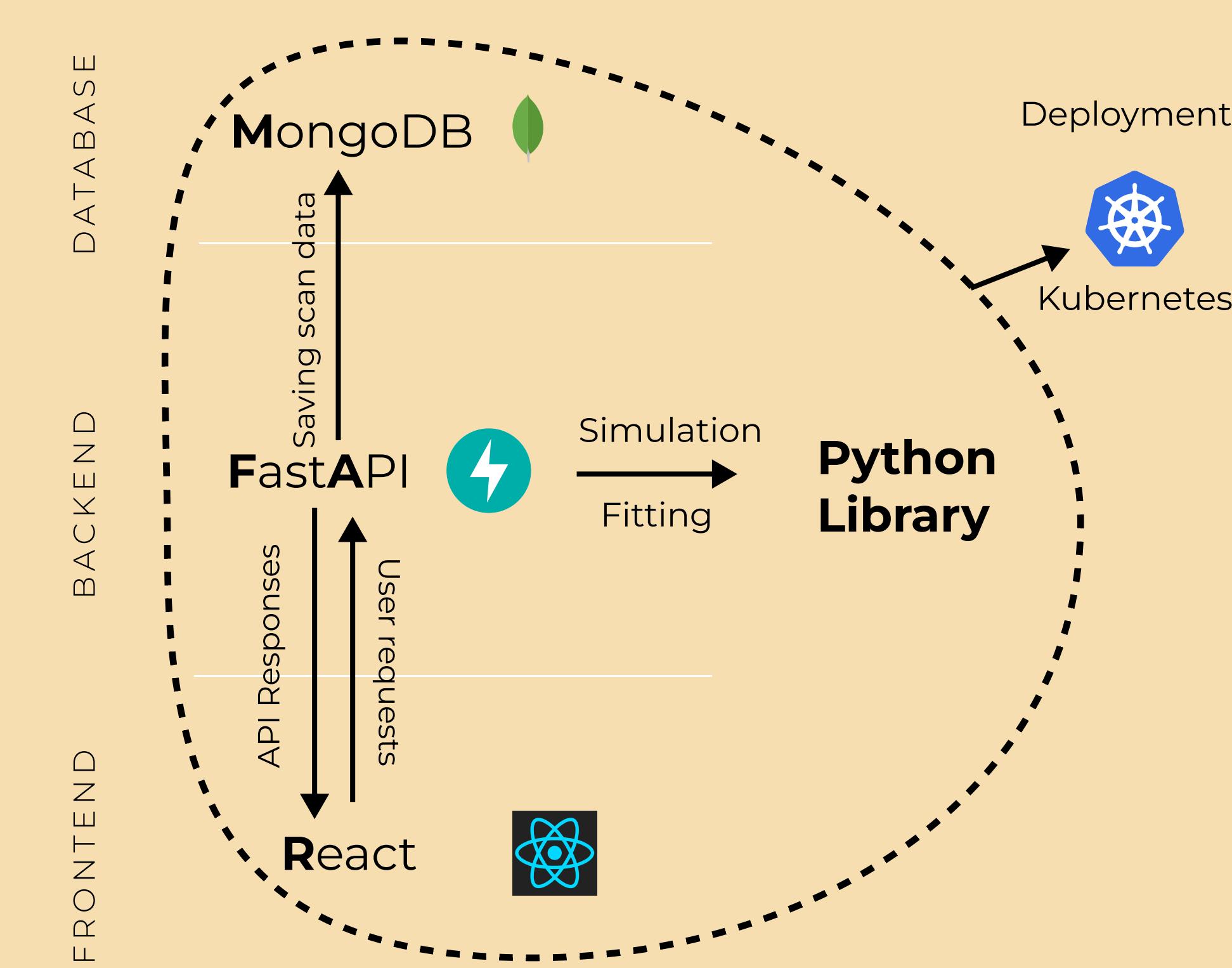
of developer's time spent on maintenance issues

opportunity cost of legacy code

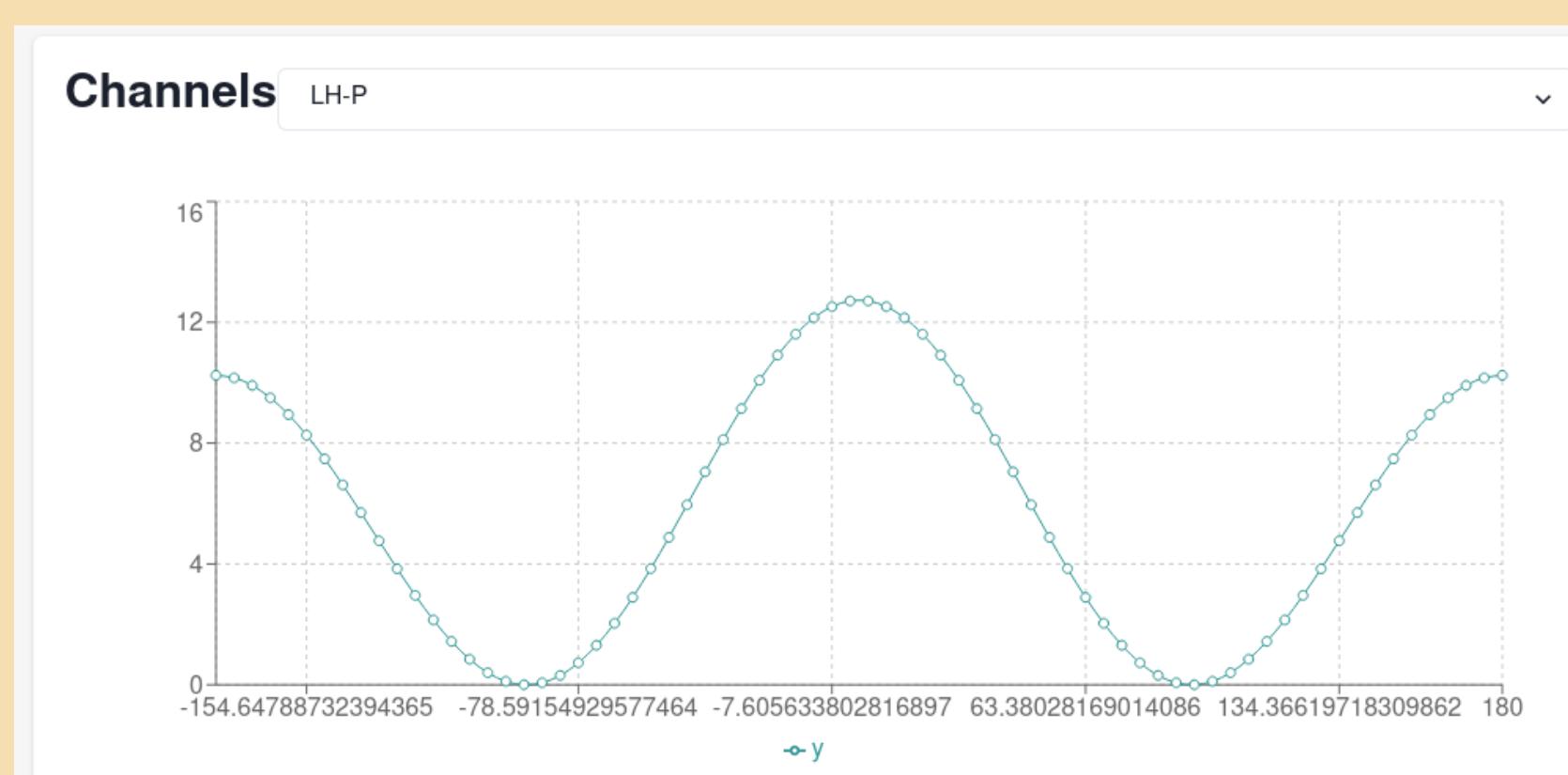
Python Library for simulation

- The previous codebase successfully refactored into a **modern**, highly **maintainable** and **user-friendly** version.
- This codebase also **successfully addresses** the **issues** discussed in the previous section. This has been achieved by -
 - Improved Design
 - Simplified user workflows
 - Additional features
 - Allows for future expansion

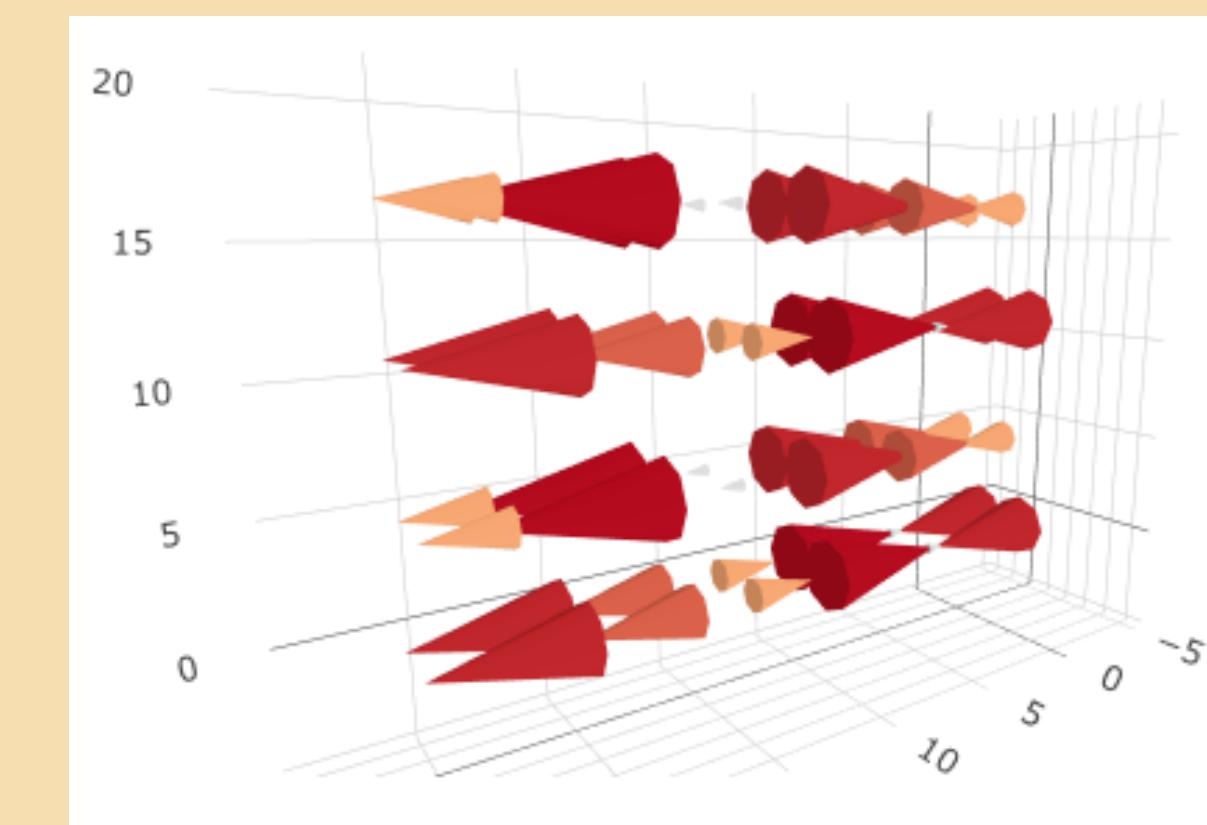
Web Application



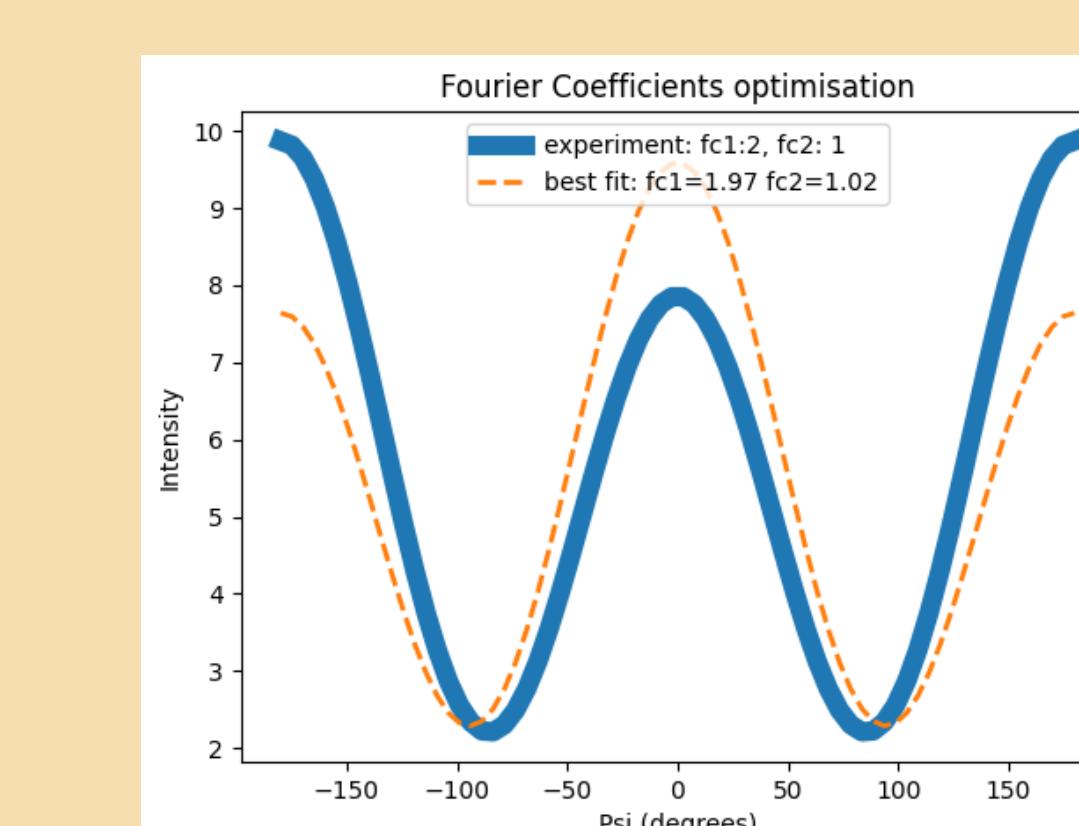
Features



Intensity vs. Azimuth
Visualization



Magnetic Moment
Visualization



Obtaining
best-fit
parameters



Additional Features

- Informative Errors
- Add Multiple Scans
- Downloadable Results