

Reproducibility Working Group

Chairs: Andrew McCluskey (ESS) & Christy Kinane (ISIS)

2022 AGM – Priors and Posteriors Paper

feature articles



JOURNAL OF
APPLIED
CRYSTALLOGRAPHY

ISSN 1600-5767

Received 16 September 2022
Accepted 28 November 2022

Edited by A. Barty, DESY, Hamburg, Germany

¹This work was developed as a part of the Open Reflectometry Standards Organisation Workshop in 2022, with contributions from all authors as part of a round-table discussion.

Keywords: reflectometry; reflectivity; Bayesian analysis; FAIR data standards.

Advice on describing Bayesian analysis of neutron and X-ray reflectometry¹

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As a result of the availability of modern software and hardware, Bayesian analysis is becoming more popular in neutron and X-ray reflectometry analysis. The understandability and replicability of these analyses may be harmed by inconsistencies in how the probability distributions central to Bayesian methods are represented in the literature. Herein advice is provided on how to report the results of Bayesian analysis as applied to neutron and X-ray reflectometry. This includes the clear reporting of initial starting conditions, the prior probabilities, the results of any analysis and the posterior probabilities that are the Bayesian equivalent of the error bar, to enable replicability and improve understanding. It is believed that this advice, grounded in the authors' experience working in the field, will enable greater analytical reproducibility in the work of the reflectometry community, and improve the quality and usability of results.

1. Introduction

Neutron and X-ray reflectometry are powerful tools to probe the interfacial structure of materials (Lovell & Richardson, 1999). However, as a result of the 'phase problem' the analysis of these techniques is ill-posed in nature, as there are multiple

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Looking forward

Continuing to harvest information about calibrations and reference samples, so please reach out to myself or Christy



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Calibrations

In this page, we are looking to harvest information about calibrations that are performed at neutron reflectometry instruments. For a given calibration, please include the following information:

- What is being calibrated?
- How is the calibration performed?
- An example of the calibrated data and details of how you get this information
- References/Code for the above would be great!

Once you add your calibration, please include yourself in the authors of this page.

Things to get you thinking: (if you calibrate/measure something not on this list then please let us know)

1. How do you measure the total flux of your beamline?
2. How do you measure the TOF flight distance of your beamline with neutrons (and without?) Neutron TOF only
3. How do you measure the wavelength or wavelengths of your beamline? Similar to 2 but for monochromatic beamlines.
4. How do you measure the polarisation of your beamline? (TOF, monochromatic)
5. How do you check with a non-magnetic sample you get zero magnetic response with polarised neutrons, i.e your zero is zero, and to what precision? (TOF/Mono)
6. If you have a pixelated detector. How do you measure your detector corrections to then flatten the detector response? (i.e. Correct all pixels to have a similar response, this is sometimes referred to as a flood measurement)

Looking for engagement

There are things that the chairs are passionate about but we need more engagement from the community

