

Dear Rietveld method user,

Over the past half-decade, our LANL team developed several tools to tackle the challenges posed by modern high-throughput neutron and X-ray scattering instruments, mostly geared towards engineering diffraction such as texture, strain and phase fraction analysis:

- MILK, the MAUD interface language toolkit, to automate Rietveld analysis with the MAUD code [<https://github.com/lanl/MILK>]
- Mystic: constrained nonlinear optimization for scientific machine learning, UQ, and AI [<https://github.com/uqfoundation/mystic>]
- Spotlight, parallelized optimization on distributed-computing resources [<https://github.com/lanl/spotlight>]
- Cinema, interactive image-based approach to data analysis and visualization that promotes investigation of large scientific datasets [[https://github.com/cinemascience/cinema\\_debye\\_scherrer](https://github.com/cinemascience/cinema_debye_scherrer)]

This development effort aims to automate diffraction analysis towards real time analysis, reduce the time needed to analyze datasets, make inspection of Rietveld results for large numbers of refinements more efficient, etc. Ralf Hielscher, developer of the texture analysis tool MTEX, also plans to present his tool and its incorporation in diffraction experiment data analysis.

In order to familiarize the scattering community with these tools and foster collaborations around them, we are planning to hold a workshop from June 5th to 9th, 2023, at LANL in Los Alamos, NM. Besides overviews, demonstrations, and tutorials for each of these components, we plan to work with attendees on solving their own data analysis problems with these tools. Examples we plan to discuss during the workshop are a series of runs to study texture evolution during deformation as well as phase transformations. The workshop is aimed at users with at least a basic understanding of Rietveld analysis, ideally with the MAUD code. Interested attendees should also have existing datasets that could benefit from the use of the LANL tools.

While details are forthcoming, we invite interested researchers to send us their intent to attend our workshop with the following information no later than Monday April 10th, 2023:

- Citizenship (non-US citizens will need additional processing to obtain access to LANL - interested foreign nationals should contact us as soon as possible)
- 2-3 sentences about the scattering data analysis problem the attendee wishes to solve during the workshop
- If suitable, any potential pathways to seek funded collaborations to improve or adapt the LANL tools for specific problems or facilities
- We have some support for travel available; if needed, please indicate how much travel support in USD is required to attend
- If in-person attendance is not possible, please indicate your interest in participating in the presentation introducing our tools remotely. However, we do not plan to offer tutorials or hands-on sessions via remote access.

We are looking forward to hearing from you! Please feel free to share this announcement with colleagues who might be interested in this workshop.

In order to facilitate site access to LANL, please reply no later than Monday, April 10, 2023, to [sven@lanl.gov](mailto:sven@lanl.gov).

Chris, Dan, Mike & Sven