ORSO Analysis Working Group

Report to the AGM

2023-06-21

Validation of Reflectivity Kernels

- Maintenance of code infrastructure that performs this validation:
  - Github Actions
  - Scheduled every Monday at midnight
- Standard data (layer inputs, calculation outputs) stored at https://github.com/reflectivity/analysis/tree/master/validation/test
- Individual test module per kernel
  - BornAgain (C++ with Python interface, many recent upgrades)
  - RefNX, Refl1D, RefNX, GenX, Anaklasis (Python)
  - NIST Web Calculator (nodejs wrapper for javascript libraries)
- Result badges at https://github.com/reflectivity/analysis, can be used e.g. on homepages of packages

Adding new test datasets

- Early work on adding new polarised data:
  - (David Cortie)

Simple Model Language

- Support provided in orsopy
- Models can be imported and used in GenX
- Examples provided on SLDDB website https://slddb.esss.dk/slddb/
- See Artur's talk for more info

Reading ORSO standard

Import for the ORSO standard reflectometry file format implemented in analysis software (through orsopy)

- GenX
- RefNX
- Refl1D
  - (beta, also experimental NeXus .orb support)

- No more shims or errors interpreting columns

ORSO standard encoded as HDF5 (NeXus)

- Preliminary mapping proposed
- Minimal NeXus namespace (NXEntry, NXData)
- New ORSO_class attribute matches orsopy classes
- See https://github.com/reflectivity/file_format/blob/master/nexus_mapping.md
- More details during 5-minute talks on FAIR