

A NeXus/HDF5 mapping of the ORSO standard reflectivity format

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Summary

- Contains the same information encoded in the .ort (text) file
- Written from orsopy just like .ort:
 - `fileio.save_orso([datasets])` -> .ort file
 - `fileio.save_nexus([datasets])` -> .orb file
- No new application definition is specified
 - Does not use the NXRefl application definition
- Minimal NXData folder created with links to columns

https://github.com/reflectivity/file_format/blob/master/nexus_mapping.md

Datasets to HDF5

- fileio.OrsoDataset are written to top-level HDF5 group
- 'info' is the header, mapped as described in next slide
- 'data' represents the columns
 - Index of column is written to @sequence_index attribute
 - Names of subgroups match names in info.columns (matched by index)

```
/ : (HDF5 Group)
|
└─ dataset : (HDF5 Group, ORSO_class='OrsoDataset')
    └─ info : (HDF5 Group, @ORSO_class='Orso')
        └─ data_source : (HDF5 Group,
            @ORSO_class='DataSource')
            └─ ...
            └─ data : (HDF5 Group, @sequence=1)
                └─ Qz : (HDF5 Dataset, @sequence_index=0)
                └─ R : (HDF5 Dataset, @sequence_index=1)
                └─ sR : (HDF5 Dataset, @sequence_index=2)
                └─ sQz : (HDF5 Dataset, @sequence_index=3)
```

Header to HDF5

- Every Header subclass becomes HDF5 Group
 - Follows hierarchy of orsopy classes, e.g.
dataset.info.data_source.experiment becomes HDF5 Group
"dataset/info/data_source/experiment"
 - Special handling for Python lists, e.g. [Columns]
 - Group is created, with attribute @sequence = 1
 - Members of list are added as sub-groups with attribute @sequence_index=<list index>
 - String, numeric, boolean and array attributes become HDF5 Datasets
 - Value "None" becomes empty HDF5 dataset, shape = None
 - Python datetime.datetime are converted to ISO 8601 string Dataset
 - Python Enum becomes base class (int or str)

NXData folder

Additional group `plottable_data` with given these HDF5 attributes:

- `@NX_class = NXdata`
- `@axes = ['Qz']`
- `@signal = 'R'`
- `@Qz_indices = [0]`

```
/ : (HDF5 Group, @NX_class='NXroot', @default='dataset')
|
└─ dataset : (HDF5 Group, @NX_class='NXentry', @default='plottable_data',
    @ORSO_class='OrsoDataset')
    ├── info : (HDF5 Group, @ORSO_class='Orso')
    │   ├── data_source : (HDF5 Group, @ORSO_class='DataSource')
    │   │   ...
    │   └─ data : (HDF5 Group, @sequence=1)
    │       ├── Qz : (HDF5 Dataset, @sequence_index=0)
    │       ├── R : (HDF5 Dataset, @sequence_index=1)
    │       ├── sR : (HDF5 Dataset, @sequence_index=2)
    │       └─ sQz : (HDF5 Dataset, @sequence_index=3)
    └─ plottable_data (HDF5 Group, @NX_class='NXdata', @signal='R'...)
        ├── Qz : link to ../data/Qz
        ├── R : link to ../data/R
        ├── R_errors : link to ../data/sR
        └─ Qz_errors : link to ../data/sQz
```

Demo: Web Viewer

H5Web (from PANOSC)

[https://h5web.panosc.eu/h5wasm?url=https%3A%2F%2Fwww.reflectometry.org%2Fprojects%2Ffile_formats%2Fexamples%2FFreestanding SiO2 Thick NoPMMA 6K4347 UP.orb](https://h5web.panosc.eu/h5wasm?url=https%3A%2F%2Fwww.reflectometry.org%2Fprojects%2Ffile_formats%2Fexamples%2FFreestanding%2FSiO2%2FThick%2FNoPMMA%2F6K4347%2FUP.orb)

