file format for reduced reflectivity data

ASCII representation

.ort orso reflectivity text file

relation to FAIR standards realisation

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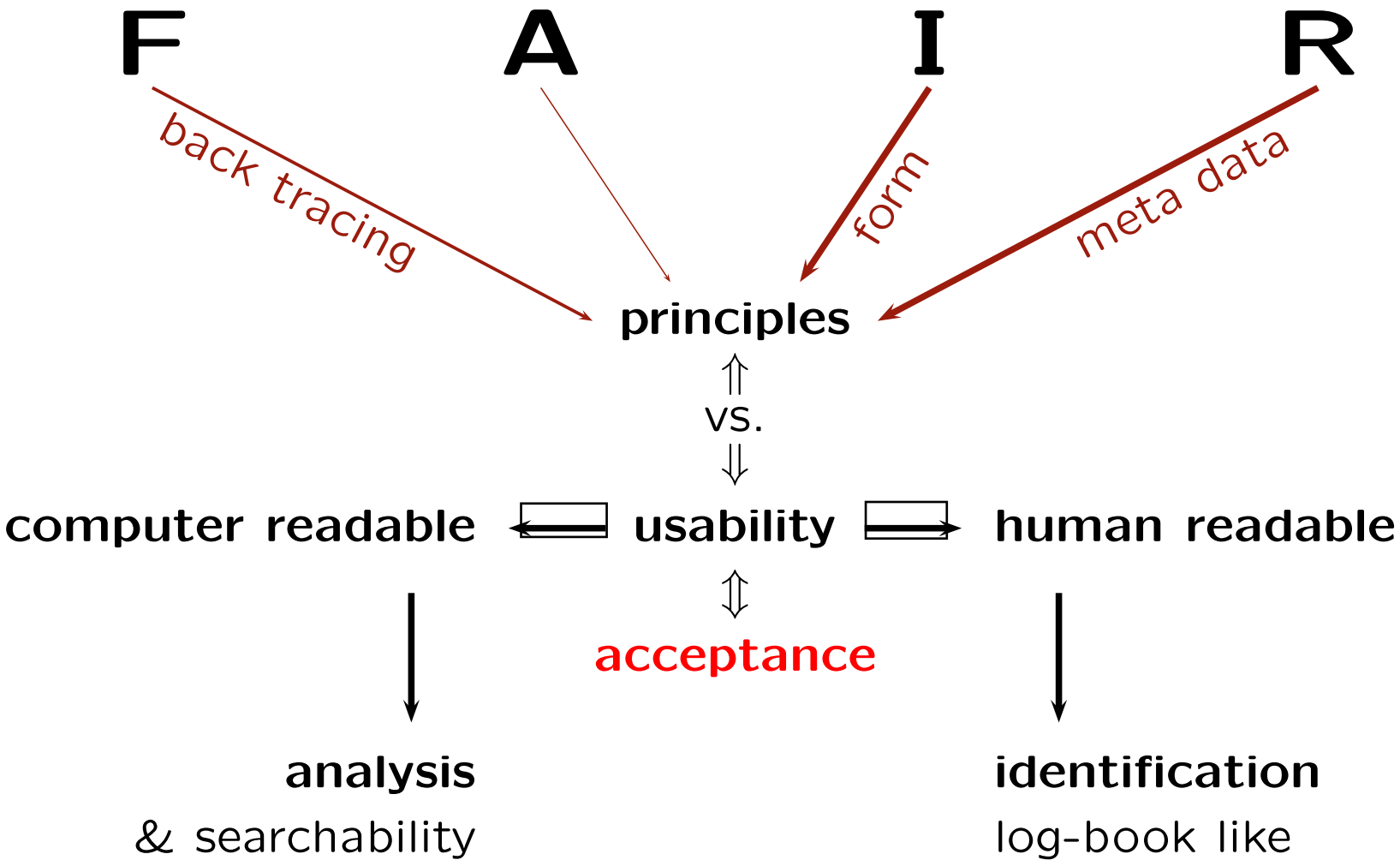
on behalf of ORSO

file format for reduced reflectivity data

principles and acceptance



file format for reduced reflectivity data

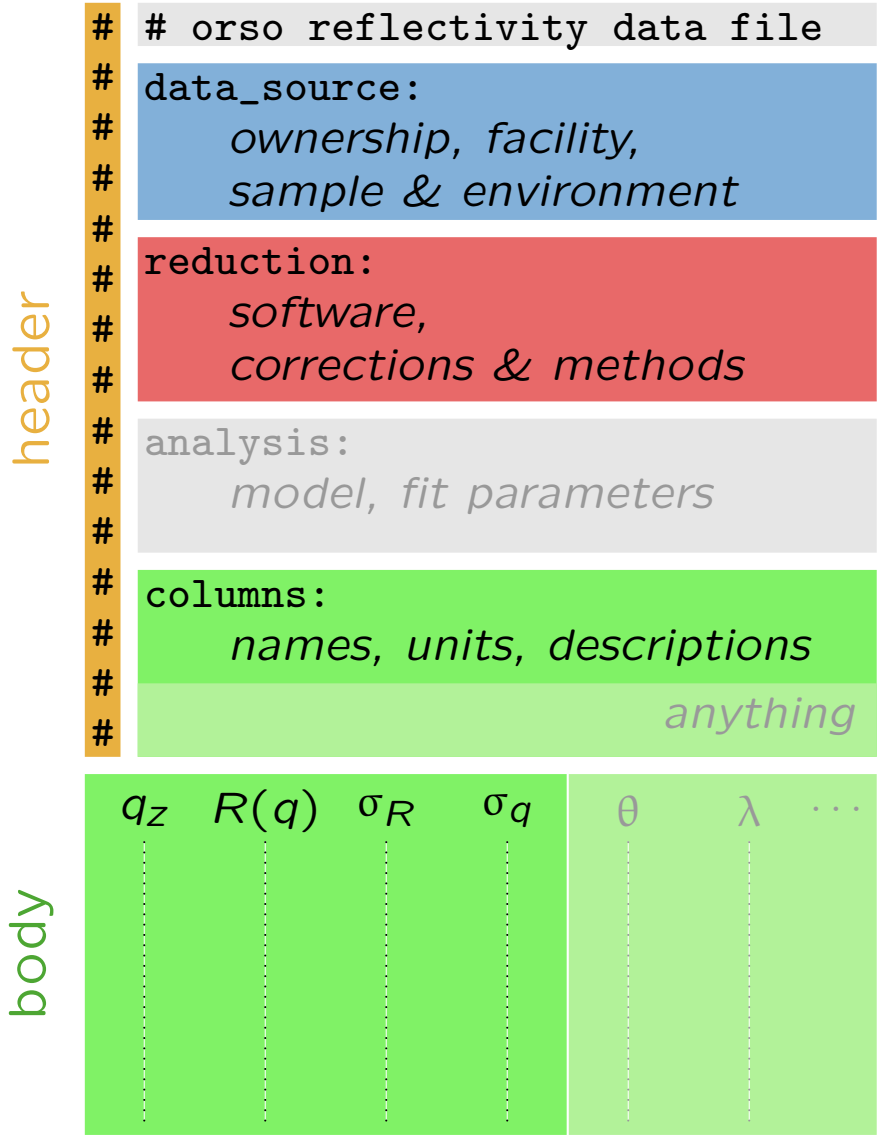
formalised structure

strict formal rules

defined entries and key words

open = expandable

recommendations



meta data

defined structure (YAML, JSON)

predefined keys

open for user-defined entries

data set

& declarations

cols $1-4$ predefined

cols $5-\infty$ free choice

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```
# # ORSO reflectivity data file | 0.1 standard | YAML enc
# # Interdiffusion in Fe | 2020-12-24 | sample fe-457-2
# data_source:
#     owner:
#         name:           Jochen Stahn
#         affiliation:    PSI, CH 5232 Villigen
#         contact:        jochen.stahn@psi.ch
#     experiment:
#         title:          Interdiffusion in Fe
#         probe:          neutron
#         facility:       PSI SINQ
#         instrument:     Amor
#         proposalID:     2021 9876
#         start_date:     2021-05-16
#     sample:
#         name:           fe-457-2
#         description:    10 x 10 mm^2
#         environment:    small in-situ furnace with impr
```

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```
# analysis:
#   software:
#     name: GenX
#     version: 3.5.6
#   script: "import models.spec_nx as model\nfrom models
#     \ fw, bc, bw\nfrom numpy import *\n\n# BEGIN Instru
#     \ import create_fp, create_fw\ninst = model.Instrum
...
#   parameters:
#   - Parameter: SiO.setD
#     Value: 1211.2966080978158
#     Fit: true
#     Min: 903.75
#     Max: 1506.25
#     Error: '-'
...
#   statistics_mcmc:
#     library: bumps
```

e.g. GENX output by Artur Glavic → no orso key words

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best practice guide in preparation

mandatory entries under debate!

- conditional information

  e.g. `proposalID` for lab x-ray sources

- multiple options

  `wavelength` vs. `photon_energy` vs. `anode`

- availability of information

  `sample.name` for in-situ prepared/modified *sample*

- practical issues

  manual input of information

- acceptance

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implementation

orsopy	python modules to read and write `.ort` files	available
model language	more useful than a sample name computer readable searchable	testing phase
validation	software to check `.ort` files	to come
in use	scipp, reductus, POLREF, eos, . . . refnx, GenX, Refl1d, easyReflectometry, . . .	

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contribution is highly appreciated!

using / testing — reflectometry.org/file_format/specification
github.com/reflectivity/orsopy

feedback on bugs / inconsistencies — Jochen.Stahn@psi.ch
request for new canonical key words — Maximilian.Skoda@stfc.ac.uk

participation in slack or on-line discussions — orso-co.slack.com

coding

thanks for listening!