

Can we work together on reflectivity analysis I?

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NIST CENTER FOR NEUTRON RESEARCH

Why are we not already?

- Communication (but here we are)
- Resources (small community)
- Instrumental specifics
- Variety of models
- Simplicity of implementation

Building reflectivity analysis: pieces

1. Model Builder / Problem Specification
2. Fitting Engine / Optimizer
3. Simultaneous fitting
4. Interactive Frontend / Visualization
5. Output format

1. Model Builder / Problem Specification

- Built-in to e.g.
 - Motofit
 - Globalfit
 - SasView
- Approaches:
 - Declarative
 - Script-based
 - GUI -> script
 - BornAgain
 - Webfit NCNR

2. Fitting Engine / Optimizer

- Bumps
 - Multiple minimizers
 - Statistical error bars
 - Parameter correlations
 - Shared with SasView
- Other options?

3. Interactive Frontend / Visualization

- Local
 - Qt 5 (e.g. SasView)
 - Wx
 - HTML / Javascript
 - Electron
 - Local webserver
- Remote
 - HTML / Javascript
 - Distributed Framework (ZeroC)

4. Output Format

- Desired
 - Reloadable
 - Traceable
 - Interoperable
- Choices
 - NXcanSAS (HDF)
 - Columnar text + rich header

Discussion Topic #1:

How to make a model builder?

What features are needed?

1. Layer definitions
2. Constraints
3. Magnetism
4. Roughness
5. Multilayers
6. ?

Are models declarative or
script-based?

Separate from the engine
frontend or included?

How many model builders
(how many types of model?)

Discussion Topic #2:

Frontend Development: local vs remote

Local frontend:

- ▶ Can be part of "batteries included" installation package
- ▶ Updates

Separation into client/server:

- ▶ Migration to distributed / cloud is greatly simplified
- ▶ Updates to backend and frontend can be separated
- ▶ Versioning is an issue
- ▶ Can still be run locally

Discussion Topic #3: Helping with model selection

Should the analysis program help select the model?

- ▶ AI / ML pre-analysis of scattering pattern
- ▶ Meta-analysis: does adding new layers increase information content of fits?
- ▶ Can we use data inversion (multiple contrast) to predetermine the overall shape of the realspace model?