

# Can we work together on reflectivity analysis I?

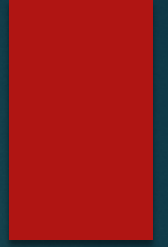
BRIAN BEN MARANVILLE & PAUL KIENZLE

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

- Builtin 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?