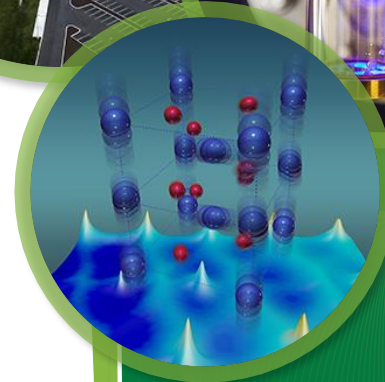# Transformation of the Liquids Reflectometer

Mathieu Doucet

NDAV

Recent Changes

- In the past two years, **all the software** for acquiring, reducing, and analyzing LR data has been replaced.

- A whole team of people worked on this:

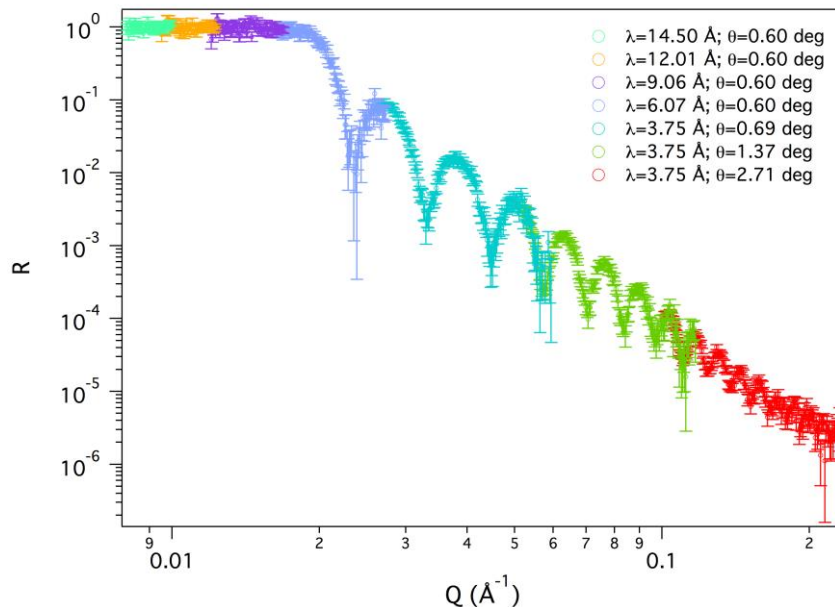| DAS	NDAV	Beamline
➢ Bogdan	➢ Jean-Christophe	➢ Jim
➢ Marie	➢ Mathieu	➢ John
➢ Matt		➢ Candice

- Our goal is to streamline the process so users can leave the lab with good reduced data, and a good **start on their analysis**.

OAK RIDGE
National Laboratory | SPALLATION NEUTRON SOURCE

Outline of a LR measurement

1. Measure scattering data.

2. Measure direct beam.

3. Reflectivity is the ratio of the two…

4. … but we need scaling factors for absolute normalization.

5. The scaling factors correct for the fact that we measure the direct beams with smaller slit openings than when we measure reflectivity.

$$R = 1 / N_{\Lambda, j} \times \left[\text{scattering} \right] / \left[D_0 \right]$$

6. For a full measurement, we may need dozens of attenuated direct beam measurements.

Legend:
- $\lambda=14.50$ Å; $\theta=0.60$ deg
- $\lambda=12.01$ Å; $\theta=0.60$ deg
- $\lambda=9.06$ Å; $\theta=0.60$ deg
- $\lambda=6.07$ Å; $\theta=0.60$ deg
- $\lambda=3.75$ Å; $\theta=0.69$ deg
- $\lambda=3.75$ Å; $\theta=1.37$ deg
- $\lambda=3.75$ Å; $\theta=2.71$ deg

θ_i (°)	Measurement	S_1 (mm)	S_2 (mm)	Attenuators
–	D_0	0.26	0.26	0
–	$A_I D_0$	0.26	0.26	1
0.60	$A_I D_j$	0.33	0.26	1

$$D_j(\lambda) = \frac{A_I D_j(\lambda)}{A_I(\lambda)} = \frac{A_I D_j(\lambda)}{A_I D_0(\lambda)} D_0(\lambda).$$

$$N_{\Lambda, j}(\lambda)$$

We need this for each one of the settings we measure!

OAK RIDGE National Laboratory | SPALLATION NEUTRON SOURCE

New Data Acquisition System

- Stable and reliable.

- Allows for live streaming of the acquired data.

- Allows for better monitoring.

- Helps guide the user through the measurement process.

- New tools allow the user to optimize the measurement process for footprint and resolution.

- It also plans the direct beam measurements needed to compute scaling factors.

- These features make users more independent.

- **It can store meta-data that fully describes the measurement.**

This is what allows us to do automated reduction!
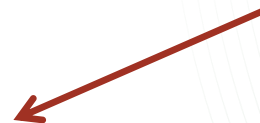
Web Monitor

- Used to follow the status of the instrument / experiment.

- Used to look at reduced data and check for error.

- Monitored by IHCs.

Automated Reduction

- Once the data is written do disk, it is catalogued and sent to auto-reduction.

- The LR auto-reduction uses a template system, but can also be run in fully automated mode.

- To use the fully automated mode, you have to follow the DAS process and fill out the boxes.

- The processing of direct beam sets used for scaling factor calculations is fully automated.
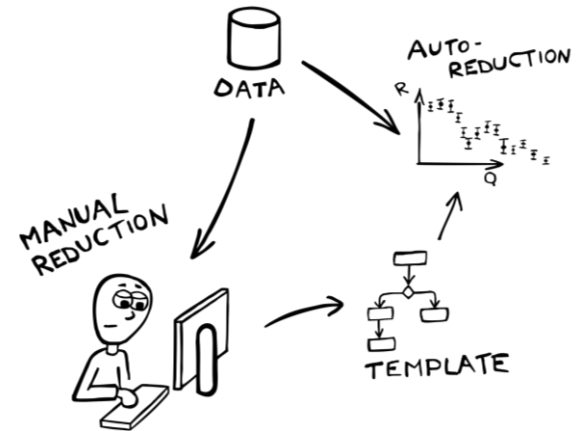

Note from the field:
I have used the fully automated mode to set up templates, but I prefer running in template mode for my own data.

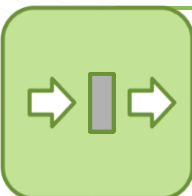OAK RIDGE National Laboratory | SPALLATION NEUTRON SOURCE

Manual Reduction - RefRed

- The application automatically sorts data runs and finds reflectivity peaks. It also matches data runs to normalization runs.

- Runs the same algorithms as the auto-reduction.

- Can be used to generate templates. A template management tool is available to easily deploy auto-reduction templates.

- Auto-reduction templates can be directly loaded in RefRed.

- Can be used to calculate scaling factors for absolute normalization.

- RefRed offers tools for browsing meta-data in Nexus files and to preview scaling factor files.
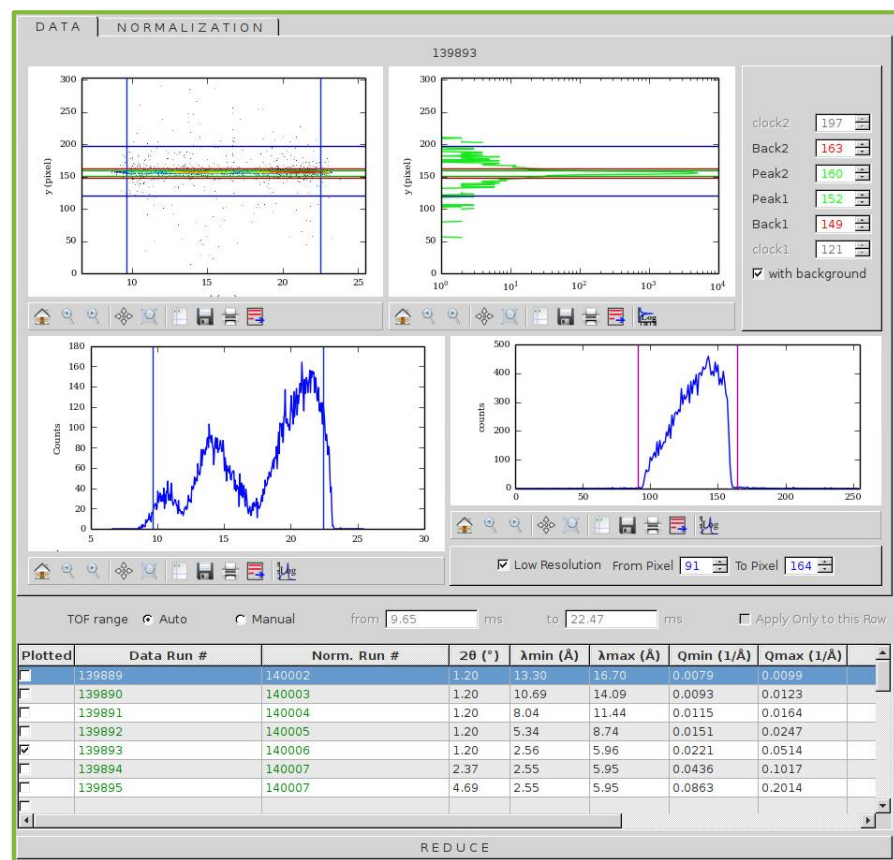
Screenshot of the new RefRed application showing the main data management tools.

Automated Reduction: types of measurements

		Automated Process
→	0-attenuator direct beams	Do nothing
⇨▯⇨	Scaling factor direct beams	Compute scaling factors (fully automated)
↘↗	Scattering data	Compute **normalized**, **merged**, and cleaned-up reflectivity
?	Other	Do nothing

Automated Reduction: outputs

- Creates the merged reflectivity data.

- Creates a configuration / template file that can be reloaded in RefRed.

- Sends the reflectivity file to the web monitor, where it appears as an interactive plot.

- Data can be downloaded from the web monitor.

- *NEW!* Links out to the new reflectivity fitting application.
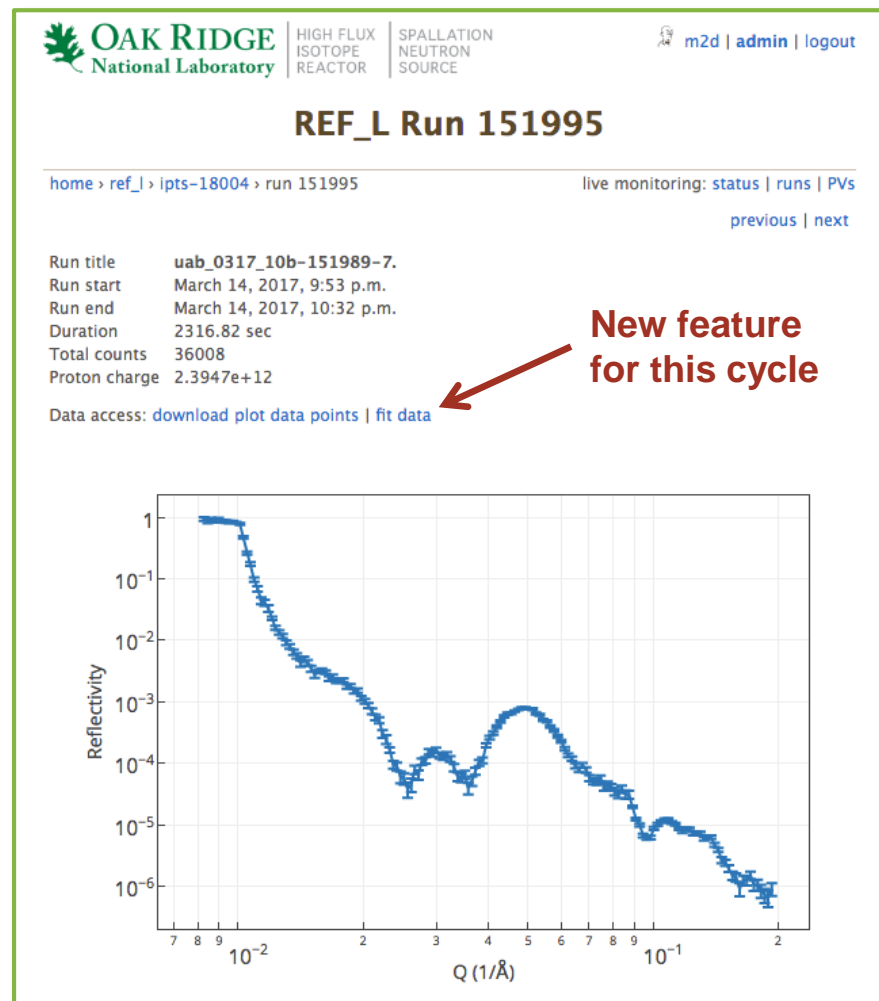
Reflectivity Fitting

- Provides an interface for Refl1D.

- Jobs are run on analysis.sns.gov.

- User can also upload reduced data.

- User can add constraints.

- Full error analysis.

- Various plots and outputs are also stored in the user's home directory on analysis.sns.gov.

Was used for the first time this week by an external user!
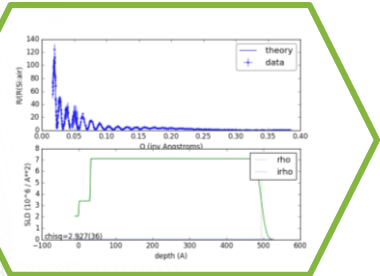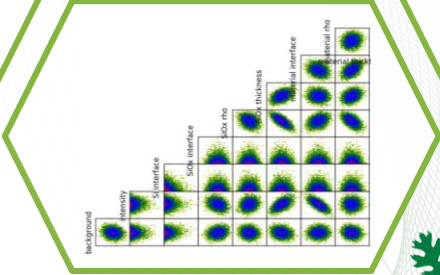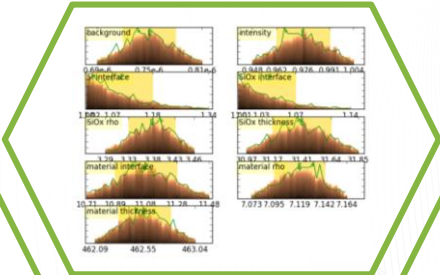
Summary
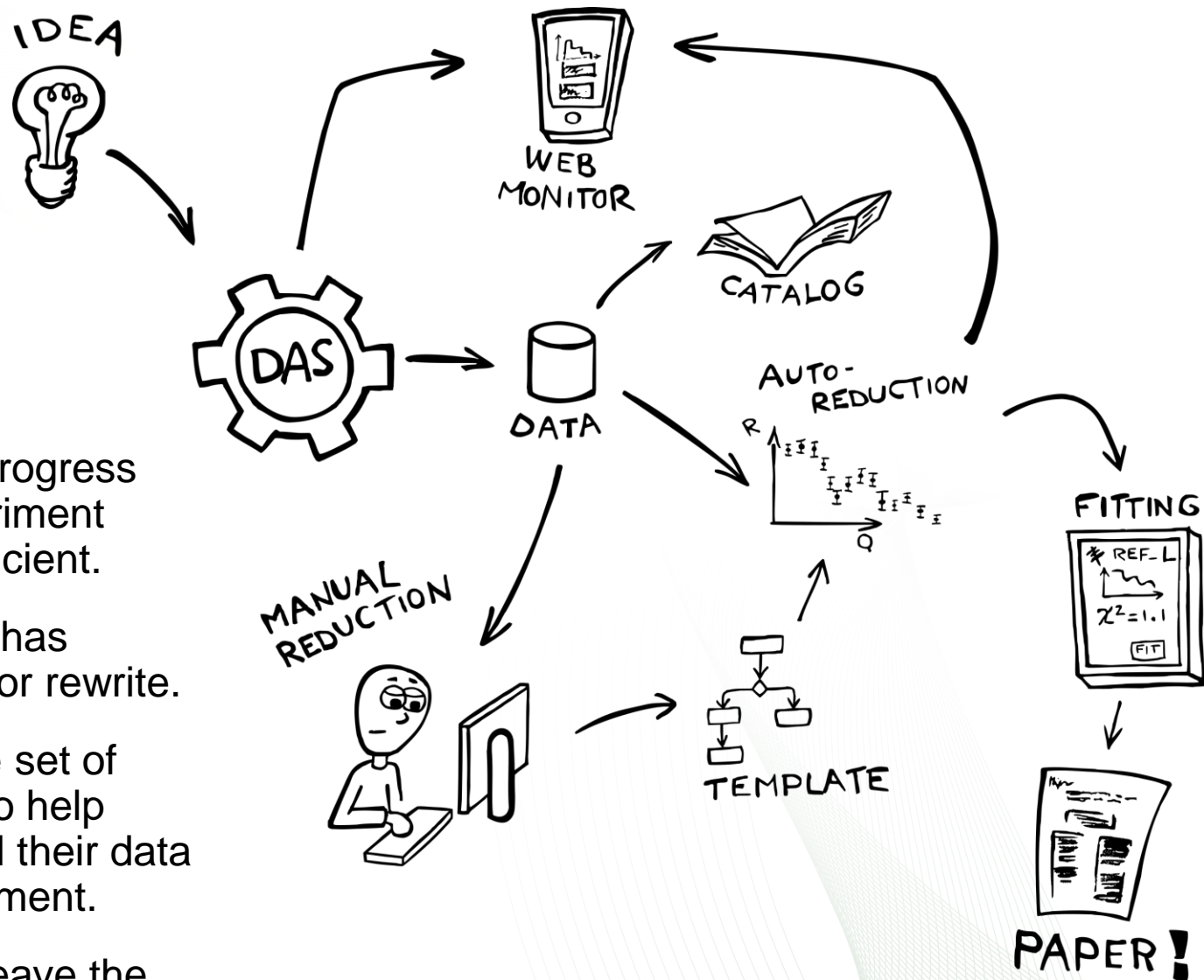
- We are making progress making the experiment process more efficient.

- The LR software has undergone a major rewrite.

- A comprehensive set of tools is in place to help users understand their data during the experiment.

- Most users can leave the lab with quality data.