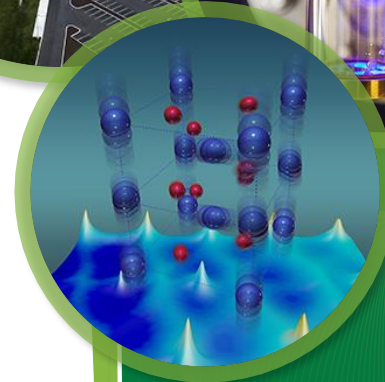


# Transformation of the Liquids Reflectometer

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
➤ Bogdan
➤ Marie
➤ Matt

NDAV
➤ Jean-Christophe
➤ Mathieu

Beamline
➤ Jim
➤ John
➤ Candice

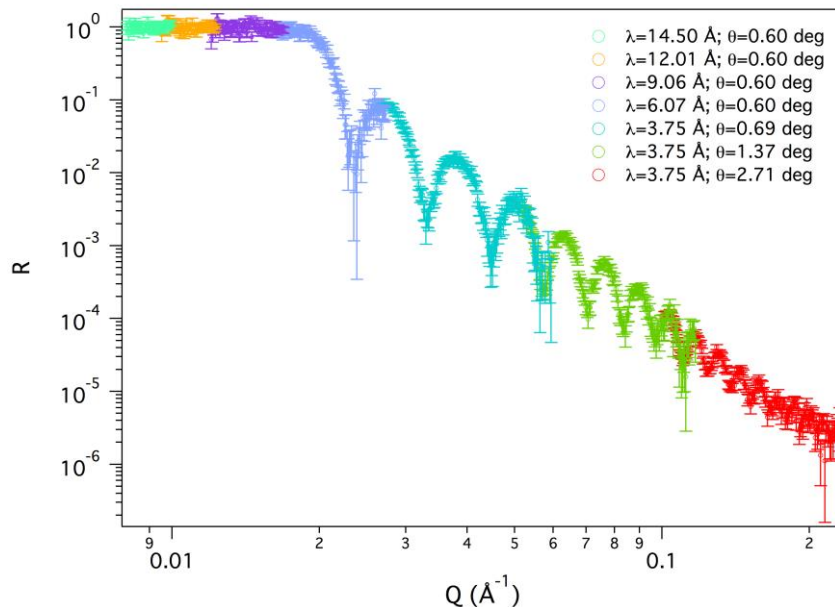
- Our goal is to streamline the process so users can leave the lab with good reduced data, and a good **start on their analysis**.

# 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.

$$R = 1 / N_{\Lambda, j} \times \left[ \text{Scattering Data} \right] / \left[ \text{Direct Beam } D_0 \right]$$

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



$\theta_i$ (°)	Measurement	$S_1$ (mm)	$S_2$ (mm)	Attenuators
–	$D_0$	0.26	0.26	0
–	$A_1 D_0$	0.26	0.26	1
0.60	$A_1 D_j$	0.33	0.26	1

$$D_j(\lambda) = \frac{A_1 D_j(\lambda)}{A_1(\lambda)} = \frac{A_1 D_j(\lambda)}{A_1 D_0(\lambda)} \underbrace{D_0(\lambda)}_{N_{\Lambda, j}(\lambda)}$$

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

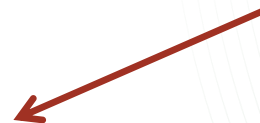
We need this for each one of the settings we measure!

# 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!**



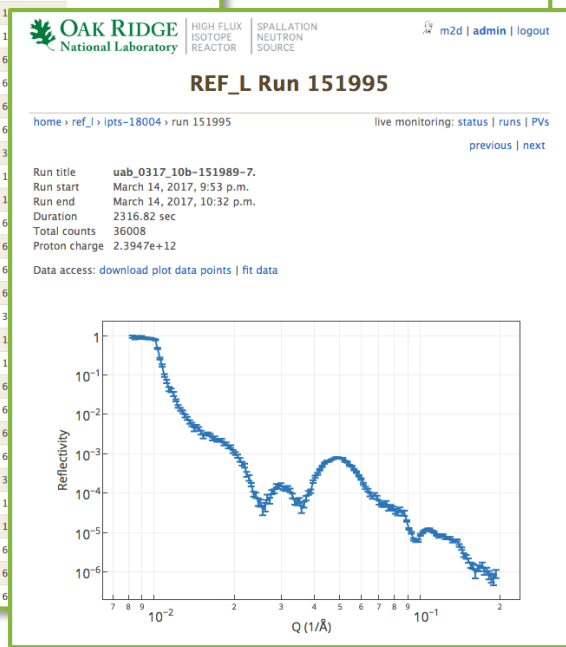
# Web Monitor

- Used to follow the status of the instrument / experiment.
- Used to look at reduced data and check for error.
- Monitored by IHCs.

OAK RIDGE National Laboratory REF\_L IPTS-18004

home > ref\_l > catalog > ipts-18004

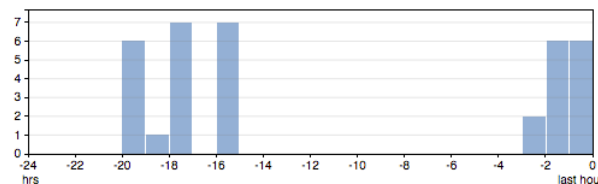
Run	Title	Duration [sec]	Total counts
152179	UAB_0317_10a-pH713b_3hr-152173-7. Mar 17, 08:27:42 - 08:38:13	630.9	3.603E+04
152178	UAB_0317_10a-pH713b_3hr-152173-6. Mar 17, 08:19:26 - 08:29:57	460.3	1
152177	UAB_0317_10a-pH713b_3hr-152173-5. Mar 17, 08:11:18 - 08:18:48	449.3	6
152176	UAB_0317_10a-pH713b_3hr-152173-4. Mar 17, 08:03:50 - 08:10:20	29.32	1
152175	UAB_0317_10a-pH713b_3hr-152173-3. Mar 17, 08:08:43 - 08:08:52	8.566	6
152174	UAB_0317_10a-pH713b_3hr-152173-2. Mar 17, 08:07:24 - 08:09:40	17.65	6
152173	UAB_0317_10a-pH713b_3hr-152173-1. Mar 17, 08:05:14 - 08:06:24	69.7	6
152172	UAB_0317_10a-pH713b-152166-7. Mar 17, 06:08:08 - 06:09:23	586.1	3
152171	UAB_0317_10a-pH713b-152166-6. Mar 17, 06:19:36 - 06:27:27	470.5	1
152170	UAB_0317_10a-pH713b-152166-5. Mar 17, 06:11:22 - 06:19:04	461.4	1
152169	UAB_0317_10a-pH713b-152166-4. Mar 17, 06:09:52 - 06:10:22	29.3	6
152168	UAB_0317_10a-pH713b-152166-3. Mar 17, 06:08:08 - 06:09:23	8.583	6
152167	UAB_0317_10a-pH713b-152166-2. Mar 17, 06:07:22 - 06:07:40	17.65	6
152166	UAB_0317_10a-pH713b-152166-1. Mar 17, 06:05:14 - 06:06:22	67.7	6
152165	UAB_0317_10a-pH713-152159-7. Mar 17, 05:21:40 - 05:29:20	649.6	3
152164	UAB_0317_10a-pH713-152159-6. Mar 17, 05:13:18 - 05:20:58	460.6	1
152163	UAB_0317_10a-pH713-152159-5. Mar 17, 05:05:09 - 05:12:43	404.8	1
152162	UAB_0317_10a-pH713-152159-4. Mar 17, 05:04:30 - 05:05:01	30.75	6
152161	UAB_0317_10a-pH713-152159-3. Mar 17, 05:03:19 - 05:04:30	8.067	6
152160	UAB_0317_10a-pH713-152159-2. Mar 17, 05:02:07 - 05:02:23	17.63	6
152159	UAB_0317_10a-pH713-152159-1. Mar 17, 04:59:59 - 05:01:09	68.63	6
152158	UAB_0317_10a-pH713-152152-7. Mar 17, 04:16:32 - 04:26:19	587	3
152157	UAB_0317_10a-pH713-152152-6. Mar 17, 04:08:02 - 04:16:43	447.8	1
152156	UAB_0317_10a-pH713-152152-5. Mar 17, 04:00:36 - 04:07:50	433.2	1
152155	UAB_0317_10a-pH713-152152-4. Mar 17, 03:59:02 - 03:59:37	34.77	6
152154	UAB_0317_10a-pH713-152152-3. Mar 17, 03:57:25 - 03:59:01	9.083	6
152153	UAB_0317_10a-pH713-152152-2. Mar 17, 03:56:38 - 03:56:53	17.15	6



## REF\_L Monitor

home > ref\_l > monitor

live monitoring: status | runs | PVs



UAB\_0317\_01\_D2O\_TempRun-152003-7.

Proposal: IPTS-18004 Run: 0

Status: Stopped Count rate: 1475

Systems: [DASMON](#) [PVStreamer](#) [Workflow](#) [Catalog](#) [Reduction](#)

Last run: 152009 from IPTS-18004 created on March 15, 2017, 12:40 p.m.

Signal/PV	Value	History	Last Updated
sequence_id	152003		March 15, 2017, 12:06 p.m.
sequence_number	0		March 15, 2017, 12:51 p.m.
sequence_total	7		March 15, 2017, 12:06 p.m.

Key	Value	Last Updated
count_rate	1475	March 15, 2017, 1:14 p.m.
paused	false	March 7, 2017, 3:35 p.m.
recording	false	March 15, 2017, 12:51 p.m.
scan_index	0	March 7, 2017, 3:35 p.m.
scanning	false	March 7, 2017, 3:35 p.m.
system_dasmon	0	March 15, 2017, 1:14 p.m.
system_pvsd	0	March 15, 2017, 1:14 p.m.
system_sms	0	March 15, 2017, 1:14 p.m.
timestamp	1.4896e+09	March 15, 2017, 1:14 p.m.
total_charge	7.10046e+11	March 15, 2017, 12:51 p.m.
total_counts	35822	March 15, 2017, 12:51 p.m.
total_time	687.257	March 15, 2017, 12:51 p.m.

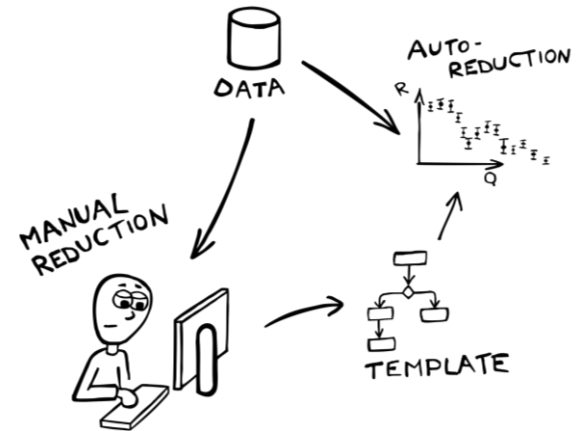


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DOE - Oak Ridge · UT-Battelle



# Automated Reduction

- Once the data is written to 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.

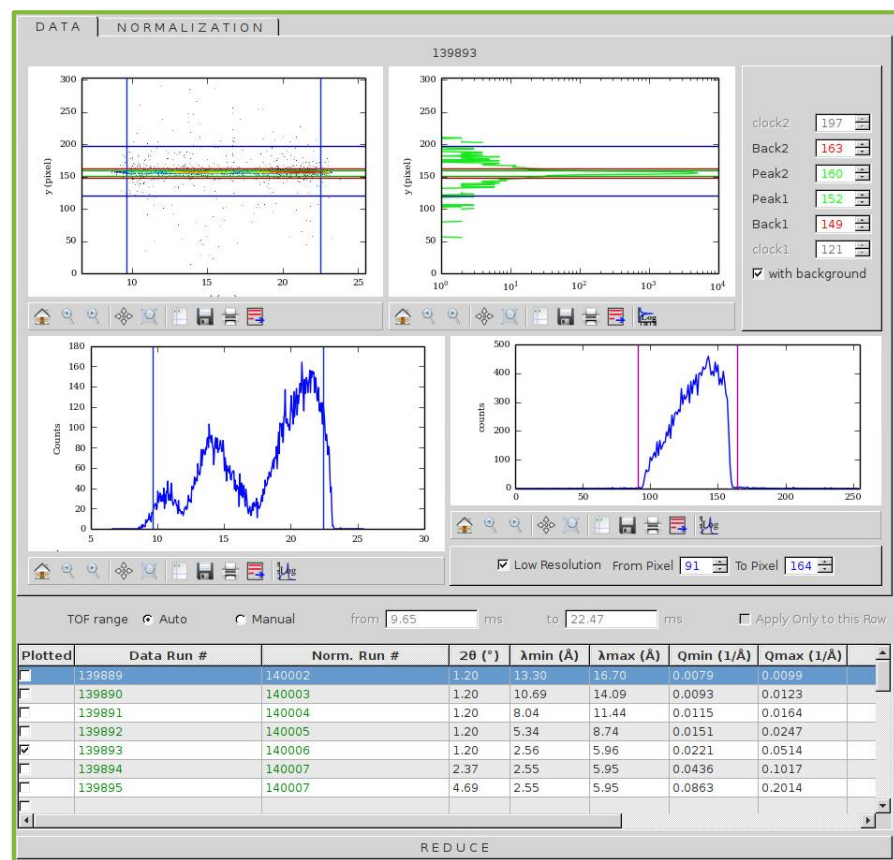


## *Note from the field:*

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


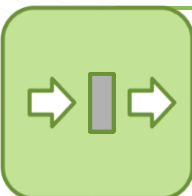


# Manual Reduction - RefRed

- 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.

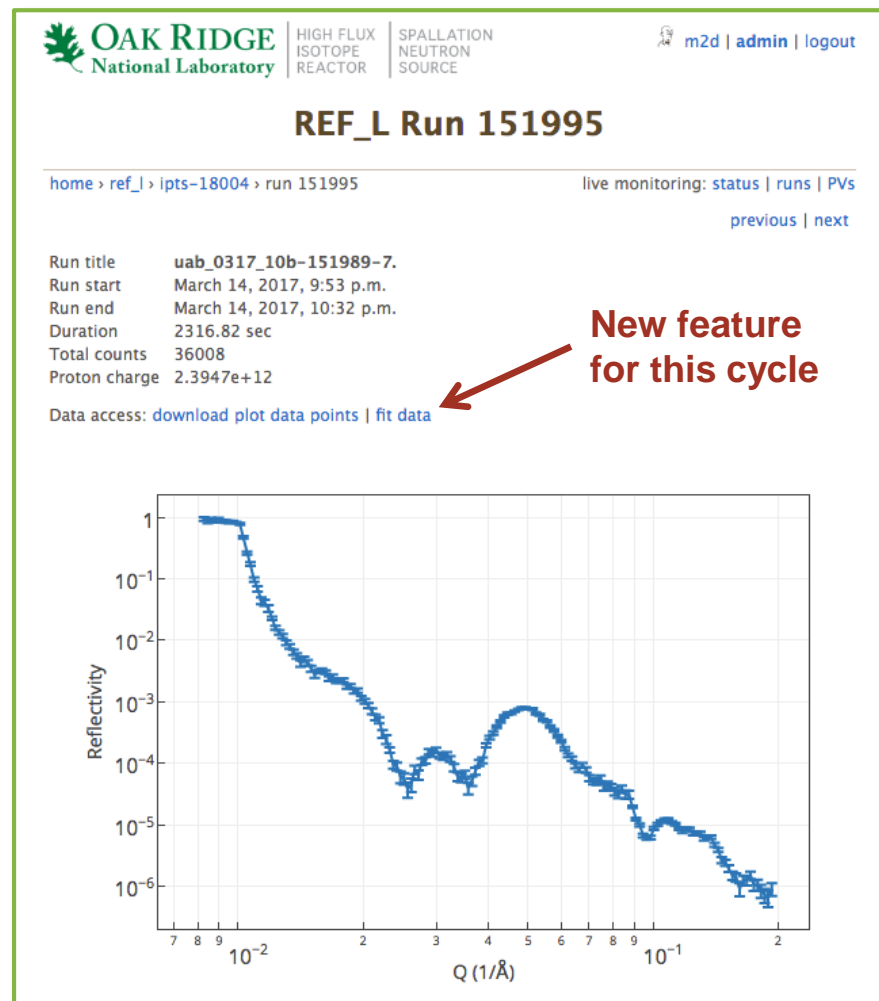
# Automated Reduction: types of measurements

		Automated Process
	0-attenuator direct beams	Do nothing
	Scaling factor direct beams	Compute scaling factors (fully automated)
	Scattering data	Compute <b>normalized, merged</b> , 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.

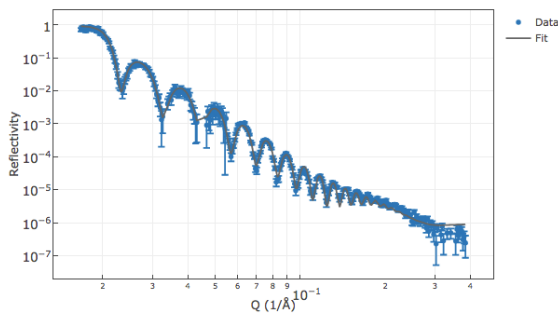
**Reflectivity Fitting**

[home](#) > [reflectivity](#) > [ref\\_1](#) | 151186

[settings](#) | [show files](#) | [show fits](#) | [download data](#) | [plot RQ<sup>2</sup> vs Q](#)

[m2d](#) | [logout](#)

**CINT Ir 30Hz-151184-3.**



**Layer model**

Checked parameters will be kept fixed during the fitting procedure.

Data:

Scale:

Background:

Neutrons scatter off the first layer on top of the following list. You can change the order of the layers by changing the layer number. The layers will be re-ordered upon submission.

Layer number	Name	Thickness (Å)	SLD (10 <sup>-6</sup> /Å <sup>2</sup> )	Roughness (Å)
Front	air	-	0.0	-
1	material	462.478	7.1312	11.003
2	SiOx	31.377	3.399	1.003
Back	Si	-	2.07	1.025

[set data](#) [fit](#) [evaluate](#)

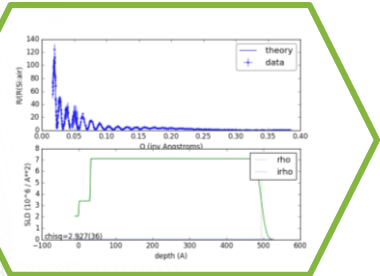
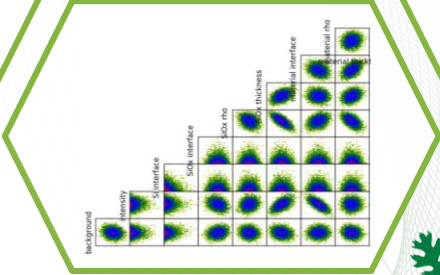
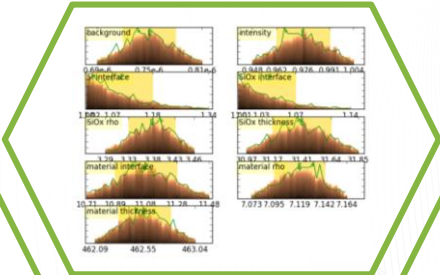
**Fitting parameters [ $\chi^2=2.927$ ]**

Q range:  to  1/Å

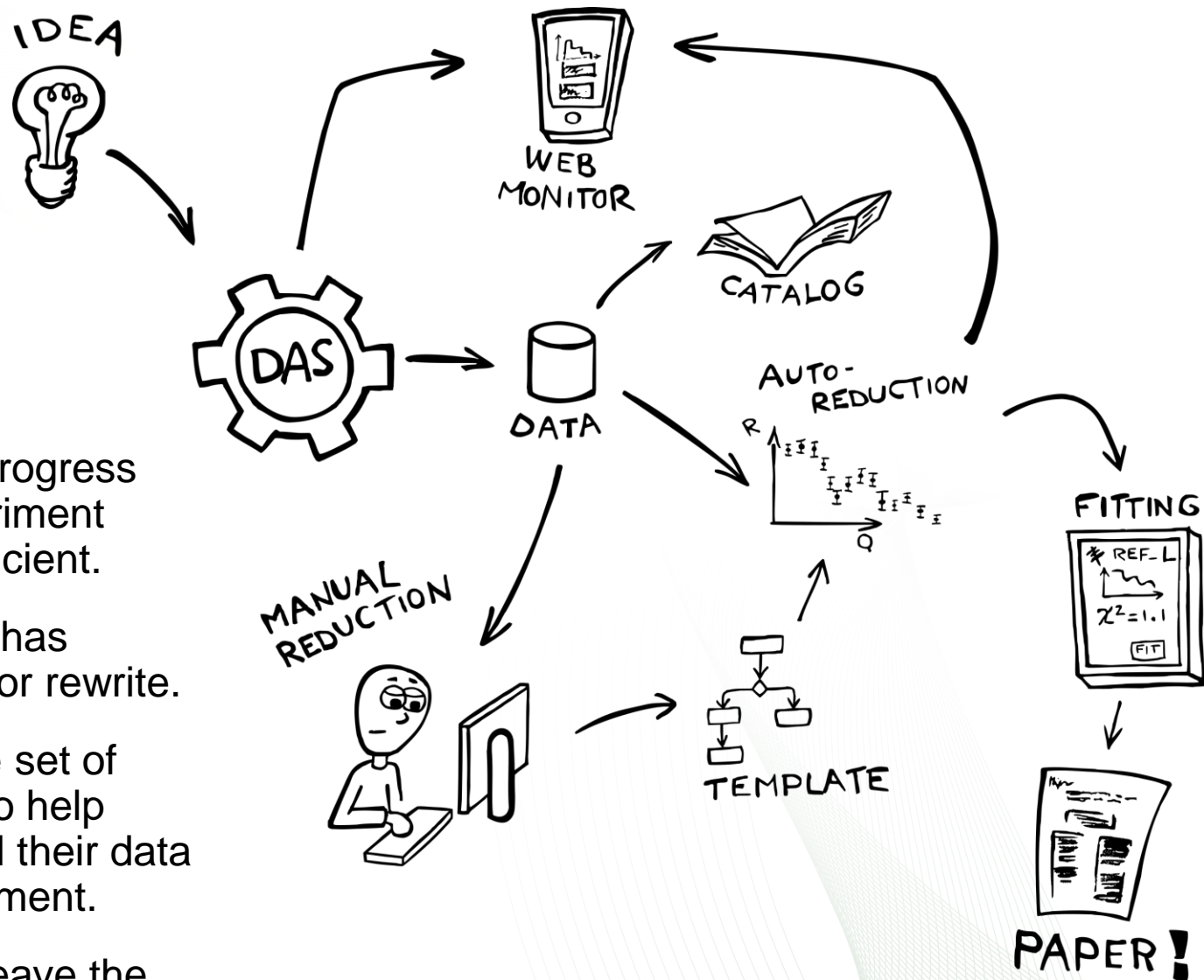
There is no **constraint** on this model.

Parameter	Value	Minimum	Maximum
scale	0.9666 ± 0.014	0.8	1.1
background	7.38e-16 ± 2.9e-08	0.0	1e-06
Front material: air			
Layer: material			
material thickness	462.478 ± 0.24	400.0	500.0
material SLD	7.1312 ± 0.023	6.0	8.0
material roughness	11.003 ± 0.19	1.0	22.0
Layer: SiOx			
SiOx thickness	31.377 ± 0.23	10.0	40.0
SiOx SLD	3.399 ± 0.045	1.0	4.0
SiOx roughness	1.003 ± 0.038	1.0	10.0
Back material: Si			
Si roughness	1.025 ± 0.091	1.0	5.0

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.