PAUL SCHERRER INSTITUT

PSI

EUROPEAN SPALLATION SOURCE

Artur Glavic :: Paul Scherrer Institut

DMSC Common Requirements

Reflectometry Software Requirements Meeting – 21.02. 2017

Outline

- **Reflectometry – Geometry, Common Terms, etc.**
- **Reduction of event mode ToF data**
- **Demonstration reduction with QuickNXS/SNS**
- **Requirements for instrument control**

Reflectometry Introduction

Specular:

$$\phi_f = 0 \qquad \alpha_i = \alpha_f \qquad Q_z = \frac{4\pi}{\lambda_n}\sin\alpha_i$$

$$\lambda_n = \frac{h \cdot ToF}{\text{distance} \cdot m_n}$$

$$R \approx \frac{I_{window} - I_{background}}{I_0(\lambda) \cdot \Delta\Theta \cdot l \cdot \sin\alpha_i}$$

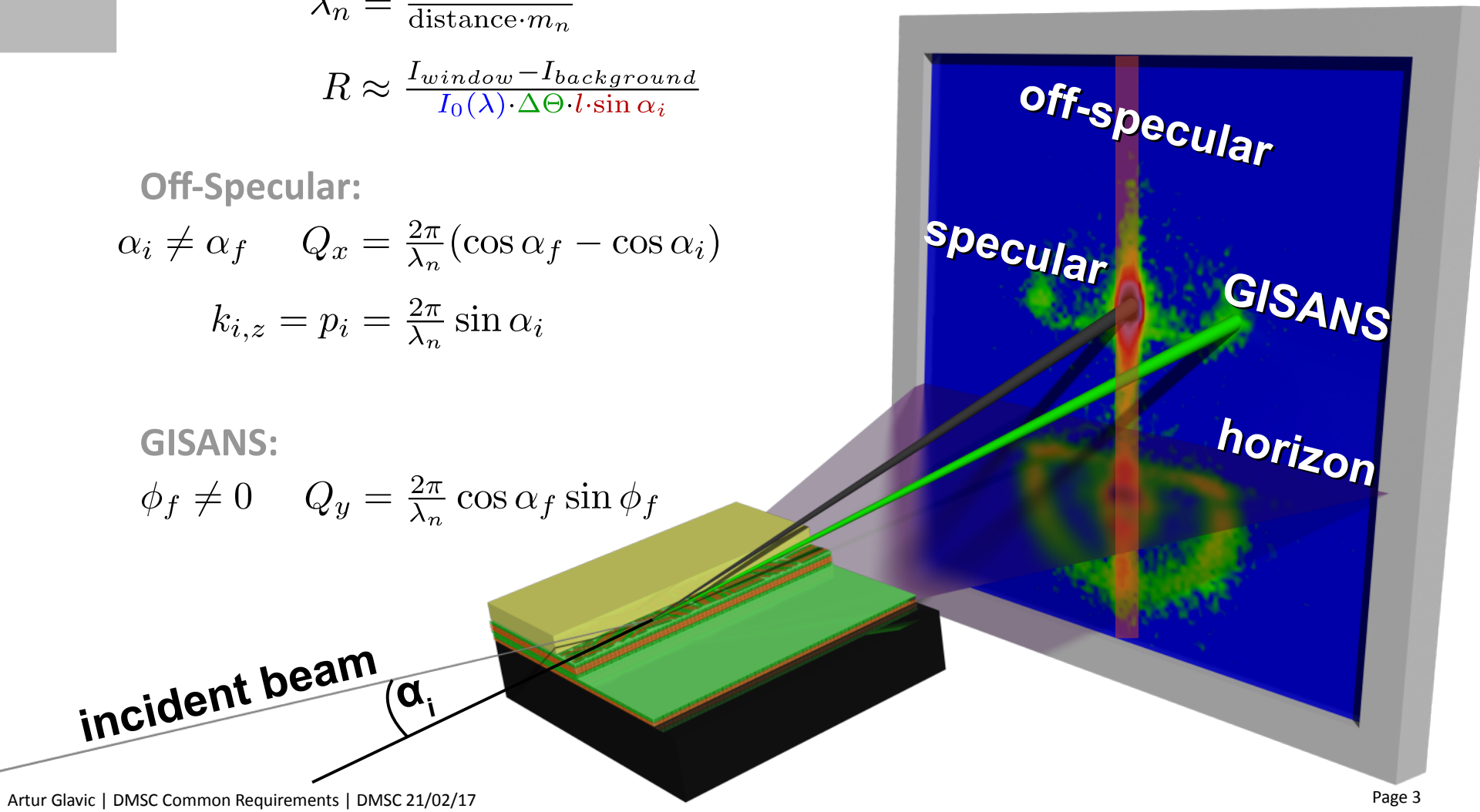
Off-Specular:

$$\alpha_i \neq \alpha_f \qquad Q_x = \frac{2\pi}{\lambda_n}(\cos\alpha_f - \cos\alpha_i)$$

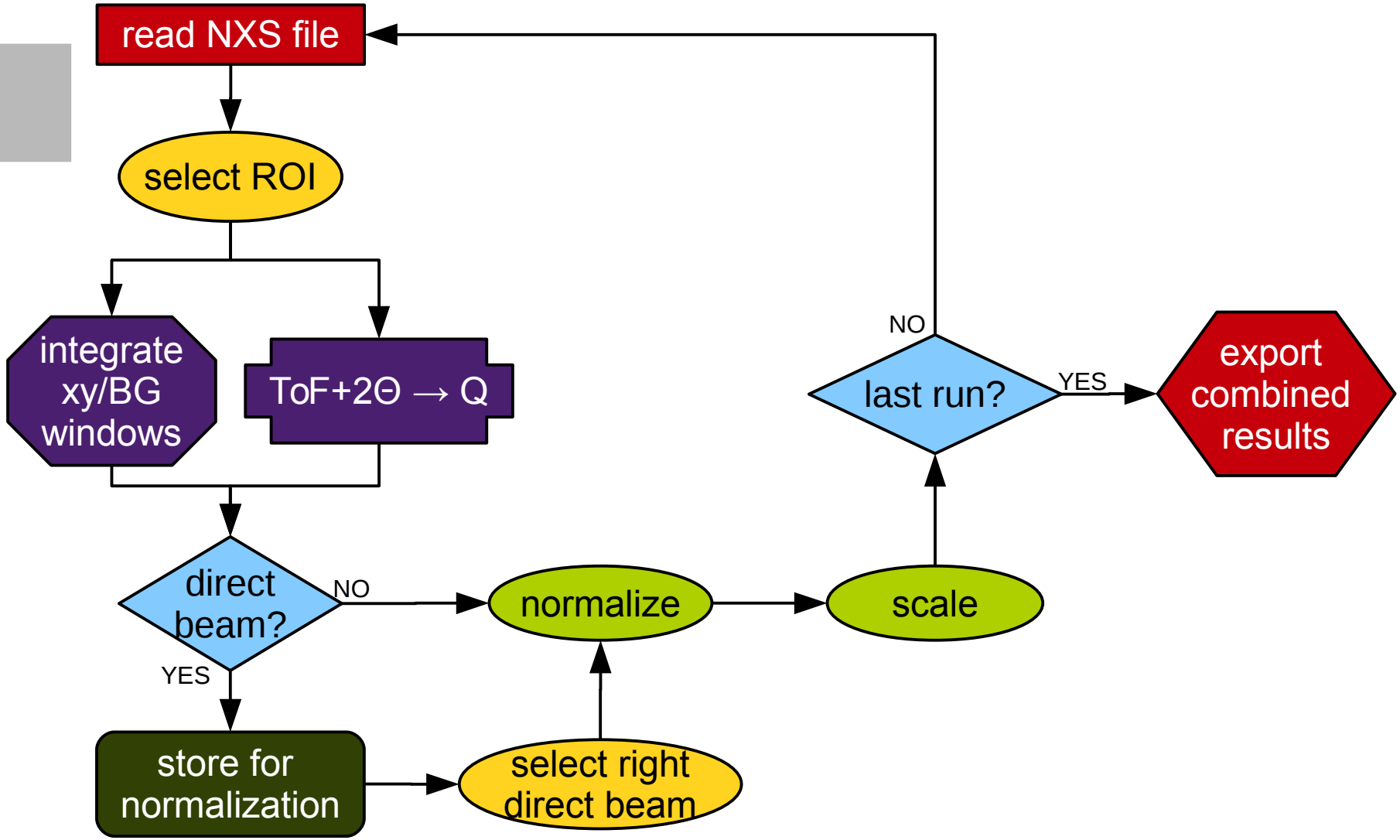
$$k_{i,z} = p_i = \frac{2\pi}{\lambda_n}\sin\alpha_i$$

GISANS:

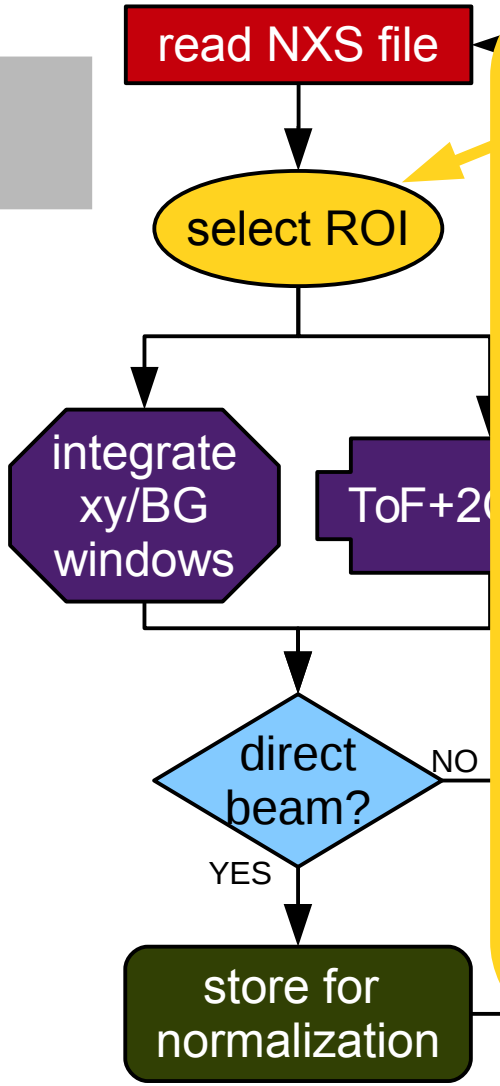
$$\phi_f \neq 0 \qquad Q_y = \frac{2\pi}{\lambda_n}\cos\alpha_f \sin\phi_f$$



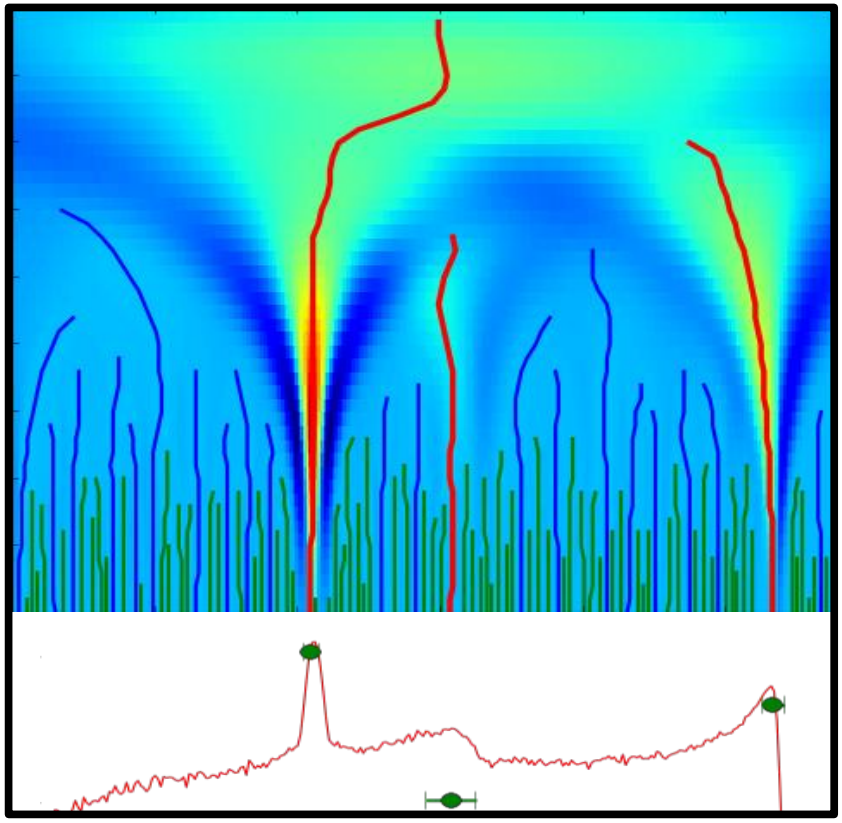
Reduction of event mode ToF data



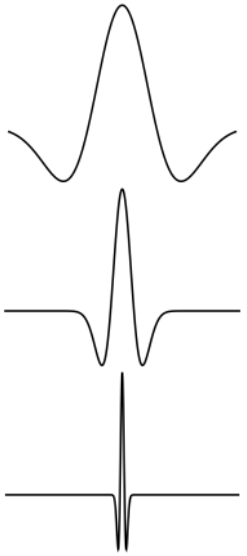
Reduction of event mode ToF data



Find peak from reflected beam using Continuous Wavelet Transform:

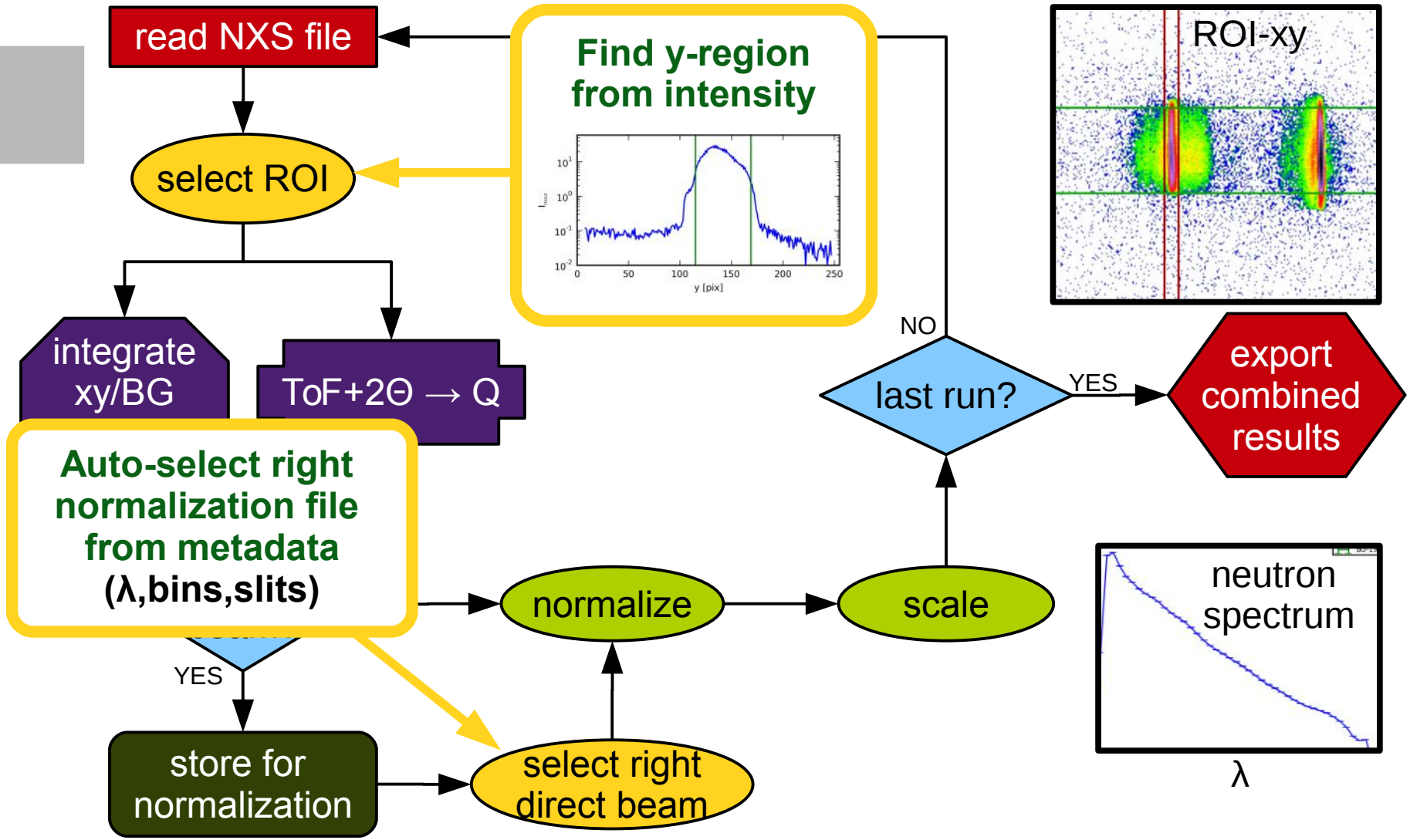


Mexican Hat wavelet



J. M. Gregoire, D. Dale and R. B. van Dover: *A wavelet transform algorithm for peak detection and application to powder x-ray diffraction data*, Rev. Sci. Inst. **82**, 015105 (2011)

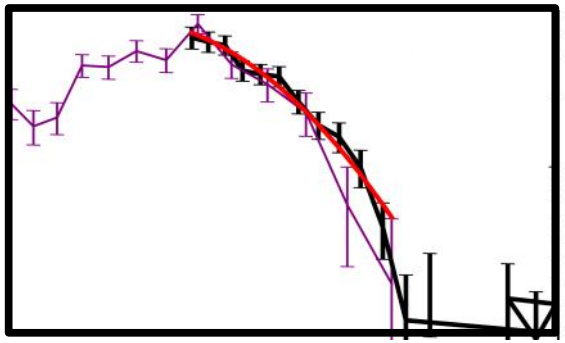
Reduction of event mode ToF data



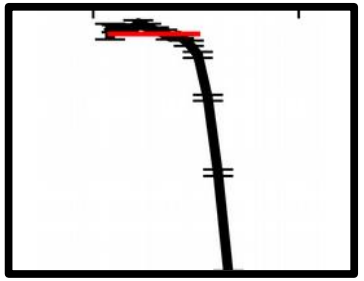
Reduction of event mode ToF data

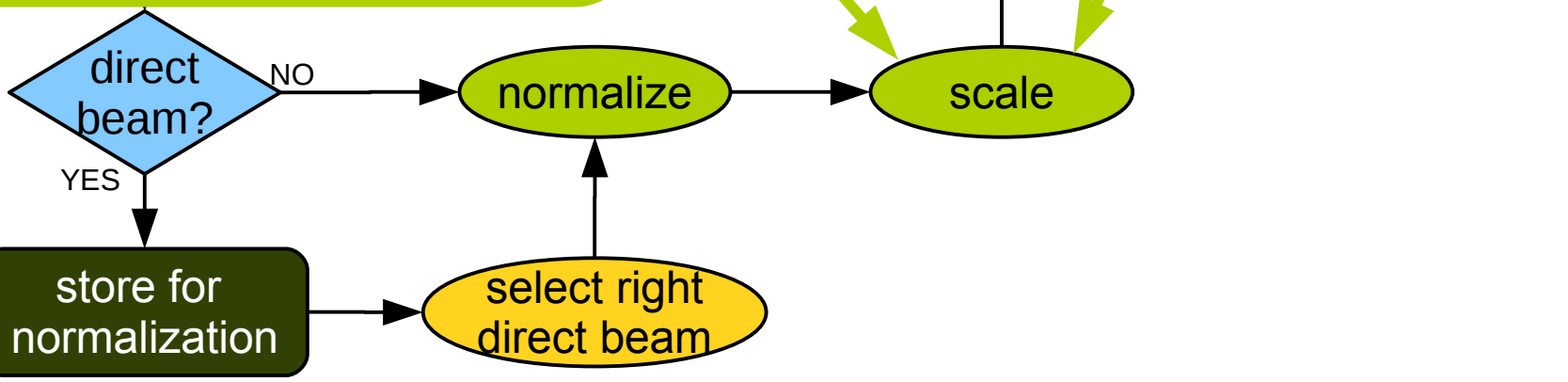
Scale subsequent runs by fitting a scaling factor and polynomial to overlapping region

$$\chi^2_{stitch} = \sum_{DS1} \frac{(\log(I_i) - p(Q_i))^2}{(\delta I_i / I_i)^2} + \sum_{DS2} \frac{(\log(I_j \cdot scale) - p(Q_j))^2}{(\delta I_j / I_j)^2}$$

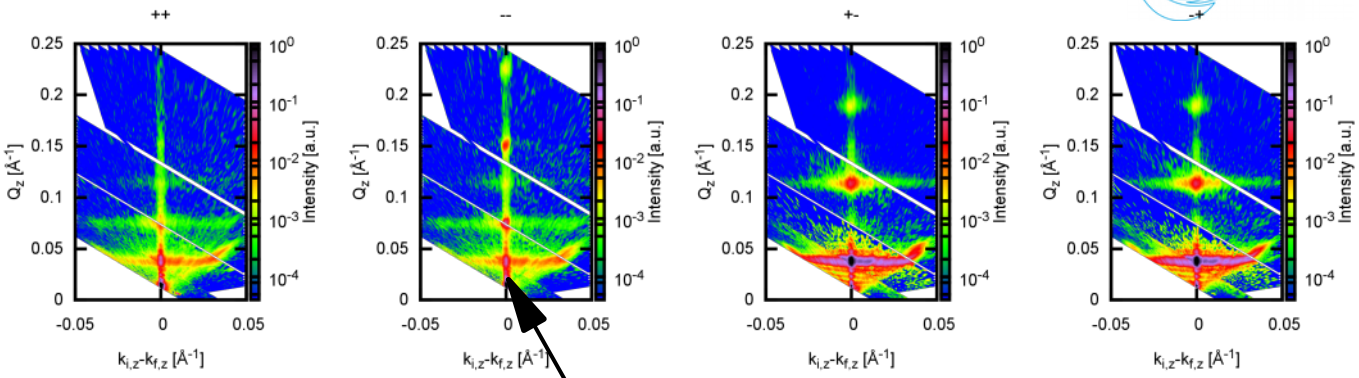


Detect total reflection and scale to 1

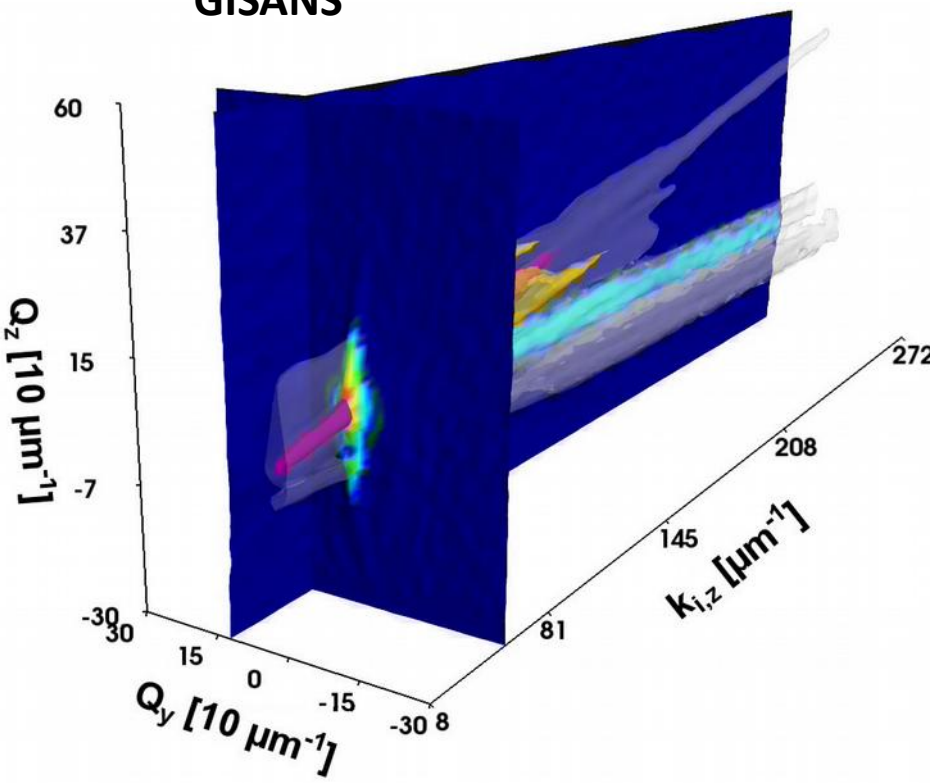




Reduction example data

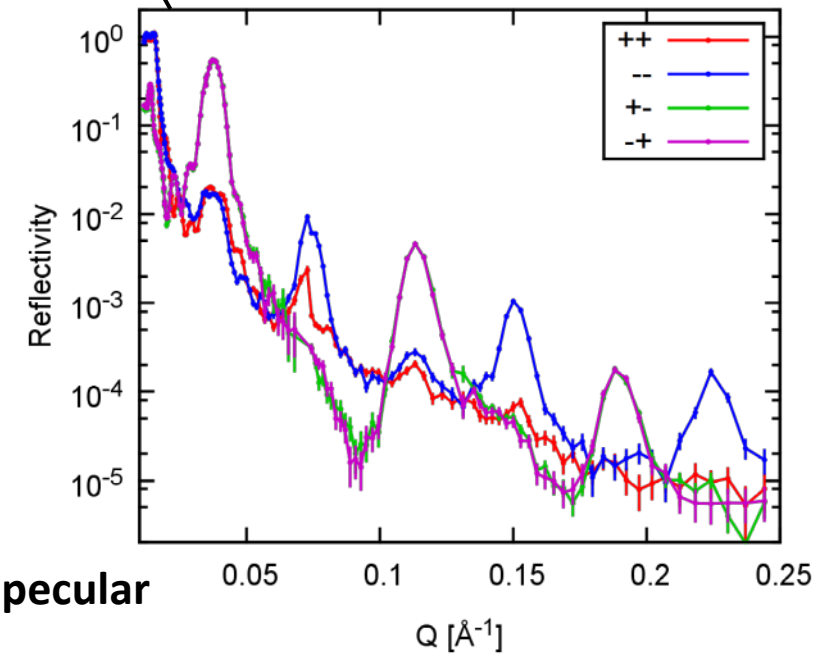


GISANS



Off-Specular

Specular



QuickNXS 0.9.63

File Reduction Automatics Tools Advanced Help

Open Number:

Histogram Event Old

REF_M_12271_histo.nxs
REF_M_12272_histo.nxs
REF_M_12273_histo.nxs
REF_M_12274_histo.nxs
REF_M_12275_histo.nxs
REF_M_12276_histo.nxs
REF_M_12277_histo.nxs
REF_M_12278_histo.nxs
REF_M_12279_histo.nxs
REF_M_12280_histo.nxs
REF_M_12281_histo.nxs
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REF_M_12297_histo.nxs
REF_M_12298_histo.nxs
REF_M_12299_histo.nxs

Reload Active File | Load Live Data

Reflectivity Extraction (Basic)

	Position	Width
Y	142.0	54.0
X	159.6	9.0
BG X	40.1	56.7
Scale 10^		1.147
Cut Pts	5	32

Reflectivity Extraction (Advanced)

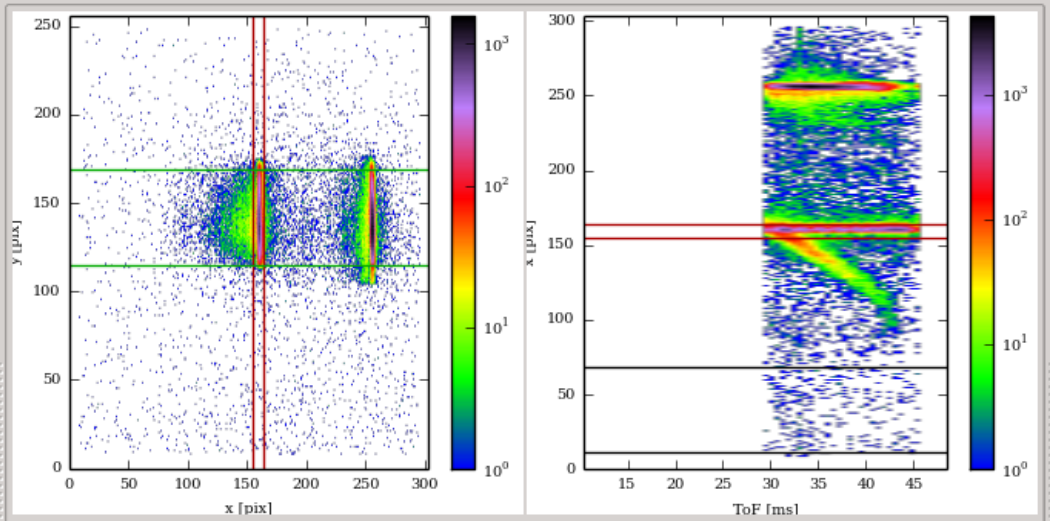
Peak Finder Algorithm

Plot Options

Colorbars default
Log Colorscale Log Y for lines
Hide Empty X-λ Maps
Norm. X-ToF/λ 2θ-φ Maps

Overview | X-Y | X-ToF | OffSpec Preview | GISANS Preview | DAS Logs | Compare

12290 (2012_2_4a_SCI) Type: Polarization Analysis Current State: ++



Direct Pixel	226.0	λ	7.00 (5.50-8.50) Å
DANGLE	5.000°	Proton Charge	1.887e+12
DANGLE0	4.500°	SANGLE	0.762°
		SANGLE-calc	0.772°

Counting Time	13579 s
Total Counts	2.2354e+05
Count Rate	16.5 cps
Counts ROI	8.001e+04

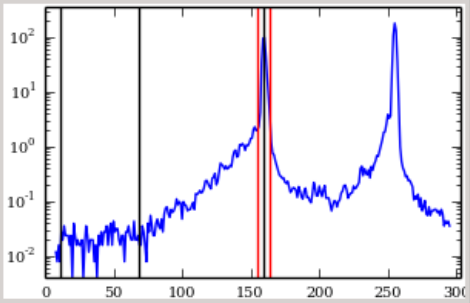
Direct Beam Runs: 12287,12288,12289 ++ -- +- -+

Data | Direct Beam

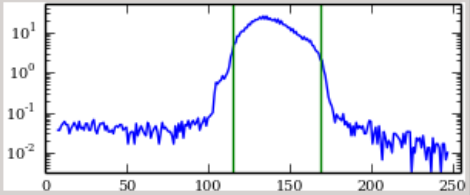
Run No.	I0	NL	NR	x0	xw	y0	yw	bg0	bgw	DPix	TTH	Dir. Run
12290	14.7231	6	33	159.6	9.0	142.0	54.0	40.1	56.7	226.0	0.5005	12287
12291	14.7231	20	19	159.6	9.0	142.0	54.0	40.1	56.7	226.0	0.5005	12288
12292	14.0281	40	3	159.6	9.0	142.0	54.0	40.1	56.7	226.0	0.5005	12289
12293	14.0281	41	2	162.6	9.0	142.0	54.0	40.1	56.7	226.0	2.0016	12289

Reduce... | Quick-Reduce (use last options)

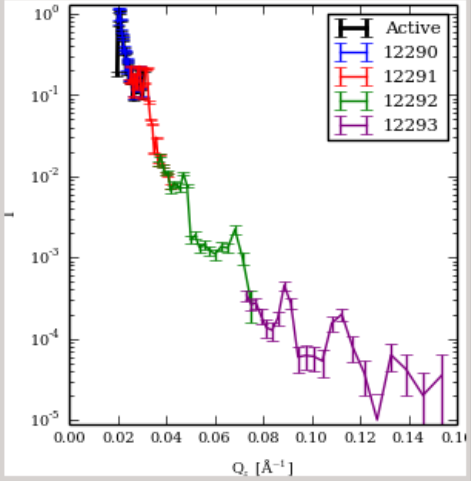
X-Projection



Y-Projection



Reflectivity



x=34.6198 y=34.6198 Cache Size: 24.4MB Empty Cache 100%

Requirements for instrument control

In addition to most neutron beamlines, typical challenges include:

- **LIVE feedback via color plots with log- and lin-scale**
  - **X-Y-I and X/Y-ToF-I are bare minimum**
- **Precise positioning of various components**
  - **Linear scans motor vs. ROI for position optimizations**
  - **Measurement of peak characteristics (position, size etc.)**
  - **Comparison of scans**
- **Concentrated high count rates on small detector area**
- **Similar user experiment planning**
  - **One or more reference measurements (direct beam, special sample)**
  - **One set of angle positions repeated for various samples/external parameters**
  - **Selection of slit parameters for specific resolution**

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Thank you for your attention!