

SANS RESOLUTION:



“Numerical evaluation, convolution and recombination of SANS instrument resolution using real-shape kernels”



Charles Dewhurst

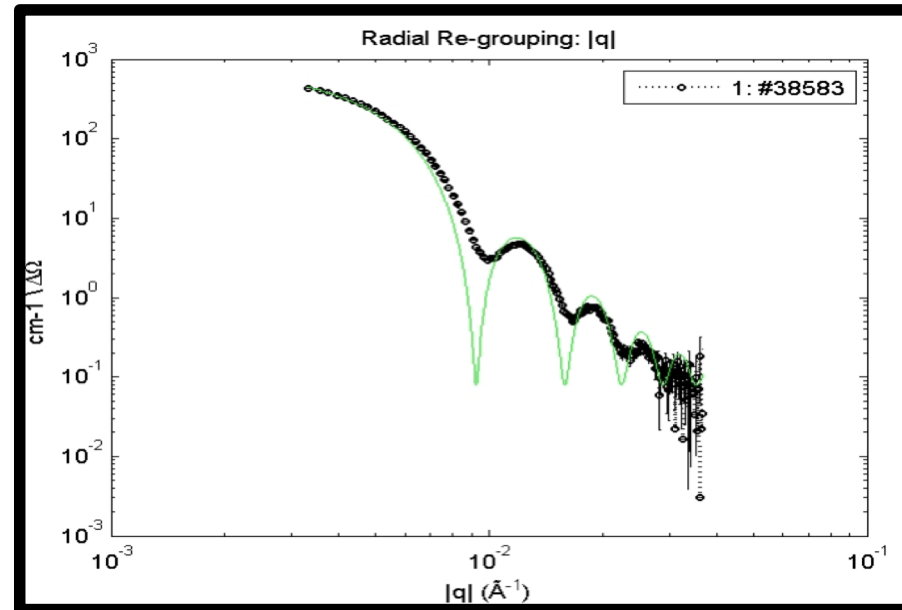
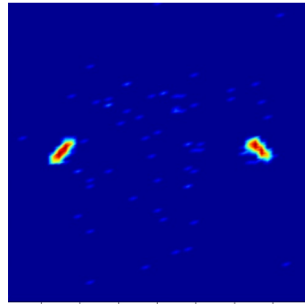
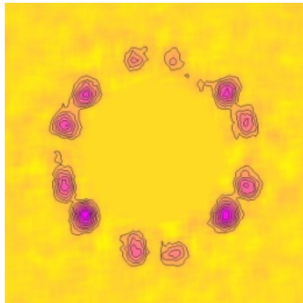
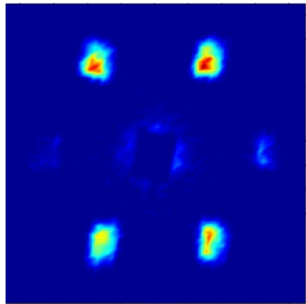
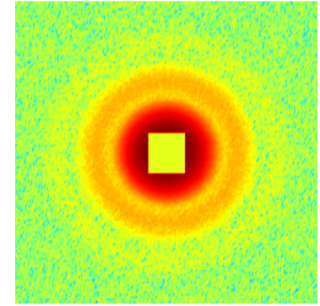
*Institut Laue-Langevin
Grenoble*

SANS resolution is by no means perfect!

- Accurate consideration of the instrument resolution in data treatment and model fitting is vital to obtain accurate structural parameters

e.g.

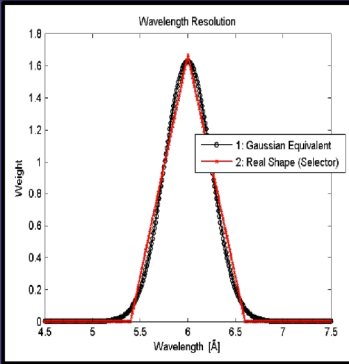
- Particle size, shape and correlations, e.g. soft-matter
- Highly ordered structures, e.g. vortex lattice, gratings, nano-structures
- Yes, even for low resolution structures, e.g. 'hairy' biological structures



The 'Classic' approach:

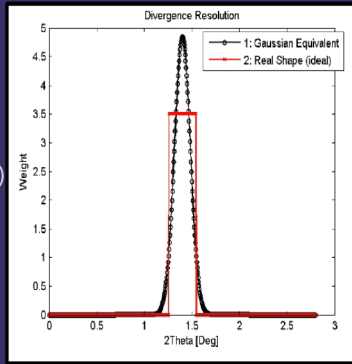
- Assume resolution components to be Gaussian \rightarrow simple analytical mathematics
- This actually works quite well – but can it be improved?

Wavelength: $\delta\lambda$



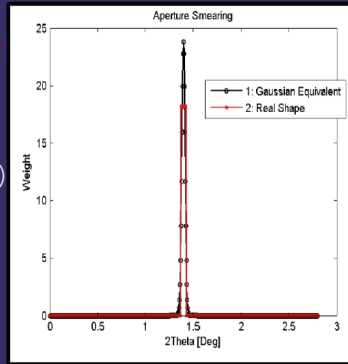
Gaussian

Divergence: $\delta\theta$



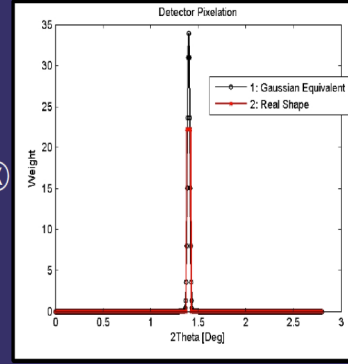
Gaussian

Aperture Smearing



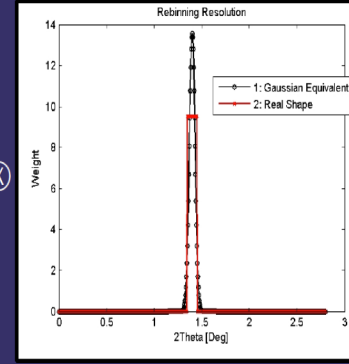
Gaussian

Detector Pixelation



Gaussian

Re-binning



Gaussian

⊗

⊗

⊗

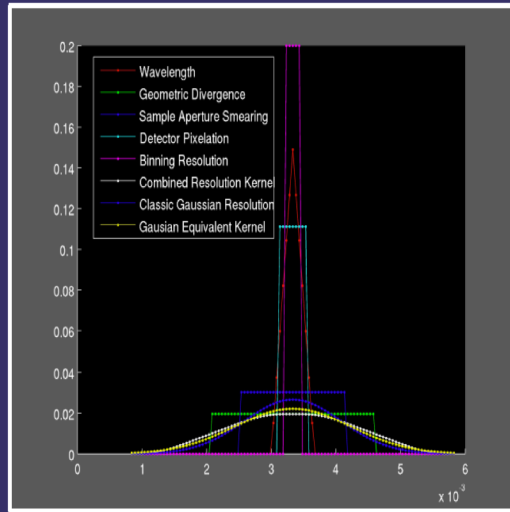
⊗

=

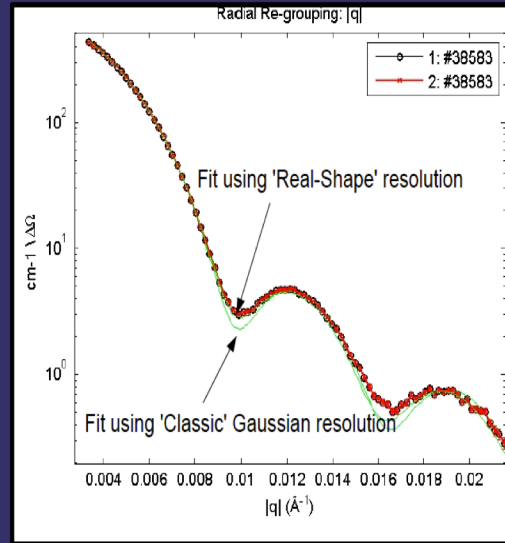
$$\sigma_q^2 = \sigma_{q-\lambda}^2 + \sigma_{q-\theta}^2 + \sigma_{q-\text{aperture}}^2 + \sigma_{q-\text{pixel}}^2 + \sigma_{q-\text{binning}}^2 + \dots \text{etc.}$$

Numerical approach:

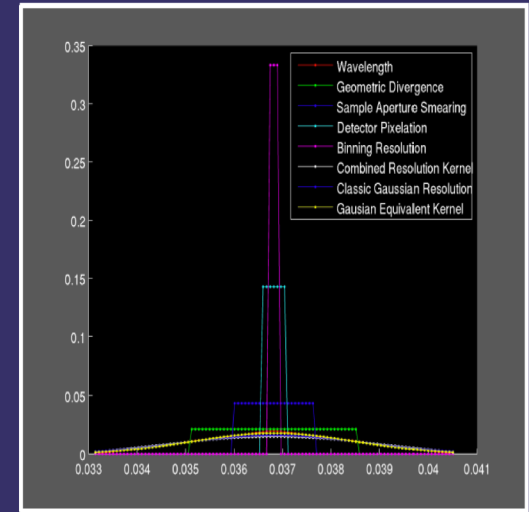
- Use the 'Real-Shape' kernels of the individual resolution components and numerically perform the convolution
- Better representation of the true instrument resolution – but more computationally intensive



Low-q resolution

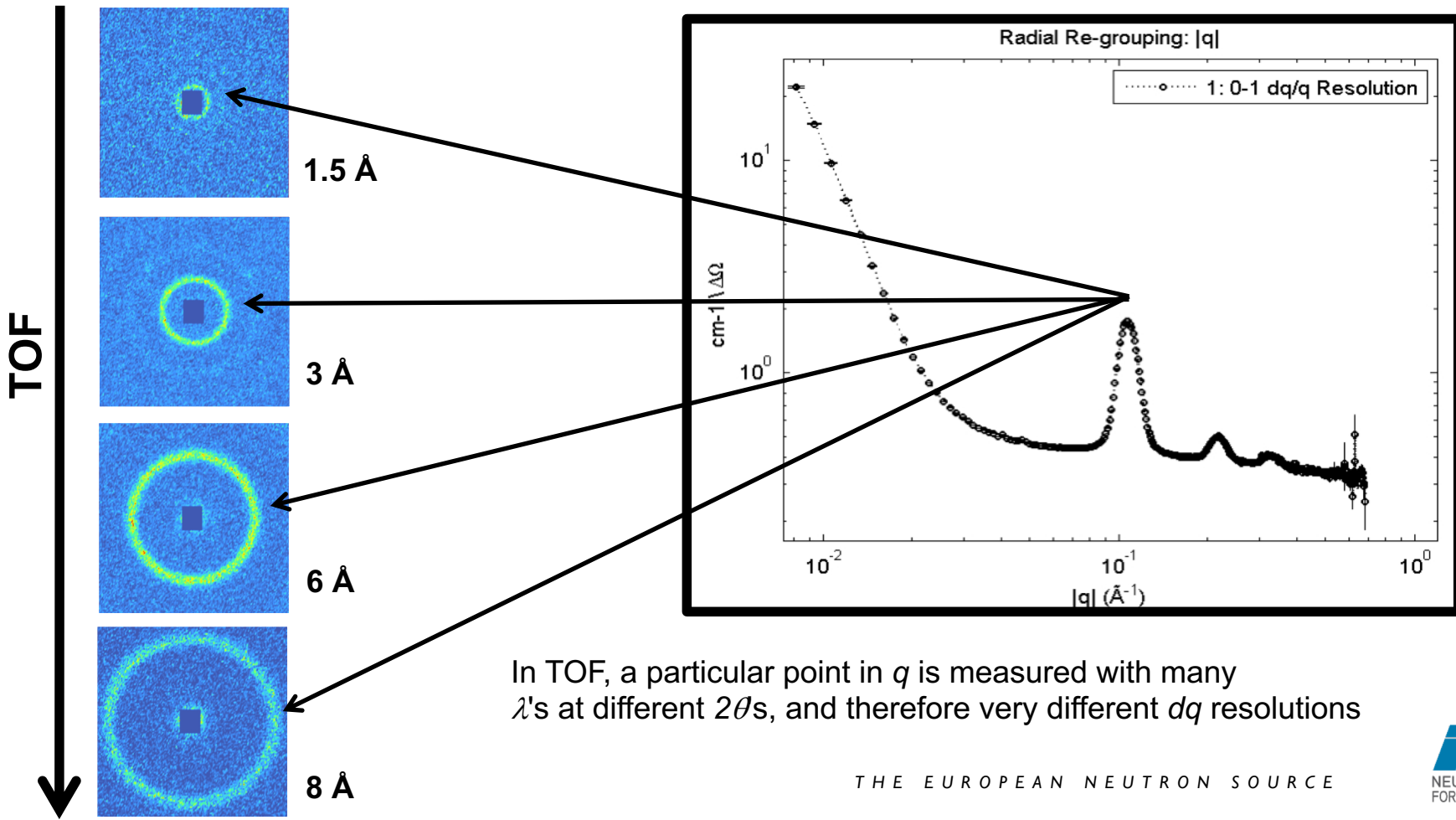


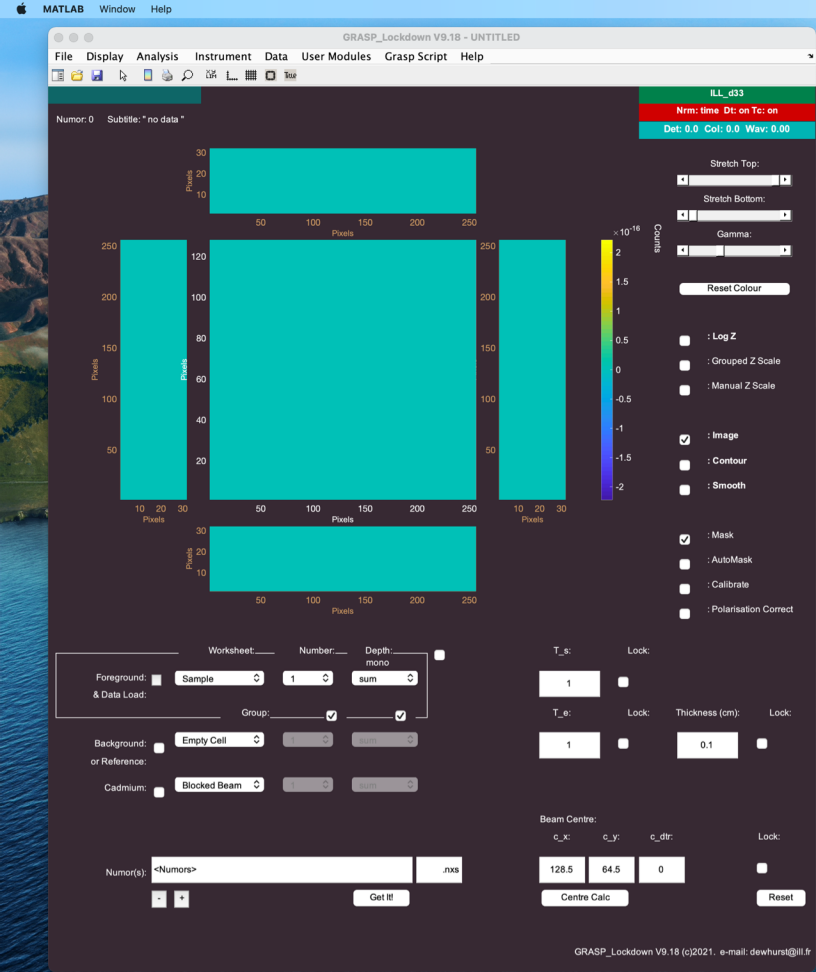
A. Rennie – PS4 latex, D33



High q resolution

Regrouping of time-of-flight SANS data





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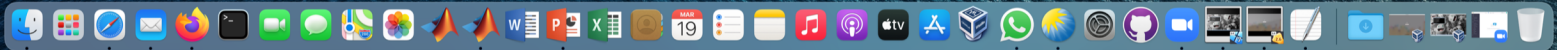
```

Loading Grasp Configuration from grasp.ini
Building Instrument List
Loading Instrument Configuration from instrument_ini/ILL_d11.ini
Loading Instrument Configuration from instrument_ini/ILL_d11_legacy128.ini
Loading Instrument Configuration from instrument_ini/ILL_d11_legacy64.ini
Loading Instrument Configuration from instrument_ini/ILL_d11_plus.ini
Loading Instrument Configuration from instrument_ini/ILL_d22.ini
Loading Instrument Configuration from instrument_ini/ILL_d22_20.ini
Loading Instrument Configuration from instrument_ini/ILL_d22_legacy.ini
Loading Instrument Configuration from instrument_ini/ILL_d22_saxs.ini
Loading Instrument Configuration from instrument_ini/ILL_d33.ini
Loading Instrument Configuration from instrument_ini/ALS_B1202.ini
Loading Instrument Configuration from instrument_ini/ANS10_Quokka.ini
Loading Instrument Configuration from instrument_ini/FRM2_KW51.ini
Loading Instrument Configuration from instrument_ini/FRM2_KW52.ini
Loading Instrument Configuration from instrument_ini/FRM2_KW53.ini
Loading Instrument Configuration from instrument_ini/FRM2_SANS1.ini
Loading Instrument Configuration from instrument_ini/LLB_PA20.ini
Loading Instrument Configuration from instrument_ini/LLB_paxy.ini
Loading Instrument Configuration from instrument_ini/LLB_tpa.ini
Loading Instrument Configuration from instrument_ini/NCNR_ng3.ini
Loading Instrument Configuration from instrument_ini/NCNR_ng7.ini
Loading Instrument Configuration from instrument_ini/NCNR_ngNexus.ini
Loading Instrument Configuration from instrument_ini/ORNL_cp2.ini
Loading Instrument Configuration from instrument_ini/SINQ_SANS_I.ini
Loading Instrument Configuration from instrument_ini/SINQ_SANS_II.ini
No handle for Exploration.ZoomIn
No handle for Exploration.ZoomOut
No handle for Exploration.Pan
Initialising Data Arrays
Looking for Instrument Detector Mask: instrument_ini/det_mask/detector_mask_det1_ILL_d33.mat
Loading Default Instrument Mask for Detector: 1 : instrument_ini/det_mask/detector_mask_det1_ILL_d33.mat
Looking for Instrument Detector Mask: instrument_ini/det_mask/detector_mask_det2_ILL_d33.mat
Loading Default Instrument Mask for Detector: 2 : instrument_ini/det_mask/detector_mask_det2_ILL_d33.mat
Looking for Instrument Detector Mask: instrument_ini/det_mask/detector_mask_det3_ILL_d33.mat
Loading Default Instrument Mask for Detector: 3 : instrument_ini/det_mask/detector_mask_det3_ILL_d33.mat
Looking for Instrument Detector Mask: instrument_ini/det_mask/detector_mask_det4_ILL_d33.mat
Loading Default Instrument Mask for Detector: 4 : instrument_ini/det_mask/detector_mask_det4_ILL_d33.mat
Looking for Instrument Detector Mask: instrument_ini/det_mask/detector_mask_det5_ILL_d33.mat
Loading Default Instrument Mask for Detector: 5 : instrument_ini/det_mask/detector_mask_det5_ILL_d33.mat
Looking for Detector Efficiency Map: instrument_ini/det_efficiency/detector_efficiency_det1_ILL_d33.mat
Loading Default Detector Efficiency Map for Detector: 1 : instrument_ini/det_efficiency/detector_efficiency_det1_ILL_d33.mat
Looking for Detector Efficiency Map: instrument_ini/det_efficiency/detector_efficiency_det2_ILL_d33.mat
Loading Default Detector Efficiency Map for Detector: 2 : instrument_ini/det_efficiency/detector_efficiency_det2_ILL_d33.mat
Looking for Detector Efficiency Map: instrument_ini/det_efficiency/detector_efficiency_det3_ILL_d33.mat
Loading Default Detector Efficiency Map for Detector: 3 : instrument_ini/det_efficiency/detector_efficiency_det3_ILL_d33.mat
Looking for Detector Efficiency Map: instrument_ini/det_efficiency/detector_efficiency_det4_ILL_d33.mat
Loading Default Detector Efficiency Map for Detector: 4 : instrument_ini/det_efficiency/detector_efficiency_det4_ILL_d33.mat
Looking for Detector Efficiency Maps: instrument_ini/det_efficiency/detector_efficiency_det5_ILL_d33.mat
Loading Default Detector Efficiency Map for Detector: 5 : instrument_ini/det_efficiency/detector_efficiency_det5_ILL_d33.mat
Attempted divide by zero using this data normalisation scheme 'time'
resetting divider = 1 in normalize_data.m

**** Params are empty ****

**** Resolution Components: ****

f >>
  
```



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File Display Analysis Instrument Data User Modules Grasp_script Help

Not over active figure (Z)

Numor: 0 Subtitle: "no data"

ILL_d22_2D
 Nm: mon Dt on Tr: on
 Det: 6.0 Col: 0.0 Wav: 0.00

Stretch Top:
 Stretch Bottom:
 Gamma:
 Reset Colour

: Log Z
 : Grouped Z Scale
 : Manual Z Scale
 : Image
 : Contour
 : Smooth
 : Mask
 : AutoMask
 : Calibrate
 : Polarisation Correct

Worksheet: _____ Number: _____ Depth: _____
 mono

Foreground:
 & Data Load:

Group:

Background:
 or Reference:

Cadmium:

Beam Centre:
 c_x: 48.8 c_y: 122.7 c_dtr: 0 c_dan: 0
 Lock:

Numor(s): .nxs
 Get It! Centre Calc Reset

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Loading Instrument Configuration from instrument_ini/det_mask/det1_ILL_d33.mat
 Loading Instrument Configuration from instrument_ini/NCNR_ng3.ini
 Loading Instrument Configuration from instrument_ini/NCNR_ng7.ini
 Loading Instrument Configuration from instrument_ini/NCNR_ngNexus.ini
 Loading Instrument Configuration from instrument_ini/ORNL_cg2.ini
 Loading Instrument Configuration from instrument_ini/SINO_SANS_I.ini
 Loading Instrument Configuration from instrument_ini/SINO_SANS_II.ini
 No handle for Exploration.ZoomIn
 No handle for Exploration.ZoomOut
 No handle for Exploration.Pan
 Initialising Data Arrays
 Looking for Instrument Detector Mask: instrument_ini/det_mask/detector_mask_det1_ILL_d33.mat
 Loading Default Instrument Mask for Detector: 1 : instrument_ini/det_mask/detector_mask_det1_ILL_d33.mat
 Looking for Instrument Detector Mask: instrument_ini/det_mask/detector_mask_det2_ILL_d33.mat
 Loading Default Instrument Mask for Detector: 2 : instrument_ini/det_mask/detector_mask_det2_ILL_d33.mat
 Looking for Instrument Detector Mask: instrument_ini/det_mask/detector_mask_det3_ILL_d33.mat
 Loading Default Instrument Mask for Detector: 3 : instrument_ini/det_mask/detector_mask_det3_ILL_d33.mat
 Looking for Instrument Detector Mask: instrument_ini/det_mask/detector_mask_det4_ILL_d33.mat
 Loading Default Instrument Mask for Detector: 4 : instrument_ini/det_mask/detector_mask_det4_ILL_d33.mat
 Looking for Instrument Detector Mask: instrument_ini/det_mask/detector_mask_det5_ILL_d33.mat
 Loading Default Instrument Mask for Detector: 5 : instrument_ini/det_mask/detector_mask_det5_ILL_d33.mat
 Looking for Detector Efficiency Map: instrument_ini/det_efficiency/detector_efficiency_det1_ILL_d33.mat
 Loading Default Detector Efficiency Map for Detector: 1 : instrument_ini/det_efficiency/detector_efficiency_det1_ILL_d33.mat
 Looking for Detector Efficiency Map: instrument_ini/det_efficiency/detector_efficiency_det2_ILL_d33.mat
 Loading Default Detector Efficiency Map for Detector: 2 : instrument_ini/det_efficiency/detector_efficiency_det2_ILL_d33.mat
 Looking for Detector Efficiency Map: instrument_ini/det_efficiency/detector_efficiency_det3_ILL_d33.mat
 Loading Default Detector Efficiency Map for Detector: 3 : instrument_ini/det_efficiency/detector_efficiency_det3_ILL_d33.mat
 Looking for Detector Efficiency Map: instrument_ini/det_efficiency/detector_efficiency_det4_ILL_d33.mat
 Loading Default Detector Efficiency Map for Detector: 4 : instrument_ini/det_efficiency/detector_efficiency_det4_ILL_d33.mat
 Looking for Detector Efficiency Map: instrument_ini/det_efficiency/detector_efficiency_det5_ILL_d33.mat
 Loading Default Detector Efficiency Map for Detector: 5 : instrument_ini/det_efficiency/detector_efficiency_det5_ILL_d33.mat
 Attempted divide by zero using this data normalisation scheme 'time'
 resetting divider = 1 in normalize_data.m

**** Params are empty ****

**** Resolution Components: ****

Initialising Data Arrays
 Looking for Instrument Detector Mask: instrument_ini/det_mask/ill_d22_mask.mat
 Loading Default Instrument Mask for Detector: 1 : instrument_ini/det_mask/ill_d22_mask.mat
 Looking for Instrument Detector Mask: instrument_ini/det_mask/
 WARNING: No Default Instrument Mask Found for Detector: 2
 Looking for Detector Efficiency Map: instrument_ini/det_efficiency/detector_efficiency_det1_ILL_d22_2D.mat
 Loading Default Detector Efficiency Map for Detector: 1 : instrument_ini/det_efficiency/detector_efficiency_det1_ILL_d22_2D.mat
 Looking for Detector Efficiency Maps: instrument_ini/det_efficiency/detector_efficiency_det2_ILL_d22_2D.mat
 Loading Default Detector Efficiency Map for Detector: 2 : instrument_ini/det_efficiency/detector_efficiency_det2_ILL_d22_2D.mat
 Attempted divide by zero using this data normalisation scheme 'mon'
 resetting divider = 1 in normalize_data.m

**** Params are empty ****

**** Resolution Components: ****

f >>

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File Display Analysis Instrument Data User Modules Grasp Script Help

Instrument
Display Instrument Configuration File
QSetup
SANS Instrument Model

ILL_d22_2D
Nm: mon On Te: on
Det: 6.0 Col: 0.0 Wav: 0.00

Stretch Top: [x]
Stretch Bottom: [x]
Gamma: [x]
Reset Colour

: Log Z
 : Grouped Z Scale
 : Manual Z Scale
 : Image
 : Contour
 : Smooth
 : Mask
 : AutoMask
 : Calibrate
 : Polarisation Correct

Worksheet: Number: Depth: mono
Foreground: Sample 1 sum
Background: Empty Cell
Cadmium: Blocked Beam

Beam Centre:
c_x: 48.8 c_y: 122.7 c_dtr: 0 c_dan: 0
Centre Calc

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Looking for Instrument Mask for Detector: 1: instrument_ini/det_mask/detector_mask_det1_ILL_d33.mat
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Loading Instrument Configuration from instrument_ini/ORNL_cg2.ini
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No handle for Exploration.Pan
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Looking for Instrument Detector Mask: instrument_ini/det_mask/detector_mask_det4_ILL_d33.mat
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Looking for Detector Efficiency Map: instrument_ini/det_efficiency/detector_efficiency_det4_ILL_d33.mat
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Loading Default Detector Efficiency Map for Detector: 5: instrument_ini/det_efficiency/detector_efficiency_det5_ILL_d33.mat
Attempted divide by zero using this data normalisation scheme 'time'
resetting divider = 1 in normalize_data.m

**** Params are empty ****

**** Resolution Components: ****

Initialising Data Arrays
Looking for Instrument Detector Mask: instrument_ini/det_mask/ill_d22_mask.mat
Loading Default Instrument Mask for Detector: 1: instrument_ini/det_mask/ill_d22_mask.mat
Looking for Instrument Detector Mask: instrument_ini/det_mask/
WARNING: No Default Instrument Mask Found for Detector: 2
Looking for Detector Efficiency Map: instrument_ini/det_efficiency/detector_efficiency_det1_ILL_d22_2D.mat
Loading Default Detector Efficiency Map for Detector: 1: instrument_ini/det_efficiency/detector_efficiency_det1_ILL_d22_2D.mat
Looking for Detector Efficiency Map: instrument_ini/det_efficiency/detector_efficiency_det2_ILL_d22_2D.mat
Loading Default Detector Efficiency Map for Detector: 2: instrument_ini/det_efficiency/detector_efficiency_det2_ILL_d22_2D.mat
Attempted divide by zero using this data normalisation scheme 'mon'
resetting divider = 1 in normalize_data.m

**** Params are empty ****

**** Resolution Components: ****
```


File Edit View Insert Tools Desktop Window Help

Mono Sample aperture: 10 [mm e]

Selector: Tri [] or Square [x] 6 10

Collimation Length (m) Bc:
 Diaphragm By:

Simulation: Subfile:

M.C. Iterations (pixel)
 Measurement Time (s)
 Sample Thickness (cm)

Add Poissonian Noise:
 Divergence Smearing:
 Delta_Lambda Smearing:
 Det Efficiency:
 Allow Inelasticity:

Scattering Model:

Scattering Model:
 Radius [Å]:
 Poly (%FWHM):
 Contrast [A-2]:
 Scale:
 Background [cm-1]:
 Background Model:
 Blocked Model:

Flux [n/cm2/s]
 Sample Transmission:

Log:

Model Scattering Data

Counts 10^0
 10^1
 10^2
 10^3
 10^4
 10^5
 10^6
 10^7
 10^8
 10^9

10^{-1} 10^0 10^1
 $|Q| \text{ \AA}^{-1}$

None

et1_I
et2_I
et3_I
et4_I
et5_I

et1_I
et2_I

File Edit View Insert Tools Desktop Window Help

Mono Sample aperture: 10 [mm e]

Selector: T₁ [] or Square [x] 6 10

Collimation Length (m) 5.6 Bc: 0

Diaphragm 40 x 55 [mm] By: 0

4

Simulation:

Auto - Off Calculate

M.C. Iterations (pixel) 10

Measurement Time (s) 600

Sample Thickness(cm): 0.1

Add Poissonian Noise:

Divergence Smearing:

Delta_Lambda Smearing:

Det Efficiency:

Allow Inelasticity:

Scattering Model:

Subfile: Sample

Scattering Model: Sphere

Radius [Å]: 60

Poly (%FWHM): 0

Contrast [A-2]: 6e-06

Scale: 0.01

Background [cm-1]: 0

Background Model: None

Blocked Model: None

Flux [n/cm²/s] 2.91e+07

Sample Transmission: 0.98843

Log: Detector_image

Model Scattering Data

Counts

$|Q| \text{ \AA}^{-1}$

None Sligger

File Edit View Insert Tools Desktop Window Help

Mono Selector: Tri [] or Square [x] 6 10 Sample aperture: 10 [mm e]

Collimation Length (m) 5.6 Bc: 0
Diaphragm 40 x 55 [mm] By: 0

Simulation: Scatterer Model: Subtitle: Sample

Auto: Off Calculate M.C. Iterations (pixel) 10
Measurement Time (s) 600
Sample Thickness (cm) 0.1
Add Poissonian Noise:
Divergence Smearing:
Delta_Lambda Smearing:
Det Efficiency:
Allow Inelasticity:

Scattering Model: Sphere
Radius [Å]: 60
Poly (%FWHM): 0
Contrast [A-2]: 6e-08
Scale: 0.01
Background [cm-1]: 0
Background Model: None
Blocked Model: None

Flux [n/cm²/s] 2.91e+07
Sample Transmission: 0.98843
Log: Direct_Beam

Model Scattering Data

Counts |Q| Å⁻¹

None Sligger

File Edit View Insert Tools Desktop Window Help

Mono Selector: Tri [] or Square [x] 6 10 Sample aperture: 10 [mm e]

Collimation Length (m) 17.6 Bc: 0
Diaphragm 40 x 55 [mm] By: 0

Simulation: Scatterer Model: Subtitle: Sample

Auto: Off Calculate M.C. Iterations (pixel) 10
Measurement Time (s) 600
Sample Thickness (cm) 0.1
Add Poissonian Noise:
Divergence Smearing:
Delta_Lambda Smearing:
Det Efficiency:
Allow Inelasticity:

Scatterer Model: Sphere
Radius [Å] 60
Poly [%FWHM] 0
Contrast [A-2] 6e-06
Scale 0.01
Background [cm-1] 0
Background Model: None
Blocked Model: None

Flux [n/cm2/s] 2.95e+06
Sample Transmission: 0.98843

Log: Detector_image

Model Scattering Data

Counts |Q| Å⁻¹ 10⁰ 10¹ 10² 10³ 10⁴ 10⁵ 10⁶ 10⁷ 10⁸ 10⁹

Note: Sligger

File Edit View Insert Tools Desktop Window Help

Mono Selector: Tri [] or Square [x] 6 10 Sample aperture: 10 [mm e]

Collimation Length (m) 2 Bc: 0
Diaphragm 40 x 55 [mm] By: 0

Simulation:

Auto: Off Calculate

M.C. Iterations (pixel) 10
Measurement Time (s) 600
Sample Thickness (cm) 0.1
Add Poissonian Noise:
Divergence Smearing:
Delta_Lambda Smearing:
Det Efficiency:
Allow Inelasticity:

Scattering Model:

Subtils: Sample
Scattering Model: Sphere
Radius [Å]: 60
Poly [%FWHM]: 0
Contrast [A-2]: 6e-08
Scale: 0.01
Background [cm-1]: 0
Background Model: None
Blocked Model: None

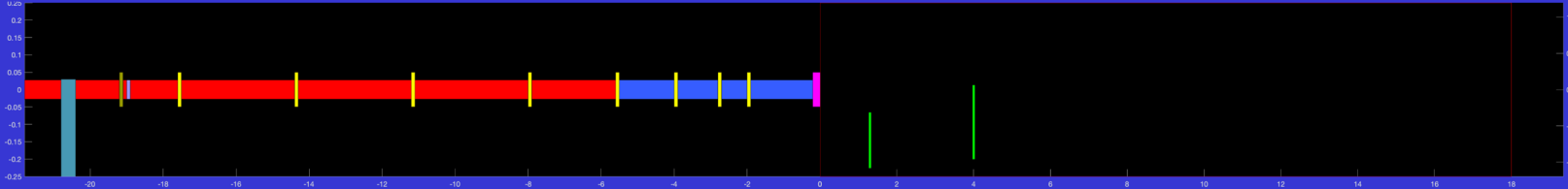
Flux [n/cm²/s] 2.25e+08
Sample Transmission: 0.98843

Log: Detector_image

Model Scattering Data

File Edit View Insert Tools Desktop Window Help

Mono Selector: Tri [] or Square [x] 6 3 Sample aperture: 10 [mm e]



Collimation Length (m) 5.6 Bc: 0
Diaphragm 40 x 55 [mm] By: 0

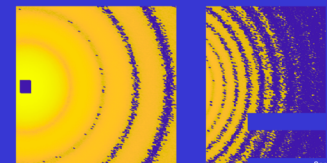
Simulation: Scattering Model:

Auto: Off Calculate

M.C. Iterations (pixel) 10
Measurement Time (s) 600
Sample Thickness (cm) 0.1

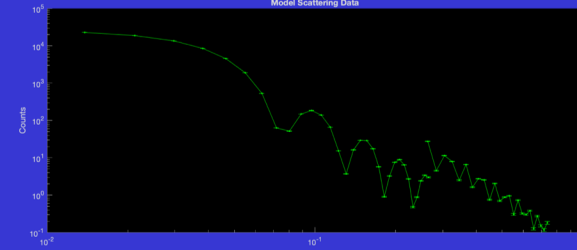
Add Poissonian Noise:
Divergence Smearing:
Delta_Lambda Smearing:
Det. Efficiency:
Allow Inelasticity:

Subfile: Sample
Scattering Model: Sphere
Radius [Å]: 60
Poly (%FWHM): 0
Contrast [A-2]: 6e-06
Scale: 0.01
Background [cm-1]: 0
Background Model: None
Blocked Model: None



Flux [n/cm2/s] 8.73e+06
Sample Transmission: 0.98843

Log: Detector_image

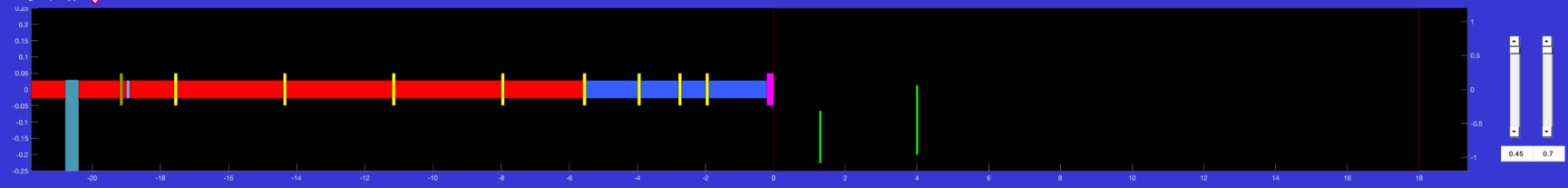


Model Scattering Data

Counts |Q| Å⁻¹

Note: Sligger

Mono Selector: Tri [] or Square [x] 6 20 Sample aperture: 10 [mm e]



Collimation Length (m) 5.6 Bc: 0
Diaphragm 40 x 55 [mm] By: 0

4

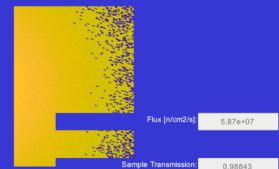
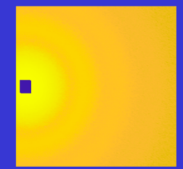
Simulation:

Auto: Off Calculate
M.C. Iterations (pixel) 10
Measurement Time (s) 600
Sample Thickness (cm) 0.1
Add Poissonian Noise:
Divergence Smearing:
Delta_Lambda Smearing:
Det Efficiency:
Allow Inelasticity:

Scattering Model:

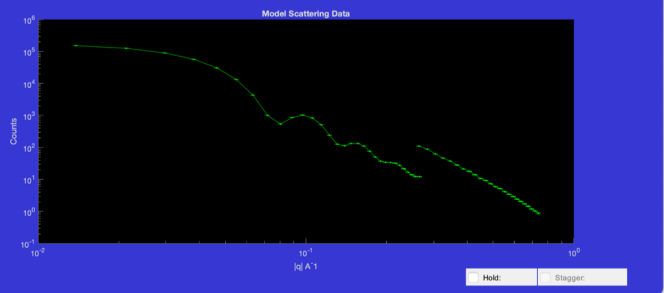
Subtils: Sample
Scattering Model: Sphere
Radius [A]: 60
Poly (%FWHM): 0
Contrast [A-2]: 6e-06
Scale: 0.01
Background [cm-1]: 0
Background Model: None
Blocked Model: None

0
0
0



Flux [n/cm2/s] 5.87e+07
Sample Transmission: 0.98843

Log: Detector_image



None Sligger

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File Display Analysis Instrument Data User Modules Grasp Script Help

ILL_d22_2D
 Nrm: non Di: off Tc: on
 Det: 4.0 Col: 5.6 Wav: 6.00

Stretch Top: [dropdown]
 Stretch Bottom: [dropdown]
 Gamma: [dropdown]
 Reset Colour

Log Z [checkbox]
 Grouped Z Scale [checkbox]
 Manual Z Scale [checkbox]
 Image [checkbox] ✓
 Contour [checkbox]
 Smooth [checkbox]
 Mask [checkbox]
 AutoMask [checkbox] ✓
 Calibrate [checkbox] ✓
 Polarisation Correct [checkbox]

Worksheet: [dropdown] Number: [dropdown] Depth: [dropdown]
 mono

Foreground: Sample [dropdown] 1 [dropdown] 1 [dropdown]
 Background: Empty Cell [dropdown] 1 [dropdown] 1 [dropdown]
 or Reference:
 Cadmium: Blocked Beam [dropdown] 1 [dropdown] 1 [dropdown]

Beam Centre:
 c_x: 48.8 c_y: 122.7 c_ctr: 0 c_dan: 0 Lock: [checkbox]
 Centre Calc [button] Reset [button]

Numer: 1,3,5,7,9 [input] [dropdown] .msx [dropdown]
 Get III [button]

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Mask Editor

Point: 1 1 [input] [input] [button]

Lines: x1 [input] [input] [button]

Box: 2 14 112 143 [input] [input] [input] [input] [button]

Circle: 64 64 10 [input] [input] [input] [button]

Clear [button] Grab Centre [button]

Sketch [button]

Averaging

Radial fract. res. bins [dq/dq]: 5 [input]

Radial bins [pixels]: 1 [input]

Angle Bin [degs]: 1 [input]

Single Depth TOF Use Sector Mask: [checkbox]
 Use Strip Mask: [checkbox]

Colors based on depth: [checkbox]
 Direct to File: [checkbox]

Pre-Av Sparse Data Filter: 0.001 [input] [button]
 Pre-Av Transmission Filter dT/T: 0.05 [input] [button]
 Pre-Av Resolution Filter dq/q: 0.5 [input] [button]
 Post-Av Stats Filter dII: 0.75 [input] [button]

Calibration Options

Detector Efficiency Correction: [checkbox] [dropdown]

Divide by Detector Efficiency Map: [checkbox] [dropdown]

Correct Relative Detector Efficiency: [checkbox]

Correct Detector Tube Parallax: [checkbox]

Calibration Method: None [radio] Direct Beam [radio] Water [radio]

Illuminated Sample % Thickness (cm): Angle (°):
 1 [input] 0.1 [input] [input]

Divide by Sample Volume: [checkbox] ✓
 Divide by Pixel Solid Angle: [checkbox] ✓
 Divide by Beam Flux (Counts / Sample Area): [checkbox] ✓

Beam Worksheet: Trans Empty ... [dropdown] 1 [input] 1 [input]

Beam ROI: X1 X2 Y1 Y2 Det:
 1 128 1 256 1 [input] [input] [input] [input] [input]
 Grab Coords [button]

HOME PLOTS APPS

Find Files Import Data Save Workspace Clear Workspace

FILE: /Users/chuck/Desktop/Dropbox/Matlab/grasp_m_lockdown

New to MATLAB? See resources for Getting Started.

```

Acquisition Time = 600 [s] Exposure Time = 600 [s]
Total Det Counts [Det:1] 103616057 Over 600secs (~172693 cps) : Relative Efficiency = 1
Total Det Counts [Det:2] 132459 Over 600secs (~221 cps) : Relative Efficiency = 1
Total Monitor Counts 600 Over 600secs (~1 cps)

***** Resolution Components: *****
Wavelength resolution d_lambda / lambda: 10 [%] FWHM of triangular shape
Effective source is Rectangular of dimensions: 40 (mm) x 55 (mm) at a distance of: 5.6 (m)
Sample aperture: assuming Circular 10 [mm] diameter
Detector 1 pixelation: x: 8 y: 4 [mm]
Detector 2 pixelation: x: 8 y: 4 [mm]

***** Numor Parameter Summary: *****
Loaded Numor(s) = 1,3,5,7,9 : Current = 1
User: "No Name"
Subtitle: "Sample"
Start: End:

Beam Parameters:
Wavelength 6(A), DeltaWav 10 (%)
Collimation 5.6 (m)
Attenuator: 0, Attenuation value: 1 : Auto-correction: on

Detectors:
Rear:
Det1: 4 [m] Detcalc: 4 [m]

***** Detector Efficiency Correction *****
DAN1 Offset: 0.25 [m] BY1: 0
DAN2 Offset: 0 [m] BY2: 0
DAN3 Offset: 0 [m] BY3: 0
DAN4 Offset: 0 [m] BY4: 0
DAN5 Offset: 0 [m] BY5: 0
DAN6 Offset: 0 [m] BY6: 0
DAN7 Offset: 0 [m] BY7: 0
DAN8 Offset: 0 [m] BY8: 0
DAN9 Offset: 0 [m] BY9: 0
DAN10 Offset: 0 [m] BY10: 0

N/A; T_sample = N/A
PS1 N/A [A] N/A [V] : PS2 N/A [A] N/A [V] : PS3 N/A [A] N/A [V]

600 [s] Exposure Time = 600 [s]
Det:1] 103616057 Over 600secs (~172693 cps) : Relative Efficiency = 1
Det:2] 132459 Over 600secs (~221 cps) : Relative Efficiency = 1
Monitor Counts 600 Over 600secs (~1 cps)

***** Resolution Components: *****
Wavelength resolution d_lambda / lambda: 10 [%] FWHM of triangular shape
Effective source is Rectangular of dimensions: 40 (mm) x 55 (mm) at a distance of: 5.6 (m)
Sample aperture: assuming Circular 10 [mm] diameter
Detector 1 pixelation: x: 8 y: 4 [mm]
Detector 2 pixelation: x: 8 y: 4 [mm]
  
```


GRASP_Lockdown V9.18 - UNTITLED

File Display Analysis Instrument Data User Modules Grasp Script Help

Not over active figure (Z)

Numor: 1 Subtitle: *Sample*

ILL_d22_2D
Nrm: mon Di: off Tc: on
Det: 4.0 Col: 5.6 Wav: 6.00

Stretch Top: [x]
Stretch Bottom: [x]
Gamma: [x]
Reset Colour

Log Z
Grouped Z Scale
Manual Z Scale

Image
Contour
Smooth

Mask
AutoMask
Calibrate
Polarisation Correct

Worksheet: _____ Number: _____ Depth: _____
mono

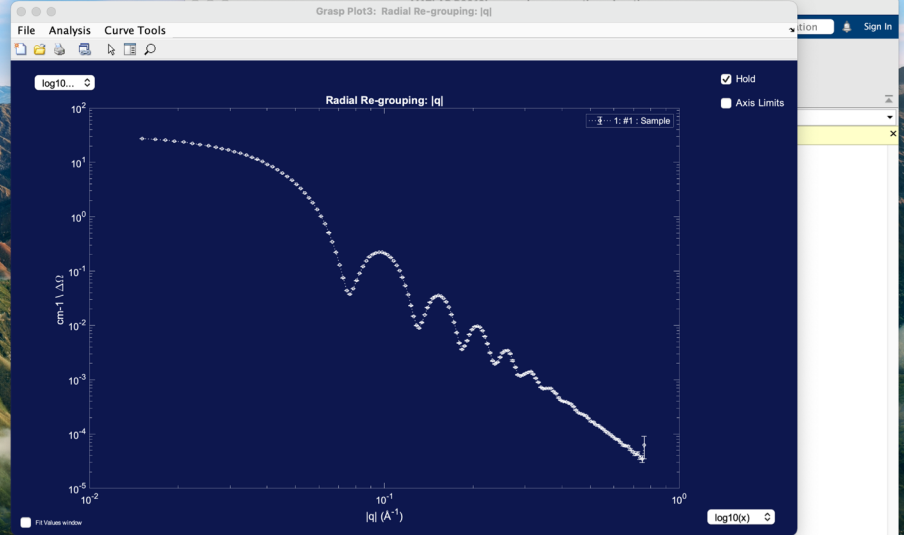
Foreground: Sample 1 1
Background: Empty Cell 1 1
Cadmium: Blocked Beam 1 1

T_s: Lock: 1
T_e: Lock: 1 Thickness (cm): 0.1 Lock:

Beam Centre:
c_x: 48.8 c_y: 122.7 c_ctr: 0 c_dan: 0 Lock:

Numor(s): 1,3,5,7,9 .nxs
Get III Reset

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Averaging

Radial fract. res. bins [dq/q]: 5
Radial bins [pixels]: 1
Angle Bin [degs]: 1

Single Depth TOF Use Sector Mask:
Use Strip Mask:

Colors based on depth:
Direct to File:

Pre-Av Sparse Data Filter: 0.001
Pre-Av Transmission Filter dT/T: 0.05
Pre-Av Resolution Filter dq/q: 0.5
Post-Av Stats Filter dII: 0.75

```

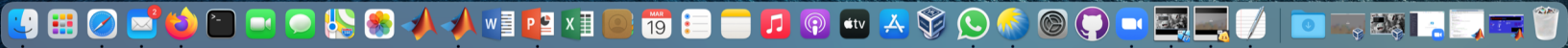
Averaging Current Display Data
Rebinning .....
Binning Version 'SPARSE'
.....done.... 0.013721[s]

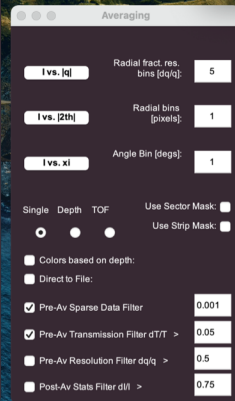
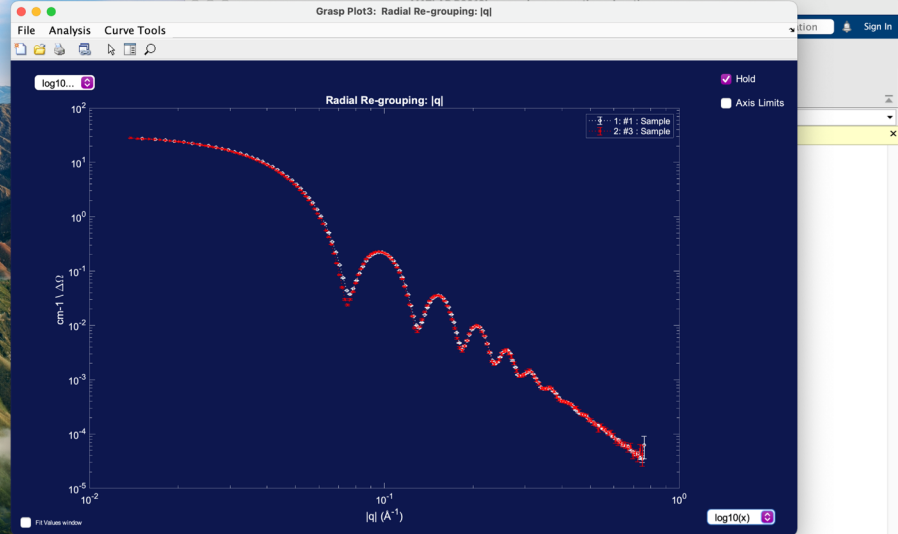
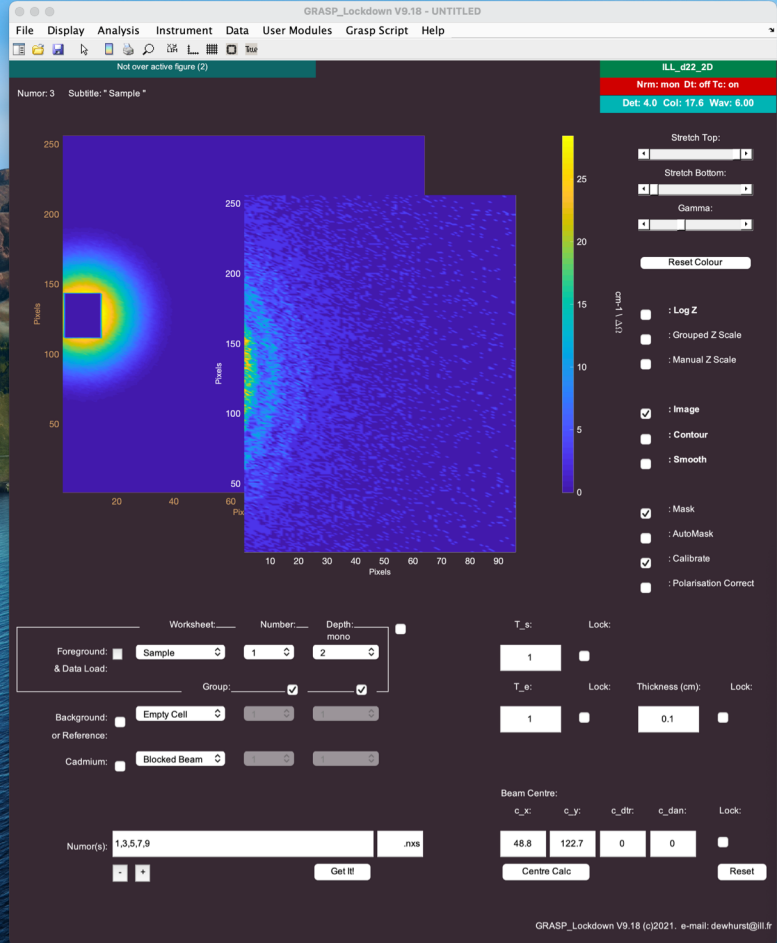
Building Real-Shape Resolution Kernel for I vs. Q data
Wavelength: Triangular (selector) Kernel
Divergence: Geometric Divergence tophat Kernel
Sample Aperture Smearing: Circular Kernel
Detector Pixelation Smearing: Top-Hat Kernel
Binning Resolution Smearing: Top-Hat Kernel

Using Real Shape Kernel (with Geometric Divergence )
Averaging Current Display Data
Rebinning .....
Binning Version 'SPARSE'
.....done.... 0.015536[s]

Building Real-Shape Resolution Kernel for I vs. Q data
Wavelength: Triangular (selector) Kernel
Divergence: Geometric Divergence tophat Kernel
Sample Aperture Smearing: Circular Kernel
Detector Pixelation Smearing: Top-Hat Kernel
Binning Resolution Smearing: Top-Hat Kernel

Using Real Shape Kernel (with Geometric Divergence )
f >>
    
```





Sample Environment:
T_set = N/A; T_reg = N/A; T_sample = N/A
Power Supplies : PS1 N/A [A] N/A [V] : PS2 N/A [A] N/A [V] : PS3 N/A [A] N/A [V]

Acquisition:
Acquisition Time = 600 [s] Exposure Time = 600 [s]
Total Det Counts [Det:1] 10467435 Over 600secs (~17446 cps) : Relative Efficiency = 1
Total Det Counts [Det:2] 13489 Over 600secs (~22 cps) : Relative Efficiency = 1
Total Monitor Counts 600 Over 600secs (~1 cps)

***** Resolution Components: *****
Wavelength resolution d_lambda / lambda: 10 [%] FWHM of triangular shape
Effective source is Rectangular of dimensions: 40 (mm) x 55 (mm) at a distance of: 17.6 (m)
Sample aperture: assuming Circular 10 [mm] diameter
Detector 1 pixelation: x: 8 y: 4 [mm]
Detector 2 pixelation: x: 8 y: 4 [mm]

Averaging Current Display Data
Rebinning

Binning Version 'SPARSE'
.....done.... 0.014605[s]

Building Real-Shape Resolution Kernel for I vs. Q data
Wavelength: Triangular (selector) Kernel
Divergence: Geometric Divergence tophat Kernel
Sample Aperture Smearing: Circular Kernel
Detector Pixelation Smearing: Top-Hat Kernel
Binning Resolution Smearing: Top-Hat Kernel

Using Real Shape Kernel (with Geometric Divergence)
f >>

GRASP_Lockdown V9.18 - UNTITLED

File Display Analysis Instrument Data User Modules Grasp Script Help

Not over active figure (Z)

ILL_d22_2D
Nrm: mon Di: off Tc: on
Det: 4.0 Col: 2.0 Wav: 6.00

Numor: 5 Subtitle: * Sample *

Stretch Top: [x]
Stretch Bottom: [x]
Gamma: [x]
Reset Colour

Log Z
Grouped Z Scale
Manual Z Scale

Image
Contour
Smooth

Mask
AutoMask
Calibrate
Polarisation Correct

Worksheet: _____ Number: _____ Depth: _____
mono

Foreground: Sample 1 3
Group: [x] [x]

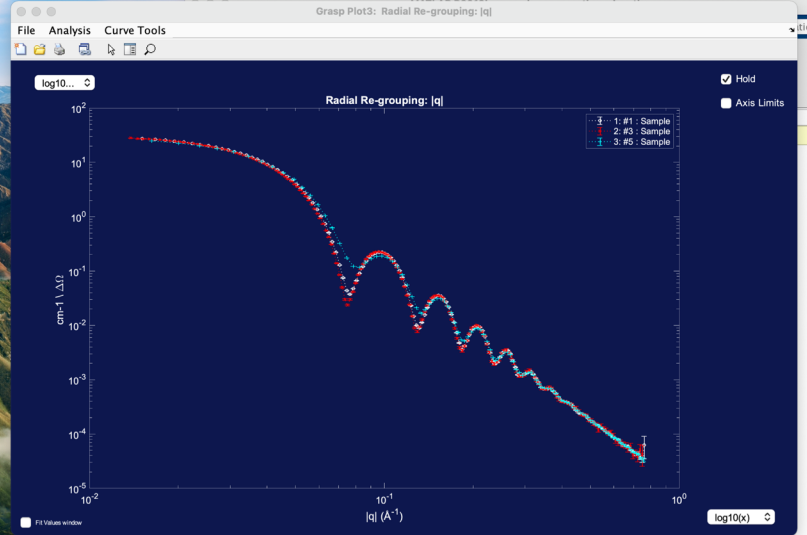
Background: Empty Cell 1 2
or Reference: Cadmium: Blocked Beam 1 2

Numor(s): 1,3,5,7,9 .nxs

T_s: Lock: 1
T_e: Lock: 1 Thickness (cm): 0.1 Lock:

Beam Centre: c_x: 48.8 c_y: 122.7 c_ctr: 0 c_dan: 0 Lock: Centre Calc Reset

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Averaging

Radial fract. res. bins [dq|q]: 5
I vs. [q]

Radial bins [pixels]: 1
I vs. [2θ]

Angle Bin [degs]: 1
I vs. x]

Single Depth TOF Use Sector Mask:
Use Strip Mask:

Colors based on depth:
Direct to File:

Pre-Av Sparse Data Filter: 0.001
Pre-Av Transmission Filter dT/T: 0.05
Pre-Av Resolution Filter dq/q: 0.5
Post-Av Stats Filter dI: 0.75

Sample Environment:
T_set = N/A; T_reg = N/A; T_sample = N/A
Power Supplies : PS1 N/A [A] N/A [V] : PS2 N/A [A] N/A [V] : PS3 N/A [A] N/A [V]

Acquisition:
Acquisition Time = 600 [s] Exposure Time = 600 [s]
Total Det Counts [Det:1] 1158354907 Over 600secs (~1930592 cps) : Relative Efficiency = 1
Total Det Counts [Det:2] 1043935 Over 600secs (~1740 cps) : Relative Efficiency = 1
Total Monitor Counts 600 Over 600secs (~1 cps)

***** Resolution Components: *****
Wavelength resolution d_lambda / lambda: 10 [%] FWHM of triangular shape
Effective source is Rectangular of dimensions: 40 (mm) x 55 (mm) at a distance of: 2 (m)
Sample aperture: assuming Circular 10 [mm] diameter
Detector 1 pixelation: x: 8 y: 4 [mm]
Detector 2 pixelation: x: 8 y: 4 [mm]

Averaging Current Display Data
Rebinning

Binning Version 'SPARSE'
.....done.... 0.014019[s]

Building Real-Shape Resolution Kernel for I vs. Q data
Wavelength: Triangular (selector) Kernel
Divergence: Geometric Divergence tophat Kernel
Sample Aperture Smearing: Circular Kernel
Detector Pixelation Smearing: Top-Hat Kernel
Binning Resolution Smearing: Top-Hat Kernel

Using Real Shape Kernel (with Geometric Divergence)
f >>

GRASP_Lockdown V9.18 - UNTITLED

File Display Analysis Instrument Data User Modules Grasp Script Help

Not over active figure (Z)

Numor: 7 Subtitle: * Sample *

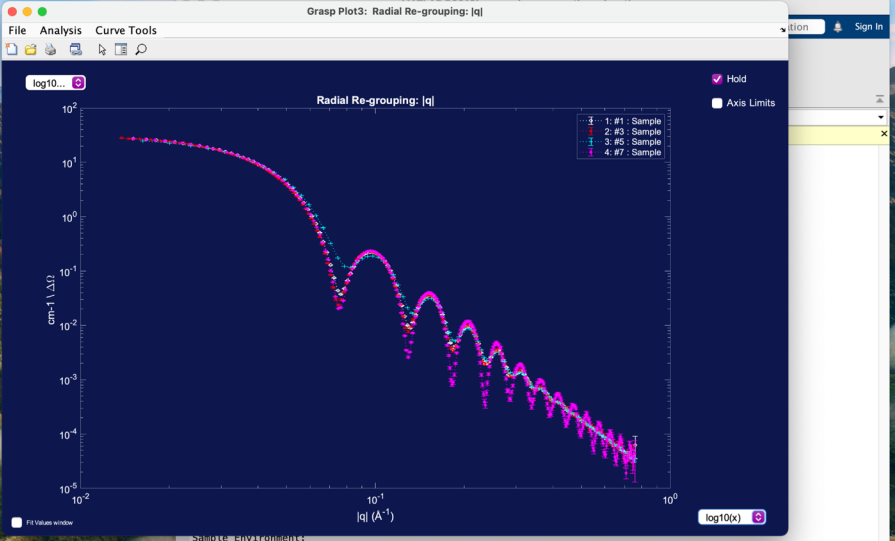
ILL_d22_2D
Nrm: mon Dt: off Tc: on
Det: 4.0 Col: 5.6 Wav: 6.00

Stretch Top: Stretch Bottom: Gamma:

: Log Z
 : Grouped Z Scale
 : Manual Z Scale
 : Image
 : Contour
 : Smooth
 : Mask
 : AutoMask
 : Calibrate
 : Polarisation Correct

Worksheet: _____ Number: _____ Depth: _____
Foreground:
Group:
Background:
or Reference: Cadmium:
Numor(s):

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Averaging

I vs. |q| Radial fract. res. bins [d|q|]:
 I vs. [2θ] Radial bins [pixels]:
 I vs. x| Angle Bin [degs]:

Single Depth TOF Use Sector Mask:
 Use Strip Mask:

Colors based on depth:
 Direct to File:

Pre-Av Sparse Data Filter
 Pre-Av Transmission Filter dT/T >
 Pre-Av Resolution Filter dq/q >
 Post-Av Stats Filter dI >

```
Sample Environment:
T_set = N/A; T_reg = N/A; T_sample = N/A
Power Supplies : PS1 N/A [A] N/A [V] : PS2 N/A [A] N/A [V] : PS3 N/A [A] N/A [V]

Acquisition:
Acquisition Time = 600 [s] Exposure Time = 600 [s]
Total Det Counts [Det:1] 30980900 Over 600secs (~51635 cps) : Relative Efficiency = 1
Total Det Counts [Det:2] 39551 Over 600secs (~66 cps) : Relative Efficiency = 1
Total Monitor Counts 600 Over 600secs (~1 cps)

***** Resolution Components: *****
Wavelength resolution d_lambda / lambda: 3 [%] FWHM of triangular shape
Effective source is Rectangular of dimensions: 40 [mm] x 55 [mm] at a distance of: 5.6 [m]
Sample aperture: assuming Circular 10 [mm] diameter
Detector 1 pixelation: x: 8 y: 4 [mm]
Detector 2 pixelation: x: 8 y: 4 [mm]

Averaging Current Display Data
Rebinning ....
Binning Version 'SPARSE'
.....done.... 0.016015[s]

Building Real-Shape Resolution Kernel for I vs. Q data
Wavelength: Triangular (selector) Kernel
Divergence: Geometric Divergence tophat Kernel
Sample Aperture Smearing: Circular Kernel
Detector Pixelation Smearing: Top-Hat Kernel
Binning Resolution Smearing: Top-Hat Kernel

Using Real Shape Kernel (with Geometric Divergence )
f_t >>
```

GRASP_Lockdown V9.18 - UNTITLED

File Display Analysis Instrument Data User Modules Grasp Script Help

Not over active figure (Z)

Numor: 9 Subtitle: * Sample *

ILL_d22_2D
Nrm: mon Dt: off Tc: on
Det: 4.0 Col: 5.6 Wav: 6.00

Stretch Top: [x] [x]
Stretch Bottom: [x] [x]
Gamma: [x] [x]
Reset Colour

: Log Z
 : Grouped Z Scale
 : Manual Z Scale

: Image
 : Contour
 : Smooth

: Mask
 : AutoMask
 : Calibrate
 : Polarisation Correct

Worksheet: _____ Number: _____ Depth: _____
mono

Foreground: Sample 1 5
Group:

Background: Empty Cell 1 1
or Reference: Cadmium: Blocked Beam 1 1

Numor(s): 1,3,5,7,9 .nxs

T_s: Lock: 1
T_e: Lock: 1 Thickness (cm): 0.1 Lock: 0.1

Beam Centre: c_x: 48.8 c_y: 122.7 c_ctr: 0 c_dan: 0 Lock: 0

Centre Calc Reset

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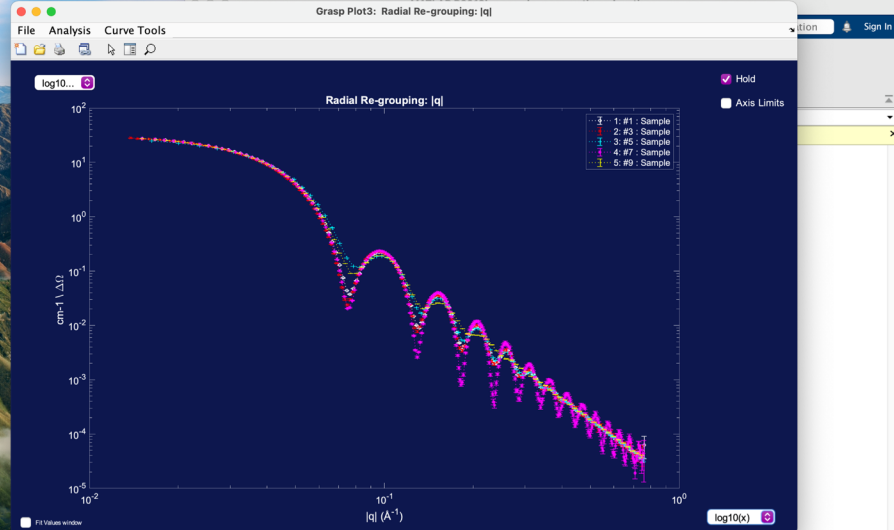
Averaging

Radial fract. res. bins [d|q]: 5
Radial bins [pixels]: 1
Angle Bin [degs]: 1

Single Depth TOF Use Sector Mask:
Use Strip Mask:

Colors based on depth:
Direct to File:

Pre-Av Sparse Data Filter 0.001
 Pre-Av Transmission Filter d/T 0.05
 Pre-Av Resolution Filter dq/q > 0.5
 Post-Av Stats Filter d/I > 0.75



Sample Environment:
T_set = N/A; T_reg = N/A; T_sample = N/A
Power Supplies : PS1 N/A [A] N/A [V] : PS2 N/A [A] N/A [V] : PS3 N/A [A] N/A [V]

Acquisition:
Acquisition Time = 600 [s] Exposure Time = 600 [s]
Total Det Counts [Det:1] 208987670 Over 600secs (~348313 cps) : Relative Efficiency = 1
Total Det Counts [Det:2] 271403 Over 600secs (~452 cps) : Relative Efficiency = 1
Total Monitor Counts 600 Over 600secs (~1 cps)

***** Resolution Components: *****
Wavelength resolution d_lambda / lambda: 20 [%] FWHM of triangular shape
Effective source is Rectangular of dimensions: 40 [mm] x 55 [mm] at a distance of: 5.6 [m]
Sample aperture: assuming Circular 10 [mm] diameter
Detector 1 pixelation: x: 8 y: 4 [mm]
Detector 2 pixelation: x: 8 y: 4 [mm]

Averaging Current Display Data
Rebinning

Binning Version 'SPARSE'
.....done.... 0.015325[s]

Building Real-Shape Resolution Kernel for I vs. Q data
Wavelength: Triangular (selector) Kernel
Divergence: Geometric Divergence tophat Kernel
Sample Aperture Smearing: Circular Kernel
Detector Pixelation Smearing: Top-Hat Kernel
Binning Resolution Smearing: Top-Hat Kernel

Using Real Shape Kernel (with Geometric Divergence)
f_t >>



GRASP_Lockdown V9.18 - UNTITLED

File Display Analysis Instrument Data User Modules Grasp Script Help

Not over active figure (Z)

Numor: 1 Subtitle: *Sample*

ILL_d22_2D
Nrm: mon Dt: off Tc: on
Det: 4.0 Col: 5.6 Wav: 6.00

Stretch Top: [x]
Stretch Bottom: [x]
Gamma: [x]
Reset Colour

Log Z
Grouped Z Scale
Manual Z Scale
Image
Contour
Smooth
Mask
AutoMask
Calibrate
Polarisation Correct

Worksheet: _____ Number: _____ Depth: _____
mono

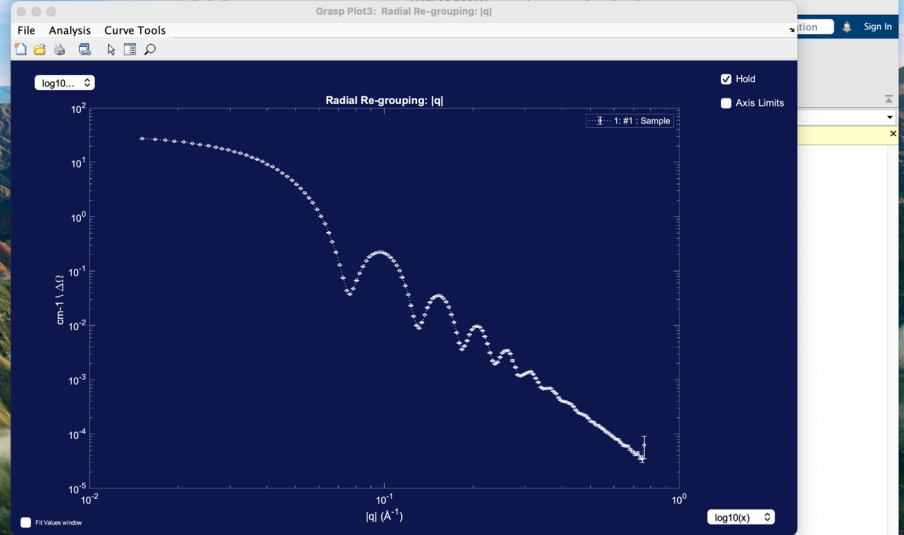
Foreground: Sample 1 1
Background: Empty Cell 1 1
Cadmium: Blocked Beam 1 1

T_s: Lock: 1
T_e: Lock: 1 Thickness (cm): 0.1 Lock: 0.1

Beam Centre:
c_x: 48.8 c_y: 122.7 c_ctr: 0 c_dan: 0 Lock: 0
Centre Calc Reset

Numor(x): 1,3,5,7,9 .nxs
Get III

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Averaging

Radial fract. res. bins [dq/q]: 5
Radial bins [pixels]: 1
Angle Bin [degs]: 1

Single Depth TOF Use Sector Mask:
Use Strip Mask:

Colors based on depth:
Direct to File:

Pre-Av Sparse Data Filter 0.001
Pre-Av Transmission Filter dT/T > 0.05
Pre-Av Resolution Filter dq/q > 0.5
Post-Av Stats Filter dII > 0.75

```

Averaging Current Display Data
Rebinning .....
Binning Version 'SPARSE'
.....done.... 0.013721[s]

Building Real-Shape Resolution Kernel for I vs. Q data
Wavelength: Triangular (selector) Kernel
Divergence: Geometric Divergence tophat Kernel
Sample Aperture Smearing: Circular Kernel
Detector Pixelation Smearing: Top-Hat Kernel
Binning Resolution Smearing: Top-Hat Kernel

Using Real Shape Kernel (with Geometric Divergence )
Averaging Current Display Data
Rebinning .....
Binning Version 'SPARSE'
.....done.... 0.015536[s]

Building Real-Shape Resolution Kernel for I vs. Q data
Wavelength: Triangular (selector) Kernel
Divergence: Geometric Divergence tophat Kernel
Sample Aperture Smearing: Circular Kernel
Detector Pixelation Smearing: Top-Hat Kernel
Binning Resolution Smearing: Top-Hat Kernel

Using Real Shape Kernel (with Geometric Divergence )
f >>
    
```



GRASP_Lockdown V9.18 - UNTITLED

File Display Analysis Instrument Data User Modules Grasp Script Help

Not over active figure (Z)

ILL_d22_2D
 Nrm: mon Dt: off Tc: on
 Det: 4.0 Col: 5.6 Wav: 6.00

Stretch Top: [x]
 Stretch Bottom: [x]
 Gamma: [x]
 Reset Colour

Log Z
 Grouped Z Scale
 Manual Z Scale
 Image
 Contour
 Smooth
 Mask
 AutoMask
 Calibrate
 Polarisation Correct

Worksheet: _____ Number: _____ Depth: _____
 mono

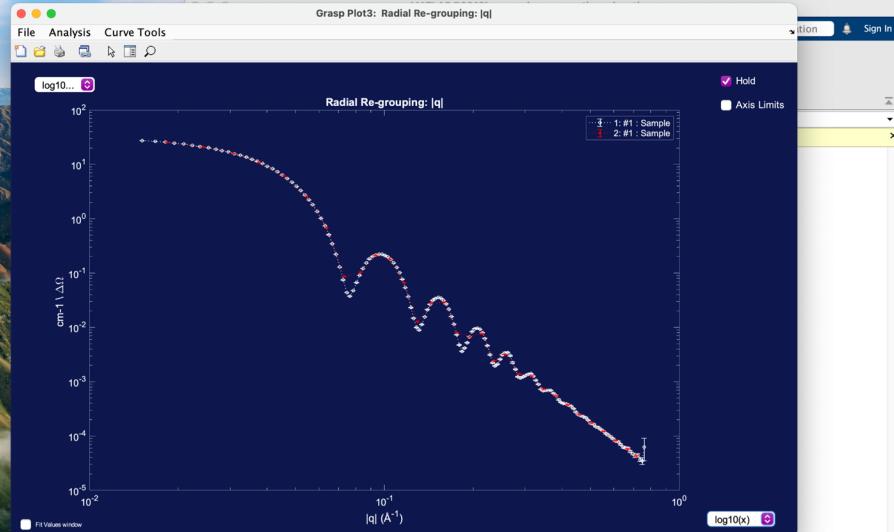
Foreground: Sample 1 1
 Background: Empty Cell 1 1
 Cadmium: Blocked Beam 1 1

T_s: Lock: 1
 T_e: Lock: Thickness (cm): 0.1 Lock: 1

Beam Centre:
 c_x: 48.8 c_y: 122.7 c_ctr: 0 c_dan: 0 Lock:
 Centre Calc Reset

Num(x): 1,3,5,7,9 .nxs
 Get III Reset

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Averaging

Radial fract. res. bins [dq/q]: 1
 I vs. [q]

Radial bins [pixels]: 1
 I vs. [2th]

Angle Bin [degs]: 1
 I vs. [x]

Single Depth TOF

Use Sector Mask:
 Use Strip Mask:

Colors based on depth:
 Direct to File:

Pre-Av Sparse Data Filter 0.001
 Pre-Av Transmission Filter dT/T > 0.05
 Pre-Av Resolution Filter dq/q > 0.5
 Post-Av Stats Filter dI > 0.75

```
Divergence: Geometric Divergence tophat Kernel
Sample Aperture Smearing: Circular Kernel
Detector Pixelation Smearing: Top-Hat Kernel
Binning Resolution Smearing: Top-Hat Kernel

Using Real Shape Kernel (with Geometric Divergence )
Averaging Current Display Data
Rebinning ....
Binning Version 'SPARSE'
.....done.... 0.015536[s]

Building Real-Shape Resolution Kernel for I vs. Q data
Wavelength: Triangular (selector) Kernel
Divergence: Geometric Divergence tophat Kernel
Sample Aperture Smearing: Circular Kernel
Detector Pixelation Smearing: Top-Hat Kernel
Binning Resolution Smearing: Top-Hat Kernel

Using Real Shape Kernel (with Geometric Divergence )
Averaging Current Display Data
Rebinning ....
Binning Version 'SPARSE'
.....done.... 0.01334[s]

Building Real-Shape Resolution Kernel for I vs. Q data
Wavelength: Triangular (selector) Kernel
Divergence: Geometric Divergence tophat Kernel
Sample Aperture Smearing: Circular Kernel
Detector Pixelation Smearing: Top-Hat Kernel
Binning Resolution Smearing: Top-Hat Kernel

Using Real Shape Kernel (with Geometric Divergence )
f >>
```



GRASP_Lockdown V9.18 - UNTITLED

File Display Analysis Instrument Data User Modules Grasp Script Help

Not over active figure (Z)

Numor: 1 Subtitle: * Sample *

ILL_d22_2D
 Nrm: mon Dt: off Tc: on
 Det: 4.0 Col: 5.6 Wav: 6.00

Stretch Top:
 Stretch Bottom:
 Gamma:
 Reset Colour

Log Z
 Grouped Z Scale
 Manual Z Scale
 Image
 Contour
 Smooth
 Mask
 AutoMask
 Calibrate
 Polarisation Correct

Worksheet: _____ Number: _____ Depth: _____
 mono

Foreground: Sample 1 1
 Background: Empty Cell 1 1
 Cadmium: Blocked Beam 1 1

Beam Centre:
 c_x: 48.8 c_y: 122.7 c_ctr: 0 c_dan: 0
 Centre Calc Reset

GRASP_Lockdown V9.18 (c)2021, e-mail: dewhurst@ill.fr

Averaging

Radial fract. res. bins [dq/dq]: 50
 Radial bins [pixels]: 1
 Angle Bin [degs]: 1

Single Depth TOF Use Sector Mask:
 Use Strip Mask:

Colors based on depth:
 Direct to File:

Pre-Av Sparse Data Filter: 0.001
 Pre-Av Transmission Filter dT/T: 0.05
 Pre-Av Resolution Filter dq/q: 0.5
 Post-Av Stats Filter dI: 0.75

Grasp Plot3: Radial Re-grouping: [q]

File Analysis Curve Tools

log10...

Radial Re-grouping: [q]

Hold
 Axis Limits

1: #1 Sample
 2: #1 Sample
 3: #1 Sample

Fit Values window log10(x)

Divergence: Geometric Divergence tophat Kernel
 Sample Aperture Smearing: Circular Kernel
 Detector Pixelation Smearing: Top-Hat Kernel
 Binning Resolution Smearing: Top-Hat Kernel

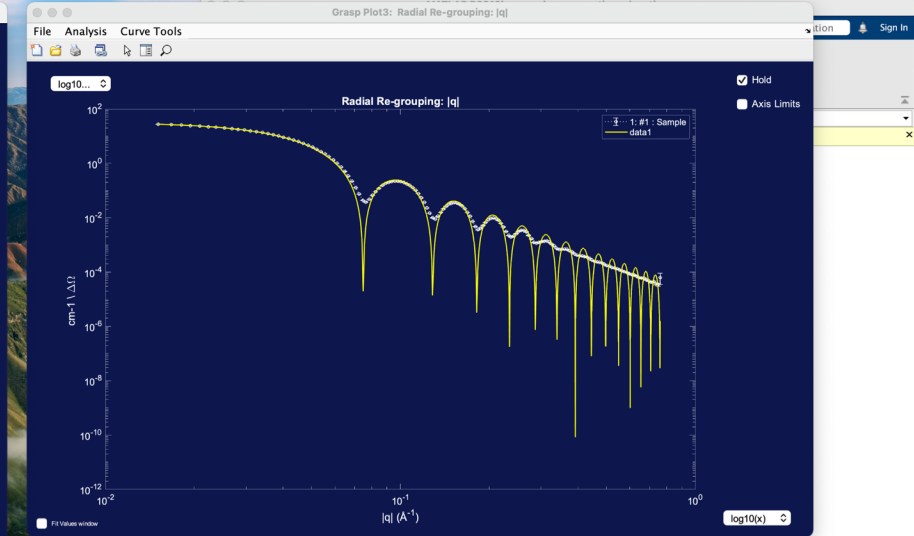
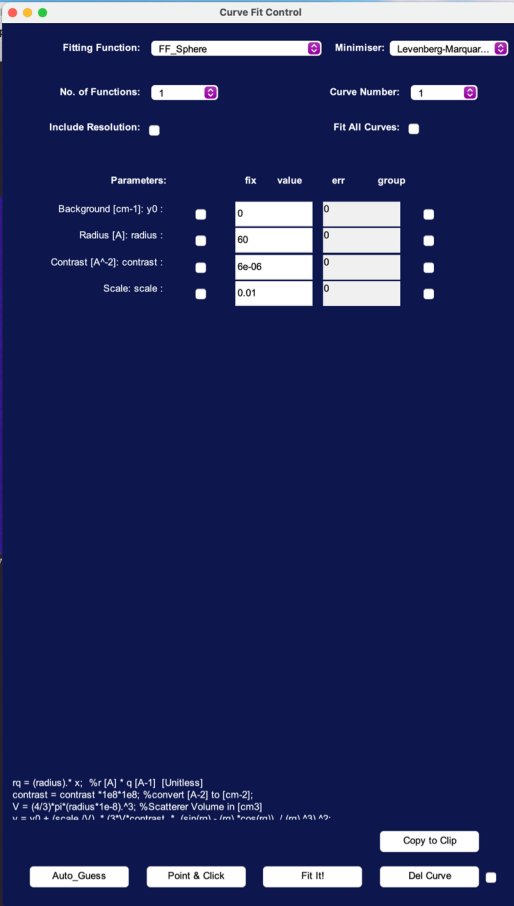
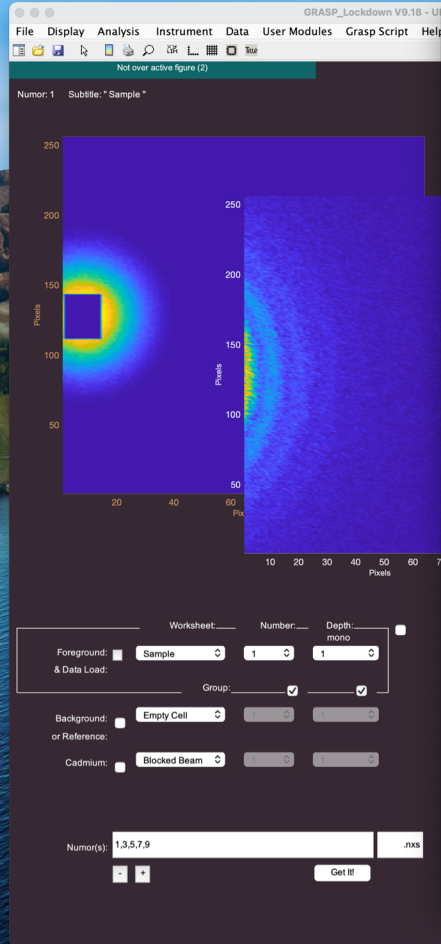
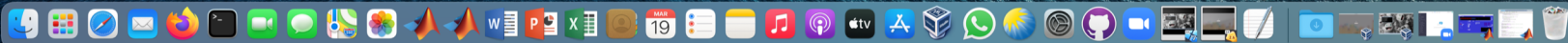
Using Real Shape Kernel (with Geometric Divergence)
 Averaging Current Display Data
 Rebinning
 Binning Version 'SPARSE'
done.... 0.025734[s]

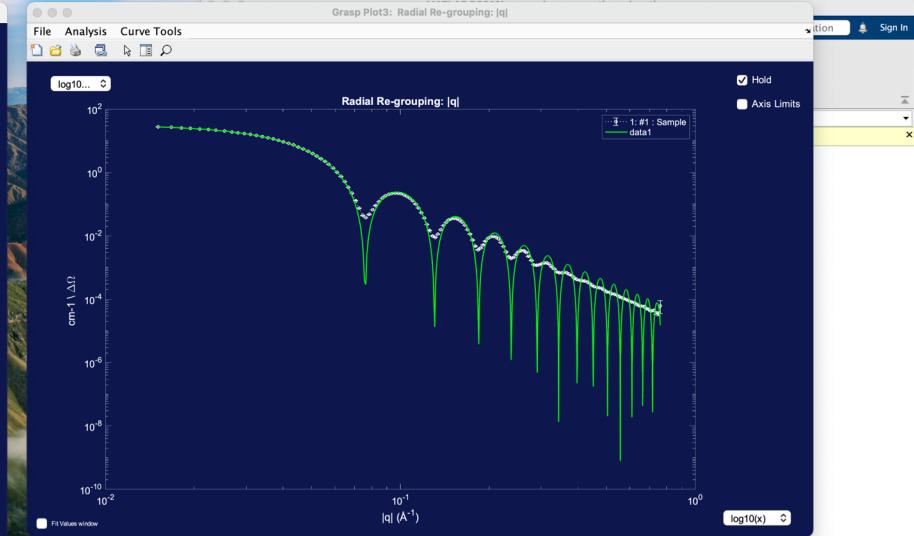
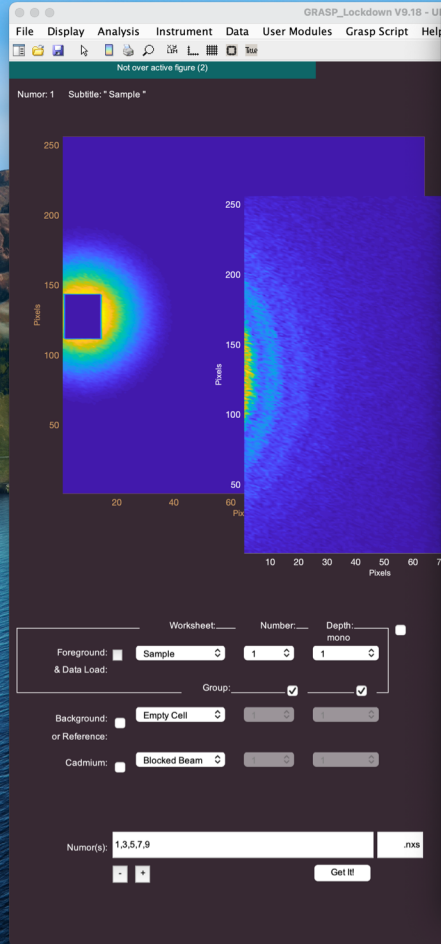
Building Real-Shape Resolution Kernel for I vs. Q data
 Wavelength: Triangular (selector) Kernel
 Divergence: Geometric Divergence tophat Kernel
 Sample Aperture Smearing: Circular Kernel
 Detector Pixelation Smearing: Top-Hat Kernel
 Binning Resolution Smearing: Top-Hat Kernel

Using Real Shape Kernel (with Geometric Divergence)
 Averaging Current Display Data
 Rebinning
 Binning Version 'SPARSE'
done.... 0.024107[s]

Building Real-Shape Resolution Kernel for I vs. Q data
 Wavelength: Triangular (selector) Kernel
 Divergence: Geometric Divergence tophat Kernel
 Sample Aperture Smearing: Circular Kernel
 Detector Pixelation Smearing: Top-Hat Kernel
 Binning Resolution Smearing: Top-Hat Kernel

Using Real Shape Kernel (with Geometric Divergence)
 f >>

or Mask: ip Mask: 



```

Iteration Time(s) Reduced Chi^2
Iteration 2 (max 100)
1 0.01 1687.449

Covariance Checking

Fitting: iteration 1
*Beginning fit (max 100 iterations)

-----
Iteration Time(s) Reduced Chi^2

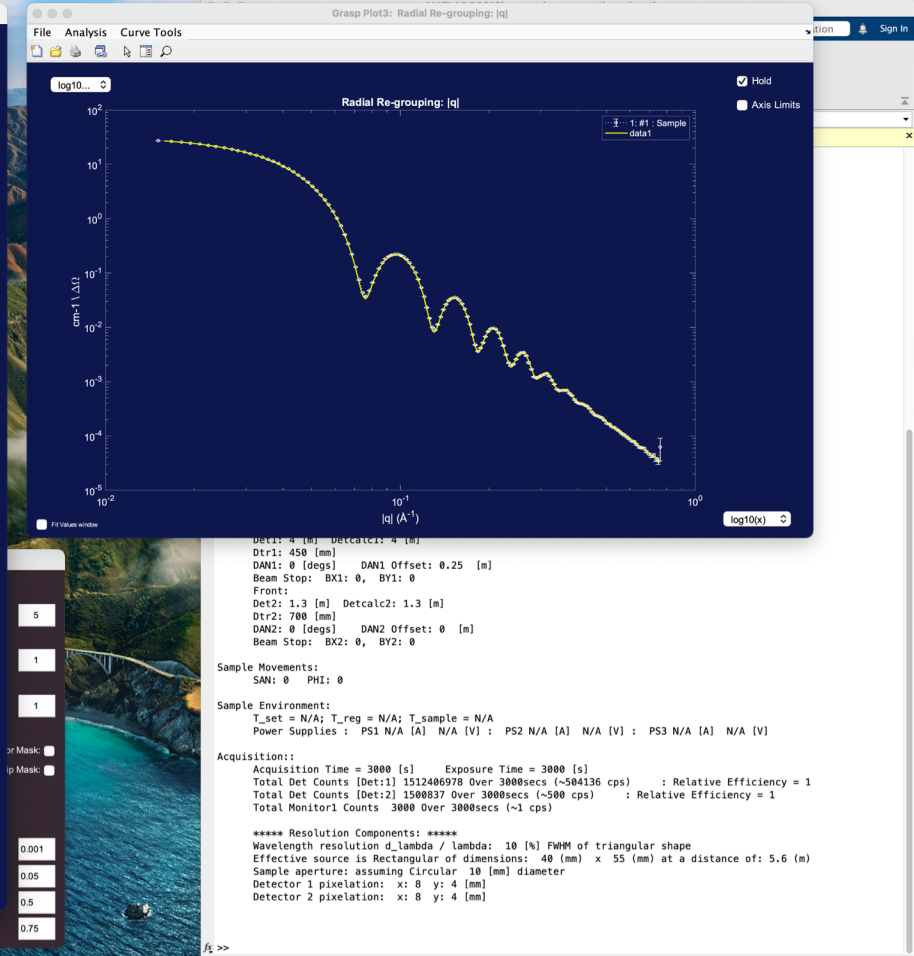
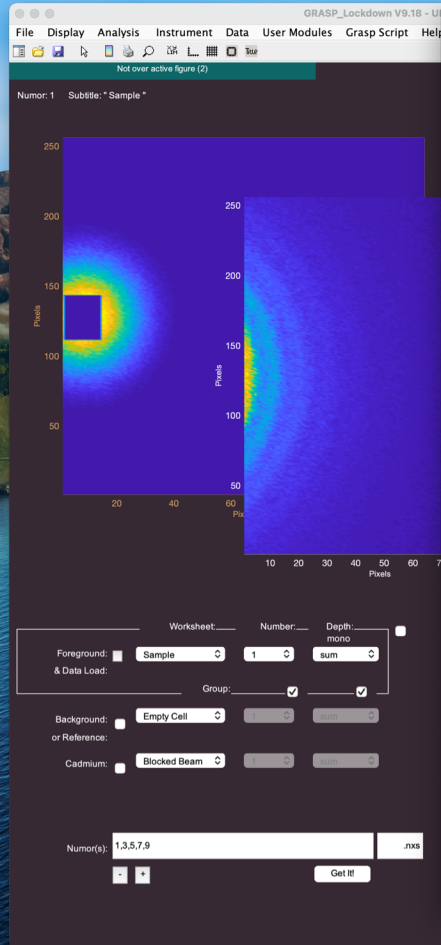
Covariance Checking

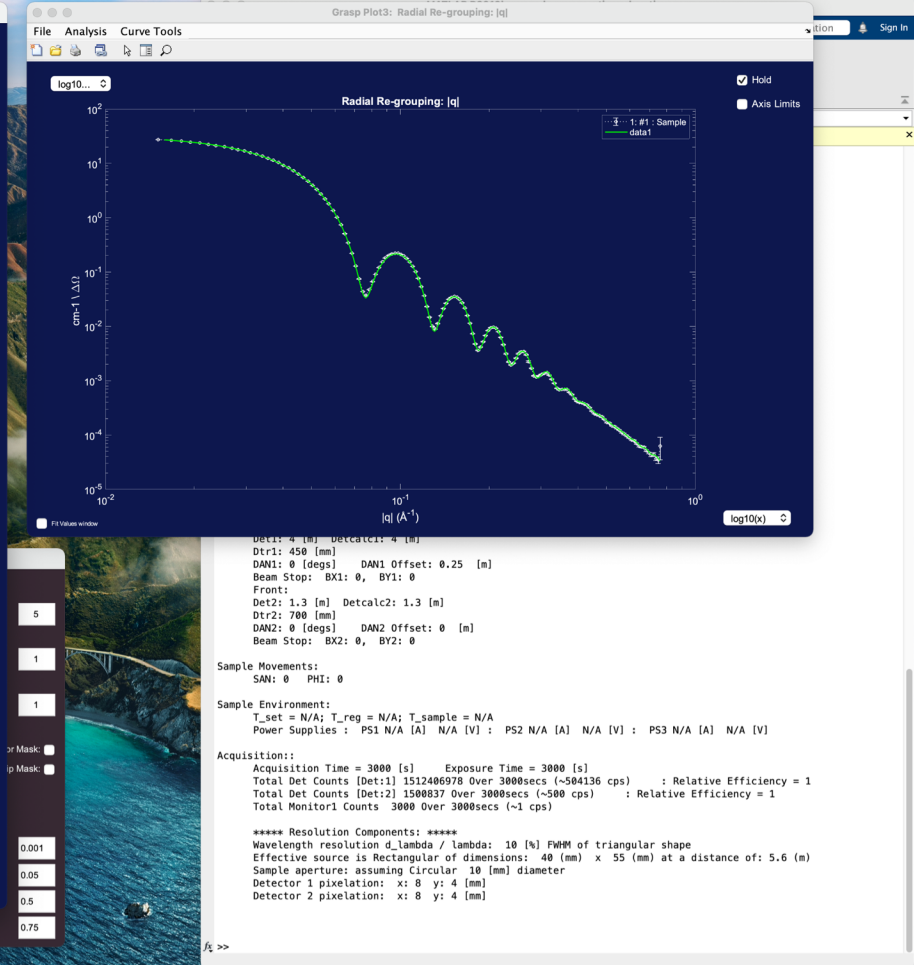
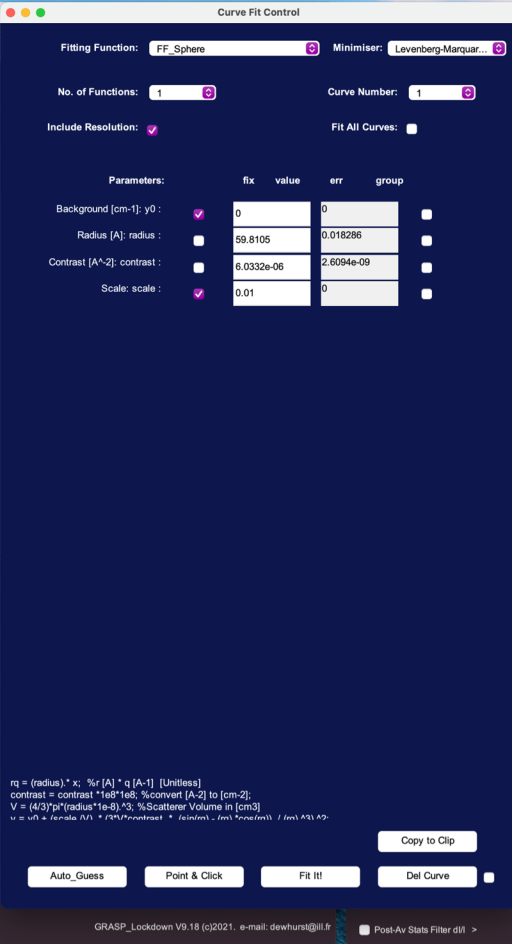
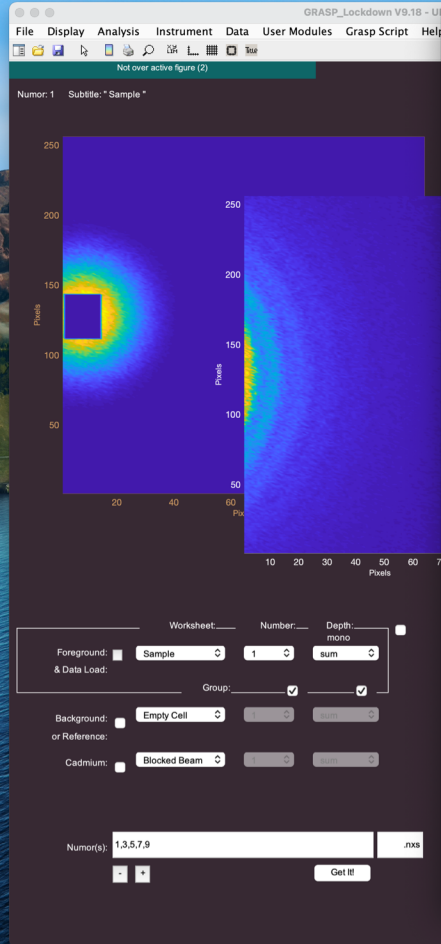
Covariance Corrected Fit Params
Chi^2 = 1687.448

f >>

```







Resolution Control

Resolution Components:

- Wavelength Spread, delta_lambda:
- Divergence, delta_theta:
 - TopHat (Geometric)
 - Measured Beam Shape(x)
- Aperture Smearing: 10 [mm]
- Detector Pixelation:
- Binning Resolution:
- Convolution Type:
 - Real Shape Kernel:
 - Gaussian Equivalent Kernel:
 - Classic Resolution:
- Show Resolution Kernels:

NOTE: For resolution calculation changes to take effect in processed data, e.g. Radial Average, I vs. Q, such processing should be remade

1D Kernel Width (n x fwhm) 2D Kernel Width (+ sigma q)

1D Kernel Finesse (points) 2D Kernel Finesse (X grid)

2D Kernel Finesse (Y grid)

& Data Load: Group:

Background: Empty Cell

or Reference:

Cadmium: Blocked Beam

Number(s):

Curve Fit Control

Fitting Function: Minimiser:

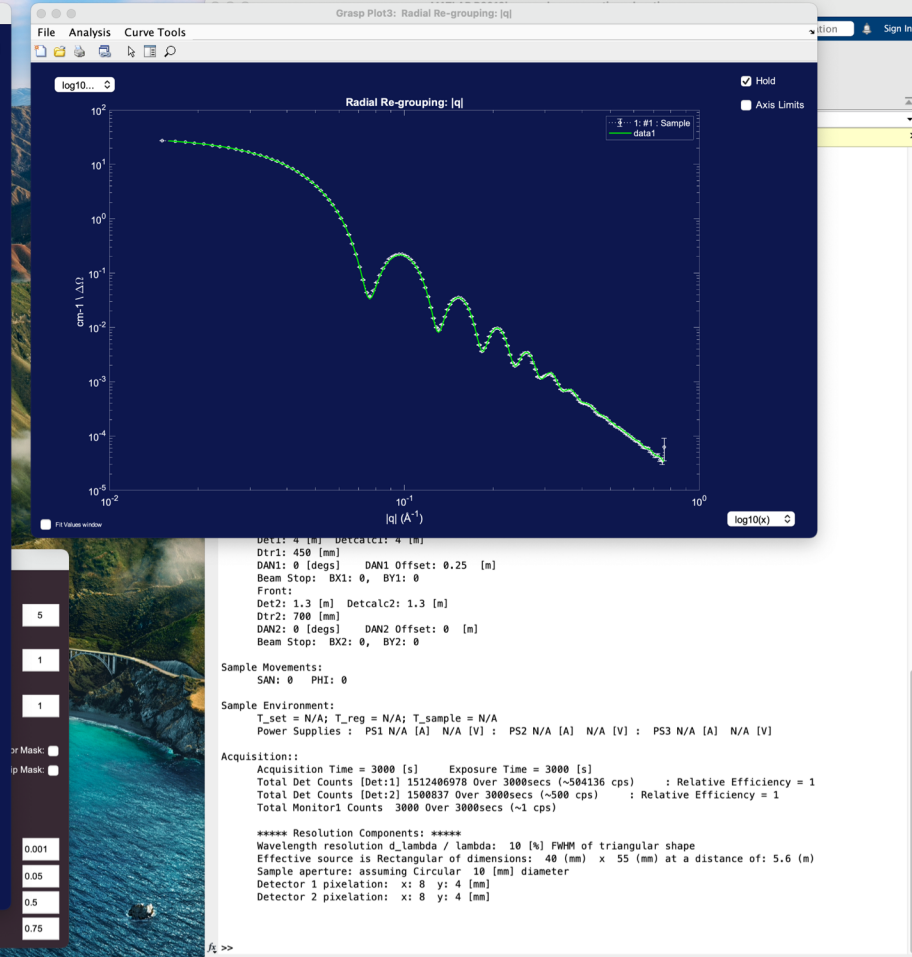
No. of Functions: Curve Number:

Include Resolution: Fit All Curves:

Parameters:	fix	value	err	group
Background [cm-1]: y0:	<input checked="" type="checkbox"/>	0	0	<input type="checkbox"/>
Radius [A]: radius:	<input type="checkbox"/>	59.8105	0.018286	<input type="checkbox"/>
Contrast [A^-2]: contrast:	<input type="checkbox"/>	6.0332e-06	2.6094e-09	<input type="checkbox"/>
Scale: scale:	<input checked="" type="checkbox"/>	0.01	0	<input type="checkbox"/>

$r_q = (\text{radius})^2 * x; \%r [A]^2 * q [A^{-1}]$ [Unitless]
 $\text{contrast} = \text{contrast} * 1e8 * 1e8; \% \text{convert} [A^{-2}] \text{ to } [cm^{-2}]$
 $V = (4/3) * pi * (\text{radius} * 1e-8)^3; \% \text{Scatterer Volume in } [cm^3]$
 $v = v0 + (\text{ends } V) * (\text{conv} * \text{contrast} + (\text{background} - \text{conv} * \text{contrast})) / (\text{im} * V) * 1e9$

GRASP_Lockdown V9.18 (c)2021. e-mail: dewhurst@ill.fr Post-Av Stats Filter dll >



Resolution Control

Resolution Components:

Wavelength Spread, delta_lambda:

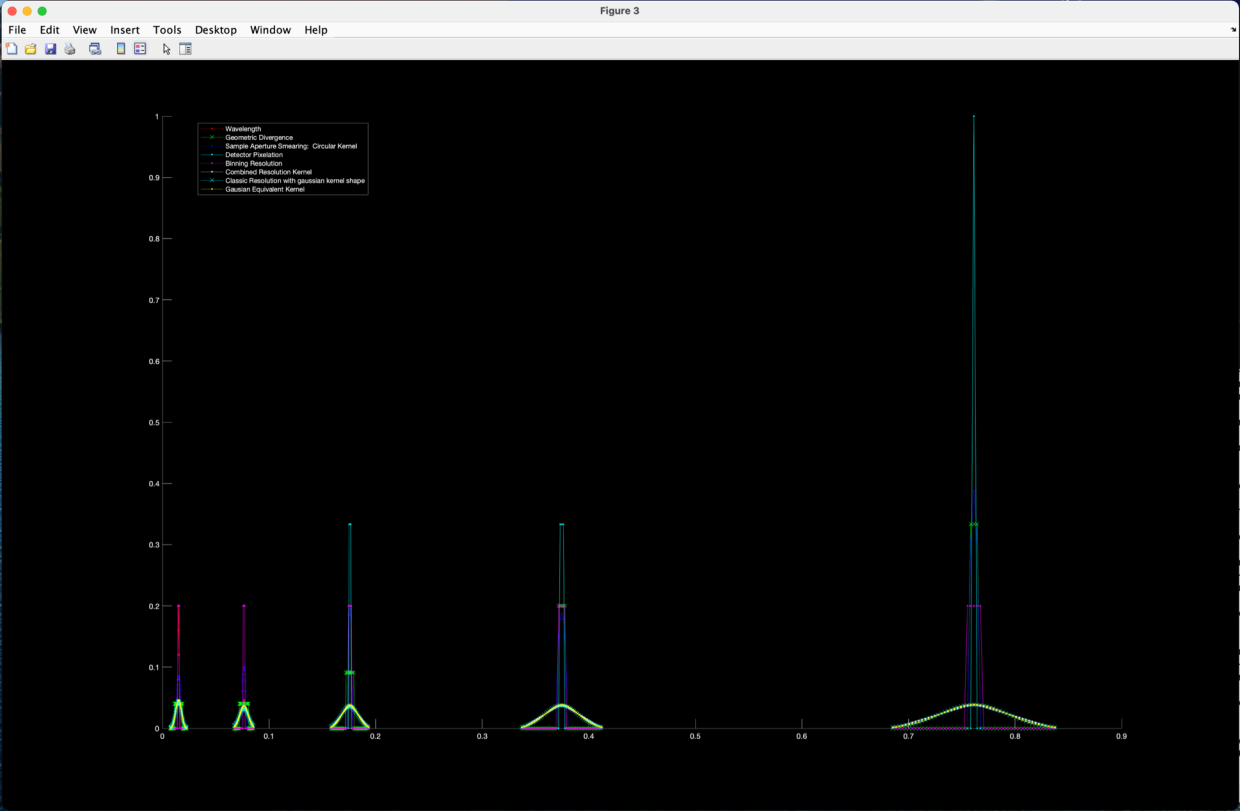
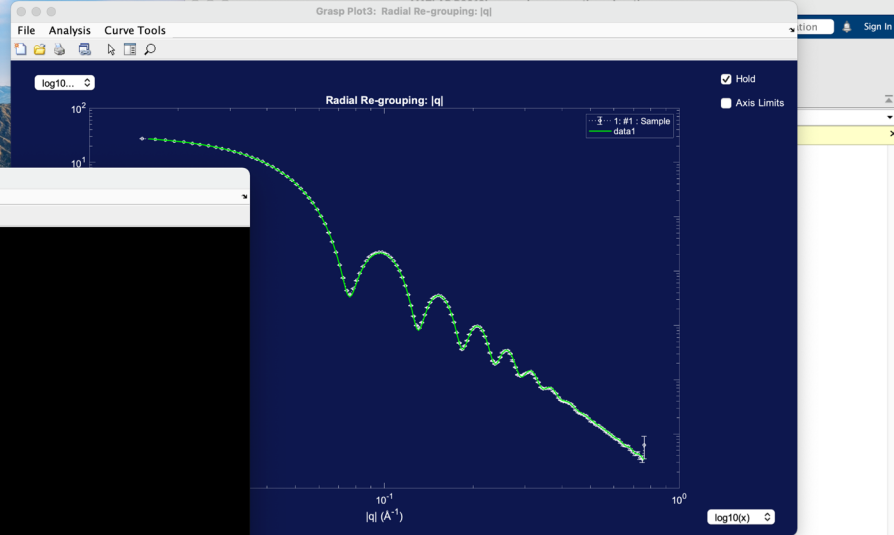
Divergence, delta_theta: TopHat (Geometric)

Curve Fit Control

Fitting Function: Minimiser:

No. of Functions: Curve Number:

Include Resolution: Fit All Curves:



```

Time(s) Reduced Chi^2
n 2 (max 100) 0.02 122.043
n 3 (max 100) 0.02 63.380
n 4 (max 100) 0.02 63.344
ce Checking
time is 0.089716 seconds.
ce Checking
iteration 1
ng fit (max 100 iterations)
Time(s) Reduced Chi^2
ce Checking
iteration 1
ng fit (max 100 iterations)
Time(s) Reduced Chi^2
ce Checking
Corrected Fit Params
63.344

```



Resolution Control

Resolution Components:

Wavelength Spread, delta_lambda:

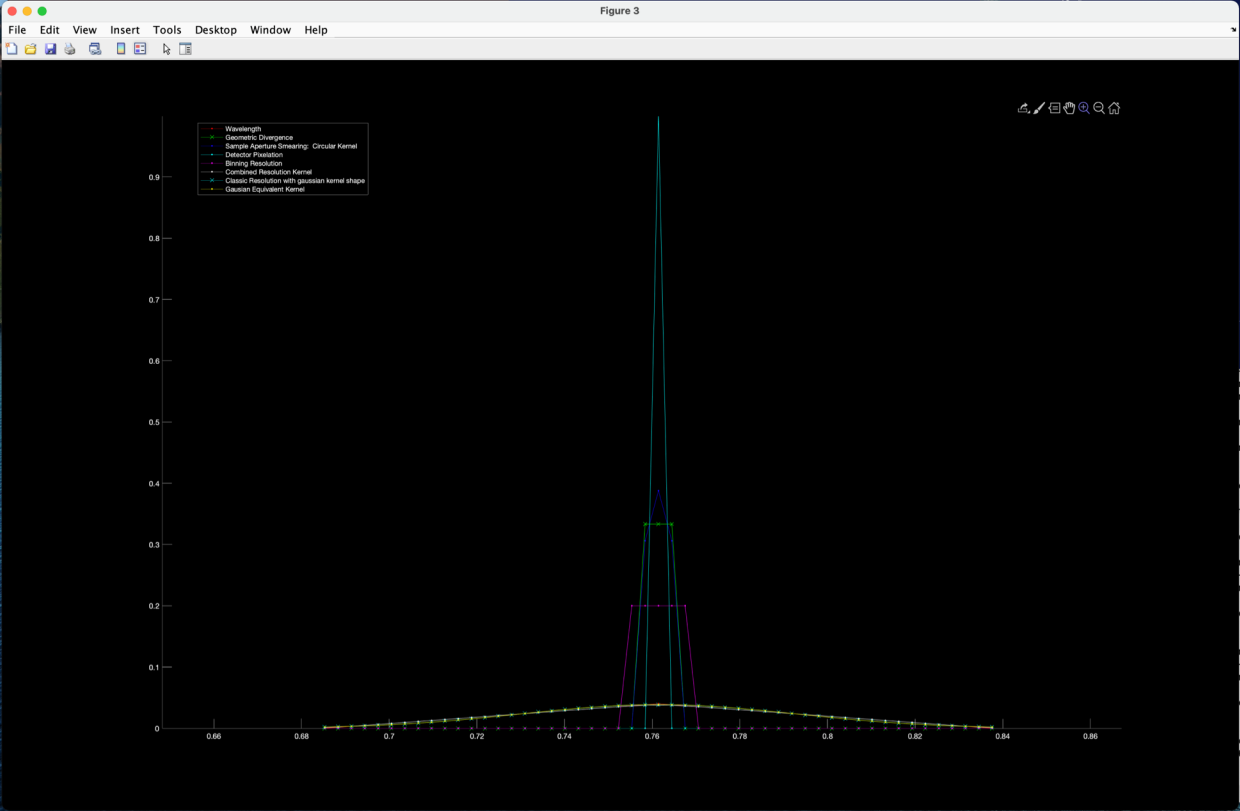
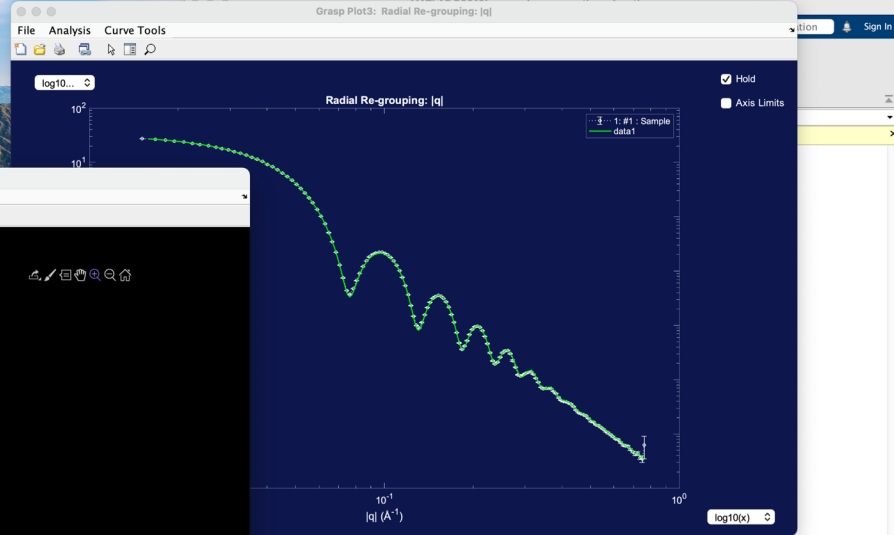
Divergence, delta_theta: TopHat (Geometric)

Curve Fit Control

Fitting Function: Minimiser:

No. of Functions: Curve Number:

Include Resolution: Fit All Curves:



```

Time(s) Reduced Chi^2
n 2 (max 100)
0.02 122.043
n 3 (max 100)
0.02 63.380
n 4 (max 100)
0.02 63.344
ce Checking
time is 0.089716 seconds.
ce Checking
iteration 1
ng fit (max 100 iterations)
Time(s) Reduced Chi^2
ce Checking
iteration 1
ng fit (max 100 iterations)
Time(s) Reduced Chi^2
ce Checking
Corrected Fit Params
63.344

```


Resolution Control

Resolution Components:

Wavelength Spread, delta_lambda:

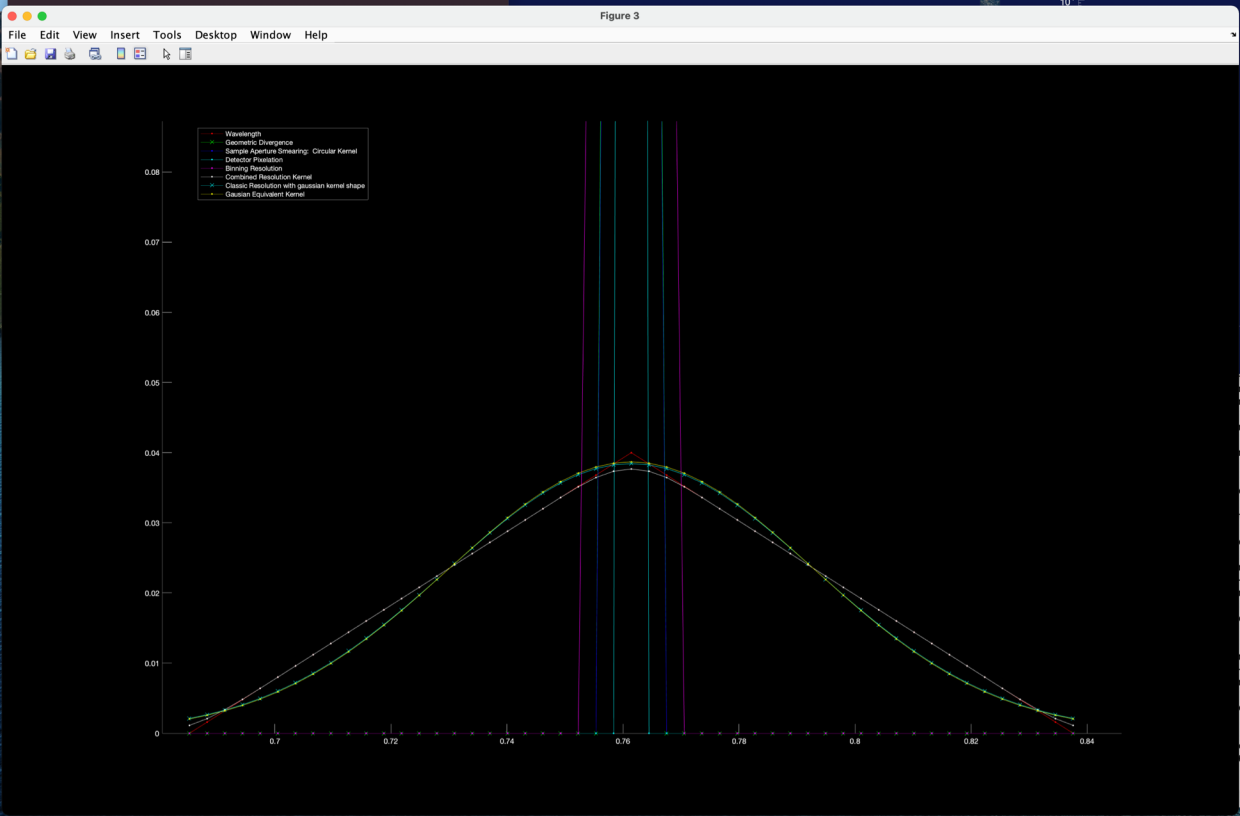
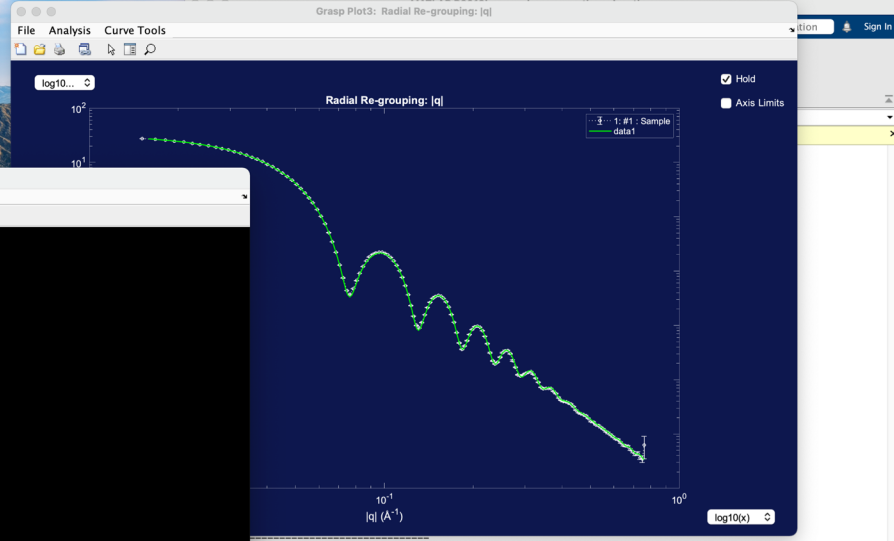
Divergence, delta_theta: TopHat (Geometric)

Curve Fit Control

Fitting Function: Minimiser:

No. of Functions: Curve Number:

Include Resolution: Fit All Curves:



```
Iteration 2 Time(s) Reduced Chi^2
Iteration 2 (max 100) 0.02 122.043
Iteration 3 (max 100) 0.02 63.380
Iteration 4 (max 100) 0.02 63.344
Iteration 5 (max 100) 0.02 63.344
Iteration 6 (max 100) 0.02 63.344
Iteration 7 (max 100) 0.02 63.344
Iteration 8 (max 100) 0.02 63.344
Iteration 9 (max 100) 0.02 63.344
Iteration 10 (max 100) 0.02 63.344
Iteration 11 (max 100) 0.02 63.344
Iteration 12 (max 100) 0.02 63.344
Iteration 13 (max 100) 0.02 63.344
Iteration 14 (max 100) 0.02 63.344
Iteration 15 (max 100) 0.02 63.344
Iteration 16 (max 100) 0.02 63.344
Iteration 17 (max 100) 0.02 63.344
Iteration 18 (max 100) 0.02 63.344
Iteration 19 (max 100) 0.02 63.344
Iteration 20 (max 100) 0.02 63.344
Iteration 21 (max 100) 0.02 63.344
Iteration 22 (max 100) 0.02 63.344
Iteration 23 (max 100) 0.02 63.344
Iteration 24 (max 100) 0.02 63.344
Iteration 25 (max 100) 0.02 63.344
Iteration 26 (max 100) 0.02 63.344
Iteration 27 (max 100) 0.02 63.344
Iteration 28 (max 100) 0.02 63.344
Iteration 29 (max 100) 0.02 63.344
Iteration 30 (max 100) 0.02 63.344
Iteration 31 (max 100) 0.02 63.344
Iteration 32 (max 100) 0.02 63.344
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Iteration 40 (max 100) 0.02 63.344
Iteration 41 (max 100) 0.02 63.344
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Iteration 43 (max 100) 0.02 63.344
Iteration 44 (max 100) 0.02 63.344
Iteration 45 (max 100) 0.02 63.344
Iteration 46 (max 100) 0.02 63.344
Iteration 47 (max 100) 0.02 63.344
Iteration 48 (max 100) 0.02 63.344
Iteration 49 (max 100) 0.02 63.344
Iteration 50 (max 100) 0.02 63.344
Iteration 51 (max 100) 0.02 63.344
Iteration 52 (max 100) 0.02 63.344
Iteration 53 (max 100) 0.02 63.344
Iteration 54 (max 100) 0.02 63.344
Iteration 55 (max 100) 0.02 63.344
Iteration 56 (max 100) 0.02 63.344
Iteration 57 (max 100) 0.02 63.344
Iteration 58 (max 100) 0.02 63.344
Iteration 59 (max 100) 0.02 63.344
Iteration 60 (max 100) 0.02 63.344
Iteration 61 (max 100) 0.02 63.344
Iteration 62 (max 100) 0.02 63.344
Iteration 63 (max 100) 0.02 63.344
Iteration 64 (max 100) 0.02 63.344
Iteration 65 (max 100) 0.02 63.344
Iteration 66 (max 100) 0.02 63.344
Iteration 67 (max 100) 0.02 63.344
Iteration 68 (max 100) 0.02 63.344
Iteration 69 (max 100) 0.02 63.344
Iteration 70 (max 100) 0.02 63.344
Iteration 71 (max 100) 0.02 63.344
Iteration 72 (max 100) 0.02 63.344
Iteration 73 (max 100) 0.02 63.344
Iteration 74 (max 100) 0.02 63.344
Iteration 75 (max 100) 0.02 63.344
Iteration 76 (max 100) 0.02 63.344
Iteration 77 (max 100) 0.02 63.344
Iteration 78 (max 100) 0.02 63.344
Iteration 79 (max 100) 0.02 63.344
Iteration 80 (max 100) 0.02 63.344
Iteration 81 (max 100) 0.02 63.344
Iteration 82 (max 100) 0.02 63.344
Iteration 83 (max 100) 0.02 63.344
Iteration 84 (max 100) 0.02 63.344
Iteration 85 (max 100) 0.02 63.344
Iteration 86 (max 100) 0.02 63.344
Iteration 87 (max 100) 0.02 63.344
Iteration 88 (max 100) 0.02 63.344
Iteration 89 (max 100) 0.02 63.344
Iteration 90 (max 100) 0.02 63.344
Iteration 91 (max 100) 0.02 63.344
Iteration 92 (max 100) 0.02 63.344
Iteration 93 (max 100) 0.02 63.344
Iteration 94 (max 100) 0.02 63.344
Iteration 95 (max 100) 0.02 63.344
Iteration 96 (max 100) 0.02 63.344
Iteration 97 (max 100) 0.02 63.344
Iteration 98 (max 100) 0.02 63.344
Iteration 99 (max 100) 0.02 63.344
Iteration 100 (max 100) 0.02 63.344
```



Resolution Control

Resolution Components:

- Wavelength Spread, delta_lambda:
- Divergence, delta_theta: TopHat (Geometric)
- Aperture Smearing: 10 [mm]
- Detector Pixelation:
- Binning Resolution:
- Convolution Type:
 - Real Shape Kernel:
 - Gaussian Equivalent Kernel:
 - Classic Resolution:
- Show Resolution Kernels:

NOTE: For resolution calculation changes to take effect in processed data, e.g. Radial Average, I vs. Q, such processing should be remade

1D Kernel Width (n x fwhm) 2D Kernel Width (+ sigma q)

1D Kernel Finesse (points) 2D Kernel Finesse (X grid)

2D Kernel Finesse (Y grid)

& Data Load: Group:

Background: Empty Cell 1 2

or Reference: Cadmium Blocked Beam 1 2

Number(s): .jxs

Curve Fit Control

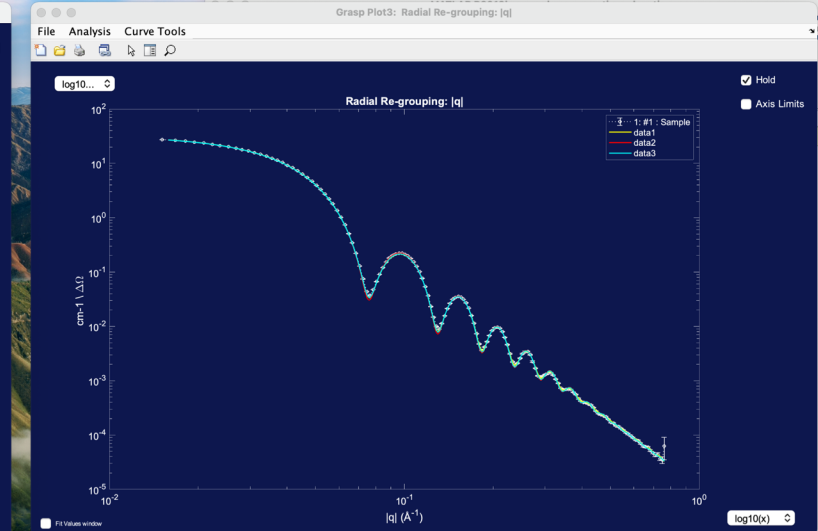
Fitting Function: Minimiser:

No. of Functions: Curve Number:

Include Resolution: Fit All Curves:

Parameters:	fix	value	err	group
Background [cm-1]: y0:	<input checked="" type="checkbox"/>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="checkbox"/>
Radius [A]: radius:	<input type="checkbox"/>	<input type="text" value="80"/>	<input type="text" value="0.016693"/>	<input type="checkbox"/>
Contrast [A^-2]: contrast:	<input type="checkbox"/>	<input type="text" value="6e-06"/>	<input type="text" value="2.4289e-09"/>	<input type="checkbox"/>
Scale: scale:	<input checked="" type="checkbox"/>	<input type="text" value="0.01"/>	<input type="text" value="0"/>	<input type="checkbox"/>

$r_q = (\text{radius})^2 \cdot x \cdot \%r [A] \cdot q [A^{-1}]$ [Unitless]
 $\text{contrast} = \text{contrast} \cdot 1e8 \cdot 1e8; \% \text{convert} [A^{-2}] \text{ to } [cm^{-2}]$
 $V = (4/3) \cdot \pi \cdot (\text{radius} \cdot 1e-8)^3 \cdot \% \text{Scatterer Volume in } [cm^3]$
 $v = v0 + (vnds \cdot N) \cdot \% \text{CPU} \cdot \text{contrast} \cdot (1 + \sin(\text{phi})) \cdot \cos(\text{theta}) / \text{Im}(\text{P}1) \cdot \text{P}2$



5

1

1

or Mask:

ip Mask:

0.001

0.05

0.5

0.75

```

Det1: 4 [m] Detcalc1: 4 [m]
Dtr1: 450 [mm]
DAN1: 0 [degs] DAN1 Offset: 0.25 [m]
Beam Stop: BK1: 0, BY1: 0
Front:
Det2: 1.3 [m] Detcalc2: 1.3 [m]
Dtr2: 700 [mm]
DAN2: 0 [degs] DAN2 Offset: 0 [m]
Beam Stop: BK2: 0, BY2: 0

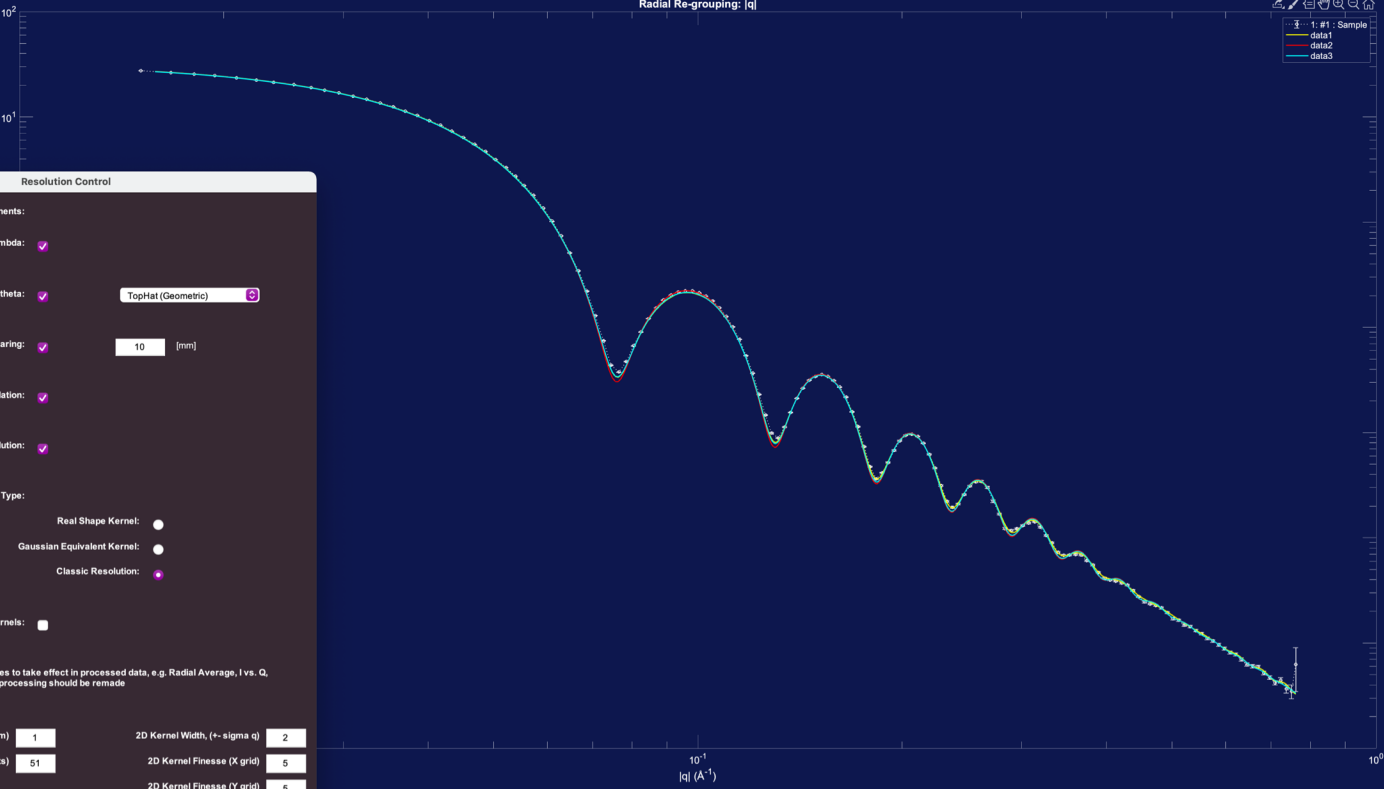
Sample Movements:
SAN: 0 PHI: 0

Sample Environment:
T_set = N/A; T_reg = N/A; T_sample = N/A
Power Supplies : PS1 N/A [A] N/A [V] : PS2 N/A [A] N/A [V] : PS3 N/A [A] N/A [V]

Acquisition:
Acquisition Time = 600 [s] Exposure Time = 600 [s]
Total Det Counts [Det1] 103616057 Over 600secs (~172693 cps) : Relative Efficiency = 1
Total Det Counts [Det2] 132459 Over 600secs (~221 cps) : Relative Efficiency = 1
Total Monitor1 Counts 600 Over 600secs (~1 cps)

***** Resolution Components: *****
Wavelength resolution_d_lambda / lambda: 10 [%] FWHM of triangular shape
Effective source is Rectangular of dimensions: 40 (mm) x 55 (mm) at a distance of: 5.6 (m)
Sample aperture: assuming Circular: 10 [mm] diameter
Detector 1 pixelation: x: 8 y: 4 [mm]
Detector 2 pixelation: x: 8 y: 4 [mm]
    
```

log₁₀(y)



- Hold
- Axis Limits

Resolution Control

Resolution Components:

Wavelength Spread, delta_lambda:

Divergence, delta_theta: TopHat (Geometric)

Aperture Smearing: 10 [mm]

Detector Pixelation:

Binning Resolution:

Convolution Type:

Real Shape Kernel:

Gaussian Equivalent Kernel:

Classic Resolution:

Show Resolution Kernels:

NOTE: For resolution calculation changes to take effect in processed data, e.g. Radial Average, I vs. Q, such processing should be remade

1D Kernel Width, (n x fwhm)

2D Kernel Width, (+- sigma q)

1D Kernel Finesse (points)

2D Kernel Finesse (X grid)

2D Kernel Finesse (Y grid)

log₁₀(x)

GRASP_Lockdown V9.18 - UNTITLED

File Display Analysis Instrument Data User Modules Grasp Script Help

Not over active figure (1)

Numer: 0 Subtitle: "no data"

ILL_d33
Nm: mon Dt: on Tc: on
Det: 6.0 Col: 0.0 Wav: 0.00

Stretch Top: [x] [x]
Stretch Bottom: [x] [x]
Gamma: [x] [x]
Reset Colour

: Log Z
 : Grouped Z Scale
 : Manual Z Scale
 : Image
 : Contour
 : Smooth
 : Mask
 : AutoMask
 : Calibrate
 : Polarisation Correct

Worksheet: _____ Number: _____ Depth: mono
Foreground: Sample 1 sum
Background: Empty Cell
Cadmium: Blocked Beam

T_s: 1 Lock:
T_e: 1 Lock:
Thickness (cm): 0.1 Lock:

Beam Centre:
c_x: 128.5 c_y: 64.5 c_dtr: 0 Lock:
Centre Calc Reset

Numer(x): 1,3,5,7,9 .nxs
Get III

GRASP_Lockdown V9.18 (c)2021, e-mail: dewhurst@ill.fr



MATLAB R2019b - non-degree granting education use

HOME PLOTS APPS

Q Search Documentation Sign In

New New Variable
Script Live Script New Open Compare Import Save
Data Workspace Clear Workspace

CODE ENVIRONMENT RESOURCES

FILE

Users > chuck > Desktop > Dropbox > Matlab > grasp_m_lockdown >

New to MATLAB? See resources for Getting Started.

```
***** Resolution Components: *****  
Wavelength resolution_d_lambda / lambda: 10 [%] FWHM of triangular shape  
Effective source is Rectangular of dimensions: 40 [mm] x 55 [mm] at a distance of: 5.6 [m]  
Sample aperture: assuming Circular 10 [mm] diameter  
Detector 1 pixelation: x: 8 y: 4 [mm]  
Detector 2 pixelation: x: 8 y: 4 [mm]
```

Initialising Data Arrays
Looking for Instrument Detector Mask: instrument_ini/det_mask/ill_d22_msk.mat
Loading Default Instrument Mask for Detector: 1 : instrument_ini/det_mask/ill_d22_msk.mat
Looking for Instrument Detector Mask: instrument_ini/det_mask/
WARNING: No Default Instrument Mask Found for Detector: 2
Looking for Detector Efficiency Map: instrument_ini/det_efficiency/detector_efficiency_det1_ILL_d22_2D.mat
Loading Default Detector Efficiency Map for Detector: 1 : instrument_ini/det_efficiency/detector_efficiency_det1_ILL_d22_2D.mat
Looking for Detector Efficiency Map: instrument_ini/det_efficiency/detector_efficiency_det2_ILL_d22_2D.mat
Loading Default Detector Efficiency Map for Detector: 2 : instrument_ini/det_efficiency/detector_efficiency_det2_ILL_d22_2D.mat
Attempted divide by zero using this data normalisation scheme 'mon'
resetting divider = 1 in normalize_data.m

***** Params are empty *****

```
***** Resolution Components: *****
```

Initialising Data Arrays
Looking for Instrument Detector Mask: instrument_ini/det_mask/detector_mask_det1_ILL_d33.mat
Loading Default Instrument Mask for Detector: 1 : instrument_ini/det_mask/detector_mask_det1_ILL_d33.mat
Looking for Instrument Detector Mask: instrument_ini/det_mask/detector_mask_det2_ILL_d33.mat
Loading Default Instrument Mask for Detector: 2 : instrument_ini/det_mask/detector_mask_det2_ILL_d33.mat
Looking for Instrument Detector Mask: instrument_ini/det_mask/detector_mask_det3_ILL_d33.mat
Loading Default Instrument Mask for Detector: 3 : instrument_ini/det_mask/detector_mask_det3_ILL_d33.mat
Looking for Instrument Detector Mask: instrument_ini/det_mask/detector_mask_det4_ILL_d33.mat
Loading Default Instrument Mask for Detector: 4 : instrument_ini/det_mask/detector_mask_det4_ILL_d33.mat
Looking for Instrument Detector Mask: instrument_ini/det_mask/detector_mask_det5_ILL_d33.mat
Loading Default Instrument Mask for Detector: 5 : instrument_ini/det_mask/detector_mask_det5_ILL_d33.mat
Looking for Detector Efficiency Map: instrument_ini/det_efficiency/detector_efficiency_det1_ILL_d33.mat
Loading Default Detector Efficiency Map for Detector: 1 : instrument_ini/det_efficiency/detector_efficiency_det1_ILL_d33.mat
Looking for Detector Efficiency Map: instrument_ini/det_efficiency/detector_efficiency_det2_ILL_d33.mat
Loading Default Detector Efficiency Map for Detector: 2 : instrument_ini/det_efficiency/detector_efficiency_det2_ILL_d33.mat
Looking for Detector Efficiency Map: instrument_ini/det_efficiency/detector_efficiency_det3_ILL_d33.mat
Loading Default Detector Efficiency Map for Detector: 3 : instrument_ini/det_efficiency/detector_efficiency_det3_ILL_d33.mat
Looking for Detector Efficiency Map: instrument_ini/det_efficiency/detector_efficiency_det4_ILL_d33.mat
Loading Default Detector Efficiency Map for Detector: 4 : instrument_ini/det_efficiency/detector_efficiency_det4_ILL_d33.mat
Looking for Detector Efficiency Map: instrument_ini/det_efficiency/detector_efficiency_det5_ILL_d33.mat
Loading Default Detector Efficiency Map for Detector: 5 : instrument_ini/det_efficiency/detector_efficiency_det5_ILL_d33.mat
Attempted divide by zero using this data normalisation scheme 'mon'
resetting divider = 1 in normalize_data.m

***** Params are empty *****

```
***** Resolution Components: *****
```

f >>

File Edit View Insert Tools Desktop Window Help

TOF: Min: 0 Max: 20 Resolution: 2-4 Rear: 11.0357 [%] Spacing: 2.114 [m] #TOF: 100 Width [s]: 0.0009655 Sample aperture: 10 [mm e]

Selector: Tri [] or Square [x]

Collimation Length (m): 7.8 Bc: 0
Diaphragm: 30 x 30 [mm] By: 0

Simulation: Auto - Off M.C. Iterations (pixel): 10 Measurement Time (s): 1200 Sample Thickness (cm): 0.1 Add Poissonian Noise: Divergence Smearing: Delta_Lambda Smearing: Det Efficiency: Allow Inelasticity:

Scattering Model: Subtitle: Sample Scattering Model: Sphere Radius [Å]: 60 Poly [%FWHM]: 0 Contrast [Å⁻²]: 6e-06 Scale: 0.01 Background [cm⁻¹]: 0 Background Model: None Blocked Model: None

Flux [n/cm²/s]: 0 Sample Transmission: 1 Log: Detector_image

Model Scattering Data

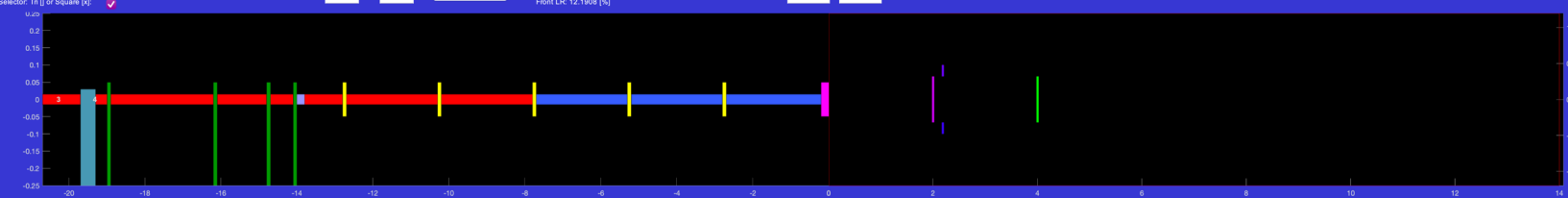
NOTE: Sligger

Thinking!

File Edit View Insert Tools Desktop Window Help

TOF: Min: 0 Max: 20 Resolution: 2-4 Rear: 11.0357 [%] Spacing: 2.114 [m] #TOF: 100 Width [s]: 0.000965 Sample aperture: 10 [mm e]

Selector: Tri [] or Square [x]



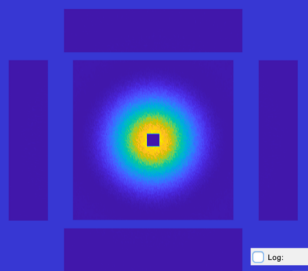
Collimation Length (m): 7.8 Bc: 0
Diaphragm: 30 x 30 [mm] By: 0

Simulation:

M.C. Iterations (pixel): 10
Measurement Time (s): 1200
Sample Thickness (cm): 0.1
Add Poissonian Noise:
Divergence Smearing:
Delta_Lambda Smearing:
Det Efficiency:
Allow Inelasticity:

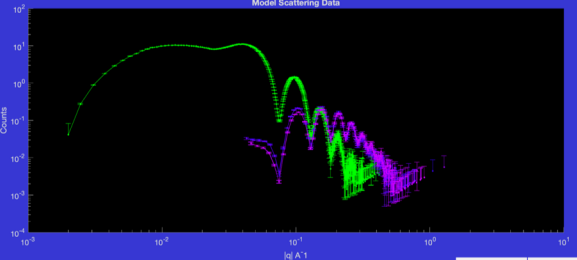
Scattering Model: Subfile:

Radius [Å]: 60
Poly [%FWHM]: 0
Contrast [A-2]: 6e-08
Scale: 0.01
Background [cm-1]: 0
Background Model:
Blocked Model:



Flux [n/cm2/s]: 2.47e+08
Sample Transmission: 0.8845
 Log:

Model Scattering Data



Counts vs |q| Å⁻¹

Note:

File Display Analysis Instrument Data User Modules Grasp Script Help

Not over active figure (1)

Numor: 14 Subtitle: "Sample"

ILL_d13
Nrm: mon Dt: off Tc: on
Det: 2.0 Col: 5.3 Wav: 0.32

Stretch Top: [x] [y]
Stretch Bottom: [x] [y]
Gamma: [x]
Reset Colour

Contours: : Log Z
 : Grouped Z Scale
 : Manual Z Scale
 : Image
 : Contour
 : Smooth

: Mask
 : AutoMask
 : Calibrate
 : Polarisation Correct

Worksheet: _____ Number: _____ Depth: _____
tof

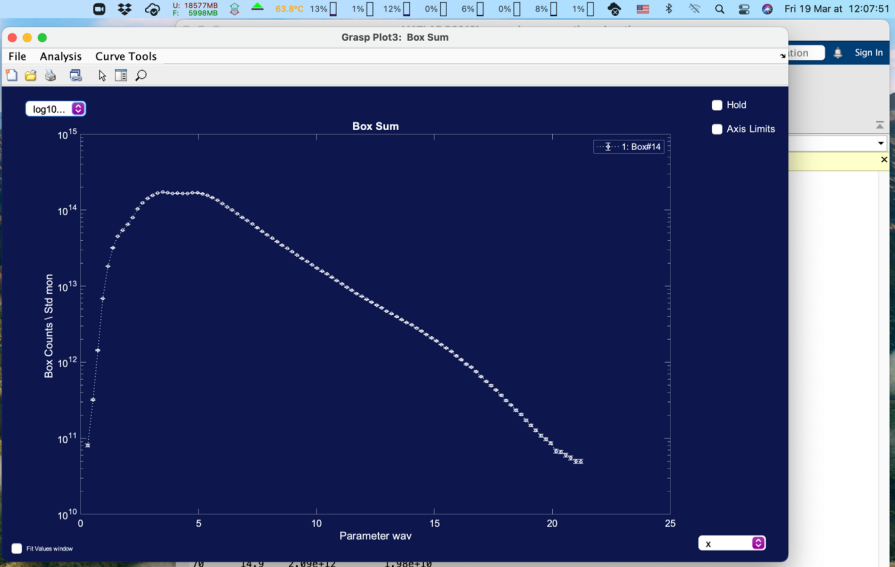
Foreground: [Trans Empty] [1] [sum]
& Data Load: _____ Group:

Background: _____
or Reference: _____
Cadmium: _____

Beam Centre: c_x: _____ c_y: _____ c_dtr: _____ Lock:
128.4252 64.5164 0

Numor(s): 14 [] .nxs
Centre Calc [] Reset []

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Boxes

Box:	x1	x2	y1	y2	Det
1	114	144	56	71	1
2	0	0	0	0	1
3	0	0	0	0	1
4	0	0	0	0	1
5	0	0	0	0	1
6	0	0	0	0	1
x					

Parameter: wav Sum_Boxes Box_Norm

Q-Lock Theta-2/Theta

Do!!!

70	14.9	2.89e+12	1.98e+10
71	15.1	1.91e+12	1.9e+10
72	15.3	1.71e+12	1.79e+10
73	15.5	1.55e+12	1.7e+10
74	15.7	1.38e+12	1.61e+10
75	15.9	1.22e+12	1.51e+10
76	16.1	1.08e+12	1.43e+10
77	16.4	9.39e+11	1.33e+10
78	16.6	8.57e+11	1.27e+10
79	16.8	7.5e+11	1.19e+10
80	17	6.46e+11	1.1e+10
81	17.2	5.58e+11	1.02e+10
82	17.4	4.95e+11	9.64e+09
83	17.6	4.29e+11	8.98e+09
84	17.8	3.68e+11	8.32e+09
85	18	3.12e+11	7.66e+09
86	18.3	2.73e+11	7.17e+09
87	18.5	2.34e+11	6.63e+09
88	18.7	2.05e+11	6.21e+09
89	18.9	1.72e+11	5.68e+09
90	19.1	1.48e+11	5.27e+09
91	19.3	1.27e+11	4.89e+09
92	19.5	1.08e+11	4.5e+09
93	19.7	9.74e+10	4.28e+09
94	19.9	8.57e+10	4.01e+09
95	20.2	6.79e+10	3.57e+09
96	20.4	6.58e+10	3.52e+09
97	20.6	6.02e+10	3.36e+09
98	20.8	5.51e+10	3.22e+09
99	21	4.96e+10	3.05e+09
100	21.2	4.94e+10	3.05e+09

GRASP_Lockdown V9.18 - UNTITLED

File Display Analysis Instrument Data User Modules Grasp Script Help

Not over active figure (1)

Numor: 13 Subtitle: "Sample"

ILL: d33
 Nrm: mon Dt: off Tc: on
 Det: 2.0 Col: 5.3 Wav: 1.58

Stretch Top: [x] [y]
 Stretch Bottom: [x] [y]
 Gamma: [x]
 Reset Colour

Log Z
 Grouped Z Scale
 Manual Z Scale

Image
 Contour
 Smooth

Mask
 AutoMask
 Calibrate
 Polarisation Correct

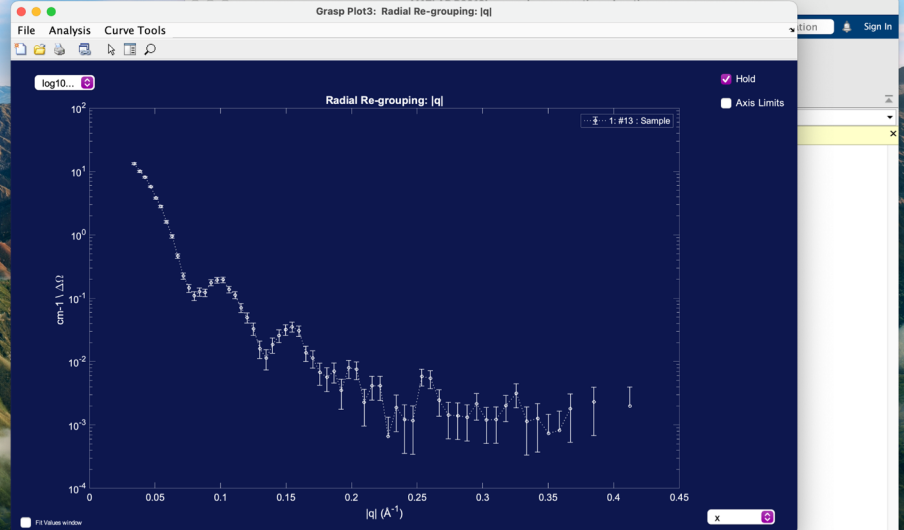
Worksheet: Number: Depth: T_s: Lock: T_e: Lock: Thickness (cm): Lock:

Foreground: Sample 1 7
 Background: Empty Cell 1 1
 Cadmium: Blocked Beam 1 1

Beam Centre: c_x: c_y: c_dtr: Lock: 128.4989 64.4995 0

Numor(s): 13 Get III Reset

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Effective source is Square of dimensions: 30 (mm) x 30 (mm) at a distance of: 5.3 (m)
 Sample aperture: assuming Circular: 10 (mm) diameter
 Detector 1 pixelation: x: 2.5 y: 5 (mm)
 Wavelength resolution d_λ / λ Detector 2: 12.1908 [%] FWHM of tophat shape
 Detector 2 pixelation: x: 5 y: 2.5 (mm)
 Wavelength resolution d_λ / λ Detector 3: 12.1908 [%] FWHM of tophat shape
 Detector 3 pixelation: x: 5 y: 2.5 (mm)
 Wavelength resolution d_λ / λ Detector 4: 12.3222 [%] FWHM of tophat shape
 Detector 4 pixelation: x: 2.5 y: 5 (mm)
 Wavelength resolution d_λ / λ Detector 5: 12.3222 [%] FWHM of tophat shape
 Detector 5 pixelation: x: 2.5 y: 5 (mm)

Averaging Current Display Data
 Rejecting detector Frame:8 ; Det: 2 due to Sparse Raw Data
 Rejecting detector Frame:8 ; Det: 3 due to Sparse Raw Data
 Rejecting detector Frame:8 ; Det: 4 due to Sparse Raw Data
 Detector 5 data empty
 Rebinning:
 Binning Version 'SPARSE'
done.... 0.011931[s]

Building Real-Shape Resolution Kernel for I vs. Q data
 Wavelength: Top-Hat (e.g. D33 TOF) Kernel
 Divergence: Geometric Divergence tophat Kernel
 Sample Aperture Smearing: Circular Kernel
 Detector Pixelation Smearing: Top-Hat Kernel
 Binning Resolution Smearing: Top-Hat Kernel

Using Real Shape Kernel (with Geometric Divergence)
 f_g >>

Averaging

Radial fract. res. bins [q|q]: 5
 I vs. [q]

Radial bins [pixels]: 1
 I vs. [2θ]

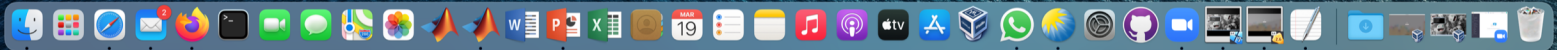
Angle Bin [degs]: 1
 I vs. x]

Single Depth TOF Use Sector Mask:

Use Strip Mask:

Colors based on depth:
 Direct to File:

Pre-Av Sparse Data Filter: 0.001
 Pre-Av Transmission Filter dT/T: 0.05
 Pre-Av Resolution Filter dq/q: 0.5
 Post-Av Stats Filter dI: 0.75



Numor: 13 Subtitle: "Sample"

ILL: d33
 Nrm: mon Dt: off Tc: on
 Det: 2.0 Col: 5.3 Wav: 3.27

Stretch Top: [x] [x]
 Stretch Bottom: [x] [x]
 Gamma: [x] [x]
 Reset Colour

Log Z
 Grouped Z Scale
 Manual Z Scale

Image
 Contour
 Smooth

Mask
 AutoMask
 Calibrate
 Polarisation Correct

Worksheet: _____ Number: _____ Depth: _____
 lof

Foreground: Sample 1 15
 & Data Load: _____

Group: [x] [x]

Background: Empty Cell
 or Reference: _____

Cadmium: Blocked Beam

Beam Centre: c_x: 128.5013 c_y: 64.4996 c_dtr: 0
 Lock: [x]

Centre Calc [x] Reset [x]

Numor(s): 13 [x] .nxs

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Averaging

Radial fract. res. bins [q|q]: 5

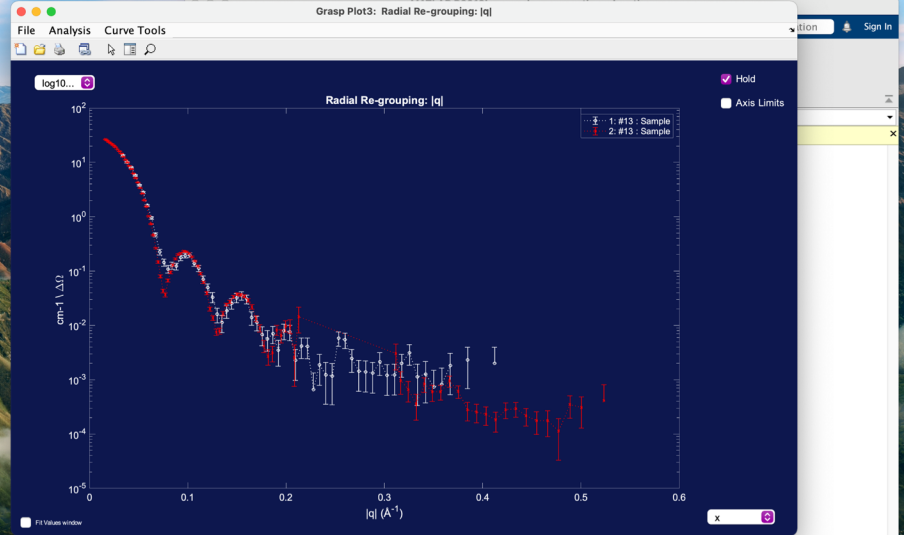
Radial bins [pixels]: 1

Angle Bin [degs]: 1

Single Depth TOF Use Sector Mask: [x]
 Use Strip Mask: [x]

Colors based on depth: [x]
 Direct to File: [x]

Pre-Av Sparse Data Filter: 0.001
 Pre-Av Transmission Filter dT/T: 0.05
 Pre-Av Resolution Filter dq/q: 0.5
 Post-Av Stats Filter dT: 0.75



```

***** Resolution Components: *****
Wavelength resolution d_lambda / lambda Detector 1: 11.0357 [%] FWHM of tophat shape
Effective source is Square of dimensions: 30 (mm) x 30 (mm) at a distance of: 5.3 (m)
Sample aperture: assuming Circular 10 (mm) diameter
Detector 1 pixelation: x: 2.5 y: 5 (mm)
Wavelength resolution d_lambda / lambda Detector 2: 12.1908 [%] FWHM of tophat shape
Detector 2 pixelation: x: 5 y: 2.5 (mm)
Wavelength resolution d_lambda / lambda Detector 3: 12.1908 [%] FWHM of tophat shape
Detector 3 pixelation: x: 5 y: 2.5 (mm)
Wavelength resolution d_lambda / lambda Detector 4: 12.3222 [%] FWHM of tophat shape
Detector 4 pixelation: x: 2.5 y: 5 (mm)
Wavelength resolution d_lambda / lambda Detector 5: 12.3222 [%] FWHM of tophat shape
Detector 5 pixelation: x: 2.5 y: 5 (mm)

Averaging Current Display Data
Rejecting detector Frame:16 ; Det: 2 due to Sparse Raw Data
Rejecting detector Frame:16 ; Det: 3 due to Sparse Raw Data
Rebinning .....
Binning Version 'SPARSE'
.....done..... 0.014133[s]

Building Real-Shape Resolution Kernel for I vs. Q data
Wavelength: Top-Hat (e.g. D33 TOF) Kernel
Divergence: Geometric Divergence tophat Kernel
Sample Aperture Smearing: Circular Kernel
Detector Pixelation Smearing: Top-Hat Kernel
Binning Resolution Smearing: Top-Hat Kernel

Using Real Shape Kernel (with Geometric Divergence )
f >>
    
```

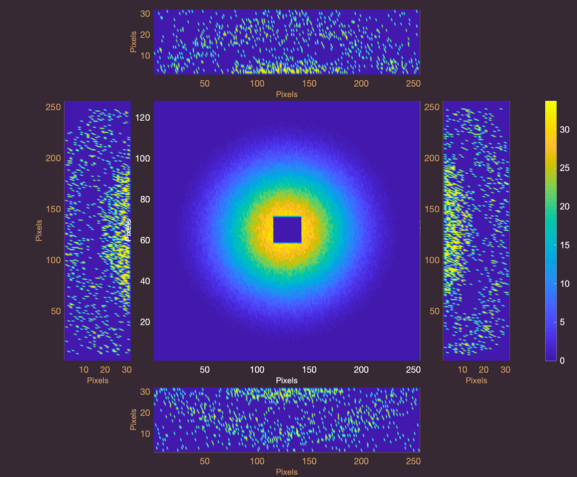
GRASP_Lockdown V9.18 - UNTITLED

File Display Analysis Instrument Data User Modules Grasp Script Help

Not over active figure (1)

Numor: 13 Subtitle: "Sample"

ILL_d33
Nrm: mon Dt: off Tc: on
Det: 2.0 Col: 5.3 Wav: 6.44



Stretch Top: [x] Stretch Bottom: [x] Gamma: [x] Reset Colour

Log Z [] Grouped Z Scale [] Manual Z Scale [] Image [x] Contour [] Smooth [] Mask [x] AutoMask [] Calibrate [x] Polarisation Correct []

Worksheet: _____ Number: _____ Depth: _____
 Foreground: [Sample] [1] [30]
 Background: [Empty Cell] [1] [30]
 Cadmium: [Blocked Beam] [1] [30]

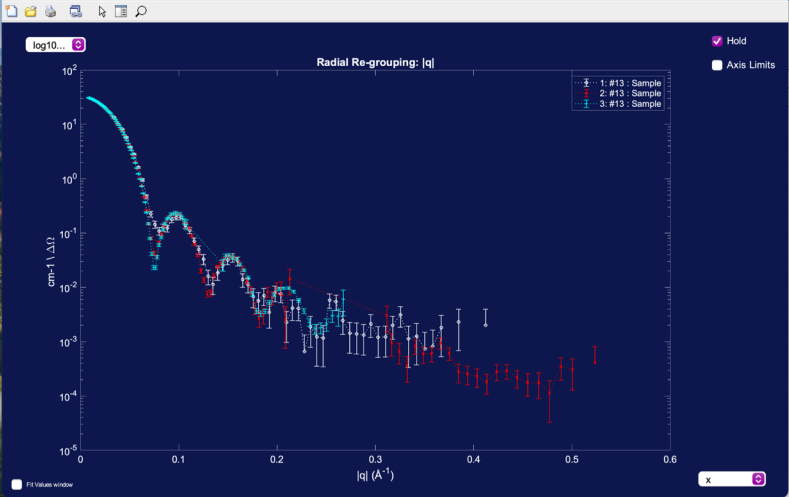
Beam Centre: c_x: 128.4976 c_y: 64.4996 c_dtr: 0

Numor(s): [13] [OK] [Cancel]

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Grasp Plot3: Radial Re-grouping: [q]

File Analysis Curve Tools



log10... [x] Radial Re-grouping: [q] Hold [x] Axis Limits []

1: #13 Sample
 2: #13 Sample
 3: #13 Sample

Fit Values window

Total Monitor Counts 6 Over 0secs (~inf cps)

***** Resolution Components: *****
 Wavelength resolution d_{λ} / λ diameter Detector 1: 11.0357 [%] FWHM of tophat shape
 Effective source is Square of dimensions: 30 (mm) x 30 (mm) at a distance of: 5.3 (m)
 Sample aperture: assuming Circular: 10 [mm] diameter
 Detector 1 pixelation: x: 2.5 y: 5 [mm]
 Wavelength resolution d_{λ} / λ diameter Detector 2: 12.1908 [%] FWHM of tophat shape
 Detector 2 pixelation: x: 5 y: 2.5 [mm]
 Wavelength resolution d_{λ} / λ diameter Detector 3: 12.1908 [%] FWHM of tophat shape
 Detector 3 pixelation: x: 5 y: 2.5 [mm]
 Wavelength resolution d_{λ} / λ diameter Detector 4: 12.3222 [%] FWHM of tophat shape
 Detector 4 pixelation: x: 2.5 y: 5 [mm]
 Wavelength resolution d_{λ} / λ diameter Detector 5: 12.3222 [%] FWHM of tophat shape
 Detector 5 pixelation: x: 2.5 y: 5 [mm]

Averaging Current Display Data
 Rebinning:

Binning Version 'SPARSE'
done.... 0.017563[s]

Building Real-Shape Resolution Kernel for I vs. Q data
 Wavelength: Top-Hat (e.g. D33 TOF) Kernel
 Divergence: Geometric Divergence tophat Kernel
 Sample Aperture Smearing: Circular Kernel
 Detector Pixelation Smearing: Top-Hat Kernel
 Binning Resolution Smearing: Top-Hat Kernel

Using Real Shape Kernel (with Geometric Divergence)
 f_g >>

Averaging

Radial fract. res. bins [d|q]: [5]

Radial bins [pixels]: [1]

Angle Bin [deg]: [1]

Single [] Depth [] TOF [] Use Sector Mask: []
 Use Strip Mask: []

Colors based on depth: [] Direct to File: []

Pre-Av Sparse Data Filter: [0.001]
 Pre-Av Transmission Filter dT/T: [0.05]
 Pre-Av Resolution Filter dq/q: [0.5]
 Post-Av Stats Filter dI: [0.75]



File Display Analysis Instrument Data User Modules Grasp Script Help

Not over active figure (1)

Numor: 13 Subtitle: "Sample"

ILL: d33
 Nrm: mon Dt: off Tc: on
 Det: 2.0 Col: 5.3 Wav: 12.77

Stretch Top: [x] [x]
 Stretch Bottom: [x] [x]
 Gamma: [x]
 Reset Colour

: Log Z
 : Grouped Z Scale
 : Manual Z Scale
 : Image
 : Contour
 : Smooth

: Mask
 : AutoMask
 : Calibrate
 : Polarisation Correct

Worksheet: _____ Number: _____ Depth: _____
 foreground: Sample 1 60
 Background: Empty Cell
 Cadmium: Blocked Beam

Beam Centre: c_x: 128.4955 c_y: 64.4977 c_dtr: 0
 Centre Calc Reset

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Averaging

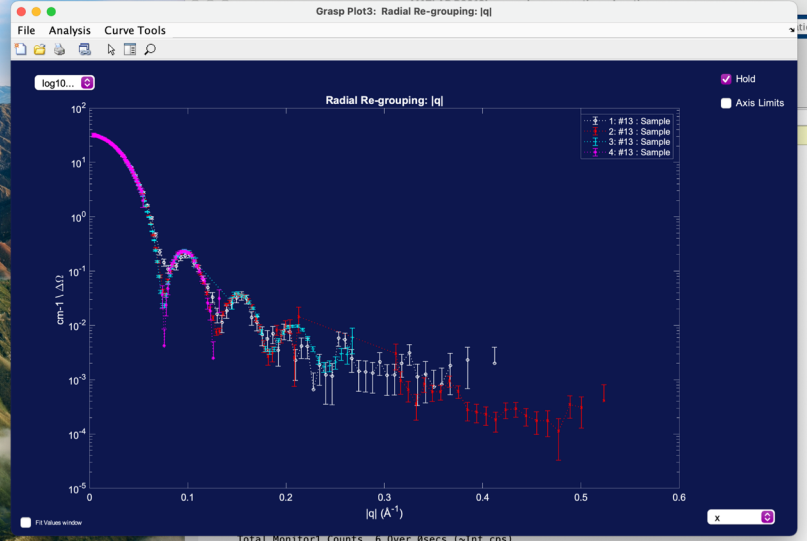
Radial fract. res. bins [dq|q]: 5
 Radial bins [pixels]: 1
 Angle Bin [degs]: 1

Single Depth TOF Use Sector Mask:

Use Strip Mask:

Colors based on depth:
 Direct to File:

Pre-Av Sparse Data Filter 0.001
 Pre-Av Transmission Filter dT/T > 0.05
 Pre-Av Resolution Filter dq/q > 0.5
 Post-Av Stats Filter dT/d > 0.75



Total Monitor Counts 6 Over 0sec (~inf cps)

**** Resolution Components: ****
 Wavelength resolution d_lambda / lambda Detector 1: 11.0357 [%] FWHM of tophat shape
 Effective source is Square of dimensions: 30 (mm) x 30 (mm) at a distance of: 5.3 (m)
 Sample aperture: assuming Circular: 10 [mm] diameter
 Detector 1 pixelation: x: 2.5 y: 5 [mm]
 Wavelength resolution d_lambda / lambda Detector 2: 12.1908 [%] FWHM of tophat shape
 Detector 2 pixelation: x: 5 y: 2.5 [mm]
 Wavelength resolution d_lambda / lambda Detector 3: 12.1908 [%] FWHM of tophat shape
 Detector 3 pixelation: x: 5 y: 2.5 [mm]
 Wavelength resolution d_lambda / lambda Detector 4: 12.3222 [%] FWHM of tophat shape
 Detector 4 pixelation: x: 2.5 y: 5 [mm]
 Wavelength resolution d_lambda / lambda Detector 5: 12.3222 [%] FWHM of tophat shape
 Detector 5 pixelation: x: 2.5 y: 5 [mm]

Averaging Current Display Data
 Rebinning
 Binning Version 'SPARSE'
done.... 0.017731[s]

Building Real-Shape Resolution Kernel for I vs. Q data
 Wavelength: Top-Hat (e.g. D33 TOF) Kernel
 Divergence: Geometric Divergence tophat Kernel
 Sample Aperture Smearing: Circular Kernel
 Detector Pixelation Smearing: Top-Hat Kernel
 Binning Resolution Smearing: Top-Hat Kernel

Using Real Shape Kernel (with Geometric Divergence)
 f >>

GRASP_Lockdown V9.18 - UI

File Display Analysis Instrument Data User Modules Grasp Script Help

Not over active figure (1)

Numer: 13 Subtitle: "Sample"

Worksheet: _____ Number: _____ Depth: _____
 foreground: Sample 1 60
 Background: Empty Cell
 Cadmium: Blocked Beam

Number(s): 13

Get III

Curve Fit Control

Fitting Function: FF_Sphere Minimiser: Levenberg-Marquar...

No. of Functions: 1 Curve Number: 1

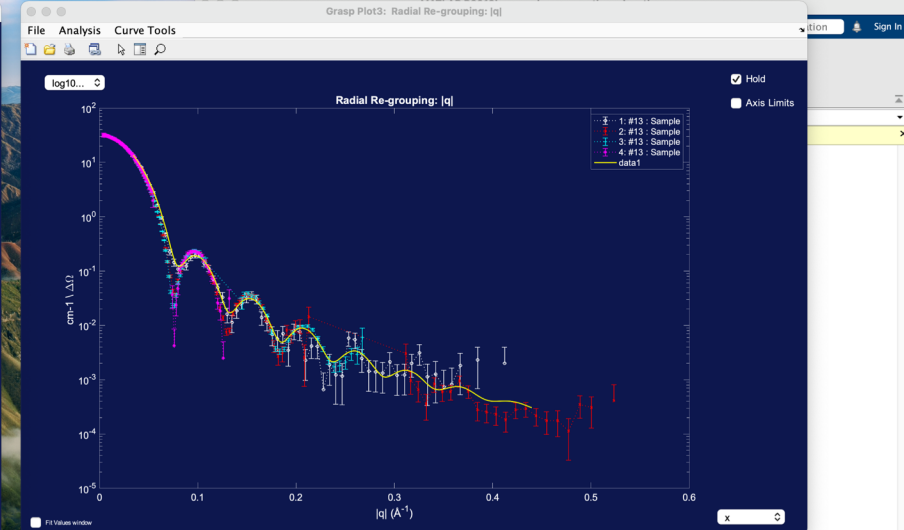
Include Resolution: Fit All Curves:

Parameters:	fix	value	err	group
Background [cm-1]: y0:	<input checked="" type="checkbox"/>	0	0	<input type="checkbox"/>
Radius [A]: radius:	<input type="checkbox"/>	60	0	<input type="checkbox"/>
Contrast [A^-2]: contrast:	<input type="checkbox"/>	6e-06	0	<input type="checkbox"/>
Scale: scale:	<input checked="" type="checkbox"/>	0.01	0	<input type="checkbox"/>

$r_1 = (\text{radius}) * x$; $\%r [A] * q [A^{-1}]$ [Unitless]
 $\text{contrast} = \text{contrast} * 1e8 * 1e8$; $\% \text{convert} [A^{-2}] \text{ to } [cm^{-2}]$;
 $V = (4/3) * pi * (\text{radius} * 1e-8)^3$; $\% \text{Scatterer Volume in } [cm^3]$
 $v = v_0 * (1 + \text{radius} * V) * CM * \text{contrast} * (1 + \text{radius} * 1e-8) * (1 + \text{radius} * 1e-8) / (1 + \text{radius} * 1e-8)$

Copy to Clip

Auto_Guess Point & Click Fit III Del Curve



Wavelength resolution d_{λ} / λ Detector 1: 11.8357 [%] FWHM of tophat shape
 Effective source is Square of dimensions: 30 (mm) x 30 (mm) at a distance of: 5.3 (m)
 Sample aperture: assuming Circular 10 [mm] diameter
 Detector 1 pixelation: x: 2.5 y: 5 [mm]
 Wavelength resolution d_{λ} / λ Detector 2: 12.1908 [%] FWHM of tophat shape
 Detector 2 pixelation: x: 5 y: 2.5 [mm]
 Wavelength resolution d_{λ} / λ Detector 3: 12.1908 [%] FWHM of tophat shape
 Detector 3 pixelation: x: 5 y: 2.5 [mm]
 Wavelength resolution d_{λ} / λ Detector 4: 12.3222 [%] FWHM of tophat shape
 Detector 4 pixelation: x: 2.5 y: 5 [mm]
 Wavelength resolution d_{λ} / λ Detector 5: 12.3222 [%] FWHM of tophat shape
 Detector 5 pixelation: x: 2.5 y: 5 [mm]

Averaging Current Display Data
 Rebinning
 Binning Version 'SPARSE'
done..... 0.017731[s]

Building Real-Shape Resolution Kernel for I vs. Q data
 Wavelength: Top-Hat (e.g. D33 TOF) Kernel
 Divergence: Geometric Divergence tophat Kernel
 Sample Aperture Smearing: Circular Kernel
 Detector Pixelation Smearing: Top-Hat Kernel
 Binning Resolution Smearing: Top-Hat Kernel

Using Real Shape Kernel (with Geometric Divergence)
 Loading 1D Fitting List
 Loading 1D Fit Function: ----General Functions----
 Loading 1D Fit Function: FF_Sphere

fg >>

GRASP_Lockdown V9.18 - UI

File Display Analysis Instrument Data User Modules Grasp Script Help

Not over active figure (1)

Numer: 13 Subtitle: "Sample"

Worksheet: _____ Number: _____ Depth: _____
 foreground: Sample 1 60
 Background: Empty Cell
 Cadmium: Blocked Beam

Number(s): 13

Get III

Curve Fit Control

Fitting Function: FF_Sphere Minimiser: Levenberg-Marquar...

No. of Functions: 1 Curve Number: 2

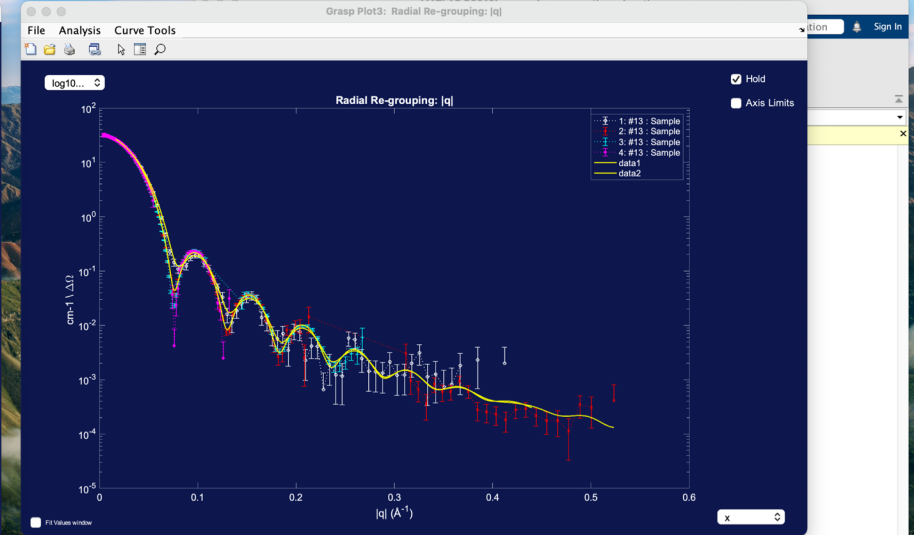
Include Resolution: Fit All Curves:

Parameters:	fix	value	err	group
Background [cm-1]: y0:	<input checked="" type="checkbox"/>	0	0	<input type="checkbox"/>
Radius [A]: radius:	<input type="checkbox"/>	60	0	<input type="checkbox"/>
Contrast [A^-2]: contrast:	<input type="checkbox"/>	6e-06	0	<input type="checkbox"/>
Scale: scale:	<input checked="" type="checkbox"/>	0.01	0	<input type="checkbox"/>

$r = (\text{radius}) * x$; $\%r [A] * q [A^{-1}]$ [Unitless]
 $\text{contrast} = \text{contrast} * 1e8 * 1e8$; $\% \text{convert} [A^{-2}] \text{ to } [\text{cm}^{-2}]$;
 $V = (4/3) * \pi * (\text{radius} * 1e-8)^3$; $\% \text{Scatterer Volume in } [\text{cm}^3]$;
 $v = v0 + (v \cdot \text{radius} * V) * \text{CMF} * \text{contrast} * (1 + \text{radius} * \text{radius}) / (\text{radius} * V)$

Copy to Clip

Auto_Guess Point & Click Fit III Del Curve



5

1

1

or Mask:
 ip Mask:

0.001
 0.05
 0.5
 0.75

Averaging Current Display Data
 Rebinning
 Binning Version 'SPARSE'
done.... 0.017731[s]

Building Real-Shape Resolution Kernel for I vs. Q data
 Wavelength: Top-Hat (e.g. D33 TOF) Kernel
 Divergence: Geometric Divergence tophat Kernel
 Sample Aperture Smearing: Circular Kernel
 Detector Pixelation Smearing: Top-Hat Kernel
 Binning Resolution Smearing: Top-Hat Kernel

Using Real Shape Kernel (with Geometric Divergence)
 Loading 1D Fitting List
 Loading 1D Fit Function: ----General Functions----
 Loading 1D Fit Function: FF_Sphere

fg >>

GRASP_Lockdown V9.18 - UI

File Display Analysis Instrument Data User Modules Grasp Script Help

Not over active figure (1)

Numer: 13 Subtitle: "Sample"

Worksheet: _____ Number: _____ Depth: _____
 foreground: Sample 1 60
 Background: Empty Cell
 Cadmium: Blocked Beam

Number(s): 13

Get III

Curve Fit Control

Fitting Function: FF_Sphere Minimiser: Levenberg-Marquar...

No. of Functions: 1 Curve Number: 3

Include Resolution: Fit All Curves:

Parameters:	fix	value	err	group
Background [cm-1]: y0:	<input checked="" type="checkbox"/>	0	0	<input type="checkbox"/>
Radius [A]: radius:	<input type="checkbox"/>	60	0	<input type="checkbox"/>
Contrast [A^-2]: contrast:	<input type="checkbox"/>	6e-06	0	<input type="checkbox"/>
Scale: scale:	<input checked="" type="checkbox"/>	0.01	0	<input type="checkbox"/>

$r_1 = (\text{radius}) * x$; $\%r [A] * q [A^{-1}]$ [Unitless]
 $\text{contrast} = \text{contrast} * 1e8 * 1e8$; $\% \text{convert} [A^{-2}] \text{ to } [cm^{-2}]$;
 $V = (4/3) * pi * (\text{radius} * 1e-8)^3$; $\% \text{Scatterer Volume in } [cm^3]$;
 $v = v_0 + (v_{\text{total}} * V) * (CM * \text{contrast} * 1e8) * (cm^3 * 1e6) / (ml * 10^3) * 10^3$

Copy to Clip

Auto_Guess Point & Click Fit III Del Curve

GRASP_Lockdown V9.18 (c)2021, e-mail: dewhurst@llnl.fr Post-Av Stats Filter dIII >

Grasp Plot3: Radial Re-grouping: [q]

File Analysis Curve Tools

log10... C

Radial Re-grouping: [q]

Hold
 Axis Limits

1: #13 Sample
 2: #13 Sample
 3: #13 Sample
 4: #13 Sample
 data1
 data2
 data3

Fit Values window

Wavelength resolution d_{λ} / λ Detector 1: 11.8357 [%] FWHM of tophat shape
 Effective source is Square of dimensions: 30 (mm) x 30 (mm) at a distance of: 5.3 (m)
 Sample aperture: assuming Circular 10 [mm] diameter
 Detector 1 pixelation: x: 2.5 y: 5 [mm]
 Wavelength resolution d_{λ} / λ Detector 2: 12.1908 [%] FWHM of tophat shape
 Detector 2 pixelation: x: 5 y: 2.5 [mm]
 Wavelength resolution d_{λ} / λ Detector 3: 12.1908 [%] FWHM of tophat shape
 Detector 3 pixelation: x: 5 y: 2.5 [mm]
 Wavelength resolution d_{λ} / λ Detector 4: 12.3222 [%] FWHM of tophat shape
 Detector 4 pixelation: x: 2.5 y: 5 [mm]
 Wavelength resolution d_{λ} / λ Detector 5: 12.3222 [%] FWHM of tophat shape
 Detector 5 pixelation: x: 2.5 y: 5 [mm]

Averaging Current Display Data
 Rebinning
 Binning Version 'SPARSE'
done.... 0.017731[s]

Building Real-Shape Resolution Kernel for I vs. Q data
 Wavelength: Top-Hat (e.g. D33 TOF) Kernel
 Divergence: Geometric Divergence tophat Kernel
 Sample Aperture Smearing: Circular Kernel
 Detector Pixelation Smearing: Top-Hat Kernel
 Binning Resolution Smearing: Top-Hat Kernel

Using Real Shape Kernel (with Geometric Divergence)
 Loading ID Fitting List
 Loading ID Fit Function: ----General Functions----
 Loading ID Fit Function: FF_Sphere

f >>

GRASP_Lockdown V9.18 - UI

File Display Analysis Instrument Data User Modules Grasp Script Help

Not over active figure (1)

Numer: 13 Subtitle: "Sample"

Worksheet: _____ Number: _____ Depth: _____
 foreground: Sample 1 60
 Background: Empty Cell
 Cadmium: Blocked Beam

Number(s): 13

Get III

Curve Fit Control

Fitting Function: FF_Sphere Minimiser: Levenberg-Marquar...

No. of Functions: 1 Curve Number: 4

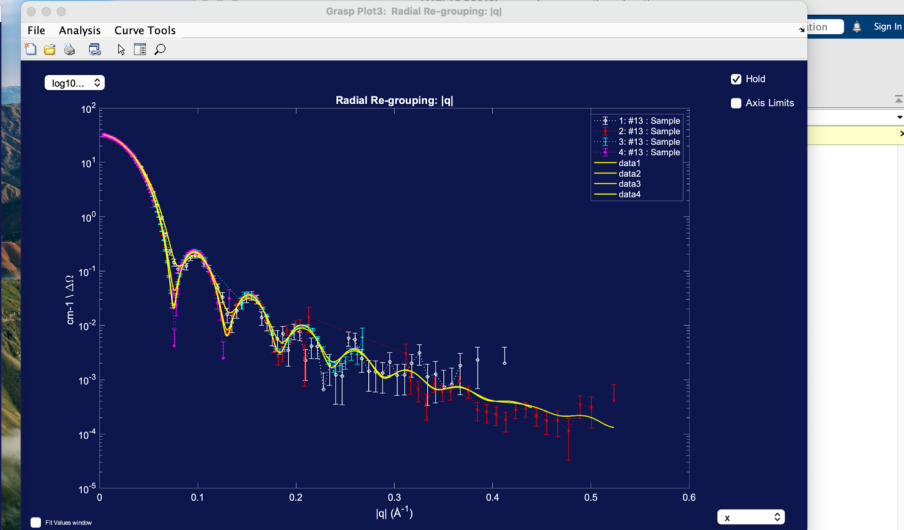
Include Resolution: Fit All Curves:

Parameters:	fix	value	err	group
Background [cm-1]: y0:	<input checked="" type="checkbox"/>	0	0	<input type="checkbox"/>
Radius [A]: radius:	<input type="checkbox"/>	60	0	<input type="checkbox"/>
Contrast [A^-2]: contrast:	<input type="checkbox"/>	6e-06	0	<input type="checkbox"/>
Scale: scale:	<input checked="" type="checkbox"/>	0.01	0	<input type="checkbox"/>

$r_1 = (\text{radius}) * x$; $\%r [A] * q [A^{-1}]$ [Unitless]
 $\text{contrast} = \text{contrast} * 1e8 * 1e8$; $\% \text{convert} [A^{-2}] \text{ to } [cm^{-2}]$;
 $V = (4/3) * pi * (\text{radius} * 1e-8)^3$; $\% \text{Scatterer Volume in } [cm^3]$
 $v = v_0 * (1 + \text{radius} * V) * CM * \text{contrast} * (1 + \text{radius} * 1e-8)^3 / (ml * V * 1e9)$

Copy to Clip

Auto_Guess Point & Click Fit III Del Curve



Wavelength resolution d_{λ} / λ Detector 1: 11.8357 [%] FWHM of tophat shape
 Effective source is Square of dimensions: 30 (mm) x 30 (mm) at a distance of: 5.3 (m)
 Sample aperture: assuming Circular 10 [mm] diameter
 Detector 1 pixelation: x: 2.5 y: 5 [mm]
 Wavelength resolution d_{λ} / λ Detector 2: 12.1908 [%] FWHM of tophat shape
 Detector 2 pixelation: x: 5 y: 2.5 [mm]
 Wavelength resolution d_{λ} / λ Detector 3: 12.1908 [%] FWHM of tophat shape
 Detector 3 pixelation: x: 5 y: 2.5 [mm]
 Wavelength resolution d_{λ} / λ Detector 4: 12.3222 [%] FWHM of tophat shape
 Detector 4 pixelation: x: 2.5 y: 5 [mm]
 Wavelength resolution d_{λ} / λ Detector 5: 12.3222 [%] FWHM of tophat shape
 Detector 5 pixelation: x: 2.5 y: 5 [mm]

Averaging Current Display Data
 Rebinning
 Binning Version 'SPARSE'
done.... 0.017731[s]

Building Real-Shape Resolution Kernel for I vs. Q data
 Wavelength: Top-Hat (e.g. D33 TOF) Kernel
 Divergence: Geometric Divergence tophat Kernel
 Sample Aperture Smearing: Circular Kernel
 Detector Pixelation Smearing: Top-Hat Kernel
 Binning Resolution Smearing: Top-Hat Kernel

Using Real Shape Kernel (with Geometric Divergence)
 Loading 1D Fitting List
 Loading 1D Fit Function: ----General Functions----
 Loading 1D Fit Function: FF_Sphere

fg >>

5

1

1

or Mask:

ip Mask:

0.001

0.05

0.5

0.75

GRASP_Lockdown V9.18 - UI

File Display Analysis Instrument Data User Modules Grasp Script Help

Not over active figure (1)

Numer: 13 Subtitle: "Sample"

Worksheet: _____ Number: _____ Depth: _____
tof

Foreground:

& Data Load: _____

Group:

Background:

or Reference: _____

Cadmium:

Numer(s):

Curve Fit Control

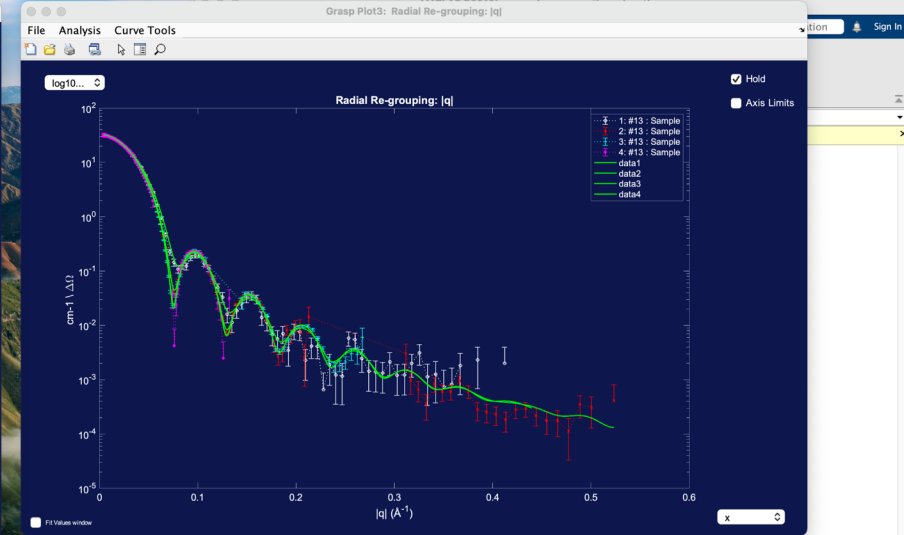
Fitting Function: Minimiser:

No. of Functions: Curve Number:

Include Resolution: Fit All Curves:

Parameters:	fix	value	err	group
Background [cm-1]: y0:	<input checked="" type="checkbox"/>	0	0	<input type="checkbox"/>
Radius [A]: radius:	<input type="checkbox"/>	60,122	0.029226	<input type="checkbox"/>
Contrast [A^-2]: contrast:	<input type="checkbox"/>	5.9859e-06	4.1300e-09	<input type="checkbox"/>
Scale: scale:	<input checked="" type="checkbox"/>	0.01	0	<input type="checkbox"/>

$r_0 = (\text{radius}) * x$; $x_r [A] * q [A^{-1}]$ [Unitless]
 $\text{contrast} = \text{contrast} * 1e8 * 1e8$; $\% \text{convert} [A^{-2}] \text{ to } [cm^{-2}]$;
 $V = (4/3) * \pi * (\text{radius} * 1e-8)^3$; $\% \text{Scatterer Volume in } [cm^3]$;
 $v = v_0 + (v_{\text{solid}} * V) * (\text{contrast} * 1e8) * (\text{radius} * 1e-8) / (m_0 * 1.21 * 10^2)$



```

1      0.03      2.175
Iteration 3 (max 100)
2      0.03      2.175
Iteration 4 (max 100)
3      0.03      2.175

Covariance Checking

Elapsed time is 0.170533 seconds.

Covariance Checking
Fitting: iteration 1
*Beginning fit (max 100 iterations)
-----
Iteration Time(s) Reduced Chi^2
Iteration 2 (max 100)
1      0.02      2.175

Covariance Checking

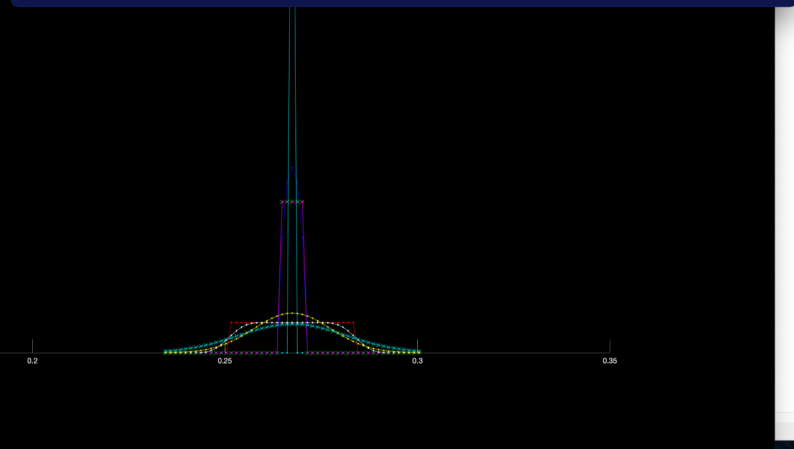
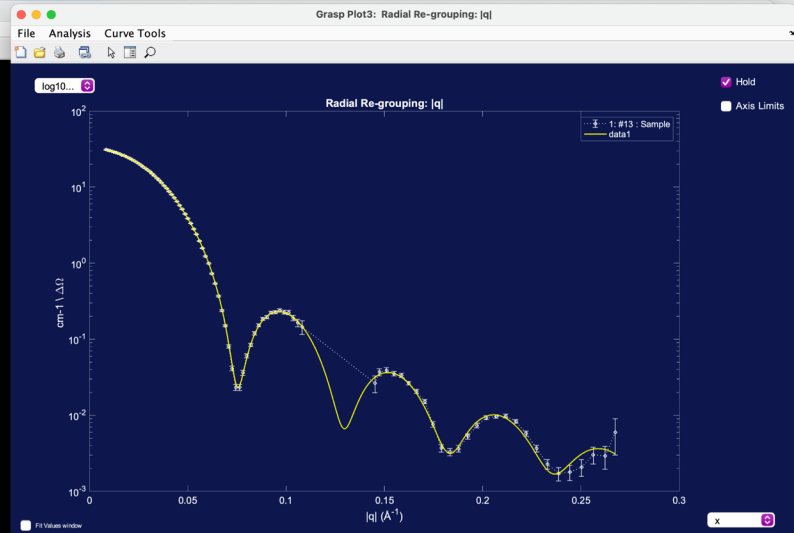
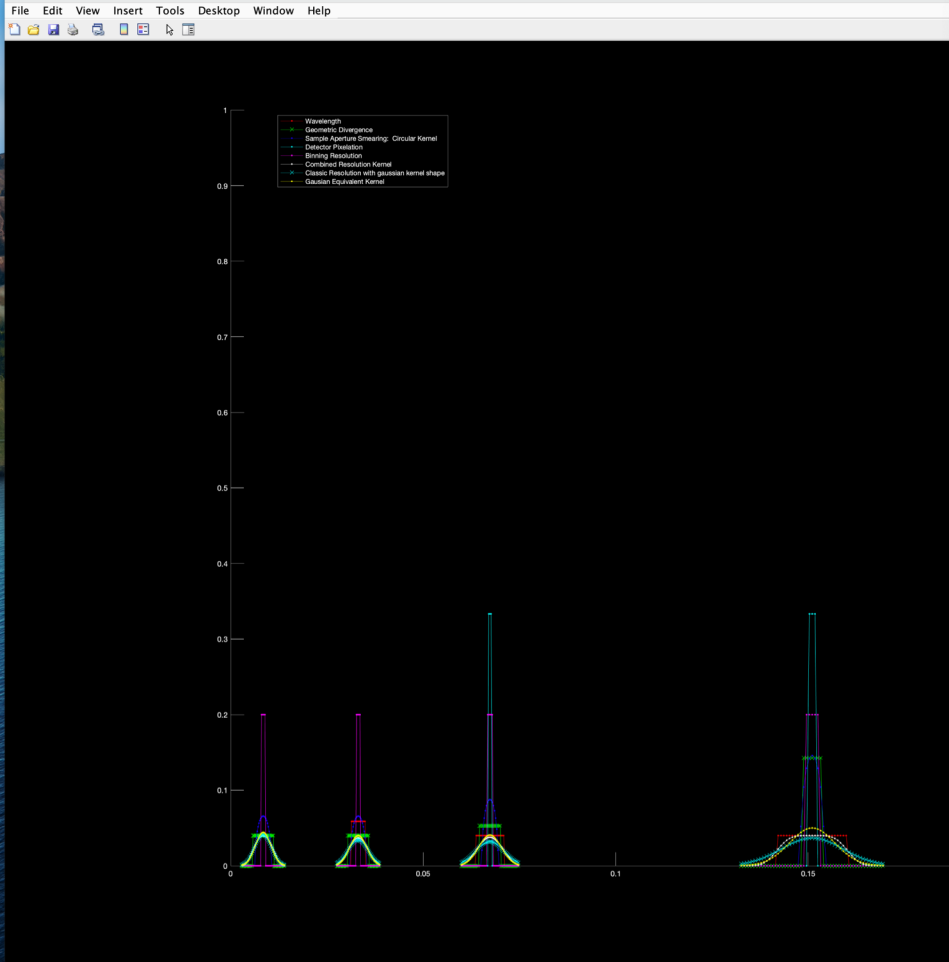
Fitting: iteration 1
*Beginning fit (max 100 iterations)
-----
Iteration Time(s) Reduced Chi^2

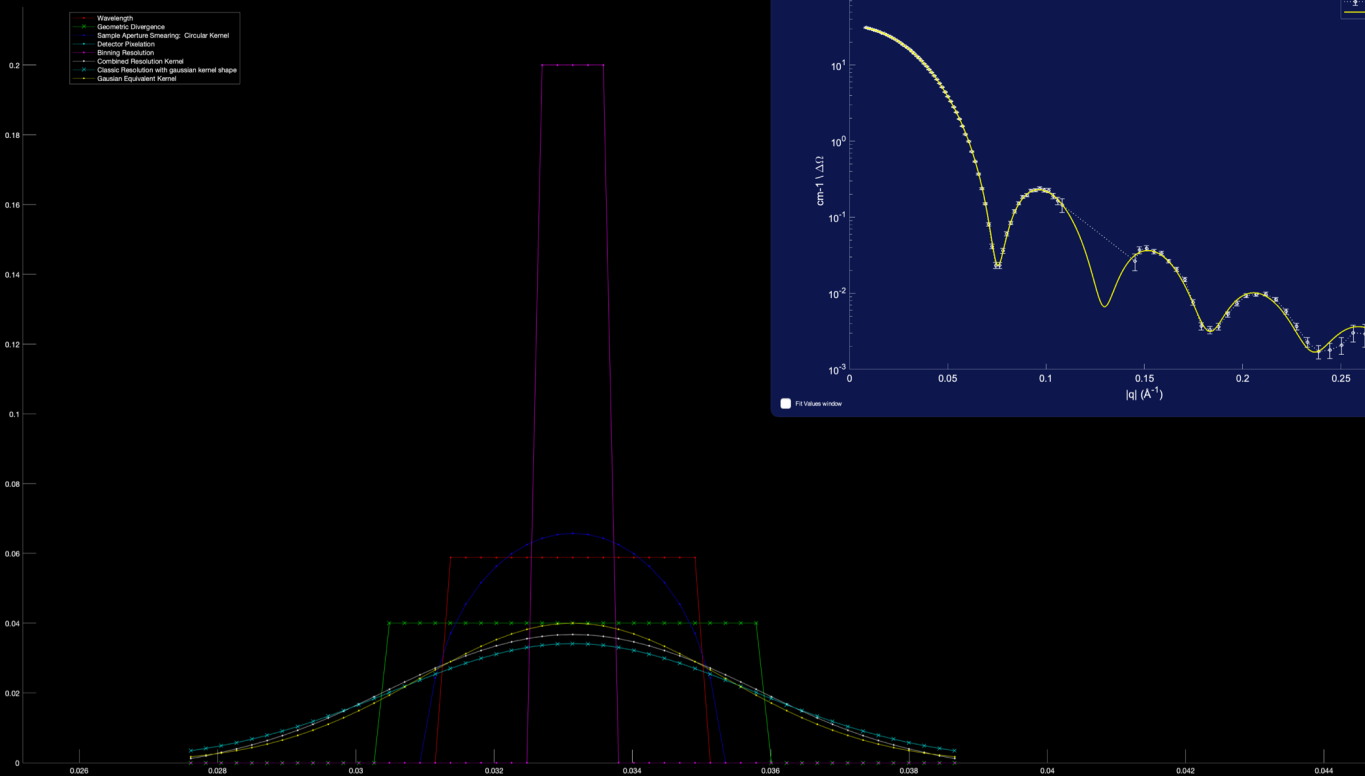
Covariance Checking

Covariance Corrected Fit Params
Chi^2 = 2.175

f >>
    
```

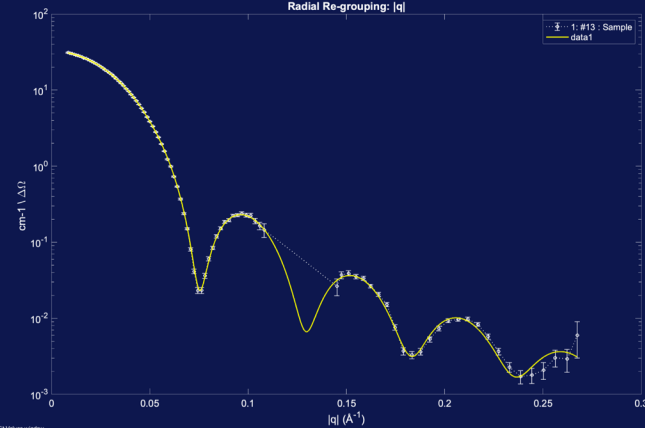
Figure 3





log10...

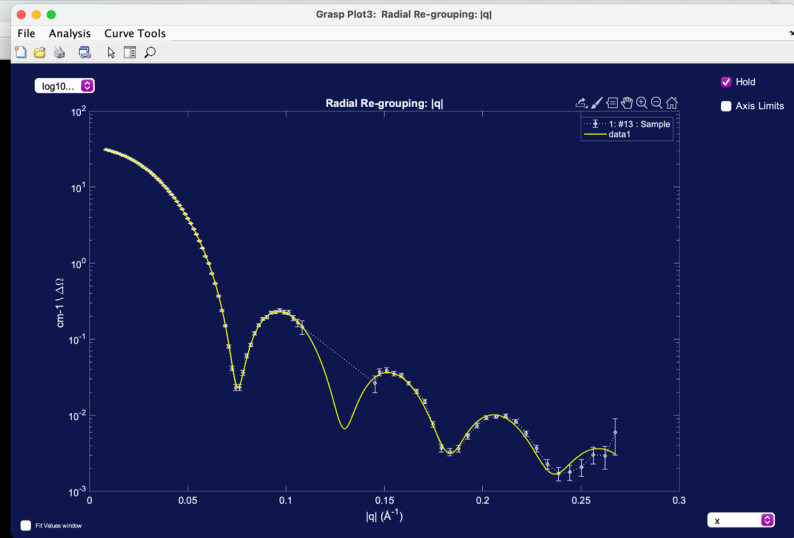
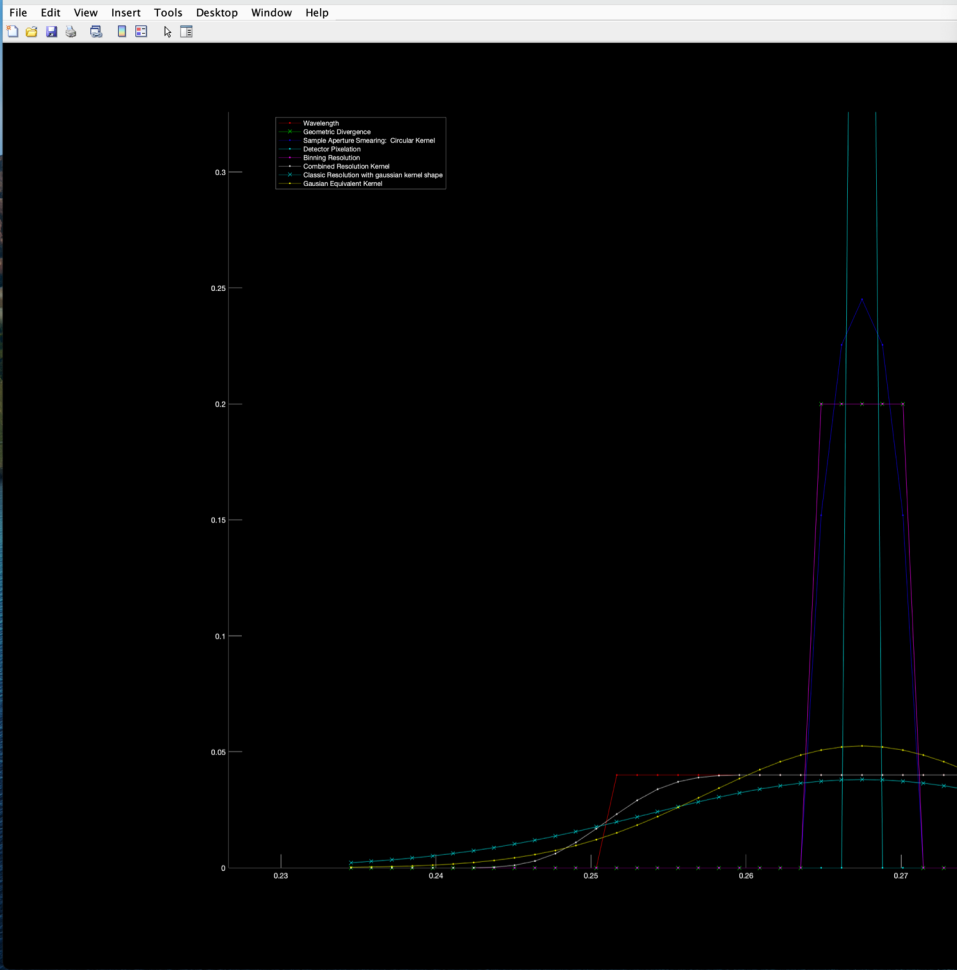
Radial Re-grouping: |q|



Fit Values window

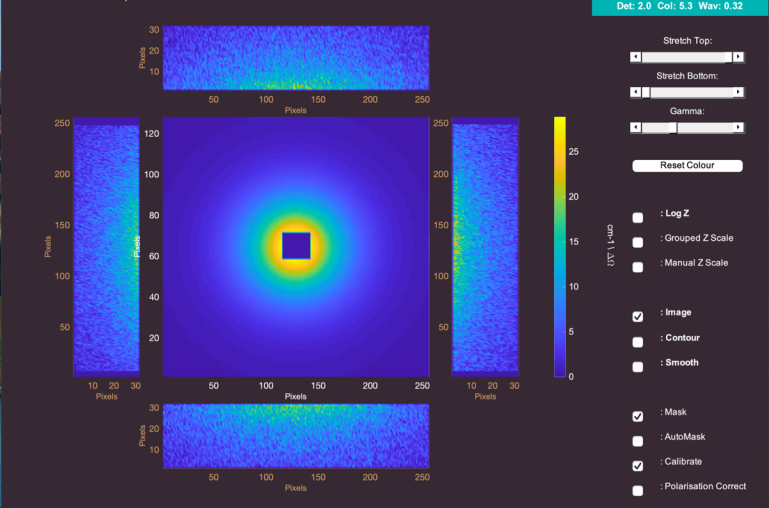
x

Figure 3



Numer: 13 Subtitle: "Sample"

ILL: d13
Nrm: mon Dt: off Tc: on
Det: 2.0 Col: 5.3 Wav: 0.32



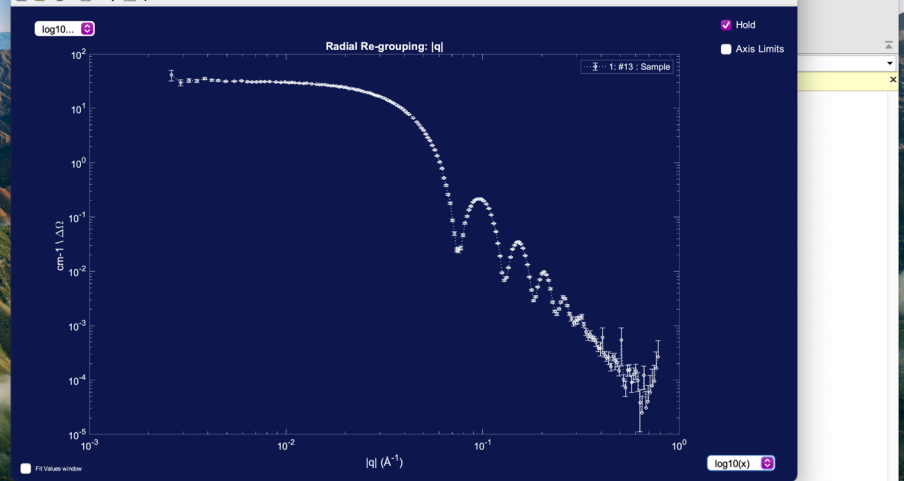
Worksheet: _____ Number: _____ Depth: _____

Foreground: Sample 1 sum
Background: Empty Cell
Cadmium: Blocked Beam

T_s: 1 Lock: _____
T_e: 1 Lock: _____ Thickness (cm): 0.1 Lock: _____

Beam Centre: c_x: 128.4252 c_y: 64.5164 c_dtr: 0 Lock: _____
Centre Calc Reset

Numer(s): 13 .nxs
Get III Reset



Averaging

Radial fract. res. bins [q|q]: 5
Radial bins [pixels]: 1
Angle Bin [degs]: 1

Single Depth TOF

Use Sector Mask:
Use Strip Mask:

Colors based on depth:
 Direct to File:

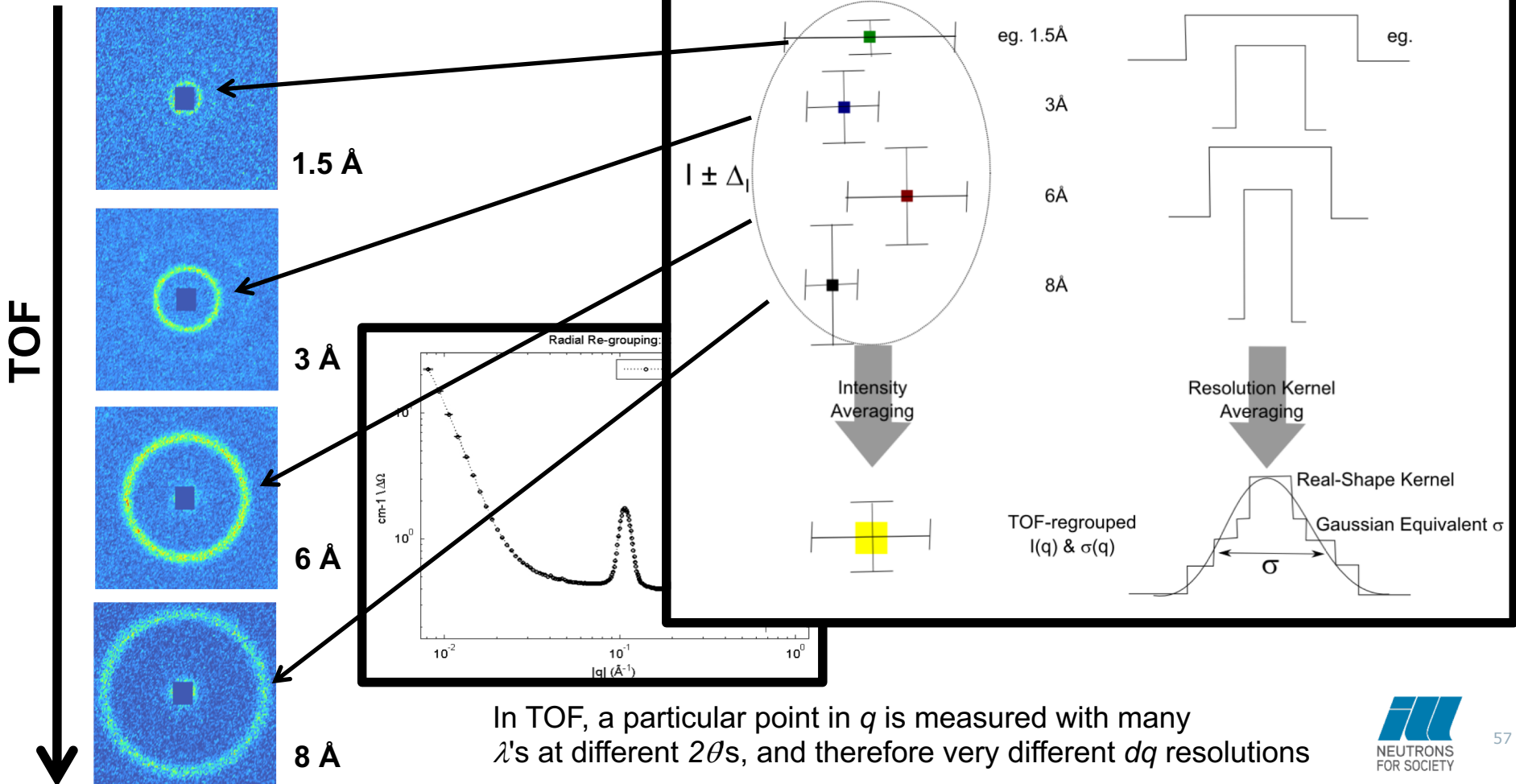
Pre-Av Sparse Data Filter 0.001
 Pre-Av Transmission Filter d/T 0.05
 Pre-Av Resolution Filter dq/q 0.5
 Post-Av Stats Filter d/I 0.75

```

Rejecting detector Frame:7 ; Det: 4 due to Sparse Raw Data
Detector 5 data empty
Rejecting detector Frame:8 ; Det: 2 due to Sparse Raw Data
Rejecting detector Frame:8 ; Det: 3 due to Sparse Raw Data
Rejecting detector Frame:8 ; Det: 4 due to Sparse Raw Data
Detector 5 data empty
Rejecting detector Frame:9 ; Det: 2 due to Sparse Raw Data
Rejecting detector Frame:9 ; Det: 3 due to Sparse Raw Data
Rejecting detector Frame:9 ; Det: 4 due to Sparse Raw Data
Rejecting detector Frame:9 ; Det: 5 due to Sparse Raw Data
Rejecting detector Frame:10 ; Det: 2 due to Sparse Raw Data
Rejecting detector Frame:10 ; Det: 3 due to Sparse Raw Data
Rejecting detector Frame:10 ; Det: 4 due to Sparse Raw Data
Detector 4 data empty
Rejecting detector Frame:14 ; Det: 5 due to Sparse Raw Data
Rejecting detector Frame:15 ; Det: 2 due to Sparse Raw Data
Rejecting detector Frame:15 ; Det: 3 due to Sparse Raw Data
Rejecting detector Frame:16 ; Det: 2 due to Sparse Raw Data
Rejecting detector Frame:16 ; Det: 3 due to Sparse Raw Data
Rejecting detector Frame:77 ; Det: 5 due to Sparse Raw Data
Rejecting detector Frame:86 ; Det: 4 due to Sparse Raw Data
Rejecting detector Frame:87 ; Det: 2 due to Sparse Raw Data
Rejecting detector Frame:95 ; Det: 2 due to Sparse Raw Data
Rejecting detector Frame:95 ; Det: 3 due to Sparse Raw Data
Detector 4 data empty
Detector 5 data empty
Rejecting detector Frame:96 ; Det: 4 due to Sparse Raw Data
Rejecting detector Frame:96 ; Det: 5 due to Sparse Raw Data
Rebinning .....
Binning Version 'FIND'
.....done.... 1.6957[s]
fg >>

```


Regrouping of time-of-flight SANS data



In TOF, a particular point in q is measured with many λ 's at different 2θ s, and therefore very different dq resolutions

