Background subtraction and normalization in SANS and SAXS

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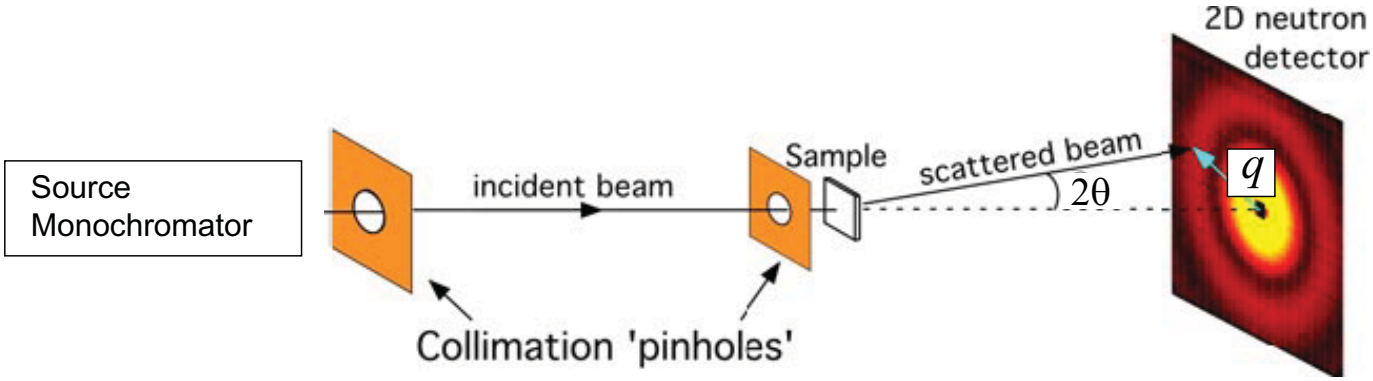
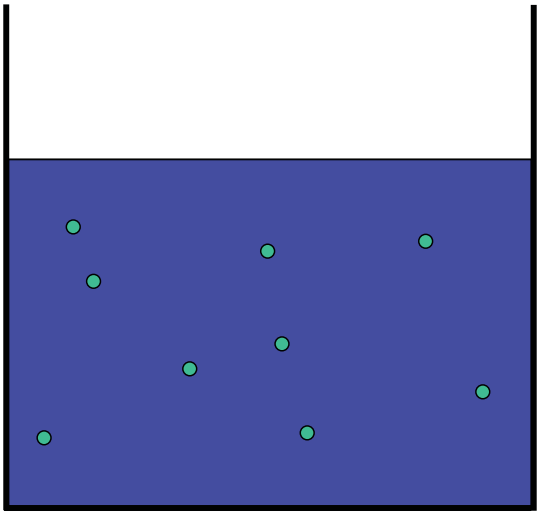
Schematic setup for small-angle scattering

Sample: Dilute solutions with 1% concentration



$$q \equiv 4\pi \sin\theta / \lambda$$

Sample



Dilute solution (1% = 10 mg/mL) of particles

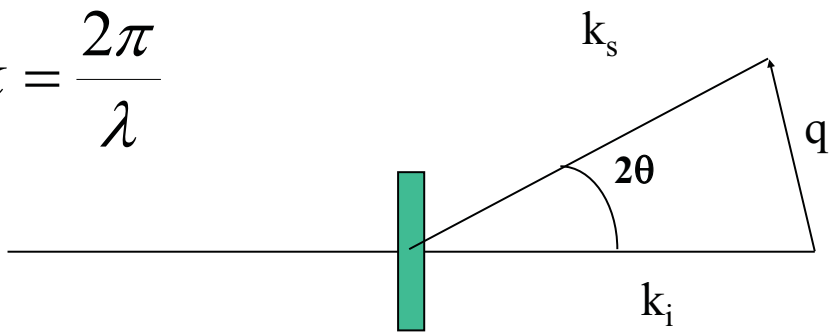
➔random orientation of particles
➔centro symmetric intensity distribution on detector

<u>Scattering vector *q*</u>

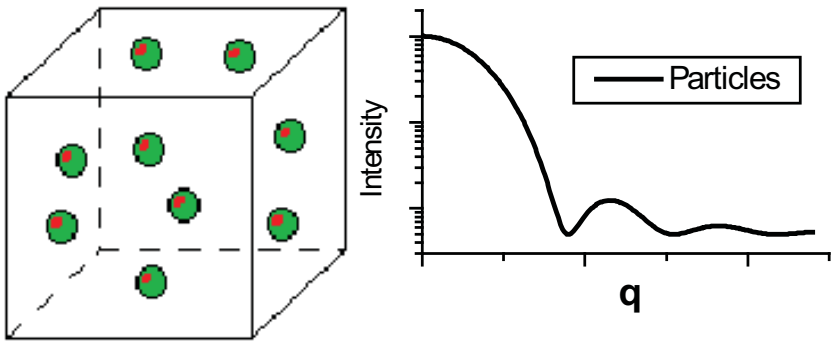
$$\boxed{q \equiv 4\pi \sin\theta / \lambda}$$

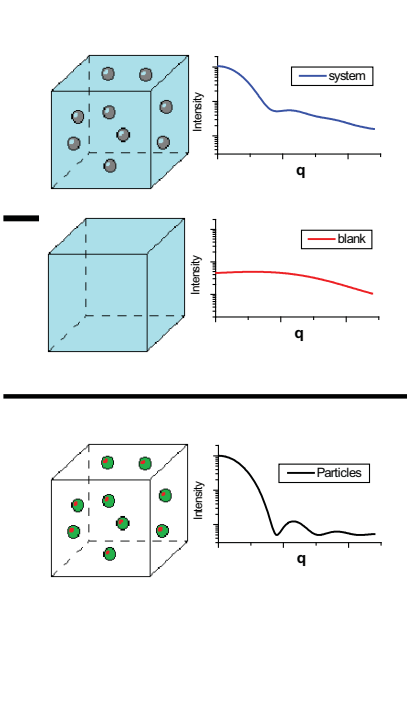
Bragg's Law: $$q = n\frac{2\pi}{d}$$

$$k = \frac{2\pi}{\lambda}$$



Data Treatment
Particles in Solution





Input data: Azimuthally averaged data

$$q_i, I(q_i), \sigma[I(q_i)] \quad i = 1,2,3,\ldots N$$

q_i calibrated

$I(q_i)$ calibrated, i.e. on absolute scale
- noisy, (smeared), truncated

$\sigma[I(q_i)]$ Statistical standard errors: Calculated from counting statistics by error propagation
- do not contain information on systematic error !!!!

Intensity and Differential Scattering Cross Section

$$I(q) = \frac{d\sigma}{d\Omega}(q)$$

number of scattered neutrons or photons per unit time, relative to the incident flux of neutron or photons, per unit solid angle at q per unit volume of the sample.

Unit : cm^{-1}

Absolute scale: SAXS

The absolute scattering of water can be calculated from the fundamental properties to be $I_{H2O}^{theory} = 0.0162\ cm^{-1}$.

$$I_{H2O} = nb^2 k_B T \chi_T$$

n: number density of molecules
b: scattering length of molecules
$k_B T$: thermal energy
χ_T: Isothermal compressibility

Convert to absolute scale using

$$\boxed{I_{abs}(q) = I(q)\frac{I_{H2O}^{theory}}{I_{H2O}^{\exp}}}$$

The same for static light scattering but toluene is usually used

Absolute scale: SANS

neutron and hydrogen parallel spins scatter very different from anti-parallel spins !

Random distribution -> incoherent scattering

$$I_{H2O}^{'theory'} = (1-T)/4\pi \; g(\lambda)$$

$g(\lambda)$ is an empirical factor
-varies with instrument and detector
-include corrections for inelactic effects anf multiple scattering

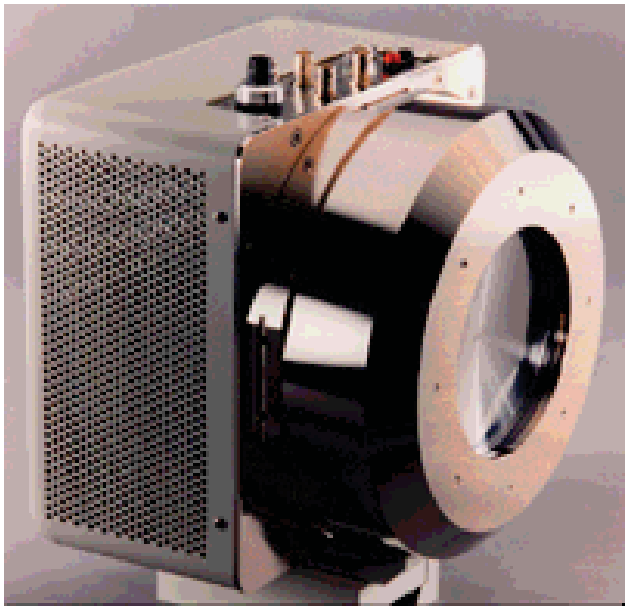
$$\boxed{I_{abs}(q) = I(q)\frac{I_{H2O}^{theory}}{I_{H2O}^{\exp}}}$$

SAXS data processing

1. SAXS NT (Bruker AXS)
   flood correction
   spatial correction
   azimuthal averaging
   (beamcenter)
   (distance calibration Ag-behenate)

2. Home-written software (SUPERSAXS package)
   conversion, inclusion of meta data
   plot
   background subtraction
   normalization (H2O)
   rebinning
   scaling…

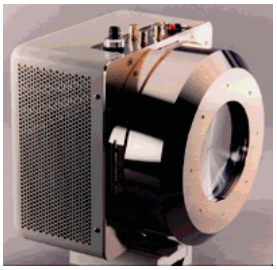
Multi-wire position sensitive detector



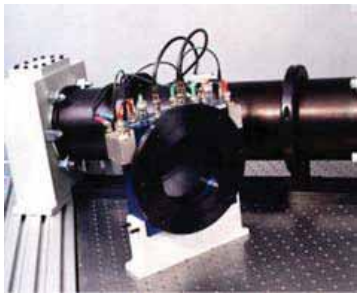
- High quantum efficinecy
- 0.5 mm (FWHM resolution)
- Saturation: 100’000 cps

11 cm

Multi-wire position sensitive detector

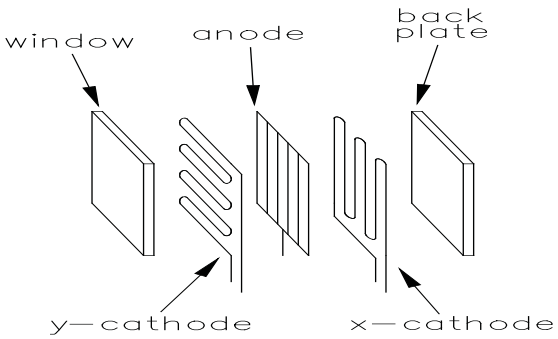


Bruker AXS’
HiSTAR detector



Gabriel type detector
sold by Molecular Metrology

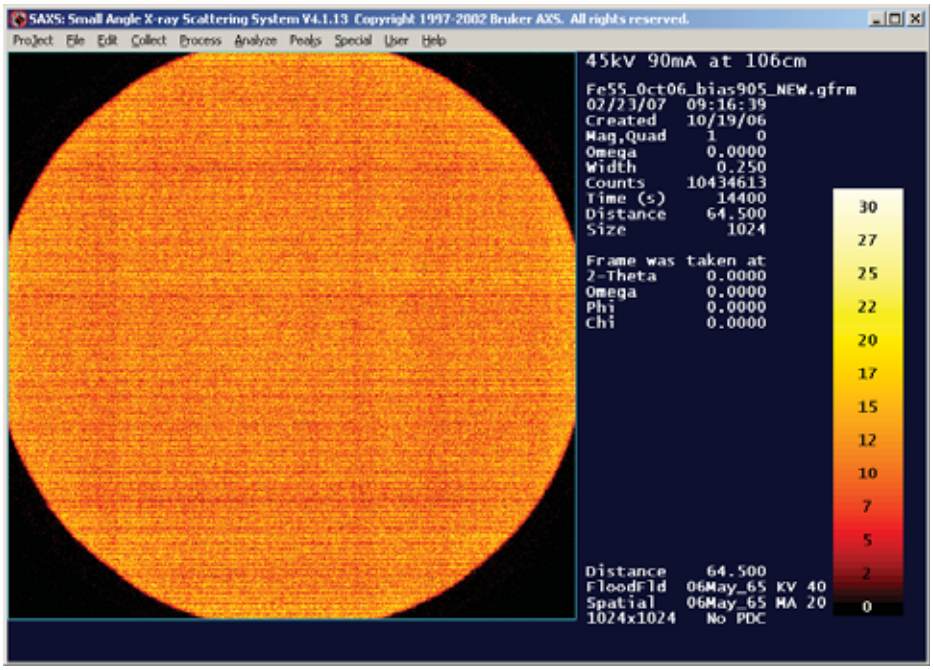
Photons converted to charge particles and electrons followed by gas amplification



Limit: about 100 000 cps

Flood correction:

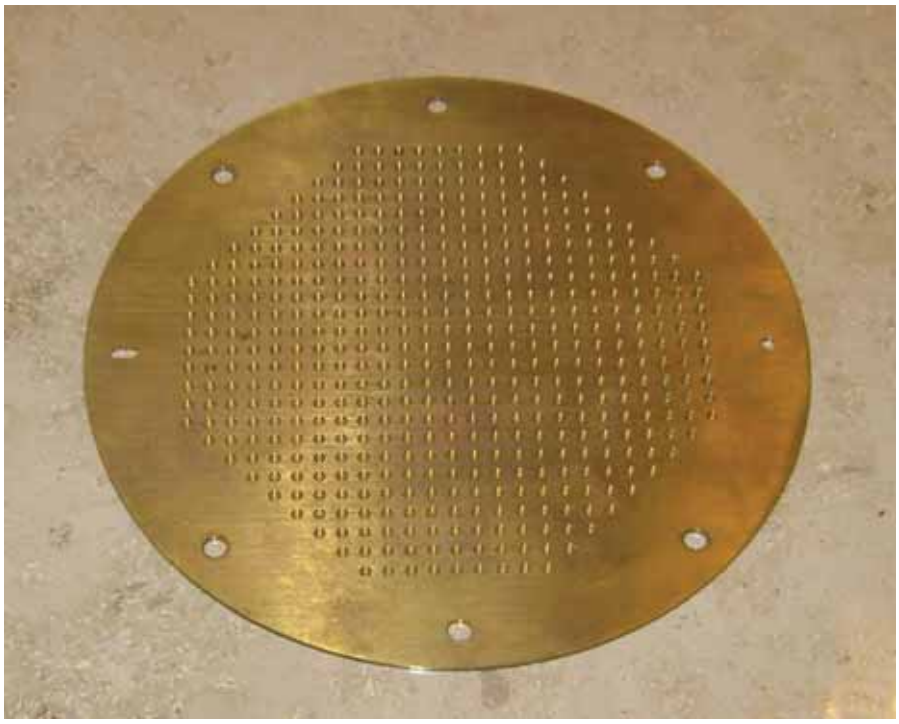
Use radioactive source ^{55}Fe decays to Mg and emits 5.8 keV x-rays (Cu Ka 8.0 keV!)



x and y projections used for correct to to uniform sensitivity

Spatial correction

Use plate with regularly spaced holes together with ^{55}Fe source



Spatial correction

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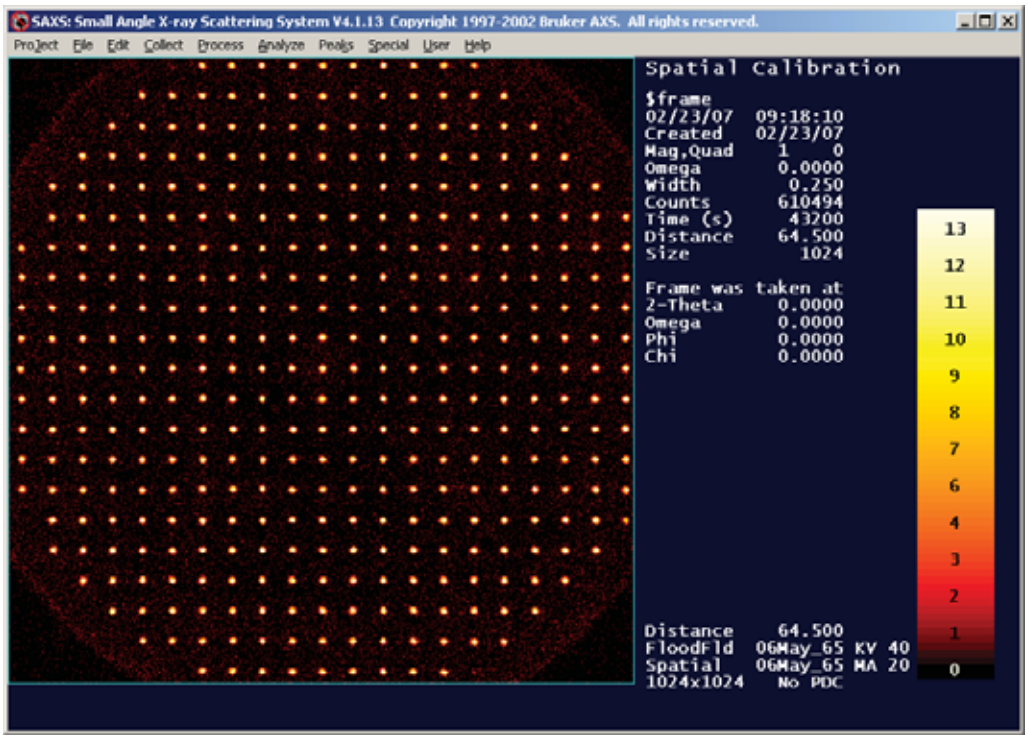
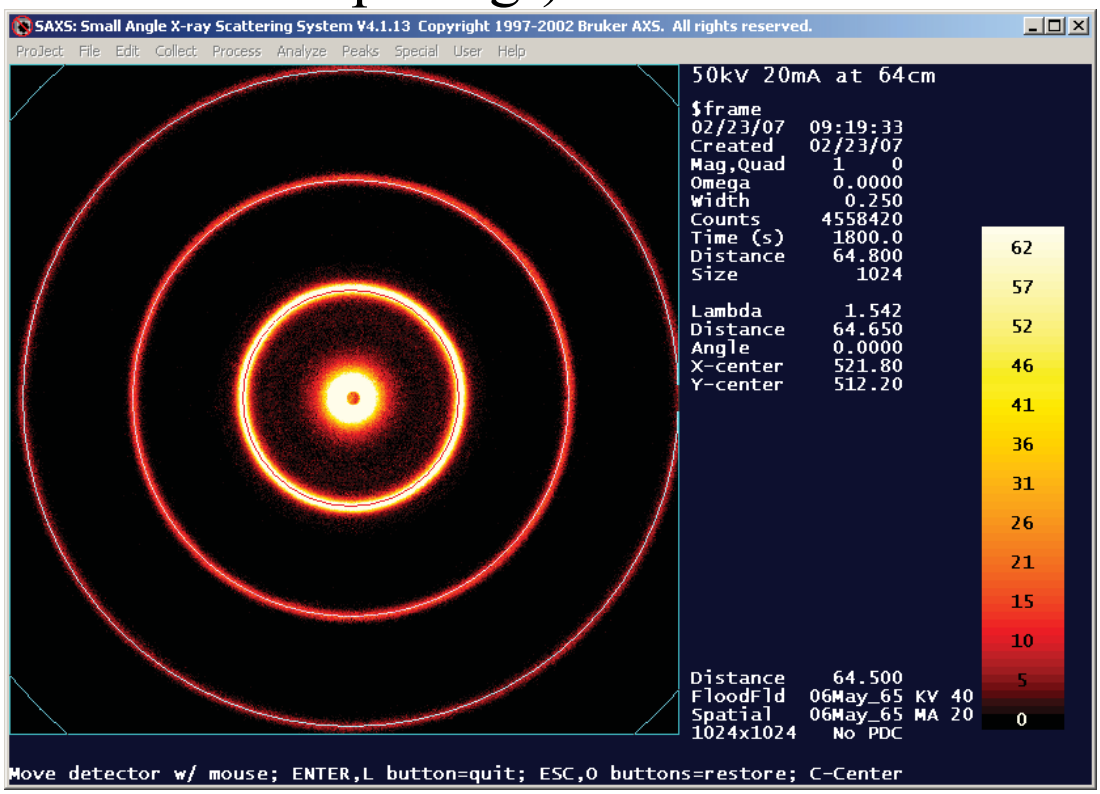
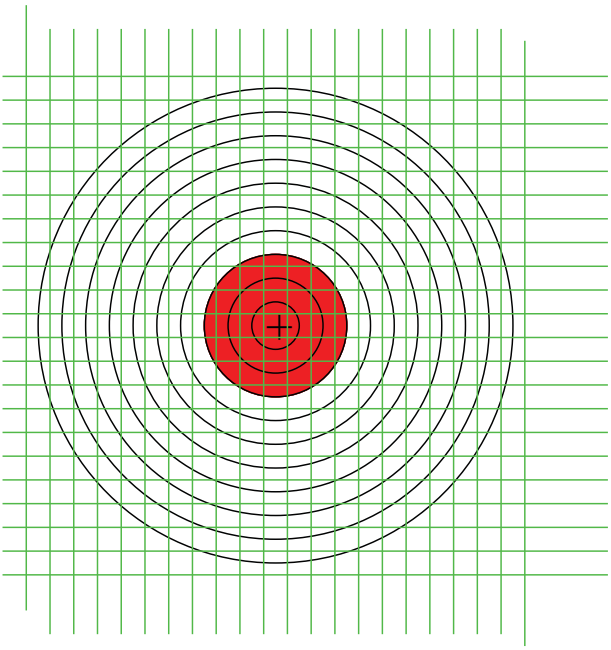


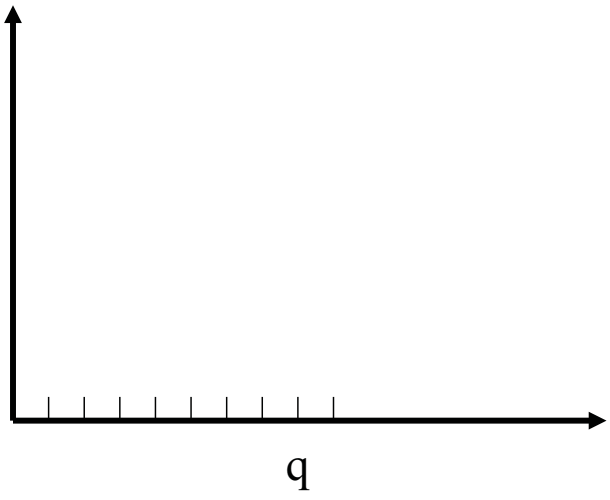
Local 'rubber' mask used for stretchin/compressing scales to map on uniform spacing

Distance calibration with Ag behenate (known lattice spacing!)

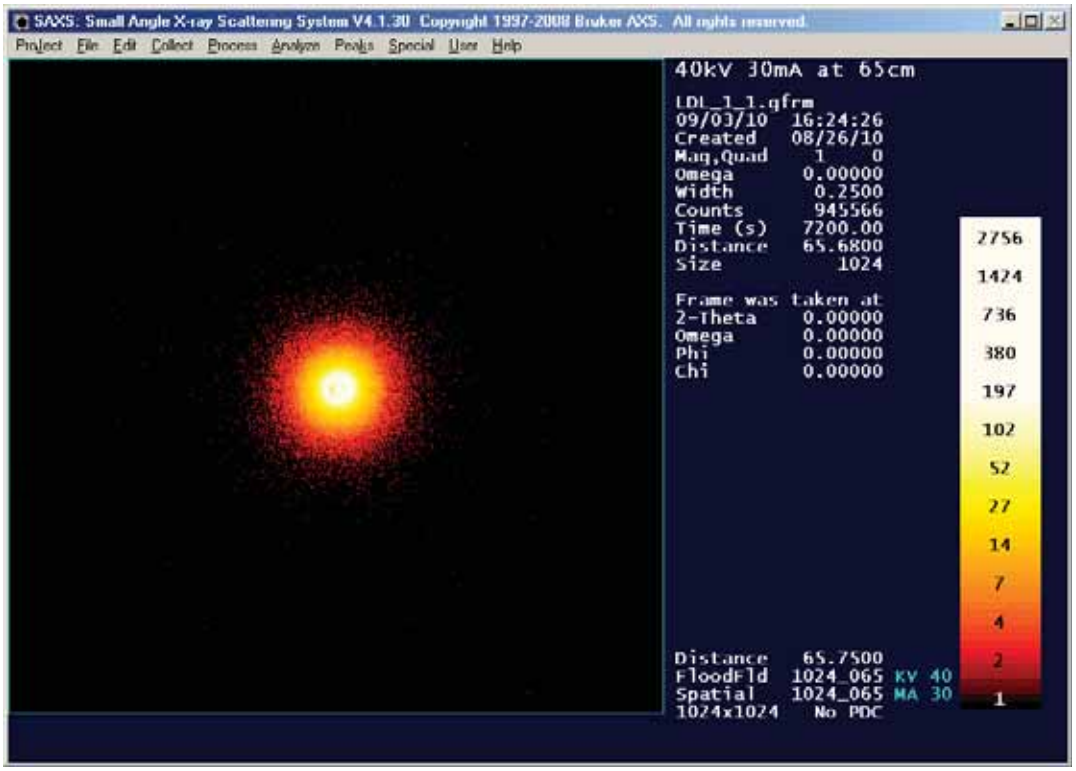


Azimuthal integration (beamcenter !)

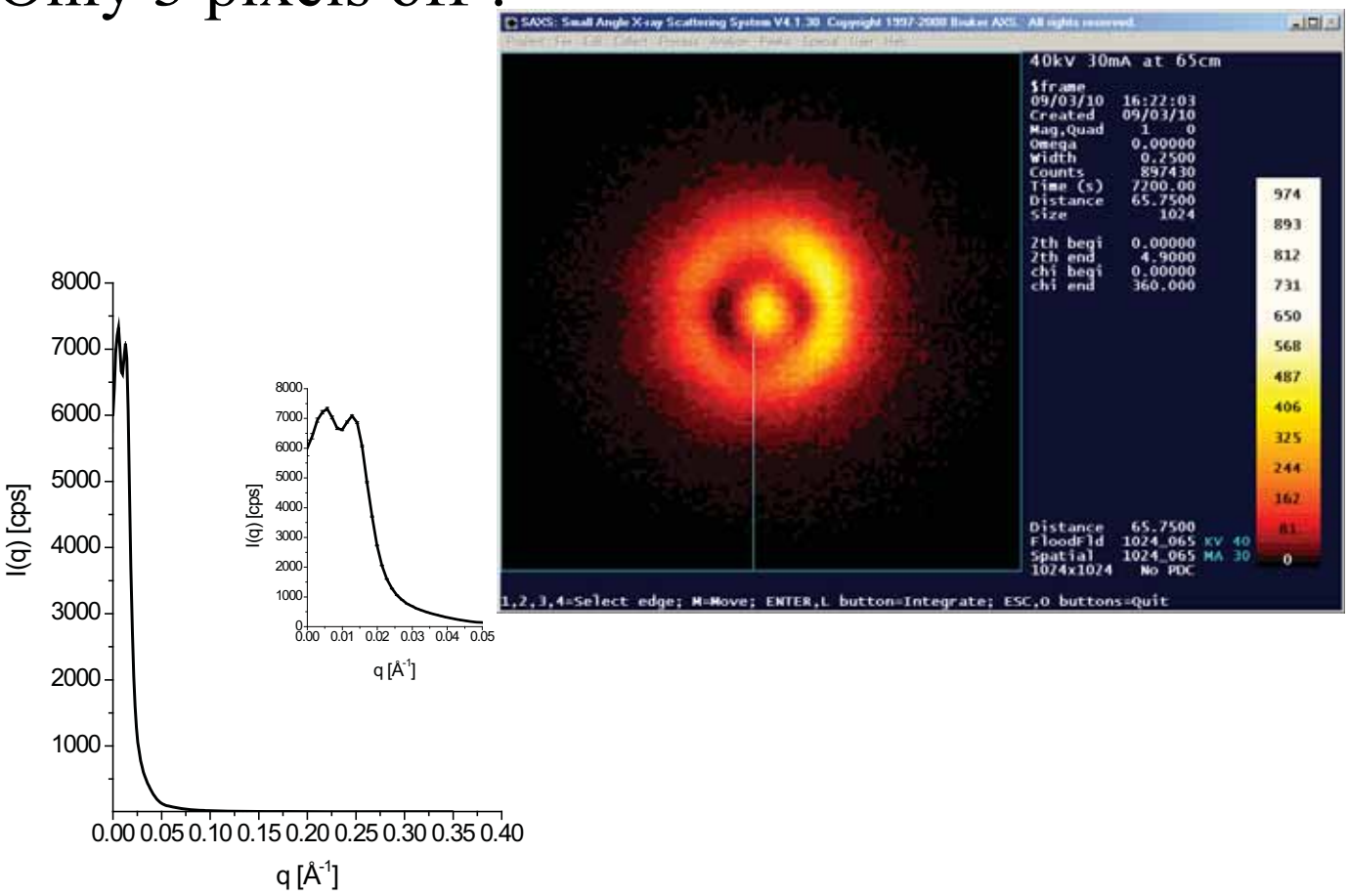




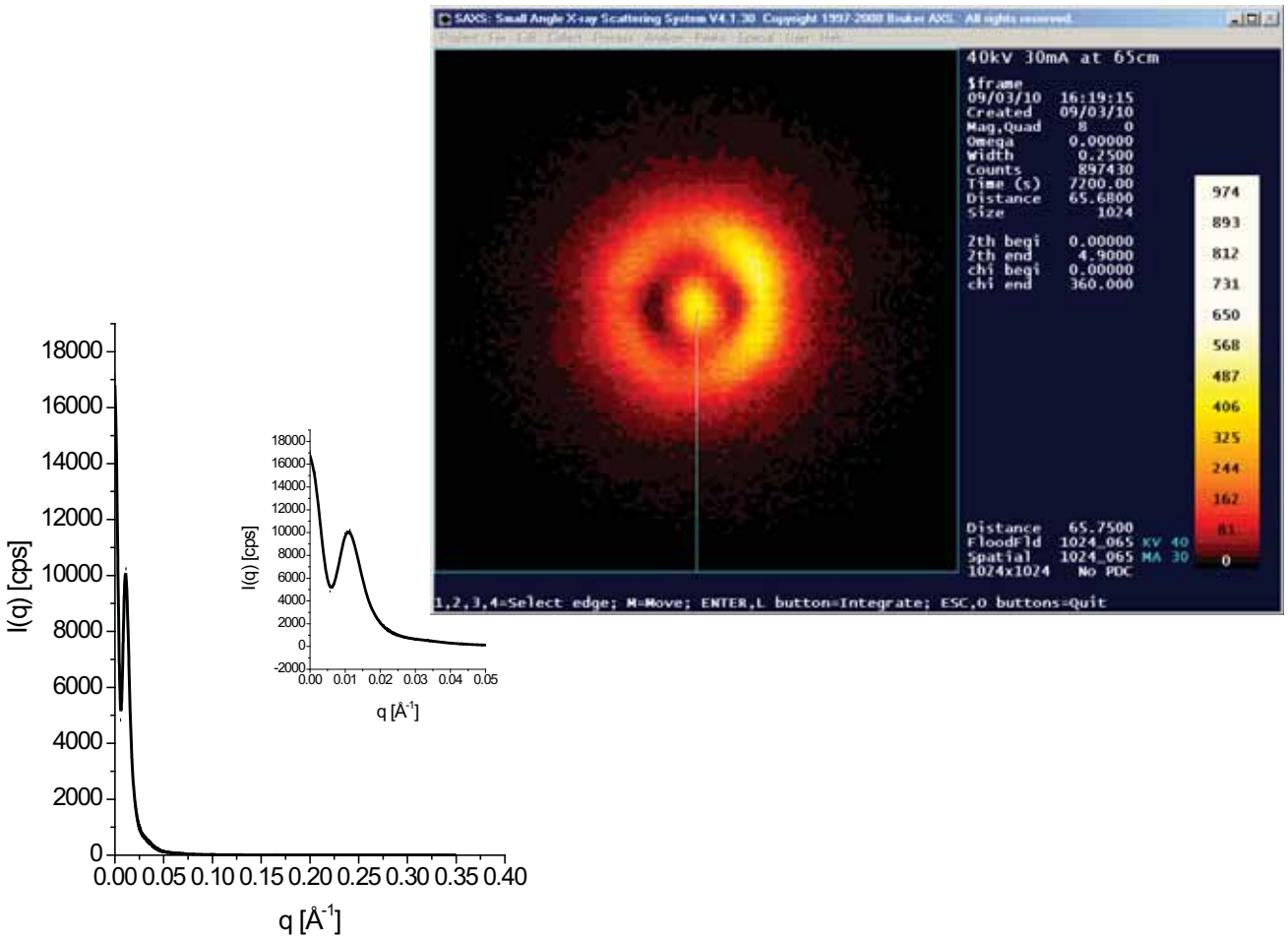
Center Misalignment

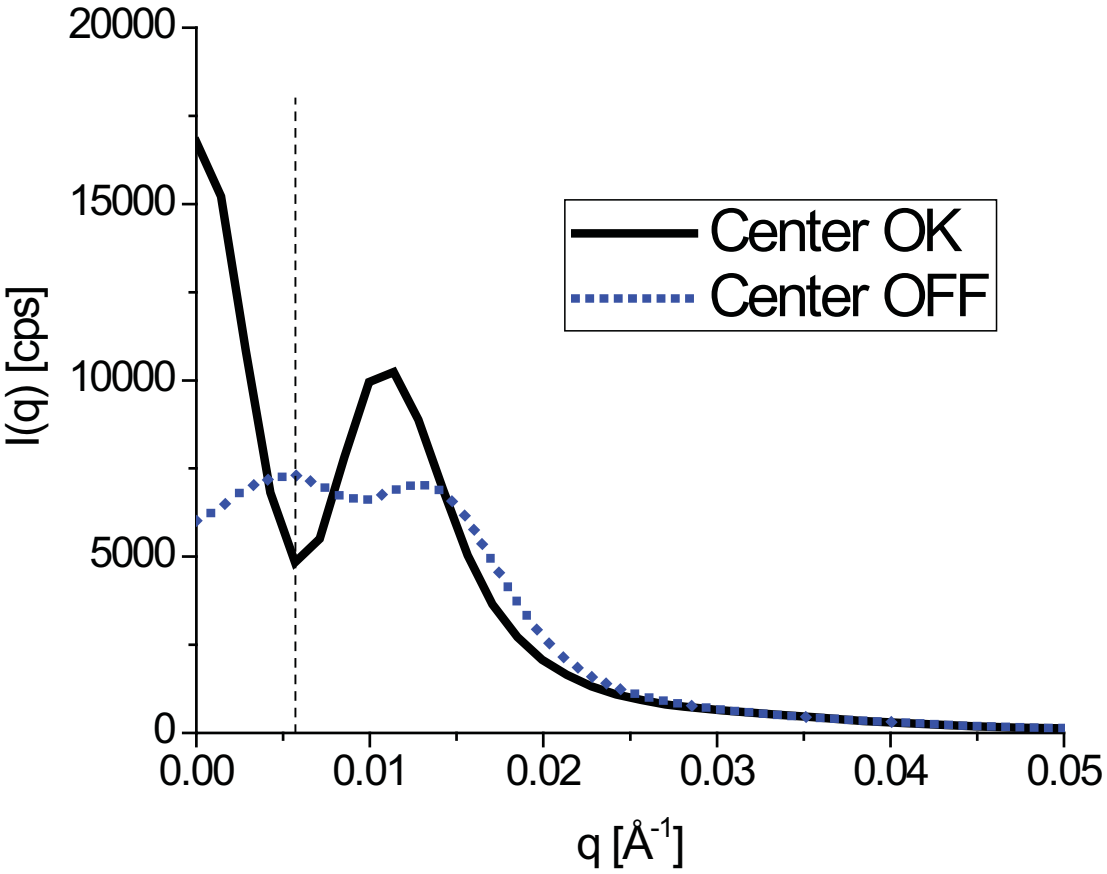


Only 3 pixels off !



Center Corrected !





Raw format: comment lines, then: theta, I, sig(I),q

```
!@!!GADDS PLOTSO FILE: Chi integration type
!@!!Title: 45kV 90mA at 64cm
!@!!Frame: $frame
!@!!Wavelengths    1.54184   1.54056   1.54439
!@!!Integration range: 2Theta: 0.100 to 4.800  Gamma: -180.000 to 180.000
!@!!Integration method: bin normalized
!@!N
!@!SS
!@!M
!@!L 0.0 0.0 0.0 0.0
!@!XDegrees
!@!YCounts
0.10 38.333706 1.547870 0.007112
0.12 100.568771 2.288812 0.008535
0.14 182.932983 2.857968 0.009957
0.16 233.431747 3.019857 0.011380
0.18 242.650208 2.902801 0.012802
0.20 234.392487 2.706550 0.014225
0.22 224.673691 2.526560 0.015647
0.24 218.917648 2.387832 0.017070
0.26 210.772476 2.251053 0.018492
0.28 204.949387 2.138994 0.019915
0.30 202.736664 2.055254 0.021337
0.32 194.081619 1.947061 0.022760
0.34 189.383942 1.865945 0.024182
```

Theta,I,sig(I),q

RAD format (.rad) q,I,sig(I),theta,

I_PE (cps)	TIME	TRANSM	D(thickness) (mm)
6752.00	6000.00	0.105800	1.80
236			
0.711200E-02	38.3337	1.54787	0.100000
0.853500E-02	100.569	2.28881	0.120000
0.995700E-02	182.933	2.85797	0.140000
0.113800E-01	233.432	3.01986	0.160000
0.128020E-01	242.650	2.90280	0.180000
0.142250E-01	234.392	2.70655	0.200000
0.156470E-01	224.674	2.52656	0.220000
0.170700E-01	218.918	2.38783	0.240000
0.184920E-01	210.772	2.25105	0.260000
0.199150E-01	204.949	2.13899	0.280000
0.213370E-01	202.737	2.05525	0.300000
0.227600E-01	194.082	1.94706	0.320000
0.241820E-01	189.384	1.86594	0.340000
0.256050E-01	186.338	1.79872	0.360000
0.270270E-01	177.610	1.70925	0.380000
0.284500E-01	174.150	1.64965	0.400000
0.298720E-01	167.297	1.57790	0.420000
0.312950E-01	152.965	1.47412	0.440000
0.327170E-01	144.600	1.40174	0.460000

RAD format (.rad) q,I,sig(I),theta,

TIME			
6000.00			
236			
0.711200E-02	38.3337	1.54787	0.100000
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0.142250E-01	234.392	2.70655	0.200000
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0.170700E-01	218.918	2.38783	0.240000
0.184920E-01	210.772	2.25105	0.260000
0.199150E-01	204.949	2.13899	0.280000
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0.327170E-01	144.600	1.40174	0.460000

Measured intensity

$$I(q) \propto \frac{d\sigma}{d\Omega}(q) dAT\langle\Phi\rangle t\varepsilon\Delta\Omega$$

counts !

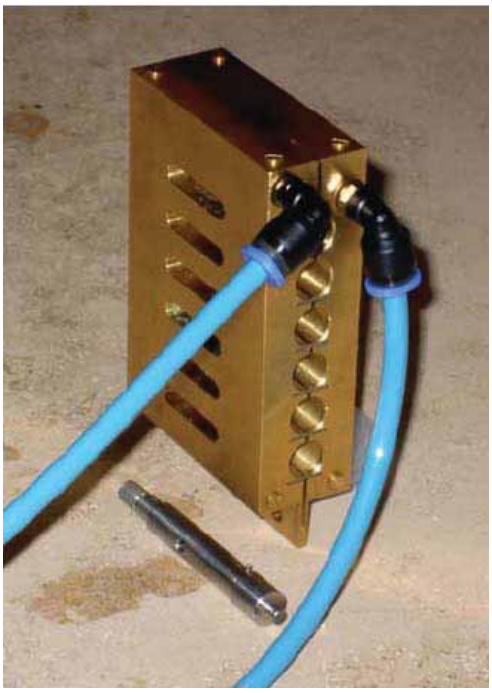
d: sample thickness
A: beam cross section area
T: sample transmission
$\langle\Phi\rangle$: average flux (photons per second)
t: measuring time
ε: detector efficiency
$\Delta\Omega$: solid angle of pixel

$$I_{abs}(q) = I(q)\frac{I_{H2O}^{theory}}{I_{H2O}^{\exp}}$$

When using same capillary for sample and water measurement:
d, A, ε, and $\Delta\Omega$ cancel

Note $\sigma(I(q)) = \sqrt{I(q)}$

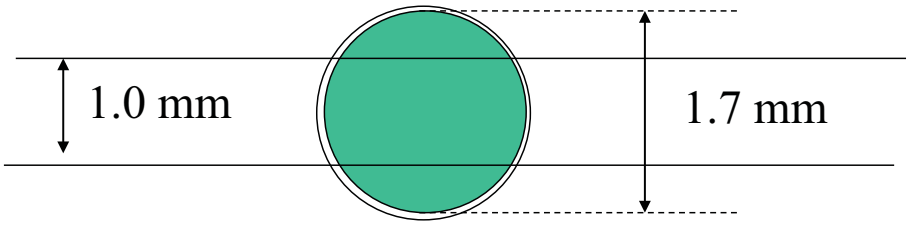
Sample holder – home-build



Quartz capillary
about 1.7 mm in diameter
wall thickness of only 0.010 mm
50 µL is enough!

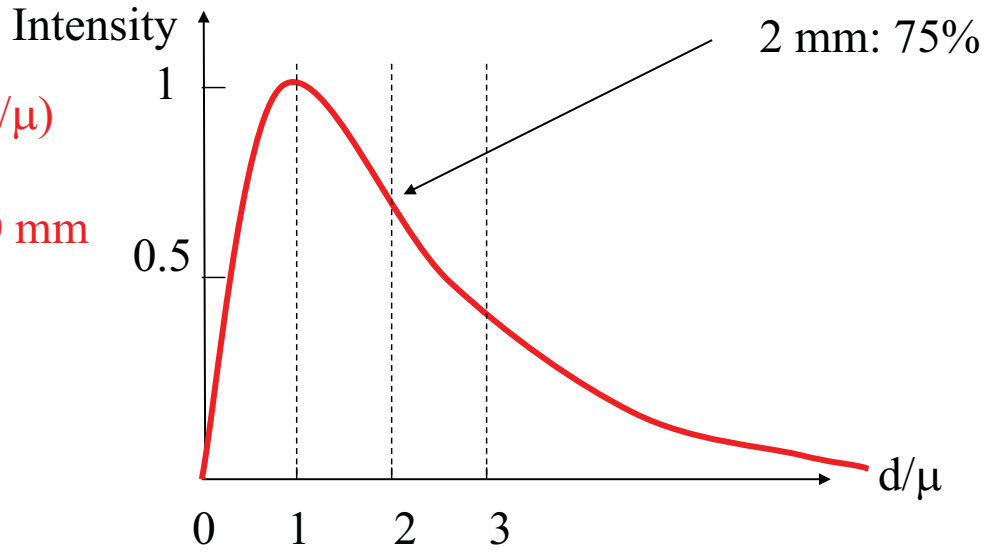
Capillary, quartz : 2 mm (actually 1.7 mm)

walls: 0.010-0.020 mm thicness



$I \propto d \exp(- d/\mu)$

Water: μ=1.0 mm



Sources of background

Solvent

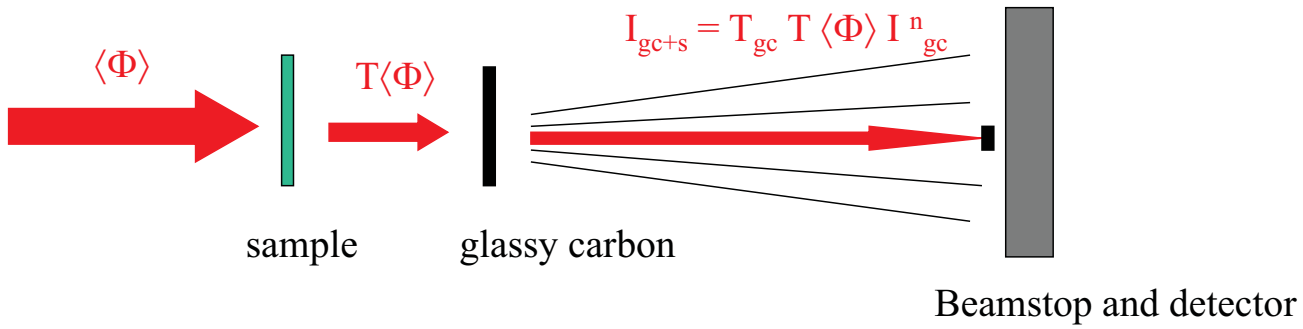
Capillary

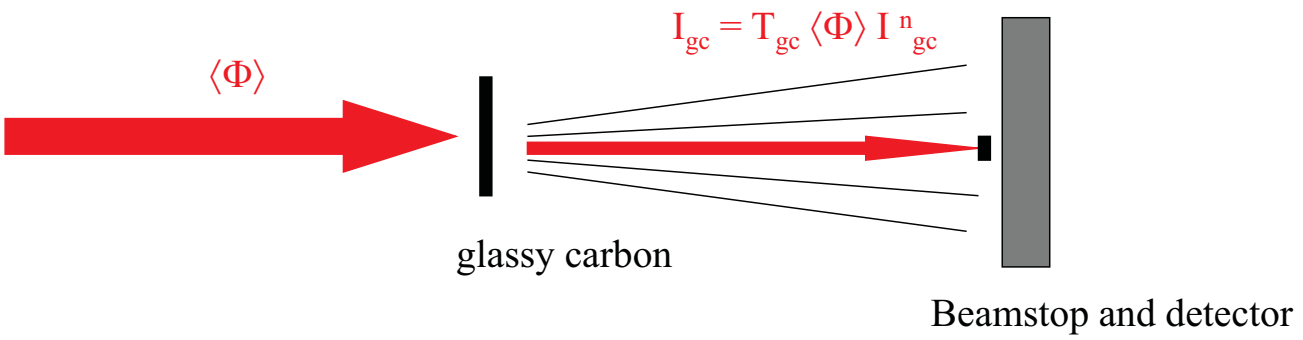
Instrument background
(parasitic scattering, fluorescence, …)

Detector noise

Normalization procedures

Normalize by $T\langle\Phi\rangle t$ ('Old' procedure for blocking beamstop)





$$T = I_{gc+s} / I_{gc}$$

Beamstop, semi-transparent 3 mm ø

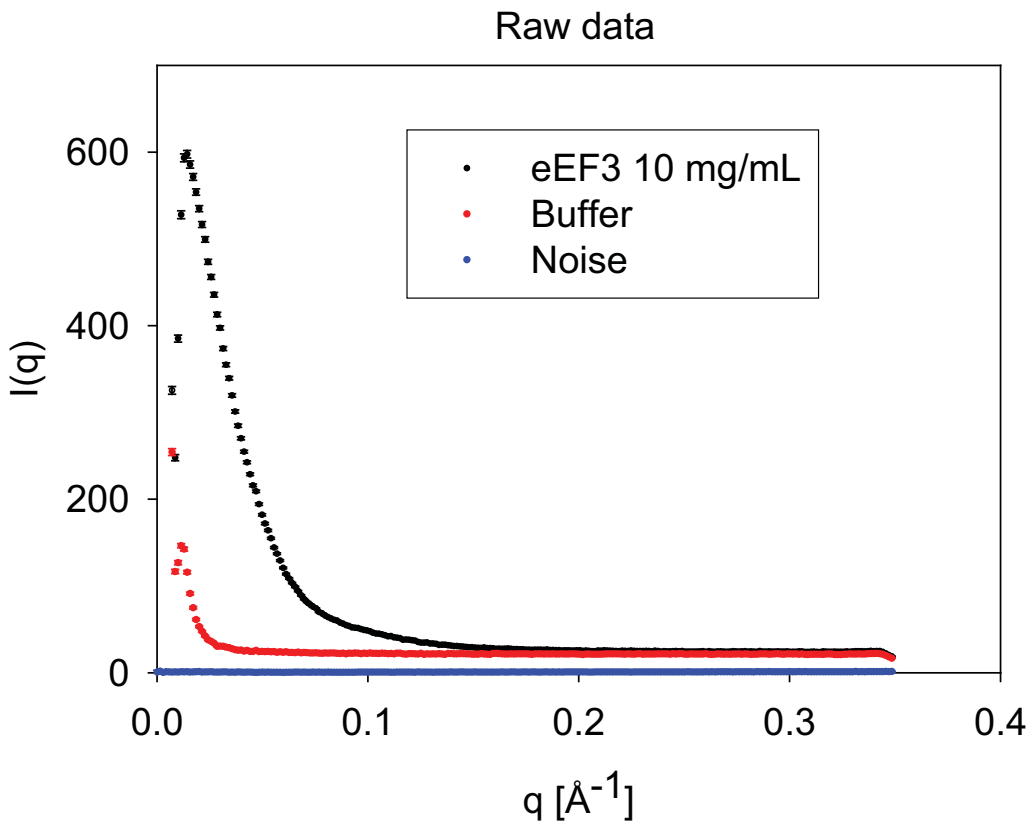
Home-build

- Semitransparent with Ni filter
- T = 1/ 50000
- 5-20 cps behind beamstop
- Monitor on detector

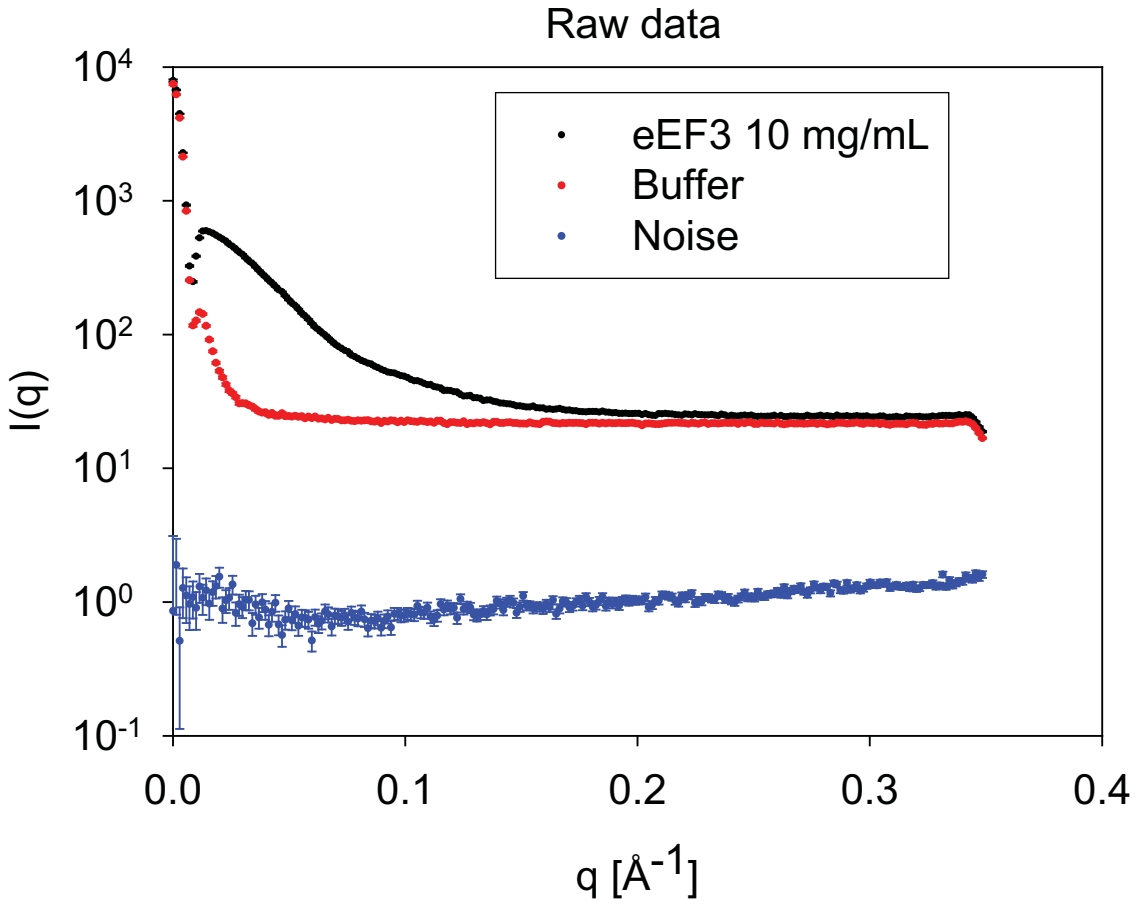
- Intensity behind beamstop prop. to transmission and integrated flux

$$I_{BS} = k\, T\, \langle\Phi\rangle\, t$$

Raw data: linear scales



Logarithmic intensity scale



Measurements required

Measure:

sample in cell, $I_m^{sample}(q)$,

solvent in cell, $I_m^{solvent}(q)$,

noise with lead at sample position $I_m^{noise}(q)$,

H_2O in cell, $I_m^{H2O}(q)$,

empty cell, $I_m^{cell}(q)$,

noise with lead at sample position $I_m^{noise}(q)$.

Normalize by integrated intensity behind beamstop…..

Data Subtraction and Normalization

Measure sample, solvent, background, H_2O, empty cell using same cell:

(1) $I_m^{sample}(q) = k\, T_s\, \Phi_s\, t_s\, I_0^{sample}(q) + k\, T_s\, \Phi_s\, t_s I_0^{solvent}(q) + t_s\, I_0^{noise}(q)$

(2) $I_m^{solvent}(q) = k\, T_{sol}\, \Phi_{sol}\, t_{sol}\, I_0^{solvent}(q) + t_{sol}\, I_0^{noise}(q)$

(3) $I_m^{noise}(q) = t_{noise}\, I_0^{noise}(q)$

---

(1) $k\, T_s\, \Phi_s\, t_s\, I_0^{sample}(q) = I_m^{sample}(q) - k\, T_s\, \Phi_s\, t_s I_0^{solvent}(q) - t_s\, I_0^{noise}(q)$

(1) $I_0^{sample}(q) = I_m^{sample}(q)/(k\, T_s\, \Phi_s\, t_s) - I_0^{solvent}(q) - t_s\, I_0^{noise}(q)/\,(k\, T_s\, \Phi_s\, t_s)$

(2) $k\, T_{sol}\, \Phi_{sol}\, t_{sol}\, I_0^{solvent}(q) = I_m^{solvent}(q) - t_{sol}\, I_0^{noise}(q)$

(2) $I_0^{solvent}(q) = I_m^{solvent}(q)/(k\, T_{sol}\, \Phi_{sol}\, t_{sol}) - t_{sol}\, I_0^{noise}(q)/(k\, T_{sol}\, \Phi_{sol}\, t_{sol})$

(3) $I_0^{noise}(q) = I_m^{noise}(q)/\, t_{noise}$

Data Subtraction and Normalization

(1)+(2): $I_0^{\text{sample}}(q) = I_m^{\text{sample}}(q)/(k\, T_s\, \Phi_s\, t_s)$

$$- [I_m^{\text{solvent}}(q)/(k\, T_{sol}\, \Phi_{sol}\, t_{sol}) - t_{sol}\, I_0^{\text{noise}}(q)/(k\, T_{sol}\, \Phi_{sol}\, t_{sol})]$$

$$- t_s\, I_0^{\text{noise}}(q)/\,(k\, T_s\, \Phi_s\, t_s)$$

use also (3): $I_0^{\text{sample}}(q) = I_m^{\text{sample}}(q)/(k\, T_s\, \Phi_s\, t_s)$

$$- [I_m^{\text{solvent}}(q)/(k\, T_{sol}\, \Phi_{sol}\, t_{sol})$$

$$- t_{sol}\, \{I_m^{\text{noise}}(q)/\, t_{noise}\}/(k\, T_{sol}\, \Phi_{sol}\, t_{sol})]$$

$$- t_s\, \{I_m^{\text{noise}}(q)/\, t_{noise}\}/\,(k\, T_s\, \Phi_s\, t_s)$$

$$= I_n^{\text{sample}}(q) - I_n^{\text{solvent}}(q)$$

$$+ t_{sol}\, I_n^{\text{noise}}(q)/(k\, T_{sol}\, \Phi_{sol}\, t_{sol})$$

$$- t_s\, I_n^{\text{noise}}(q)/\,(k\, T_s\, \Phi_s\, t_s)$$

$$= I_n^{\text{sample}}(q) - I_n^{\text{solvent}}(q)$$

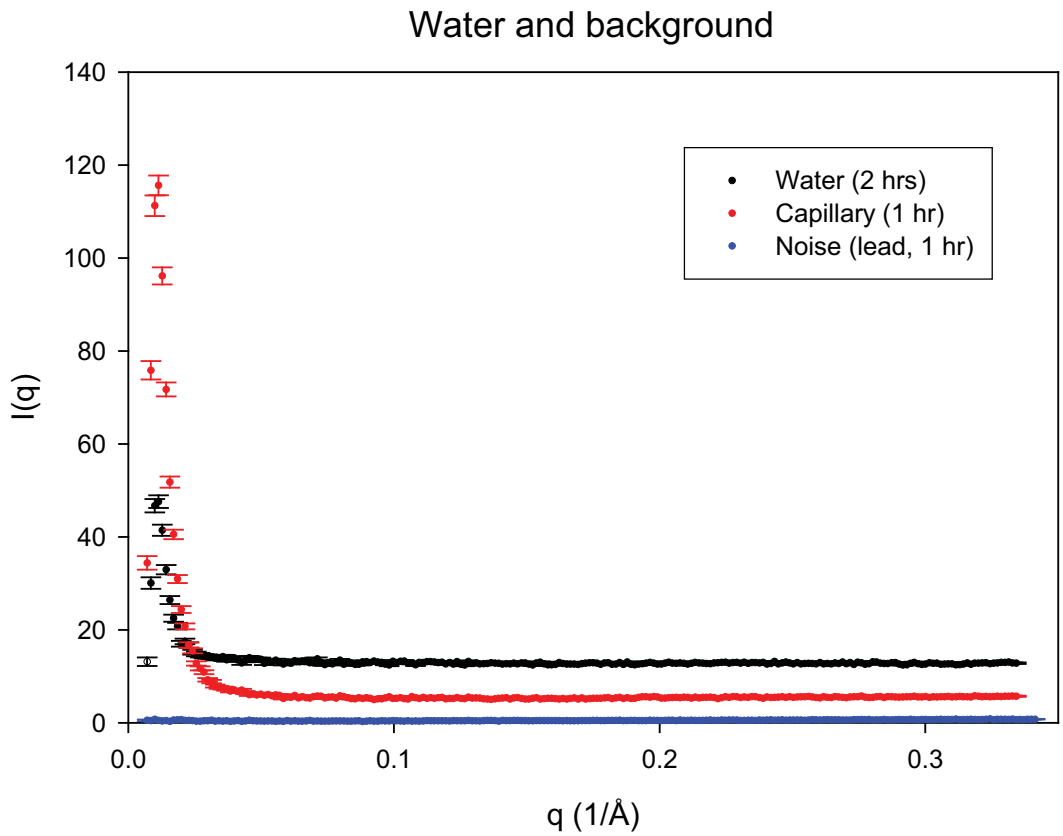
$$- I_n^{\text{noise}}(q)[t_s\,/\,(k\, T_s\, \Phi_s\, t_s) - t_{sol}/(k\, T_{sol}\, \Phi_{sol}\, t_{sol})]$$

Data Subtraction and Normalization

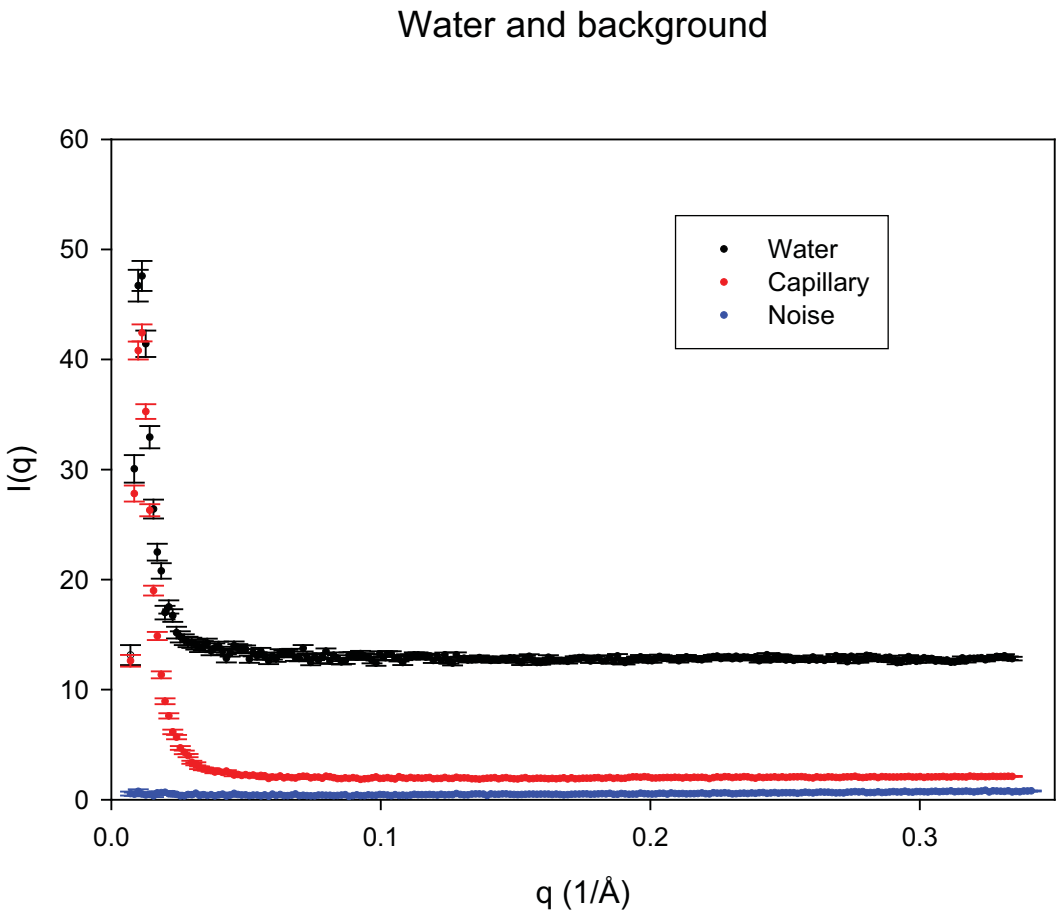
Error calculation!!!!

The same is done for water and empy cell measurements !

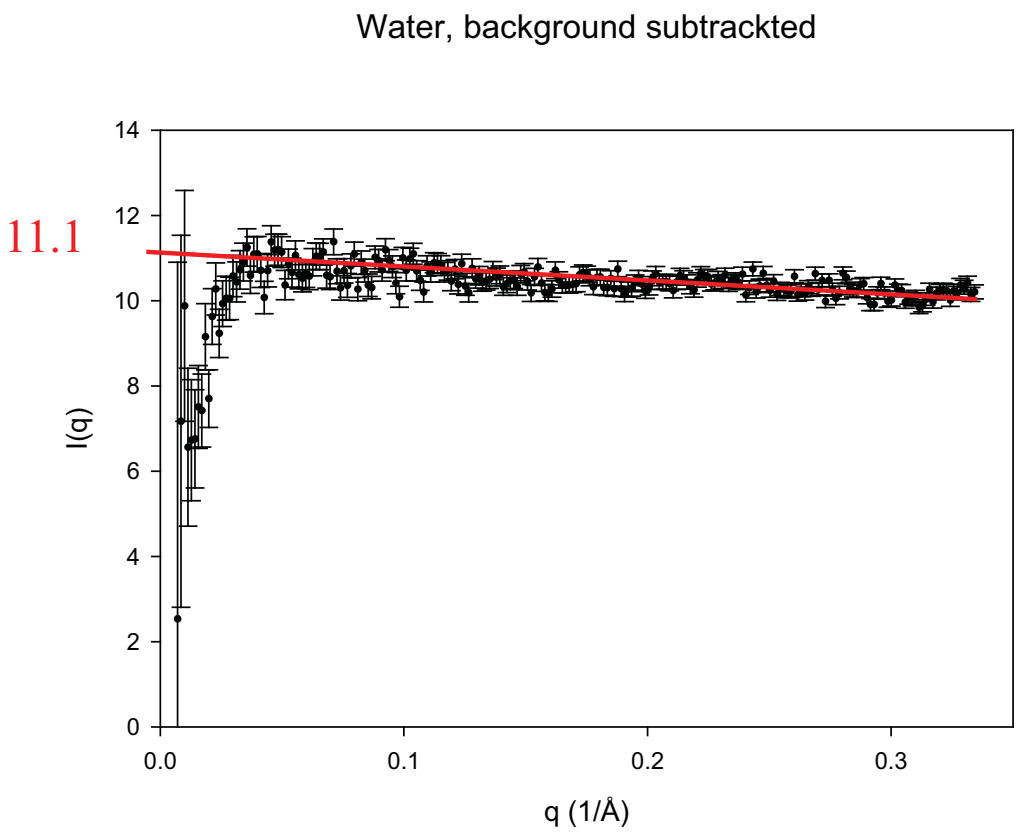
Raw water data, no normalization



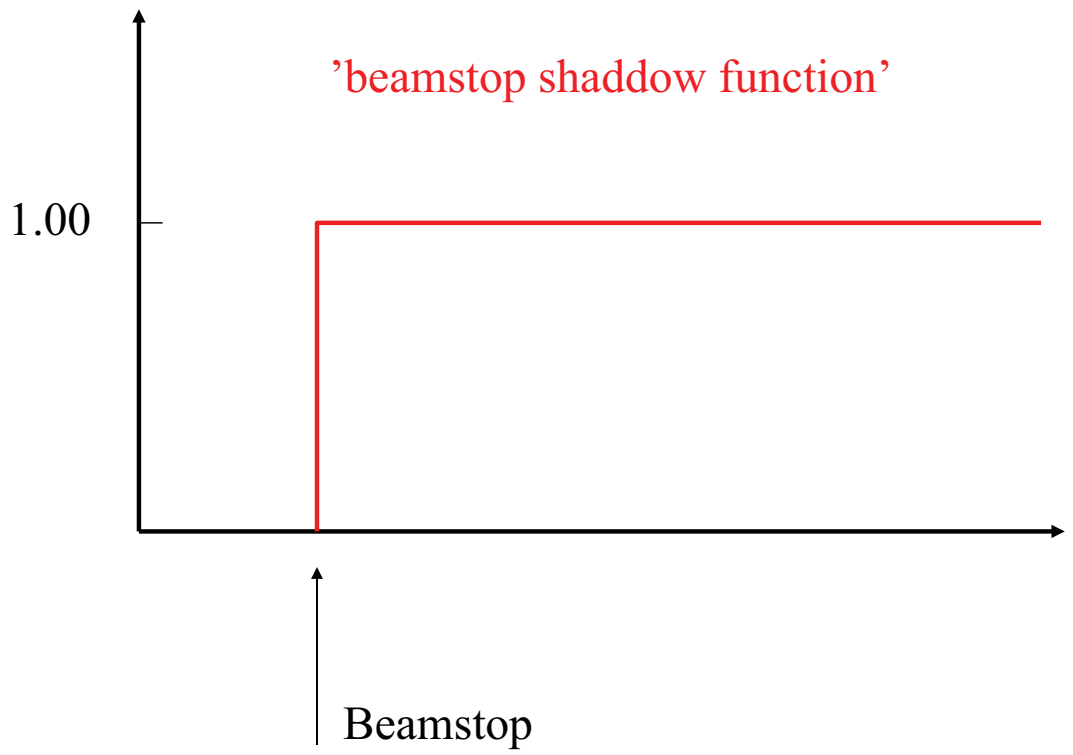
Raw water data, normalization by transmssion and time



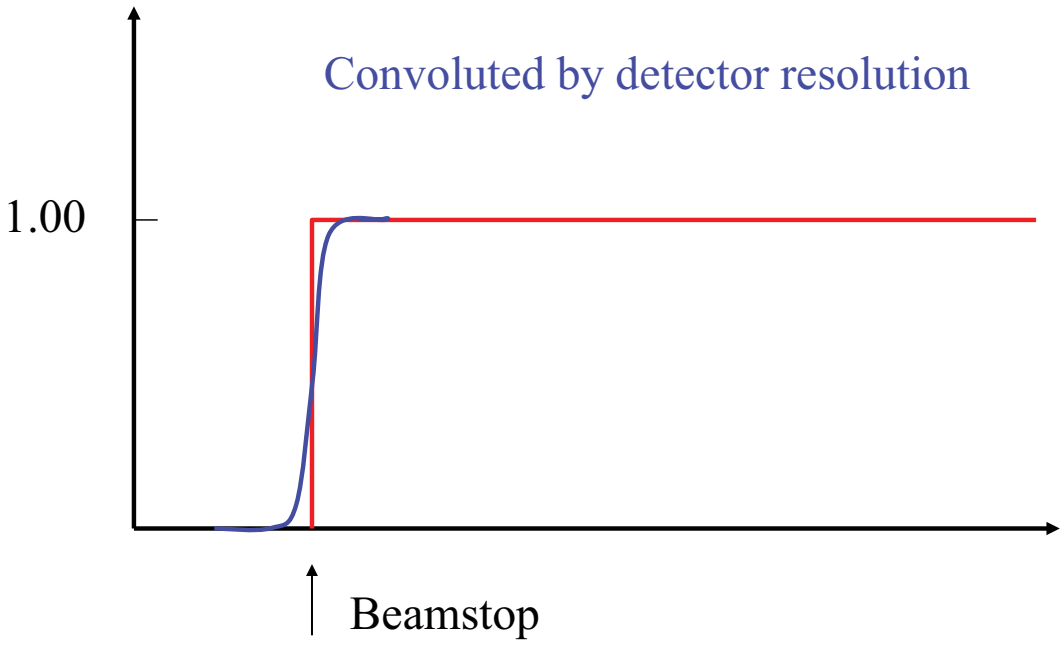
Water with extrapolation



Shaddowing by beamstop



Shaddowing by beamstop at detector



Note: Difference in BS center and q scale zero point also gives Smearing of BS edge!!!

Correction

BS(q) Beamstop response function (step)
D(q) Detector resonse function (Gaussian, FWHM=0.5 mm)
I(q) Scattering from sample, more slowly varying than BS(q) and D(q)

$$I_{meas}(q) = \int D(q-q')BS(q')I(q')dq'$$

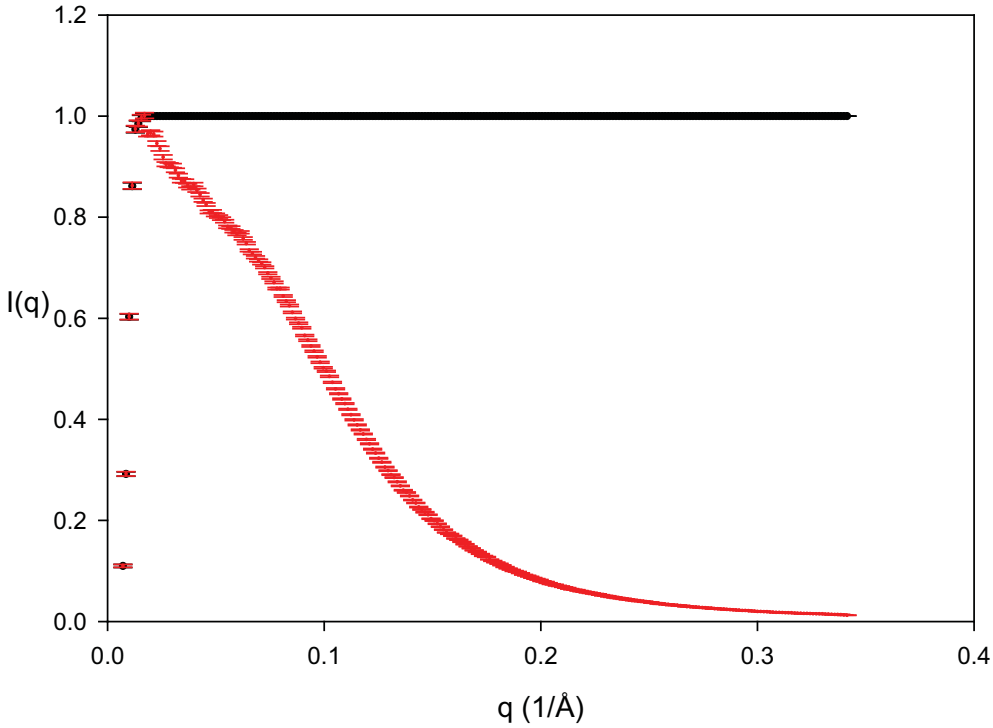
When I(q) slowly varying: $$I_{meas}(q) \approx I(q)\int D(q-q')BS(q')dq'$$

So that: $$I(q) \approx I_{meas}(q) / \int D(q-q')BS(q')dq'$$

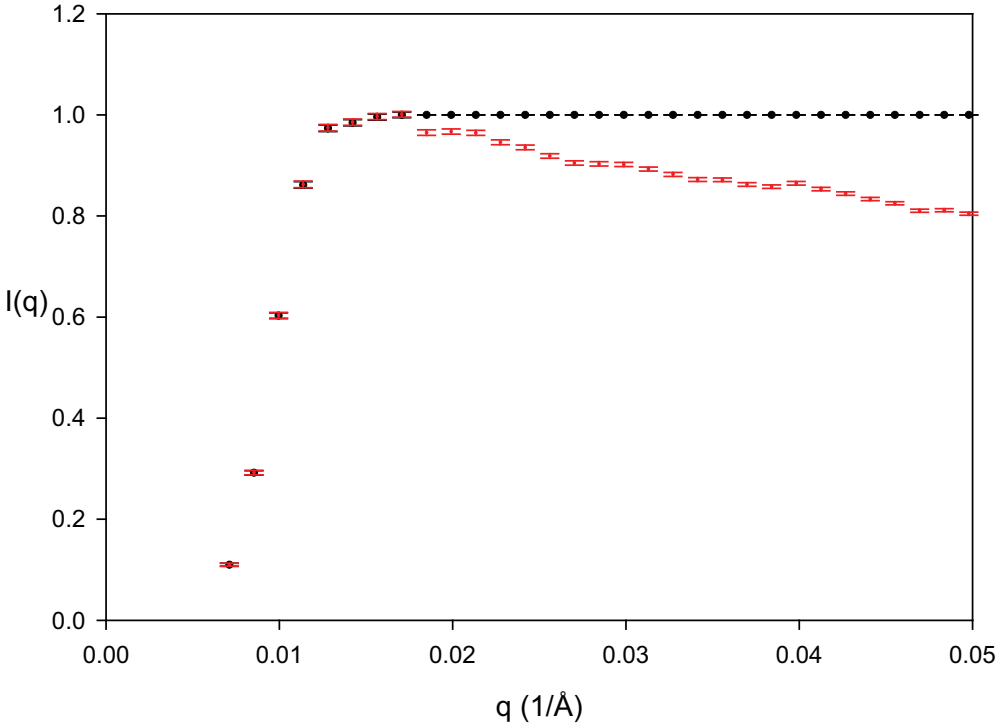
Note: For difference in BS center and q scale zero point, this correction is strickly correct!

How do we measure $\int D(q-q')BS(q')dq'$?

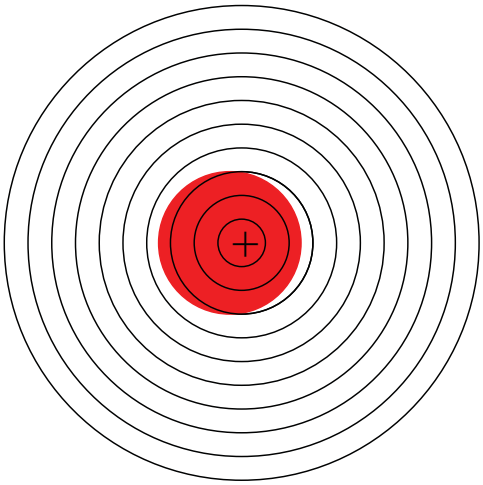
GC correction

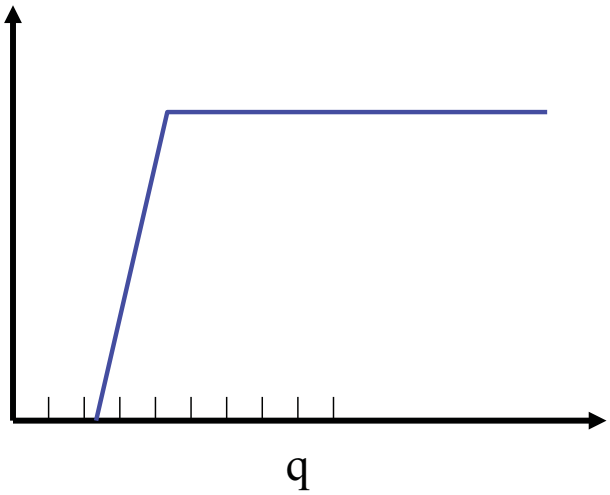


GC correction



Misalinged beamstop





The correction is striktly valid for this effect!

Calculated examples

No misalignment!

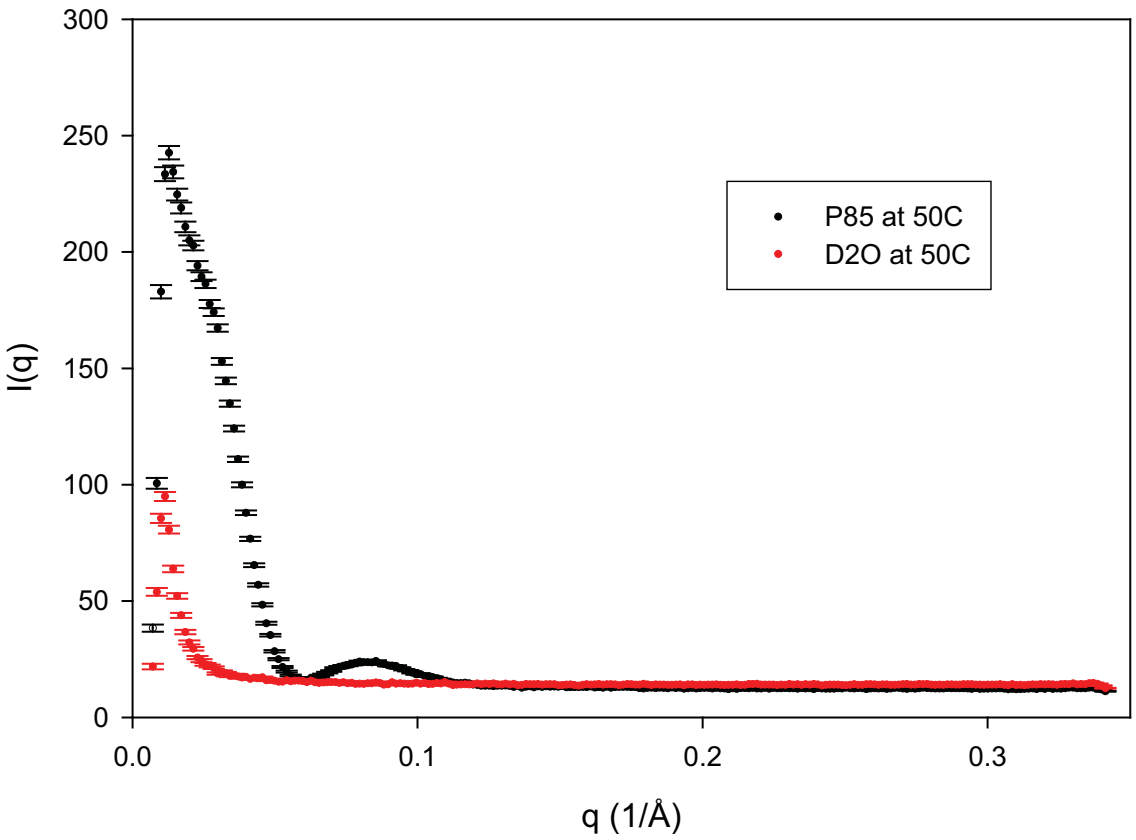
R_BS=1.4 mm, sampl-det=660 mm, q_min=0.009 1/Å
Det_FWHM=0.4 mm, Gaussian detector resolution function
Solid spheres

q (1/Å)	R=50Å corr	R=50Å uncorr	R=100Å corr	R=100Å uncorr	R=200Å corr	R=200Å uncorr	R=300 Å corr	R=300Å uncorr	R=400 Å corr	R=400Å uncorr
0.007	2%	97%	8%	97%	29%	98%	60%	99%	89%	100%
0.008	1	83	5	84	22	87	49	91	83	97
0.009	0	50	3	50	13	57	34	67	71	86
0.010	0	17	1	17	6	22	18	32	52	60
0.011	0	3	0	3	1	4	6	8	25	27
0.012	0	0	0	0	0	0	3	3	3	3
0.013	0	0	0	0	0	0	0	0	0	0

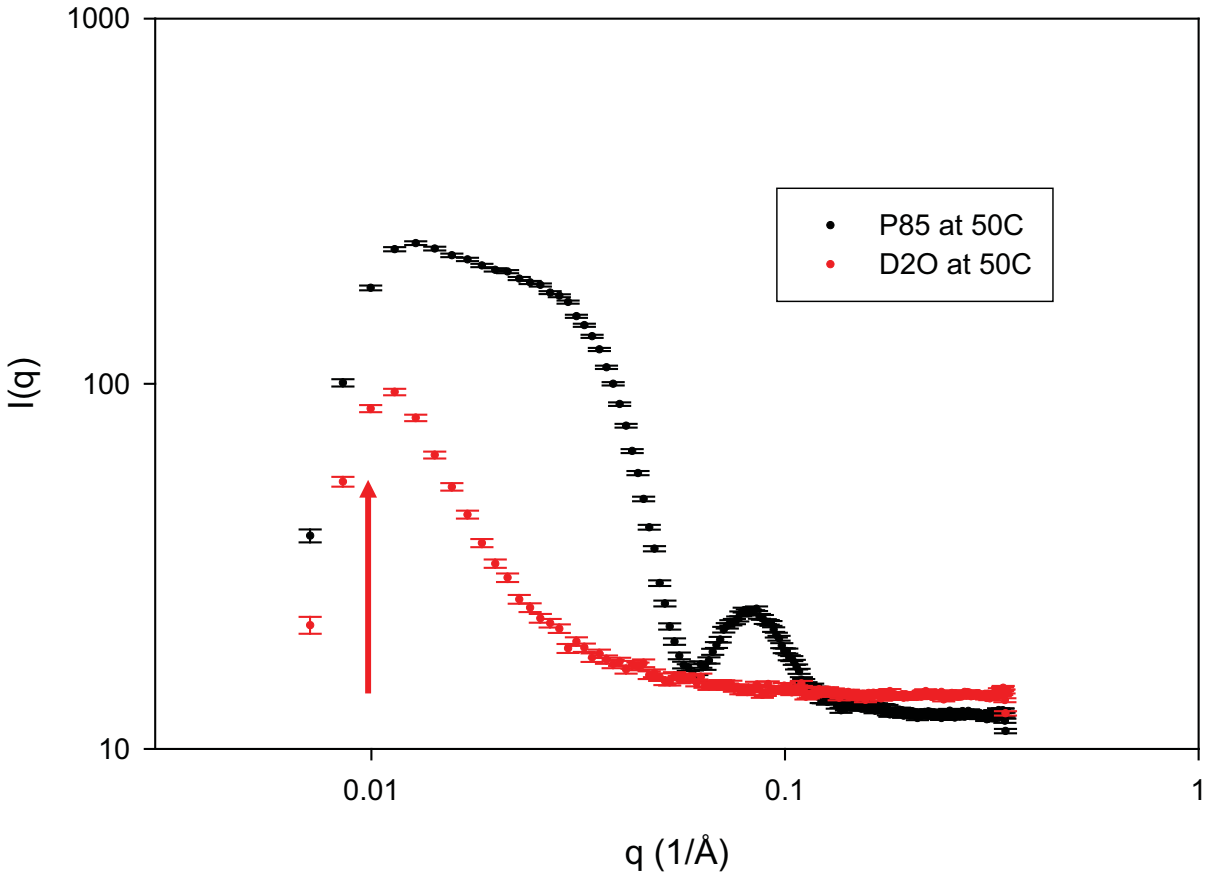
For Det_FWHM=0.15 mm, all data for q=0.010 1/Å and larger can be used for all sizes !!!!

It is very important to improve detector resolution to improve realiability of data close to q_min !!!!!

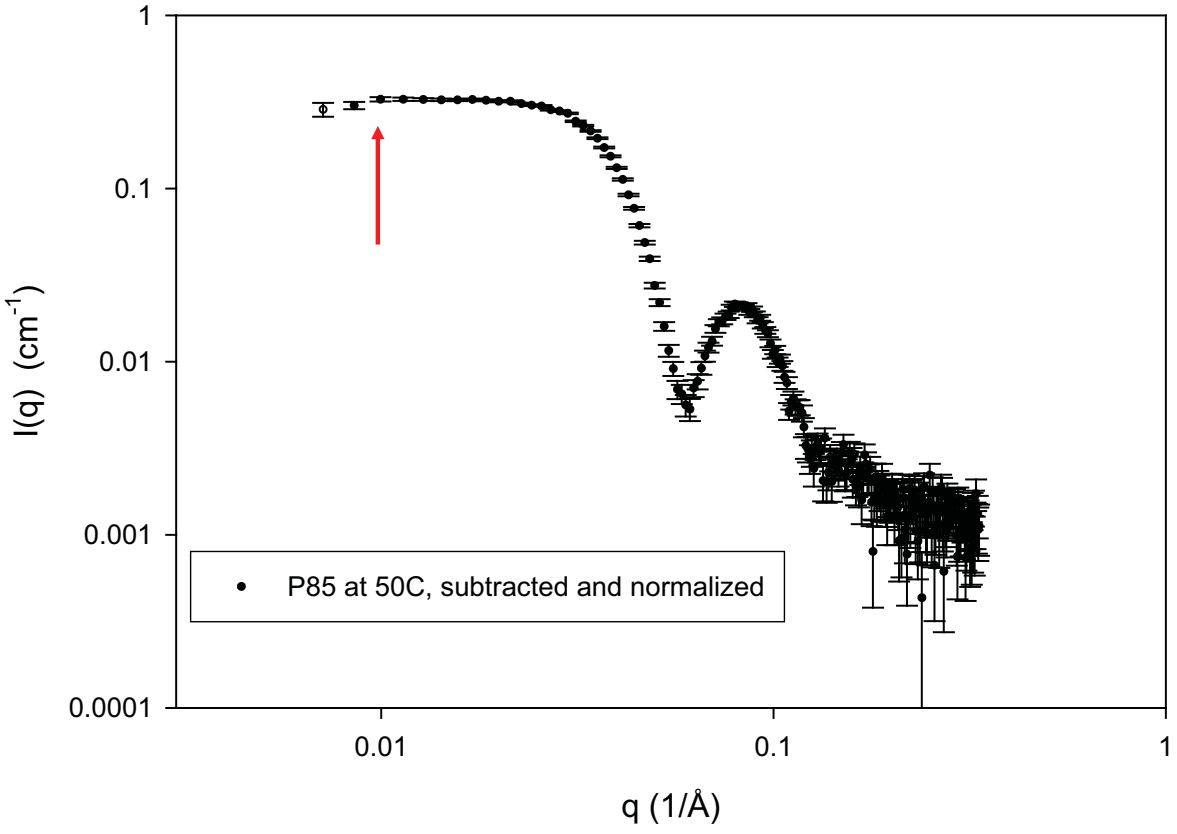
An example P85 Pluronic: EO 23-PO 40-EO 23



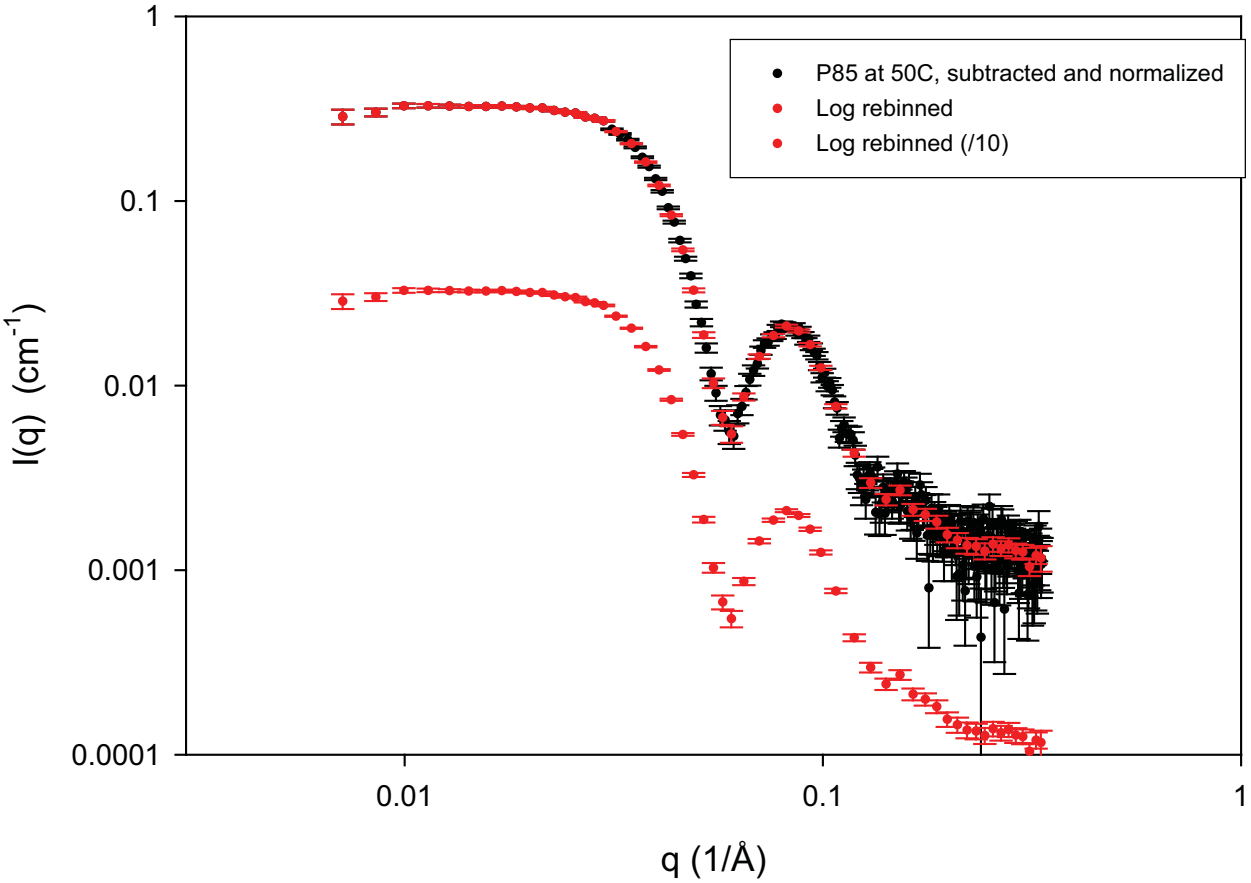
An example P85 Pluronic: Log-Log plot



An example P85 Pluronic: Subtracted, nomalized



An example P85 Pluronic: Log rebinning



Summary

- Principles of
  - calibration
  - background subtraction
  - Absolute normalization

- Now to SuperSAXS program package

S_U_P_E_R_S_A_X_S

PROGRAM PACKAGE FOR DATA TREATMENT, ANALYSIS AND MODELING

Cristiano L P Oliveira

Jan Skov Pedersen

Package characteristics

- Made in FORTRAN™ language
- Uses GNUPLOT™ Graphics interface
  - Compilable in any operating system
- Build in modular blocks
  - Easy to update, improve and integrate
- User friendly

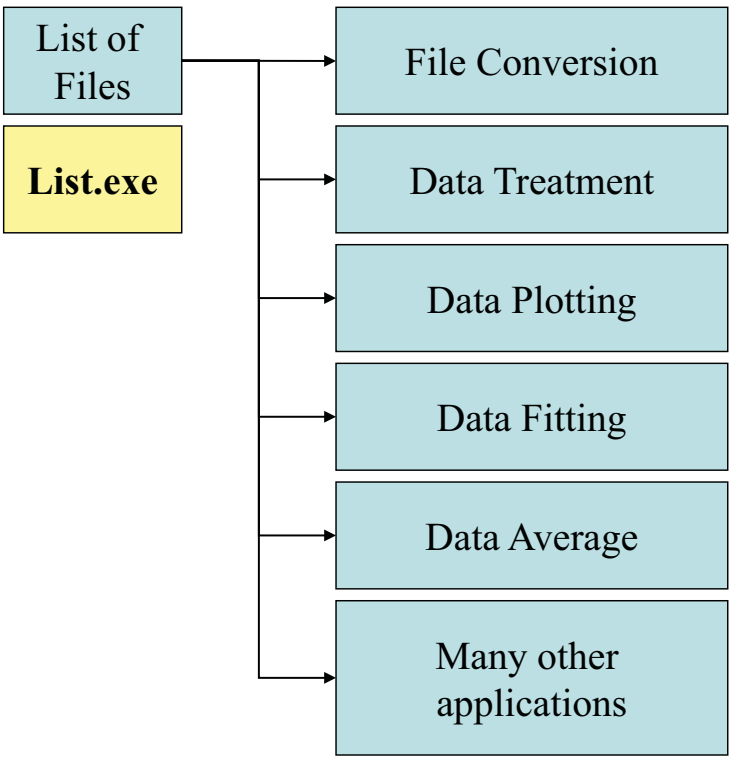
File Formats

- ***RAW files***-> Angular Integrated Data from the aquisition program
- ***RAD files***-> RAW data converted to JSP format
- ***RDN files***-> Beam stopper shadow correction file
- ***RDS files***-> Background subtracted Data
- ***RSR files***-> Rebinned data
- ***SCA files***-> Scaled Data
- ***LIS files***-> List of files for many applications

S_U_P_E_R_S_A_X_S PROGRAMS

```
MS-DOS Prompt - PROGS
C:\crislpo\AARHUS~1\Lecture\TREATM~1\RDS-RSR>PROGS
*******************************************
        S_U_P_E_R_S_A_X_S    PROGRAMS
*******************************************
List of Available Programs :
LIST.EXE     -> Creates file lists for other programs
WAVG.EXE     -> Averages RAD RDS RSR files giving chi2
WCOMP.EXE    -> Compares and rescales two input files
WCOMV.EXE    -> Converts data file to JSP format files
WIFT.EXE     -> Perform Inverse Fourier Transformation
WGNUPLOT.EXE-> Gnuplot Program  (www.gnuplot.info)
WGCNORM.EXE -> Creates a normalization file for beam
               stopper shadow correction
WLSQSAXS.EXE-> Least Squares Fitting program.
WPLOT.EXE    -> Plots JSP format files. Reads a list.
WREBINL.EXE -> Performs a logarithmically rebinning
               of input files. Reads TORAD.FIL file.
WSXH2O.EXE   -> Data treatment for water files and
               zero intensity fit
WSXSUB.EXE   -> Data treatment for SAXS data files
               and normalization to absolute scale
WTORAD.EXE   -> Converts RAW files to RAD files.
               Reads TORAD.FIL file.
If the prompt not appear, press Ctrl+C
```

List directed procedure



Easy adaptable to large scale file management

The lists can be reusable and easily changed

All steps are documented

The list have to be created

Keyboard based interaction

Converting from RAW format to RAD format

List.exe

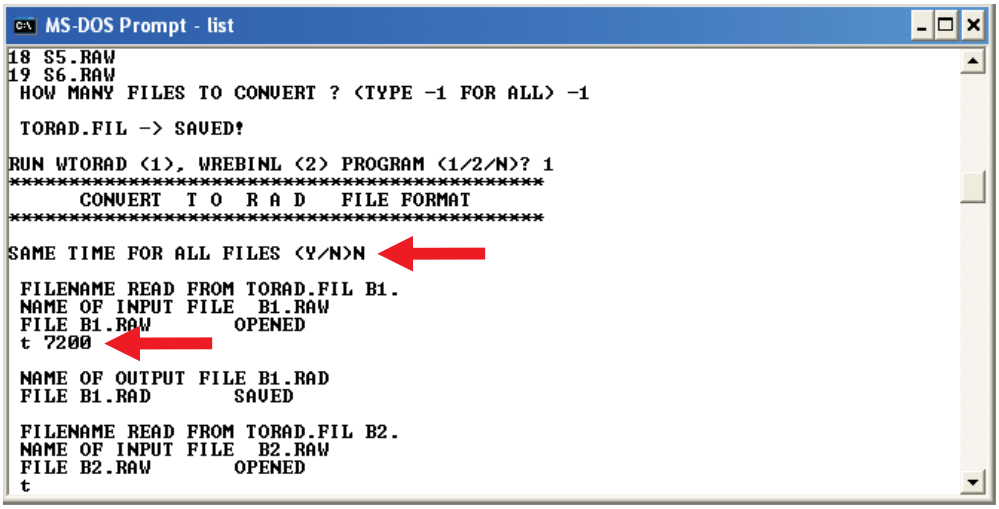
(1) Convert Files (Torad.fil)
(2) Data Treatment List File
(3) Plot List File
(4) Average List File
(5) Join Files

Type files extension
Select desired files

Select file index instead of type the file name

List Saved!
Call WTORAD

Read TORAD.FIL
Type aquisition time for each file



Data Treatment of SAXS Data

$$I_{Treated}(q)=\left[\left(\frac{I_{sample}(q)}{\Phi_s.T_s.t_s}-\frac{I_{back}(q)}{\Phi_b.T_b.t_b}-\frac{I_{noise}(q)}{t_{noise}(\Phi_s.T_s-\Phi_b.T_b)}\right)\frac{1}{I_{shadow}(q)}\right]\frac{d\Sigma/d\Omega_{water,20^oC}}{I(0)_{water,20^oC}}$$

$$\sigma_{treated}(q)=\left(\frac{\sigma_1(q)^2}{I_{shadow}(q)^2}+\left(\frac{I_{sample}(q)}{\Phi_s.A_s.t_s}\right)^2\frac{\sigma_{shadow}(q)^2}{I_{shadow}(q)^2}\right)^{1/2}$$

$$\sigma_1(q)=\sigma_{sample}(q)^2+\sigma_{back}(q)^2+\sigma_{noise}(q)^2.\left(\frac{1}{\Phi_s.A_s}-\frac{1}{\Phi_b.A_b}\right)^2$$

Bevington (1992), Data Reduction and Error Analysis for the Physical Sciences

---

- ***I(q)*** is the measured (integrated) scattering intensities
- ***Φ*** is the intensity incident beam
- ***T*** is the sample transmission
- ***t*** is the exposition time
- ***σ (q)*** is the statistical error of each point.
- $I_{shadow}(q)$, $\sigma_{shadow}(q)$ are the normalized intensity and error for the beam stopper shadow correction

Creating list for Data Treatment

List.exe

(1) Convert Files (Torad.fil)
(2) Data Treatment List File
(3) Plot List File
(4) Average List File
(5) Join Files

Creation Mode:
Stardart
Series

Select file index instead of type the file name

Select Files:
Noise file
Glassy Carbon File
Intensities Files
Buffers Files

List Saved!
Call WSXSUB

MS-DOS Prompt - list

```
 3 B2.RAD
 4 B3.RAD
 5 B4.RAD
 6 B5.RAD
 7 B6.RAD
 8 Bs1.RAD
 9 Bs2.RAD
10 Bs3.RAD
11 Bs4.RAD
12 Bs5.RAD
13 Bs6.RAD
14 LEAD_06.RAD
15 S1.RAD
16 S2.RAD
17 S3.RAD
18 S3n.RAD
19 S4.RAD
20 S5.RAD
Select Buffer file number : 3

Scale of Transmission (1=def) :

list.lis -> SAVED!

RUN WSXSUB (1), WSXH20 (2) PROGRAM (1/2/N=def)? _
```

Performing the Data Treatment

Wsxsub.exe

(1) Batch Mode
(2) Interactive Mode

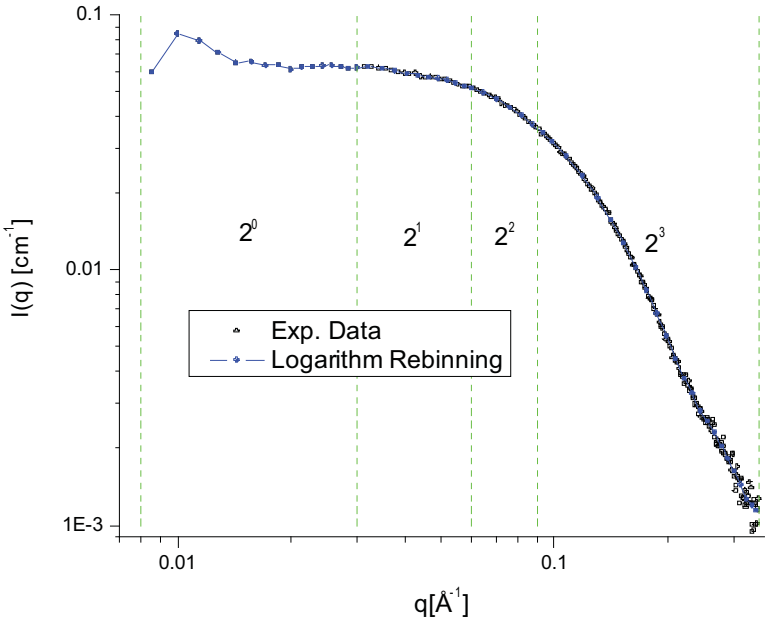
Select list of Files

Perform the Data Treatment

MS-DOS Prompt

```
Buffer File........... : B2.RAD
Scale of Transmission :  1.00000000
Output File........... : S2.RDS
**************** Data Treatment ********************
Water file for absolute norm. ......-> WATERNM.PAR
Used capillary #.................... -> 1
File 1 opened : Sample..............-> S2.RAD
File 2 opened : Background .........-> B2.RAD
Scale of Transmission ............. ->  1.00
File 3 opened : Dark Current .......-> LEAD_06.RAD
File 4 opened : Normalization File .-> 06APR_GC.RDN
File 5 Opened : Output File ........-> S2.RDS
0.951   1          DIRECT RATIO  0.99996E-02 0.10517E-01
0.969   2   DIRECT AREA-W RATIO
0.978   3   DIRECT AREA-W RATIO
1.010   4   DIRECT AREA-W RATIO
1.037   5   DIRECT AREA-W RATIO
0.987     SIMPLE RATIO OF AREAS  0.24506E+00 0.24819E+00
Smallest Value of Intensity ........->  0.00000E+00
Change Scale of Transmission (Y,N)?n

Data Treatment Finished !!!
If the prompt not appear, press Ctrl+C
^C
C:\crislpo\AARHUS~1\DATA_O~1\OTZEN\TREATM~1>_
```

Data Rebinning



Rebinning of experimental data speeds up operations with the data and also decreases the noise.

Linear rebinning (points equally spaced in linear scale) of scattering data can generate artefacts on the scattering profile

Logarithmic rebinning (points equally spaced in log scale) of scattering decreases considerably the number of points, preserving the features of experimental data

It is not recommended for curves with sharp peaks

Rebinning Experimental Data

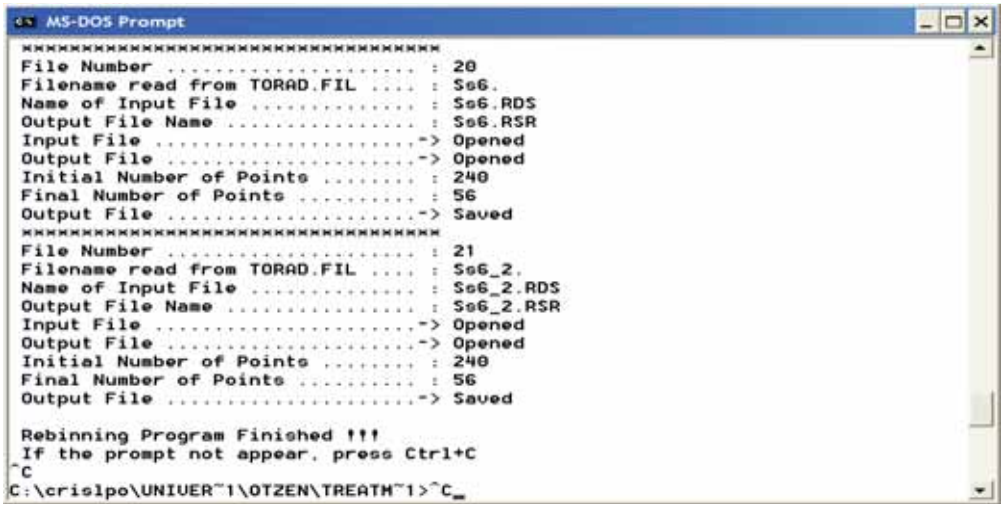
List.exe

(1) Convert Files (Torad.fil)
(2) Data Treatment List File
(3) Plot List File
(4) Average List File
(5) Join Files

Type extension RDS
Select desired files

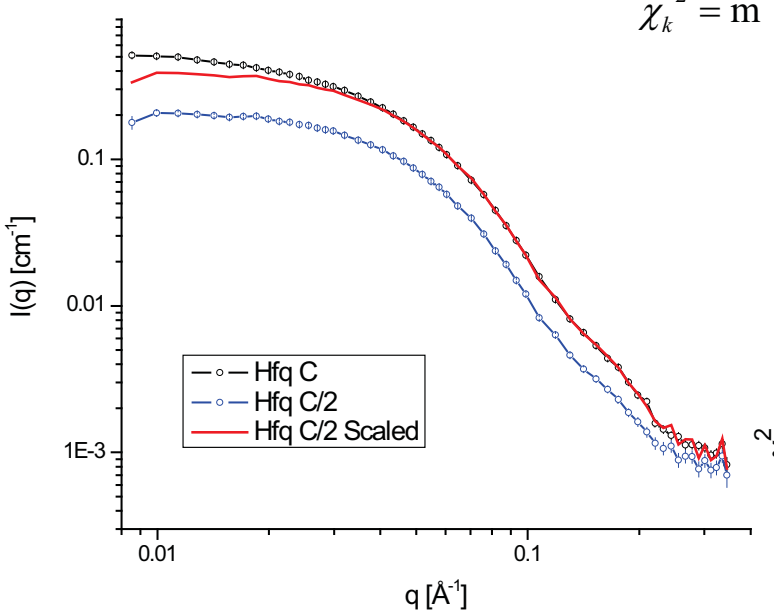
List Saved!
Call WREBINL

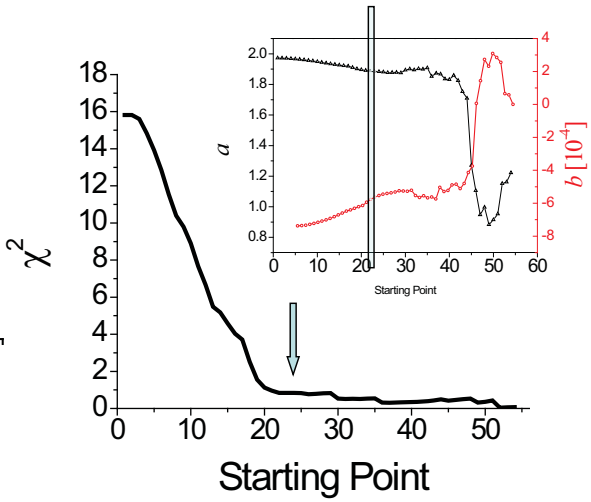
Read TORAD.FIL
Rebins the Data



Comparing and Scaling two files – Decremental Comparison

$$\chi_k^2 = m \left(\sum_{i+k-1}^{N} \left[\frac{I_{1,i}(q)}{\sigma_{1,i}} - \left(a_k + b_k \frac{I_{2,i}(q)}{\sigma_{2,i}} \right) \right]^2 \right)$$





Comparing and Scaling two files – Decremental Comparison

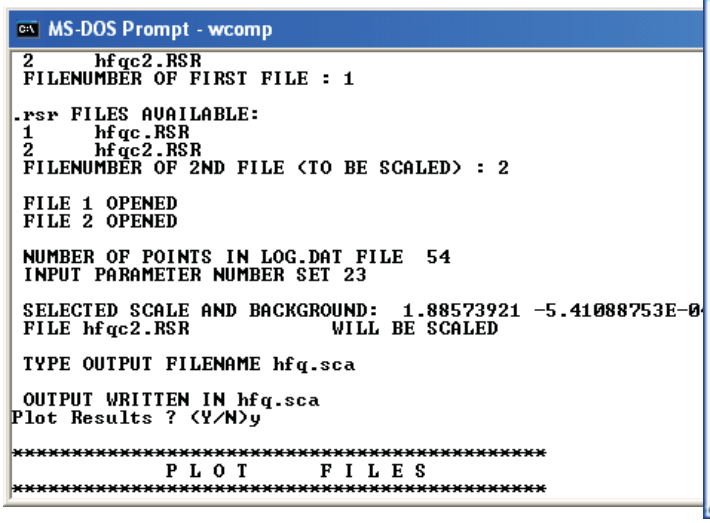
Wcomp.exe

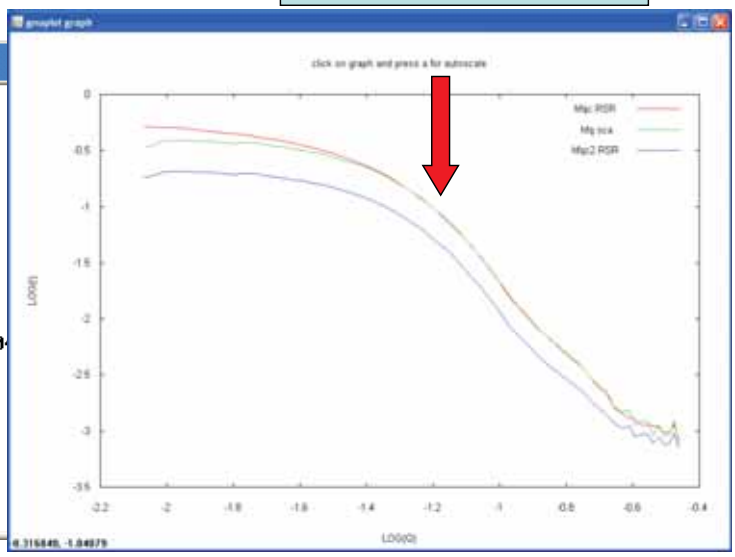
- Type file extension or
- Type file names

Select comparison index

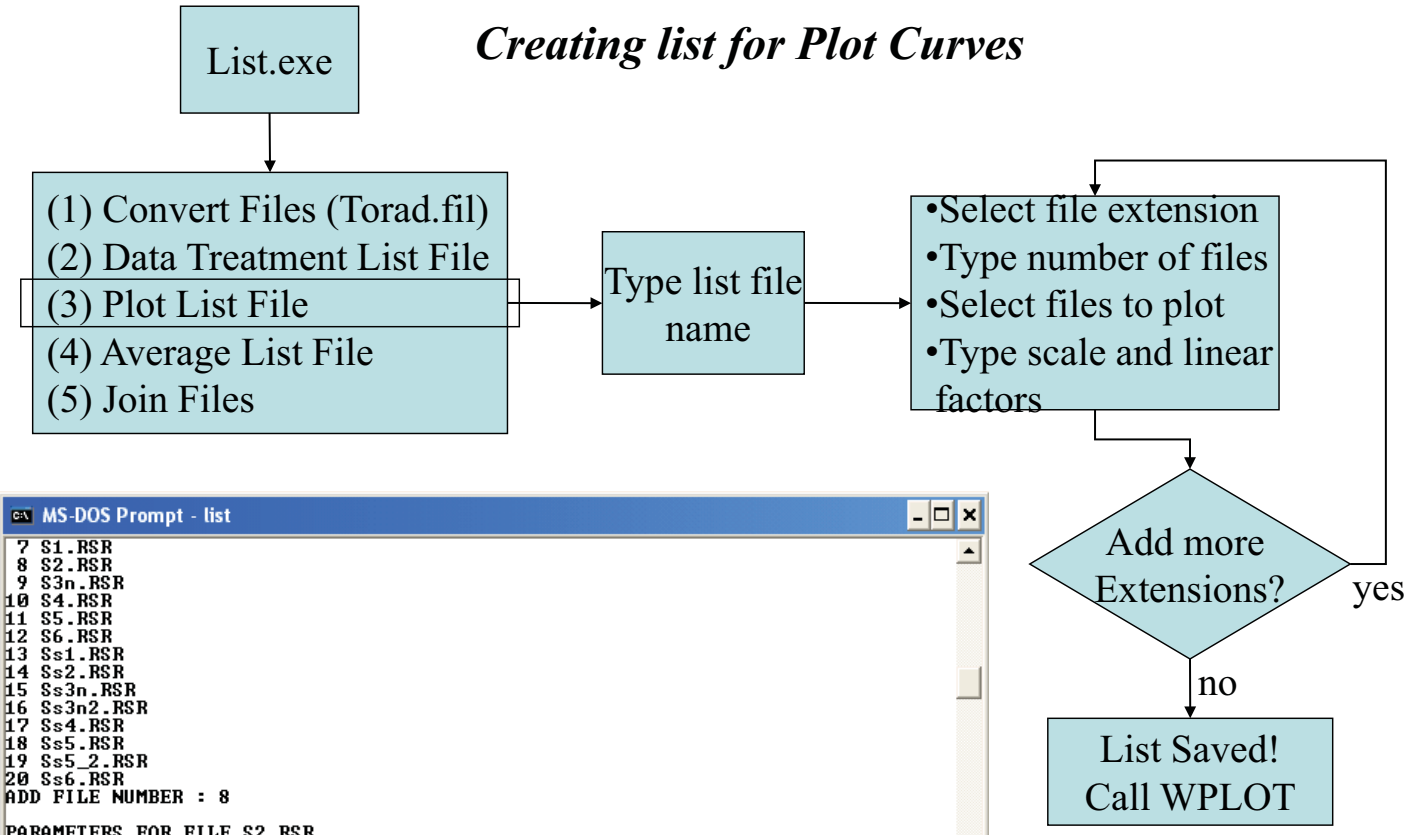
Write output file name

Plot Results



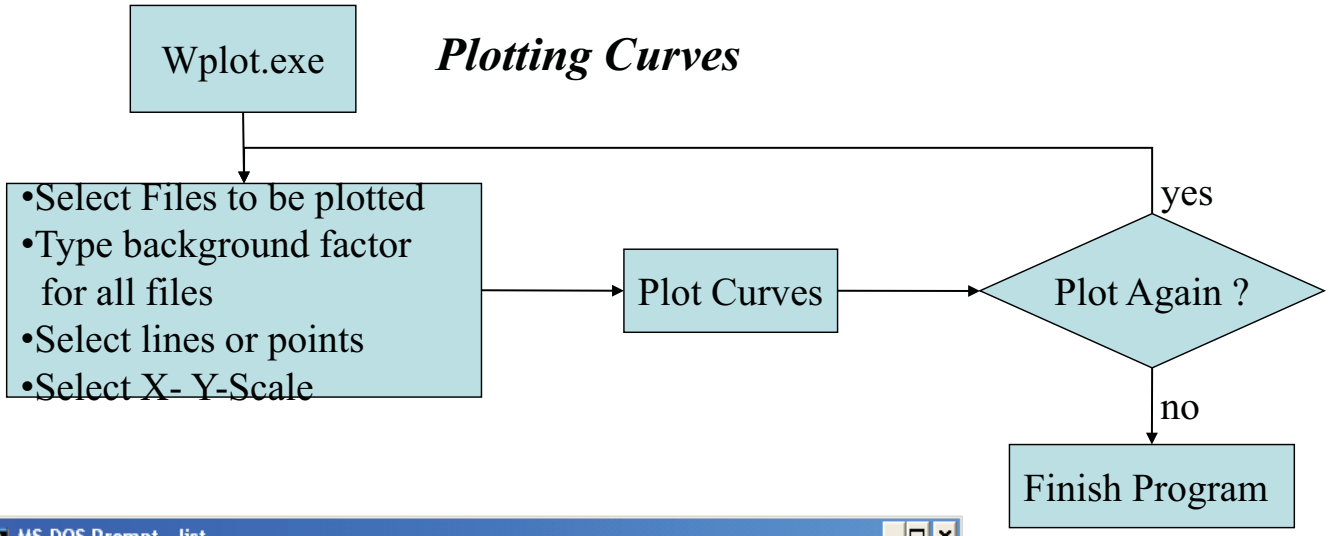


Creating list for Plot Curves




```
MS-DOS Prompt - list
 7 S1.RSR
 8 S2.RSR
 9 S3n.RSR
10 S4.RSR
11 S5.RSR
12 S6.RSR
13 Ss1.RSR
14 Ss2.RSR
15 Ss3n.RSR
16 Ss3n2.RSR
17 Ss4.RSR
18 Ss5.RSR
19 Ss5_2.RSR
20 Ss6.RSR
ADD FILE NUMBER : 8

PARAMETERS FOR FILE S2.RSR
     SCALE FACTOR (1=def) :

     BACKGROUND FACTOR (0=def) :


ADD MORE FILE EXTENSIONS TO PLOT (Y/N=def)?n

Plot Results ? (Y=def/N)y_
```

Plotting Curves




```
MS-DOS Prompt - list
 S2.RSR
S2.RSR
S2.RSR
 INPUT PREFACTOR OF Y :
1.00000000
FILE OPENED
 TIME
 1.0
56
2
 INPUT BACKGROUNDS TO BE SUBTRACTED FROM ALL FILES (0=def)

 SYMBOLS ON CURVES (1/0=def)

Which Function of Intensity;
Intensity[1], log(I)[2], log(q*I)[3], log(q*q*I)[4],1/I[5]
ln(I) [6], I*q**4[7], I*Q[8], I*Q**2[9], I*Q**-EPS/2[10], p(r)[11]: 2

Which Function of scattering vector;
q[1], q*q[2], log(q)[3] or q**4 [4] : 3

Plot Again (Y,N=def)

If the prompt not appear, press Ctrl+C
```

SUPERSAXS user manual v1.0

S_U_P_E_R_S_A_X_S

PROGRAM PACKAGE FOR DATA TREATMENT, ANALYSIS AND MODELING

19-01-2009

Written by Cristiano Luis Pinto de Oliveira (crislpo@if.usp. br)

USER MANUAL v_1.0

Future Perspectives

- Increase the applicability of the package, adding more features
- Develop the program interface
- Correct Bugs!