ESRF | The European Synchrotron

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ESRF - the European Synchrotron
Grenoble (France)

SAXS-WAXS
USAXS
ID2 TIME RESOLVED

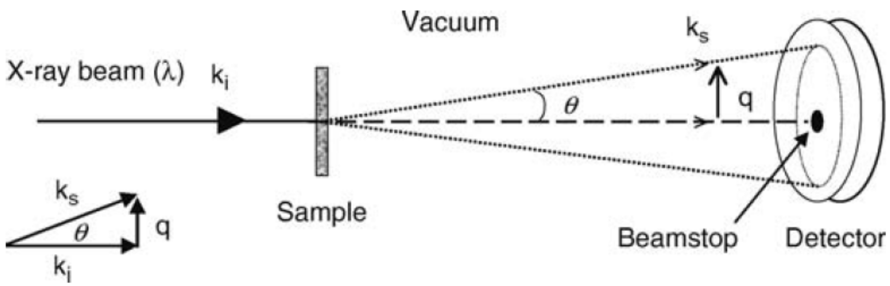
ID13
THE MICROFOCUS BEAMLINE

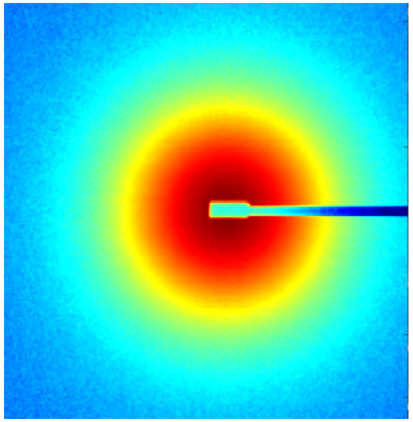
Outline

- SAXS instrumentation and theory
- SAXS data reduction and calibration
- Good practice for data recording
- SAXS data formats
- Tools for (on-line) data reduction and visualization:
  SPD, saxs programs, PyFAI, SAXSutilities

- Data Interpretation / modelling
- Form factor, Guinier / Porod law, Unified fitting, size distributions, structure factor
- Programs: SAXSutilities, IRENA, SASview, SASfit

Momentum transfer and differential scattering cross section





scattering of X-rays at small-angles originate from spatial fluctuations of the electron density within the material

Momentum transfer $$q = |\mathbf{q}| = \frac{4\pi}{\lambda}\sin(\theta/2)$$

Measured Intensity: $$I_S = i_0\, T_r\, \varepsilon\, \Delta\Omega \frac{d\sigma}{d\Omega}$$ Differential scattering cross-section

i_0 - incident flux
T_r - transmission
ε - efficiency
$\Delta\Omega$ - solid angle

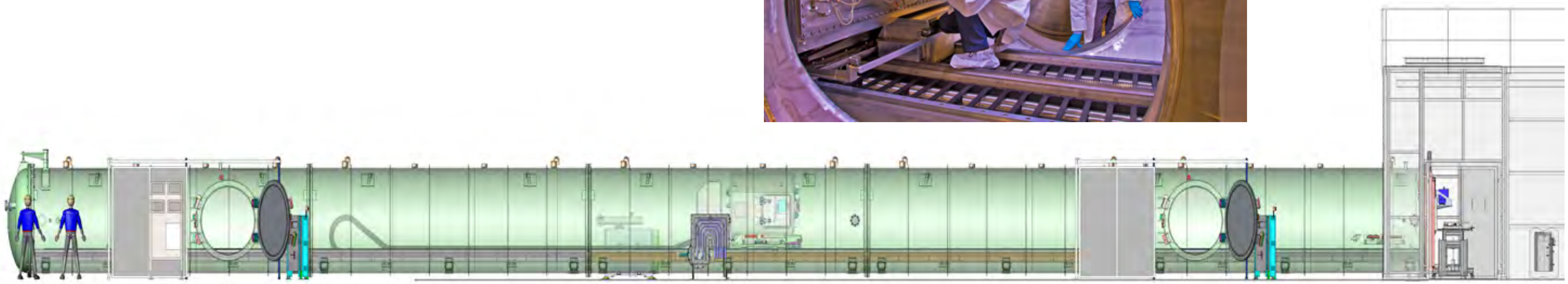
$$I(q) = \frac{d\Sigma}{d\Omega} = \frac{1}{V_{Scat}} \frac{d\sigma}{d\Omega}$$

Narayanan T. (2008) Synchrotron SAXS. In: Borsali R., Pecora R. (eds) Soft Matter Characterization. Springer https://doi.org/10.1007/978-1-4020-4465-6_17

SAXS instrumentation

SAXS, WAXS and USAXS

SAXS-WAXS
USAXS
ID2 TIME RESOLVED



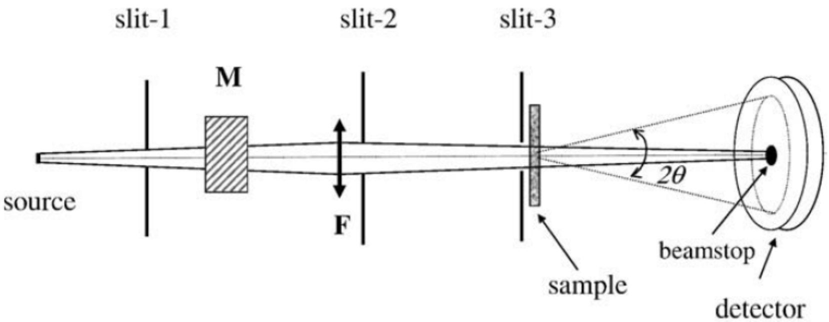
µ-beam SAXS, WAXS

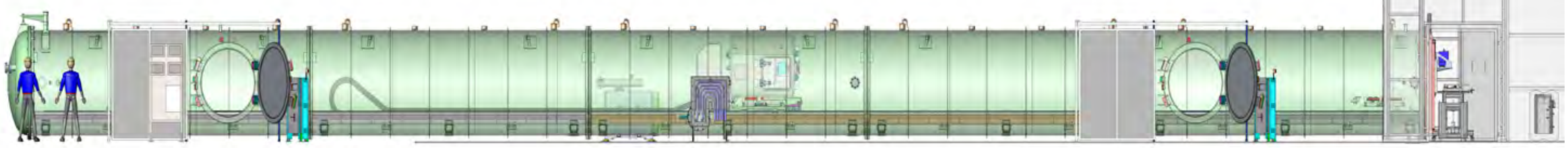
ID13
THE MICROFOCUS BEAMLINE

SAXS instrumentation

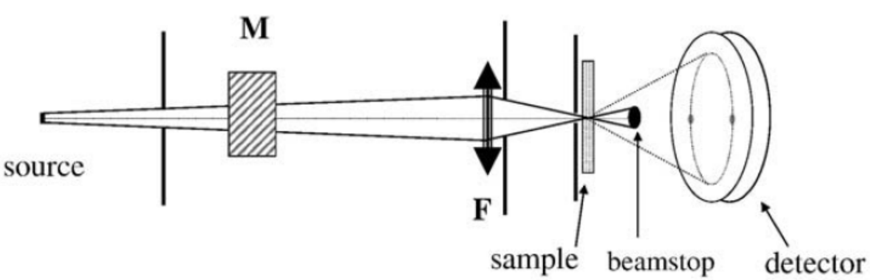
SAXS-WAXS
USAXS
ID2 TIME RESOLVED

SAXS, WAXS and USAXS





μ-beam SAXS, WAXS



ID13
THE MICROFOCUS BEAMLINE

(On-line) data reduction

(A) detector specific corrections

(B) scattering specific corrections

(C) sample and beam specific corrections

(A) detector specific corrections

CCD raw image [ADU]	i_{raw}	} identical exposure times
CCD dark image [ADU]	i_{dark}	
Flat field image [photons/ADU]	f_2	(corrected for distortion)

1. Dark image subtraction [ADU]	$i_1 = i_{raw} - i_{dark}$
2. Spatial distortion correction [ADU]	$I_2 = SPD(I_1)$
3. Division by flatfield [photons]	$i_3 = i_1 / f_2$

- Subtraction and division are done pixel by pixel
- The spatial distortion correction consists of a horizontal and vertical displacement of each pixel

4. Normalization to I0 [photons] and conversion to scattering cross section [1/sterad]

$$\left(\frac{1}{A}\right)\frac{\partial\sigma}{\partial\Omega} = \frac{\#\,Photons_{scattered}\ sterad}{\#\,Photons_{in}} = i_4 = \frac{i_3}{I_0}\cdot\frac{L_p^{\,2}}{p_1\cdot p_2}\cdot\frac{L_p}{L_0}$$

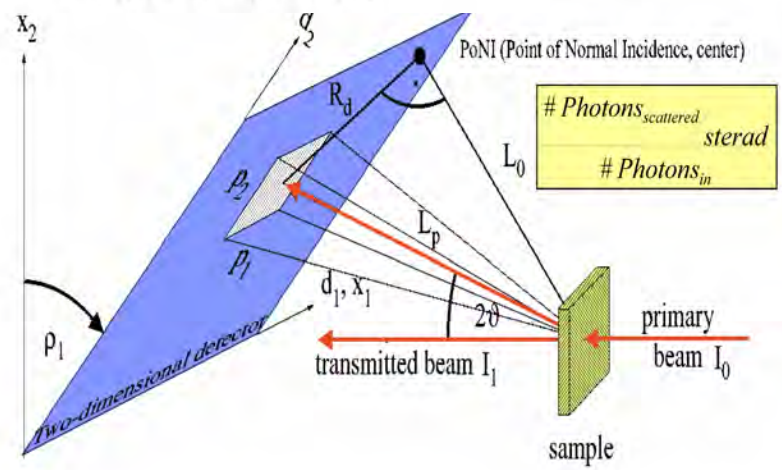
inclined surface: $\frac{L_p}{L_0}$

$1/\Delta\Omega$: $\frac{L_p^{\,2}}{p_1\cdot p_2}\cdot\frac{L_p}{L_0}$

shortest sample to detector distance L_0
sample to pixel distance L_p
pixel size p_1, p_2

(see Bösecke, Diat, J. Appl. Cryst. (1997). 30, 867-871
and Narayanan, Diat, Bösecke, NIM A 467-468 (2001) 1005-1009)

normalizing a two dimensional scattering pattern measured with a plane two-dimensional detector to absolute intensities in units of scattered photons per steradian and per incident photon, i.e. scattering cross section dσ/dΩ per sample cross section A;
to correct for absorption the normalized pattern is divided by the sample transmission T



(C) sample and beam specific corrections

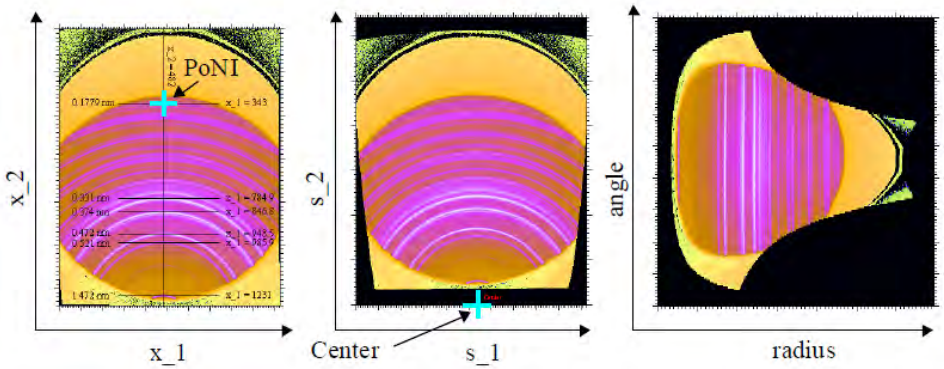
5. Normalization to transmission and scattering volume, e.g. thin film: T=I1/I0, d: sample thickness
$$i_5 = \frac{i_3}{d \cdot I_1} \cdot \frac{L_p^{\;2}}{p_1 \cdot p_2} \cdot \frac{L_p}{L_0}$$

6. Polarization correction (WAXS)

7. Reciprocal space mapping (WAXS) (Ewald sphere projections in reciprocal space, sample orientation required)

8. Azimuthal averaging

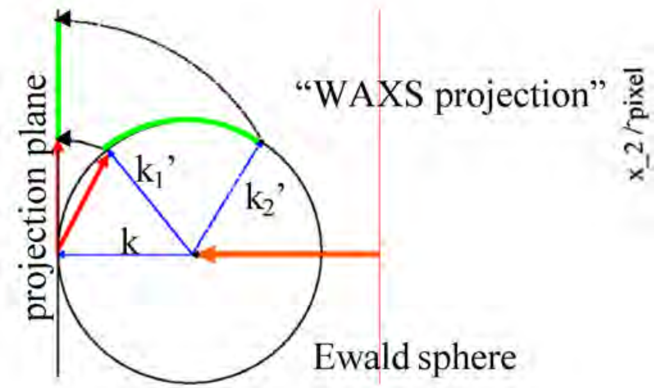
WAXS projection



raw WAXS pattern (inclination 32.5 degrees)

projected WAXS pattern

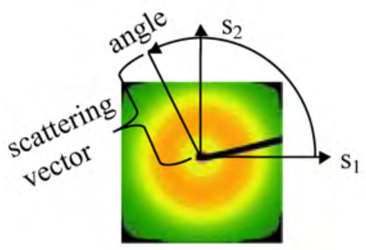
azimuthally regrouped WAXS pattern

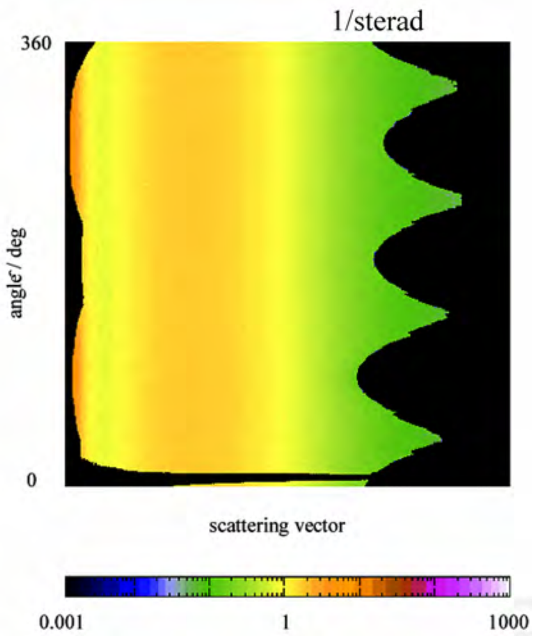


In Waxs projection the scattering pattern of a tilted detector can be geometrically analysed (azimuthal regrouping etc.) like a small angle scattering pattern.

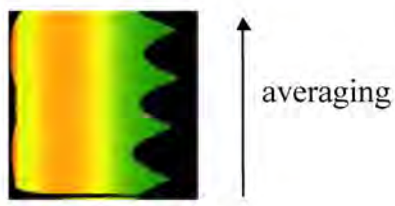
Data reduction steps

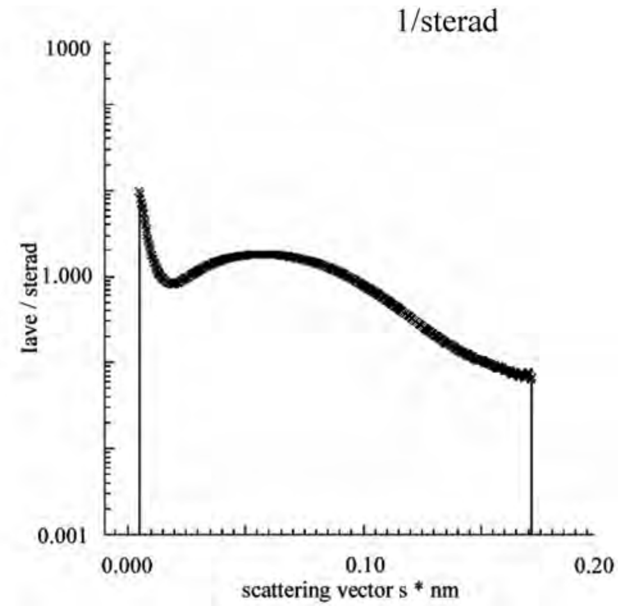
azimuthal regrouping





azimuthal averaging



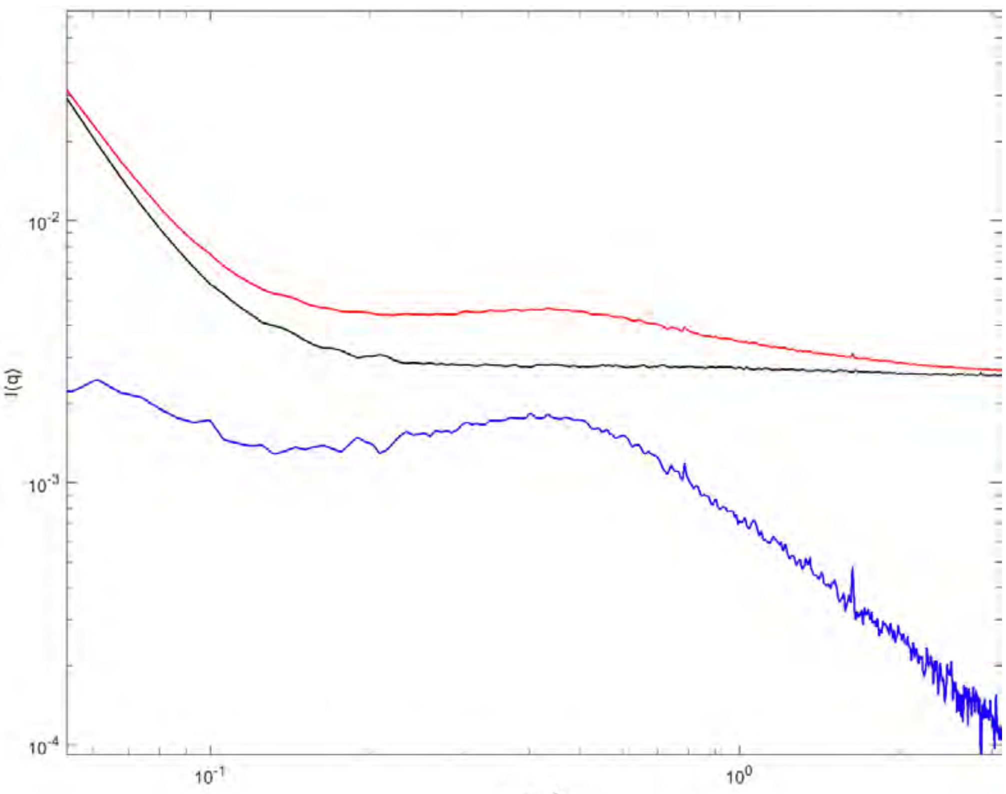


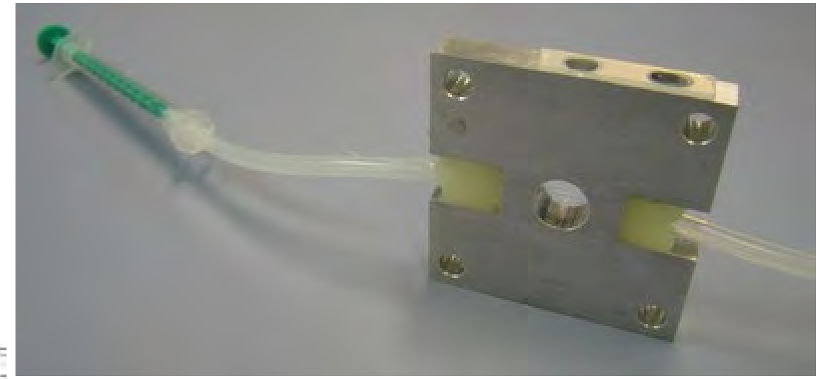
Good practice of data recording

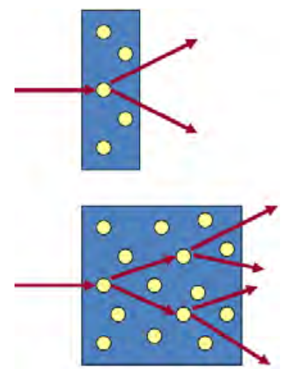
background subtraction

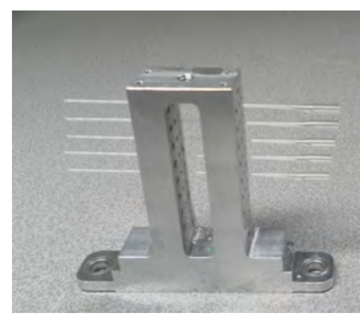
flow-through cells

radiation damage



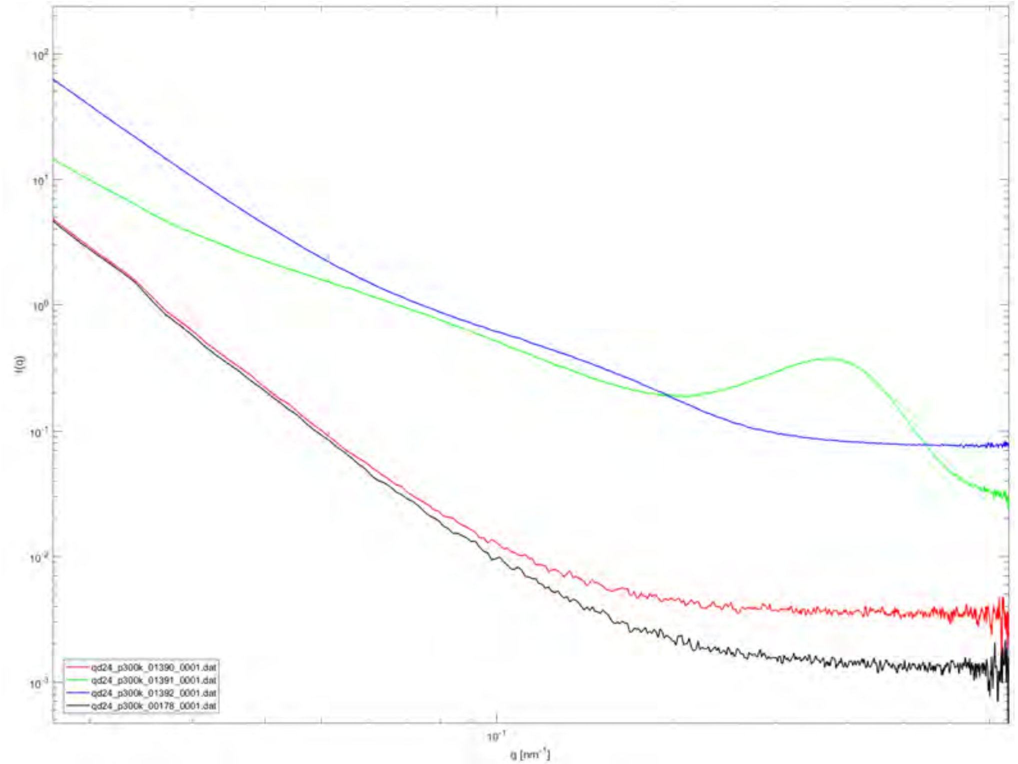






Absolute intensity calibration

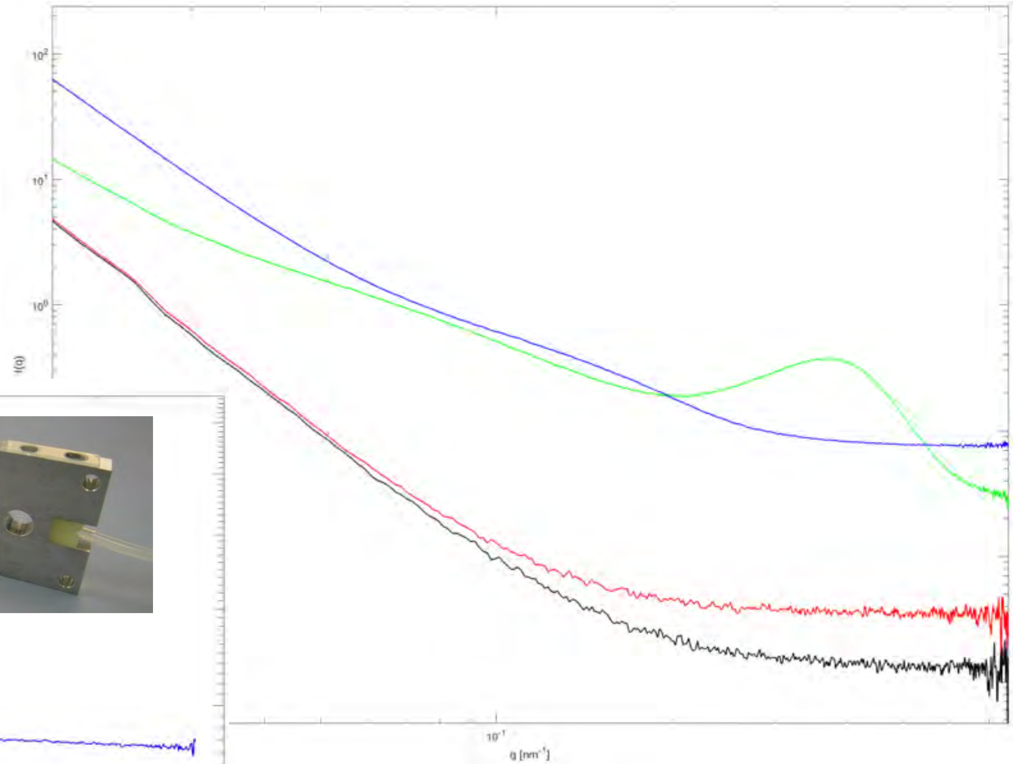
using secondary standards like water, lupolen, glassy carbon, …

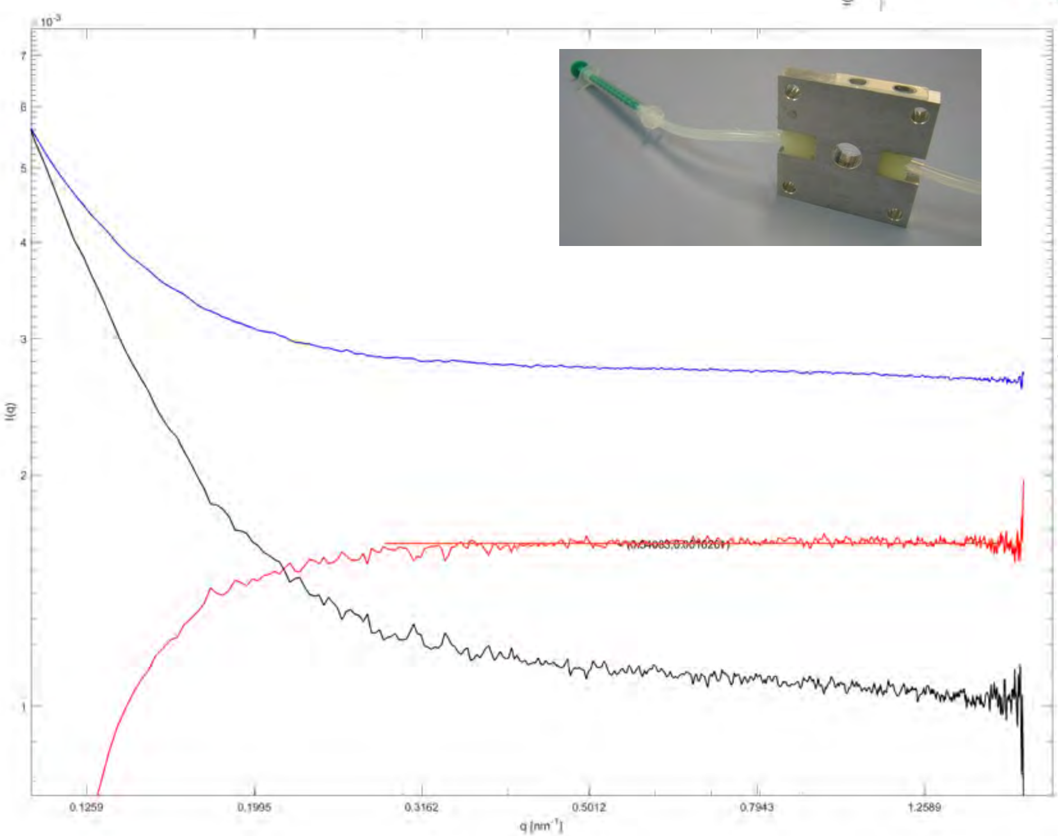


Absolute intensity calibration

using secondary standards like water, lupolen, glassy carbon, …

scattering of 1mm of water at RT: 0.00164





ID02 data and metadata concept

data.edf

```
{
EDF_DataBlockID = 1.Image.Psd ;
EDF_BinarySize = 1440256 ;
EDF_HeaderSize = 8192 ;
ByteOrder = LowByteFirst ;
DataType = FloatValue ;
Dim_1 = 1000 ;
Dim_2 = 360 ;
Dummy = -10 ;
DDummy = 0.1 ;
Offset_1 = 0 ;
Offset_2 = 0 ;
History-1 = ""C:\\Program Files (x86)\\SAXSutilitie
    C:\\Data\\SAXSutilities_Testdata\\h5/og22_saxs_
HeaderID = EH:000001:000000:000000 ;
Compression = None ;
Image = 1 ;
SaxsDataVersion = 2.40 ;
Size = 1440256 ;






}
'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7-
    '7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7-
    '7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7-
```

data.h5

- NXroot top level, one per file
  - NXentry one group per measurement
    - NXinstrument only one per NXentry
      - NXdetector
      - NXdata one NXdata group per plot
    - measurement (@NXcollection) flattened view of everything measured - only one per NXentry
      - NXdetector
      - NXdata one NXdata group per plot
        - data
        - metadata
    - NXsample
    - user (@NXuser)
    - NXprocess for analysis

understanding of the data formats (EDF, HDF5)

http://www.esrf.eu/home/UsersAndScience/Experiments/CBS/ID02/available_software.html
→ SAXS programs → SX_parametrization

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Contents

understanding of the data formats (EDF, HDF5)

SX General Parameters

- *Dim_1, Dim_2*, ... (Dim_1 default is 0, all others are 1)
- *RasterOrientation* (1 to 8 possible, 9-16 for compatibility, needs to be tested, default 1)

SX Image Parameters

- *Offset_1, Offset_2*, ... (default: 0)
- *BSize_1, BSize_2*, ... (default: 1)

SX Scattering Parameters

- *PSize_1, PSize_2*, ... (no default) [m]
- *Center_1, Center_2*, ... (PoNI in image reference system including offsets, no default)
- *SampleDistance* (no default) [m]
- *WaveLength* (no default) [m]
- *DetectorRotation_1*, *DetectorRotation_2*, *DetectorRotation_3*, ... (default: 0) [rad]

Additional SX Scattering Parameters

- *ProjectionType* (Saxs|Waxs, default: Saxs: distances proportional to tan(2ϑ))
- *AxisType_1, AxisType_2*, ...(Distance, Angle, Numerator, default: Distance)

SX Intensity Calibration and Normalization Parameters

- *Intensity0* (no default), *Intensity1* (*Intensity0*)
- *NormalizationFactor* (default 1)
- *SampleThickness* (no default)

```
{
EDF_DataBlockID = 1.Image.Psd ;
EDF_BinarySize = 1440256 ;
EDF_HeaderSize = 8192 ;
ByteOrder = LowByteFirst ;
DataType = FloatValue ;
Dim_1 = 1000 ;
Dim_2 = 360 ;
Dummy = -10 ;
DDummy = 0.1 ;
Offset_1 = 0 ;
Offset_2 = 0 ;
History-1 = ""C:\\Program Files (x86)\\SAXSuti
    C:\\Data\\SAXSutilities_Testdata\\h5/og22_
HeaderID = EH:000001:000000:000000 ;
Compression = None ;
Image = 1 ;
SaxsDataVersion = 2.40 ;
Size = 1440256 ;






}
```

'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7
'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7
'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7+Á'7

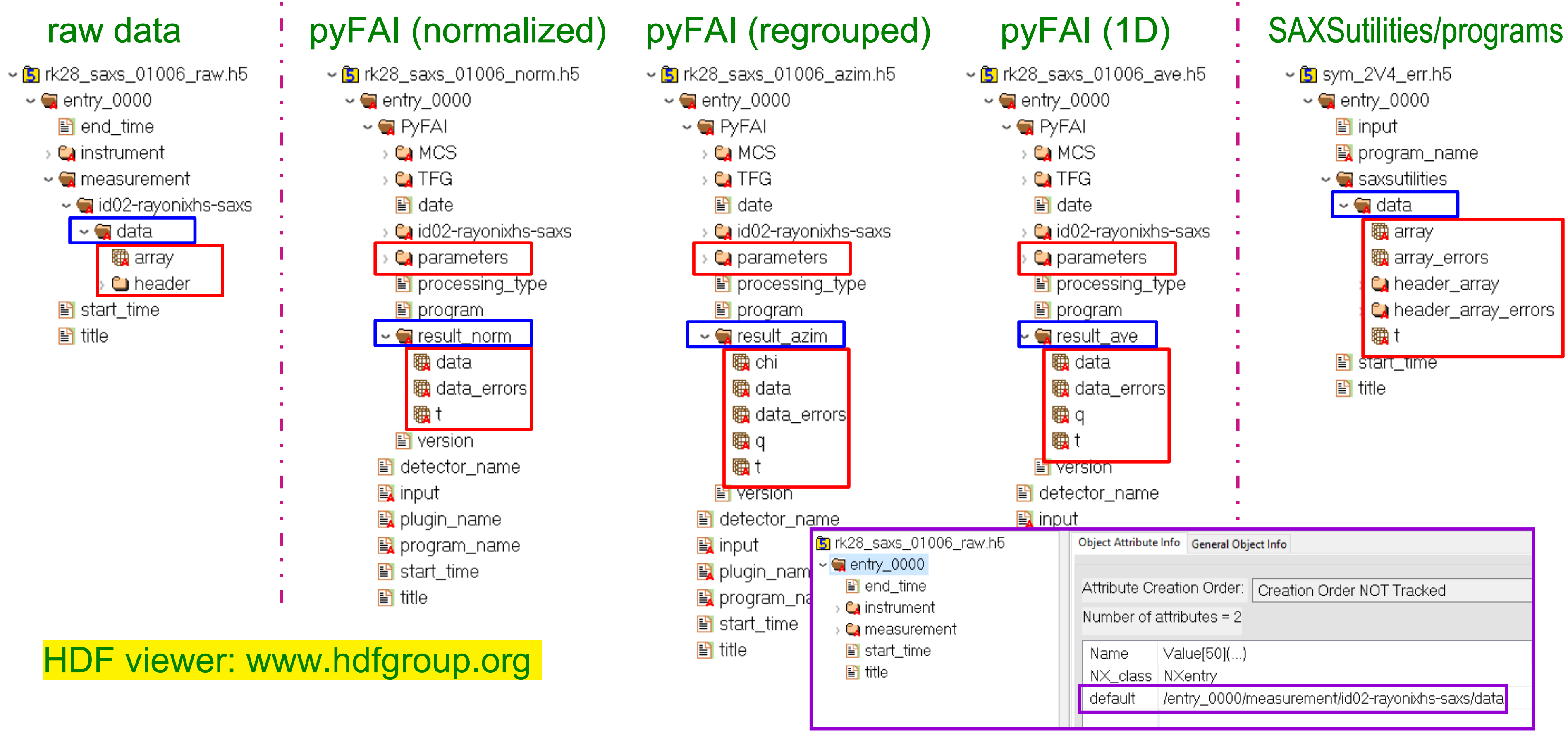
Keywords for SAXS Data in EDF Files

EDF_DataFormatVersion = 2.42

Peter Boesecke

http://www.esrf.eu/home/UsersAndScience/Experiments/CBS/ID02/available_software.html
→ SAXS programs → Saxs Format Manual

understanding of the data formats (EDF, HDF5)



NXDATA : data/data_errors (pyFAI), array/array_errors (beamline)

NOTE: “default” attributes tell you where to find data

metadata: parameters (pyFAI), header or header_array/header_array_errors

NOTE: only “header” describes NXDATA according SX_parametrization
“parameters” are only a copy of header of raw data

ID02 tools for data reduction and visualization

available programs:

+ spd
+ saxs programs
+ SAXSutilities

+ PyFAI

→ on-line and offline ←

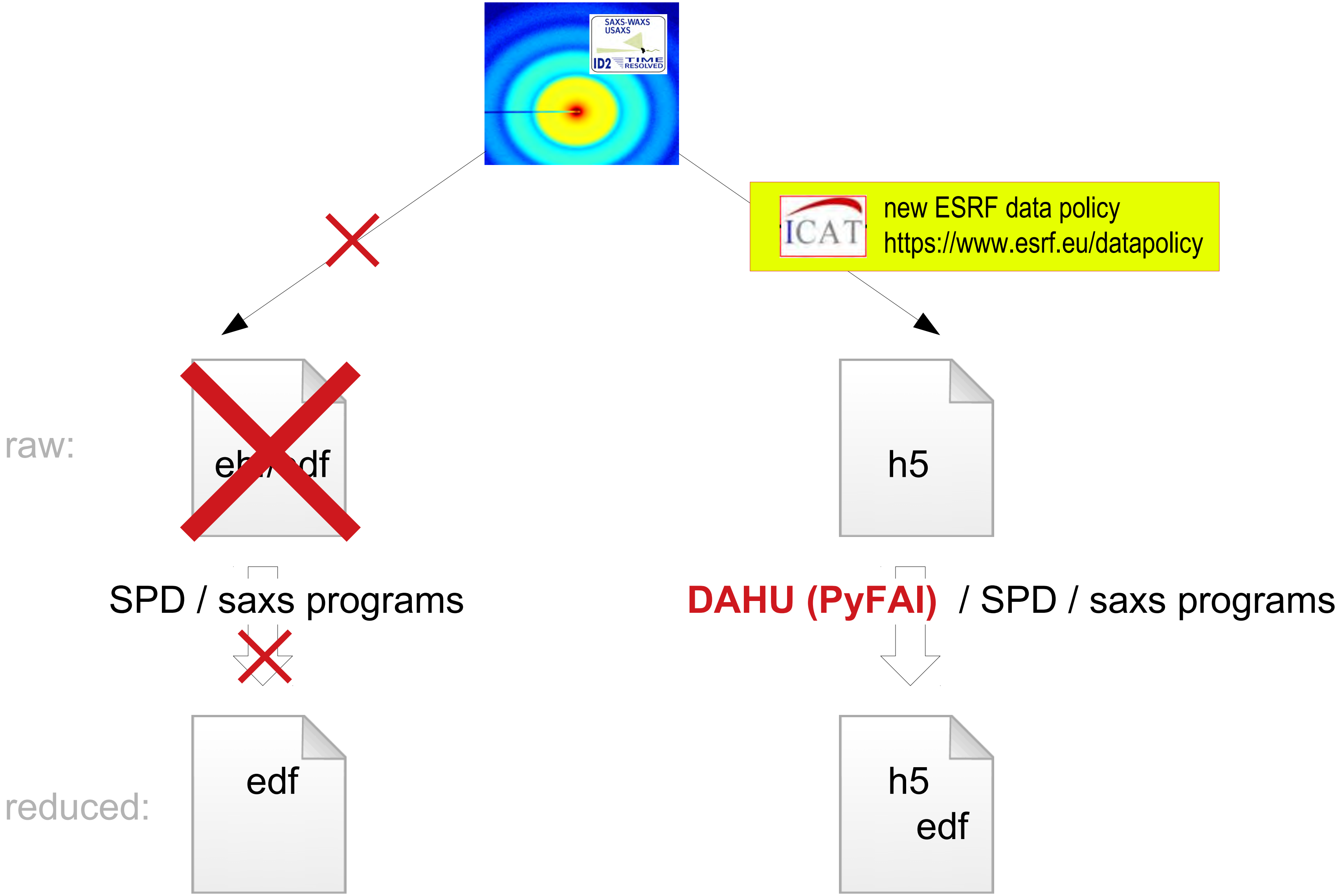
http://www.esrf.fr/home/UsersAndScience/Experiments/CBS/ID02/BeamlineDescription/DataReduction/SoftwareIntroduction.html

demonstration:

data reduction in 2D and 1D:
e.g. partial integration, averaging, subtraction, merging

typical artefacts

ID02 online data processing



SPD – saxs programs

ID02 online data reduction (SPD) package was developed by P. Boesecke, A. Sole and R. Wilcke during 2001-2005

saxs programs are command line oriented programs (C) to perform certain tasks for data reduction

propagation of statistical errors

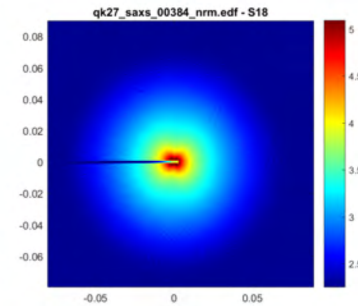
GUI is available for most common tasks in SAXSutilities

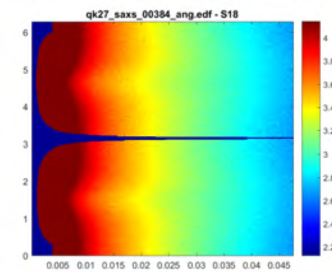
Program name	Short description
saxs_mac	standard operations on images, e.g.
	multiply by factor and add constant
saxs_add,	add, subtract, multiply, divide
saxs_sub,	several images
saxs_mul,	
saxs_div	
saxs_normn	flatfield correction and
	normalization of scattering patterns
	to absolute units in 1/sterad
saxs_waxs	waxs projection and backprojection
saxs_angle	transformation to polar coordinates
saxs_row,	row, column projection of images
saxs_col	
saxs_ascii	convert images to ascii
saxs_patch	patch images to other images
saxs_stat	calculate image statistics

P. Bösecke, "Reduction of two-dimensional small- and wide-angle X-ray scattering data," J. Appl. Cryst. 40, 423-427 (2007)

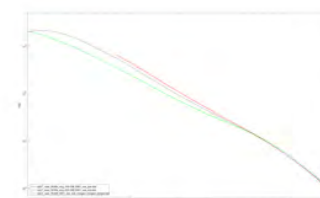
SPD – saxs programs

```
saxs_arc
        -omod n
        -i1nam ra26_saxs_%%%%%_nrm.edf,1,500
        +mask
        -i2nam mask-2m5.edf
        -onam ra26_saxs_%%%%%_nrm_azim.edf
        +pass
        -p
```






```
saxs_curve
        -alf1 80_deg
        -alf2 100_deg
        -scf 2_pi
        -head
        -hedl "q*nm [TitleBody,,1]"
        -ext .dat
        -i1nam ra26_saxs_%%%%%_nrm_azim.edf,1,500
        -onam ra26_saxs_%%%%%_nrm_80-100_ave.dat
        -p
```



Note: double the number of ‘%’ in windows bat scripts...

saxs programs

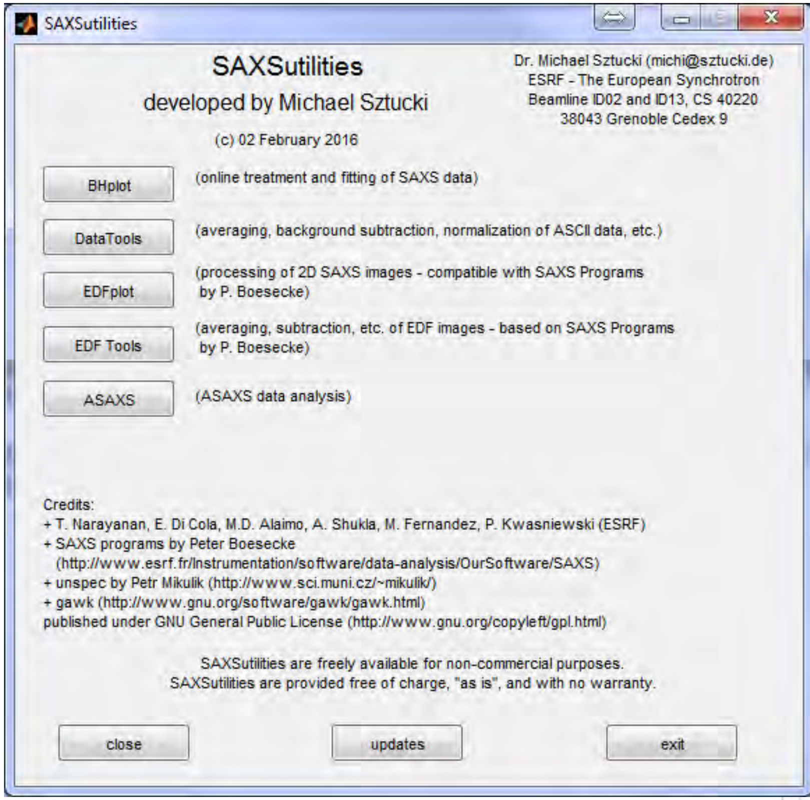
further info:

http://www.esrf.eu/home/UsersAndScience/Experiments/CBS/ID02/available_software.html
→ SAXS programs → SaxsPrograms Package Manual

PETER BOESECKE SaxsPrograms.doc 2013/01/25

P. Bösecke, "Reduction of two-dimensional small- and wide-angle X-ray scattering data," J. Appl. Cryst. 40, 423-427 (2007)

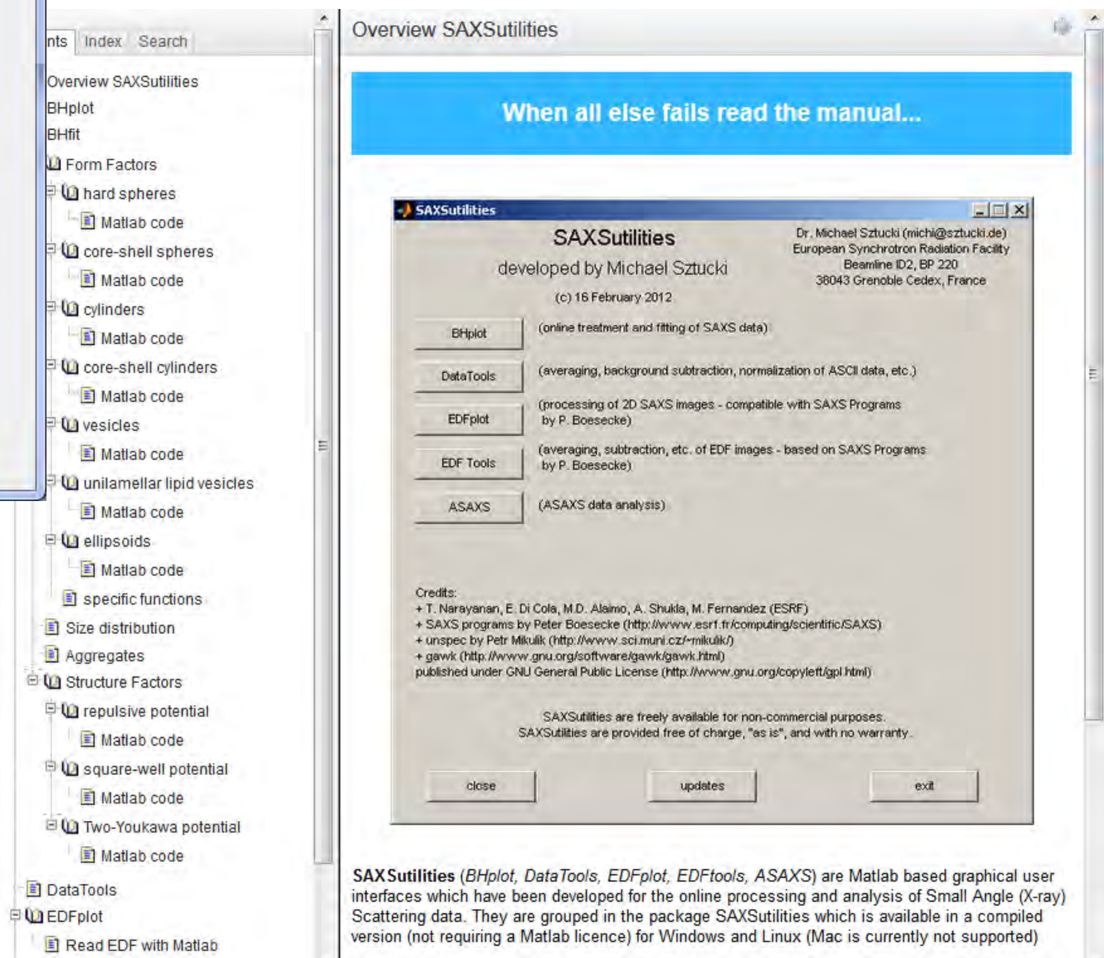
SAXSutilities(2)



NEW in spring 2020:

SAXSutilities2 developed in Python 3.6/3.7

package with Windows / Linux installer



http://www.saxsutilities.eu

SAXSutilities – SAXSutilities2 ready for restart of beamlines in spring 2020

Get latest Windows version (WindowsXP, Vista, Windows7, Windows8) :

Download and install program files using the installer (64bit): SAXSutilitiesSetup64.exe
Do not forget to install the Matlab runtime environment!!
You will be asked at the end of the installation routine to download and install this runtime environment. The installation has to be done only once.

Download 32bit version: SAXSutilitiesSetup32.exe
This version might not support all features of the 64bit version!!

Get latest Linux version *(64-bit only!)* (developed under Debian6):

New procedure since October 2013 (Matlab R2013b) !!!

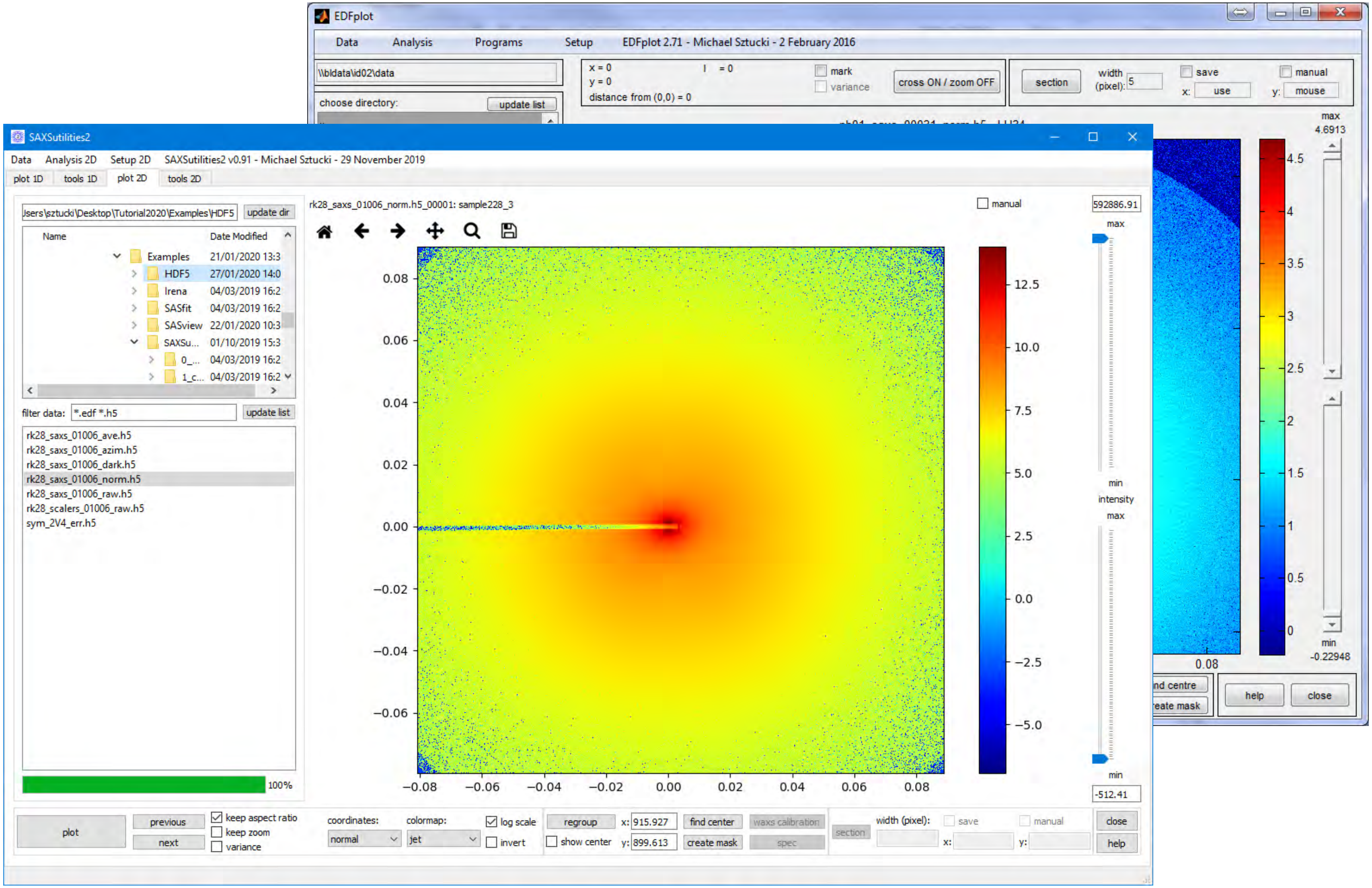
1. Download and unpack to a folder of your choice: saxsutilities.zip
   `> unzip saxsutilities.zip`
2. Download and unzip: MCRInstaller2013b_glnxa64.zip
   `> unzip MCRInstaller2013b_glnxa64.zip`
   Then, run the MCR Installer script from the directory where you unzipped the package file by entering:
   `> ./install`
   Add the environment variables **LD_LIBRARY_PATH** and **XAPPLRESDIR** to your system as indicated in the last step of the installation procedure.
   Note *that this has to be done only once for each new release of Matlab.*
3. Add an environment variable **SAXSUTILITIESPATH** to your system which points to the directory created in step 1.
4. Note that unspec by P. Mikulík has to be installed.
5. Note that saxsprograms by P. Bösecke have to be installed.
6. Note that roca by P. Bösecke has to be installed. (Since version saxs_V2.461P2.043E2.236R1.500 included in saxsprograms)
7. Start SAXSutilities from the folder created in step 1.

   You can also use a start script like:

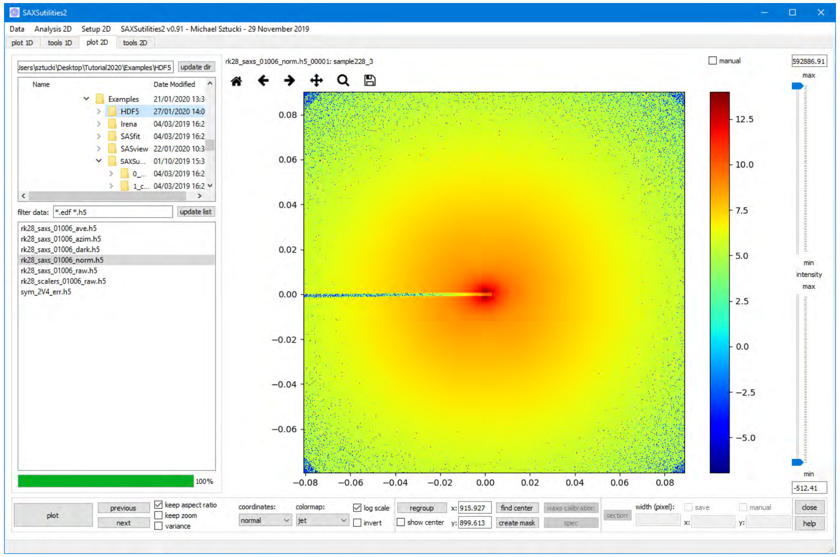
```
#!/bin/csh
setenv LD_LIBRARY_PATH [...as indicated by MCRInstaller...]
setenv XAPPLRESDIR [...as indicated by MCRInstaller...]
setenv SAXSUTILITIESPATH [/path/to/directory/of/SAXSutilities]
[/path/to/directory/of/SAXSutilities]/SAXSutilities
```

http://www.saxsutilities.eu

SAXSutilities(2) – 2D visualisation (EDFplot / plot2D)



SAXSutilities(2) – 2D visualisation (EDFplot / plot2D)



Saxs COORDINATES < ≠ > Saxs PROJECTION

Saxs PROJECTION (scattering pattern on a flat 2D detector)

$$\text{SAXS coordinate} = \frac{\text{(distance of pixel from poni on detector)}}{\text{(distance of poni from sample)}} * \frac{\text{wavelength0}}{\text{wavelength}}$$

where wavelength0 is 1e-9 m

SAXS(Saxs) coordinate ~ s*nm for 2Theta<<1

Waxs PROJECTION (projection of the scattering pattern from the EWALD sphere to a plane perpendicular to the incident beam)

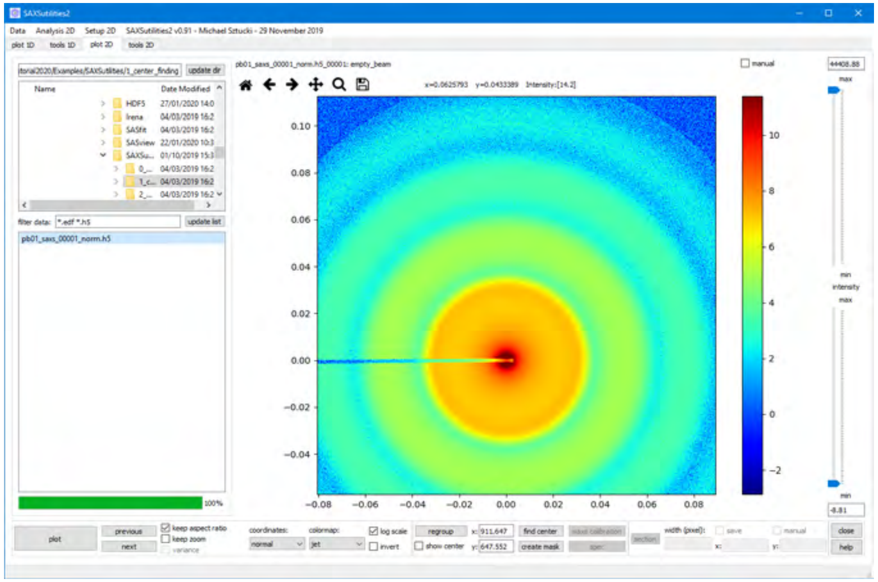
In the Waxs projection, the scattering pattern of the detector is distorted in such a way that the SAXS coordinate of the new pattern is equal to s:

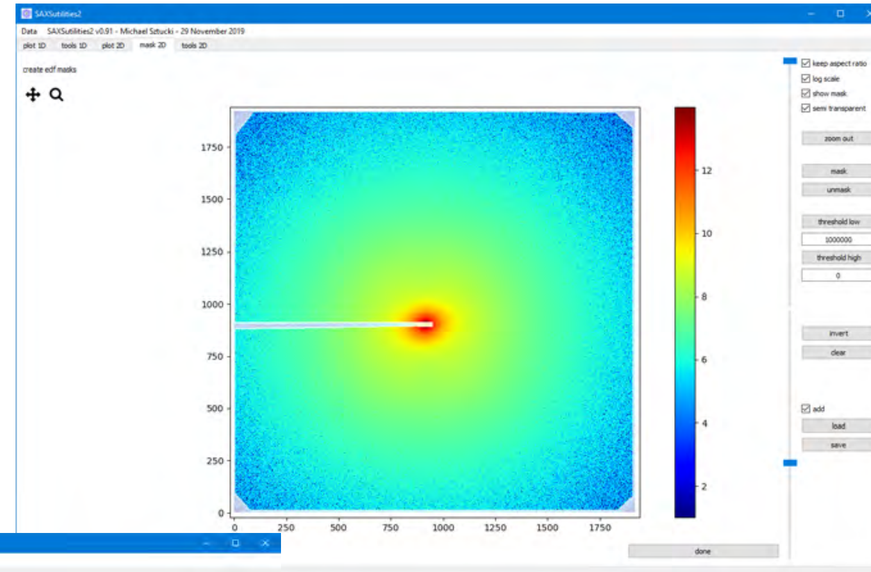
SAXS(Waxs) coordinate = s*nm

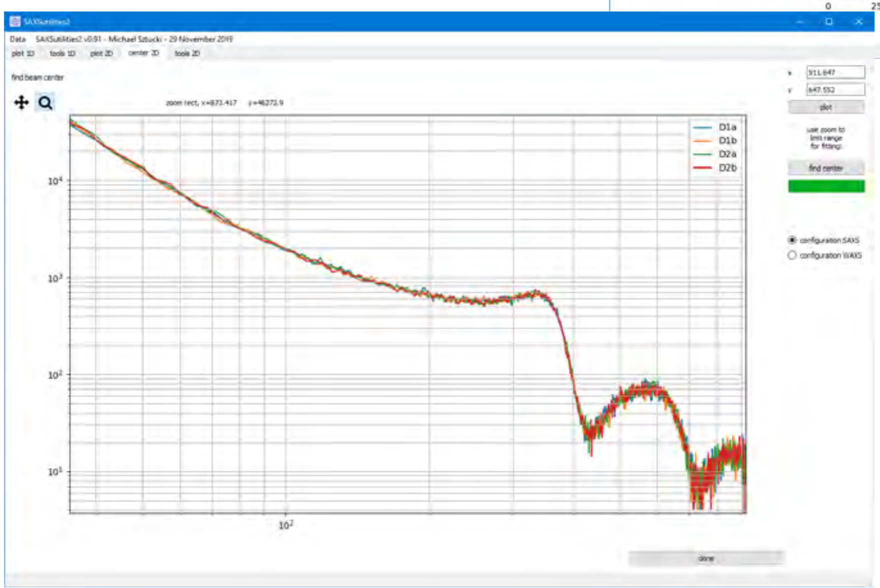
In Waxs PROJECTION the scattering pattern of a tilted detector can be geometrically analysed (azimuthal regrouping etc.) like a small angle scattering pattern.

Reference system	Applied affine coordinate transformation
Array	$f_A = f$
Image	$f_I = \text{Offset} + f$
Region	$f_B = (\text{Offset} + f) \times \text{BSize}$
Real	$f_R = (\text{Offset} + f) \times \text{PSize}$
Center	$f_C = \text{Offset} - \text{Center} + f$
Normal	$f_N = (\text{Offset} - \text{Center} + f) \times \text{PSize}$
Saxs	$f_S = \text{Normal}(\text{Offset}, \text{Center}, \text{PSize}, f)/\text{SampleDistance}/(\text{WaveLength}/\text{nm})$

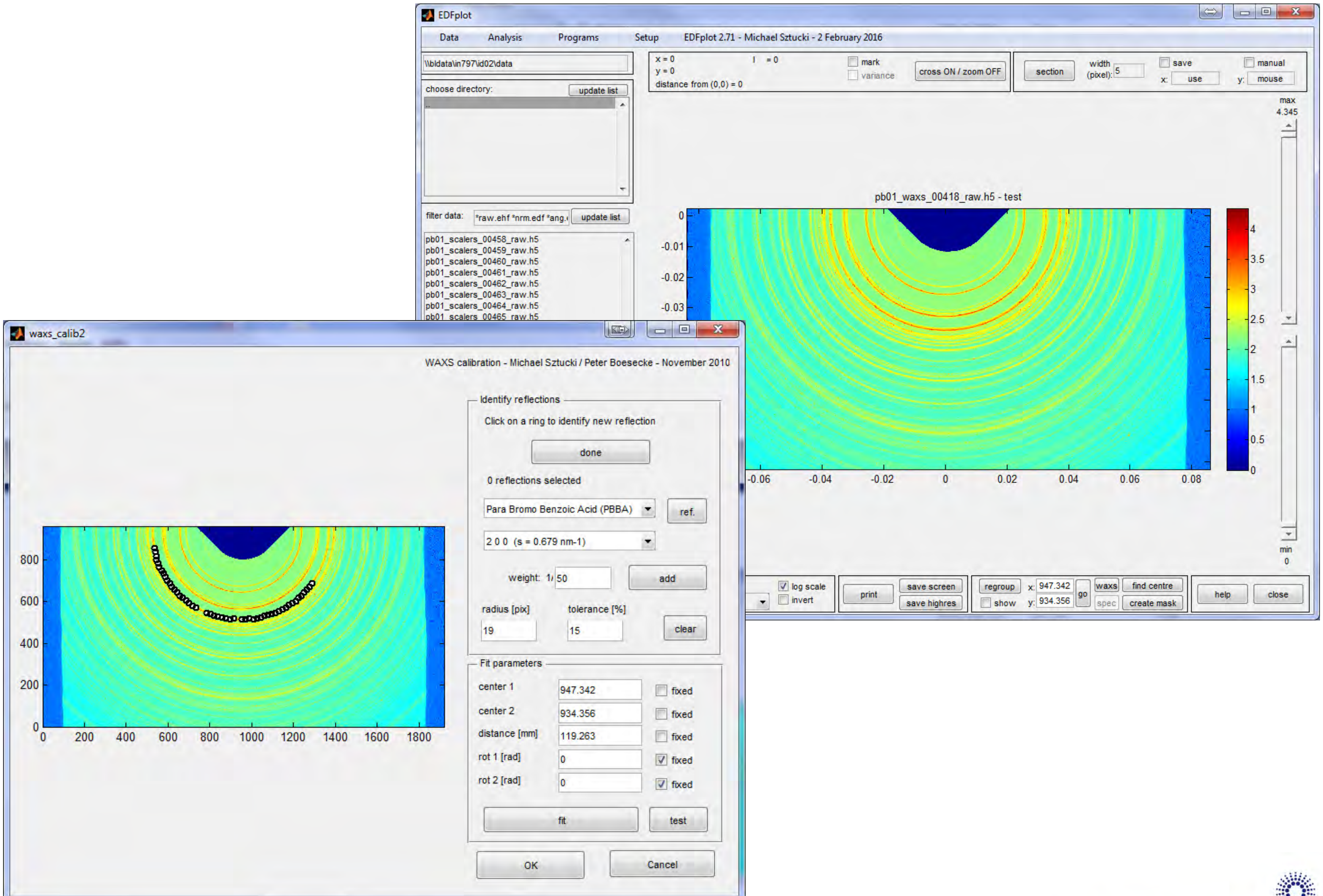
SAXSutilities(2) – 2D visualisation (EDFplot / plot2D)



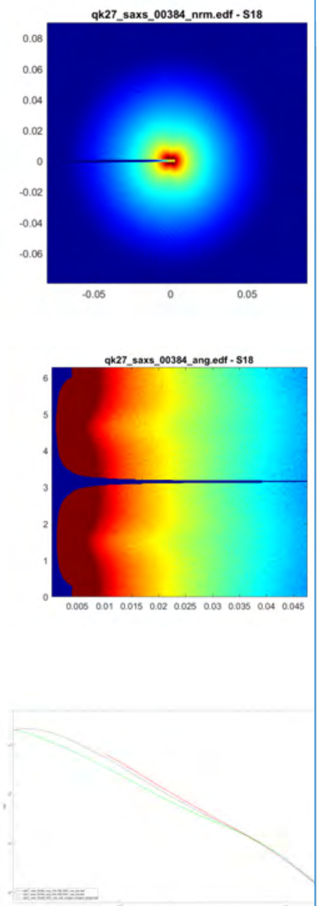


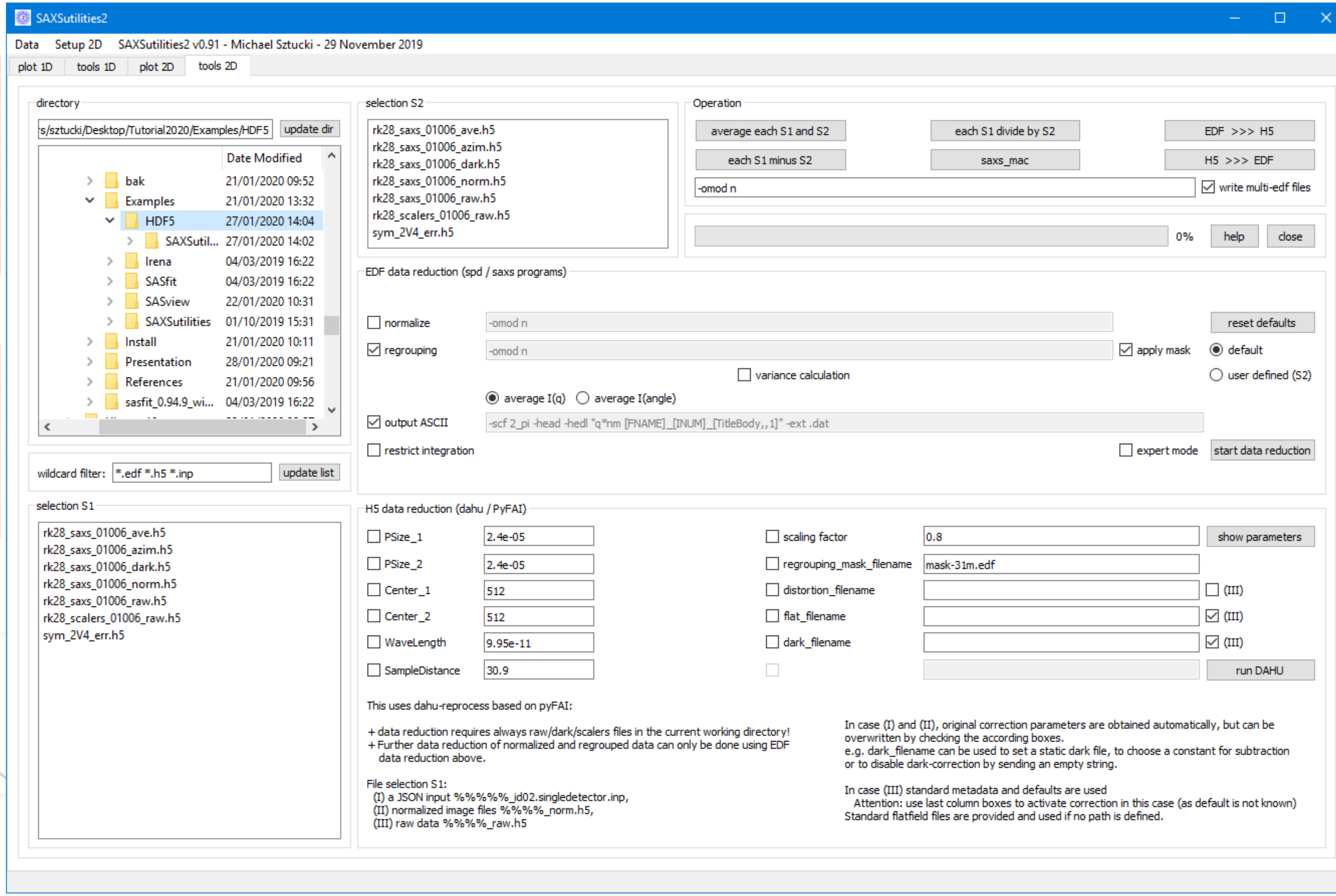


SAXSutilities – 2D visualisation (EDFplot)

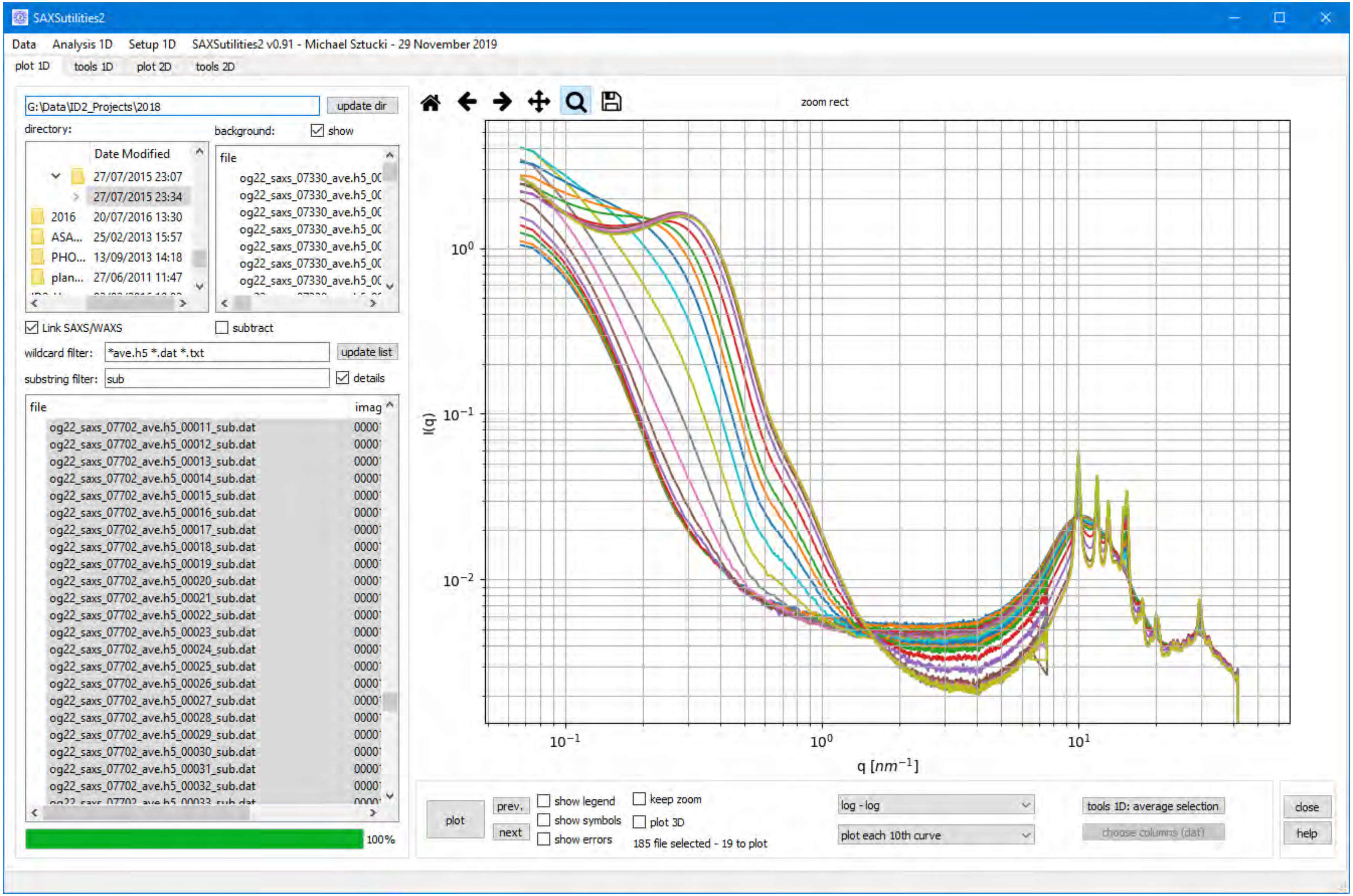


SAXSutilities(2) – 2D tools (EDFtools / tools 2D)

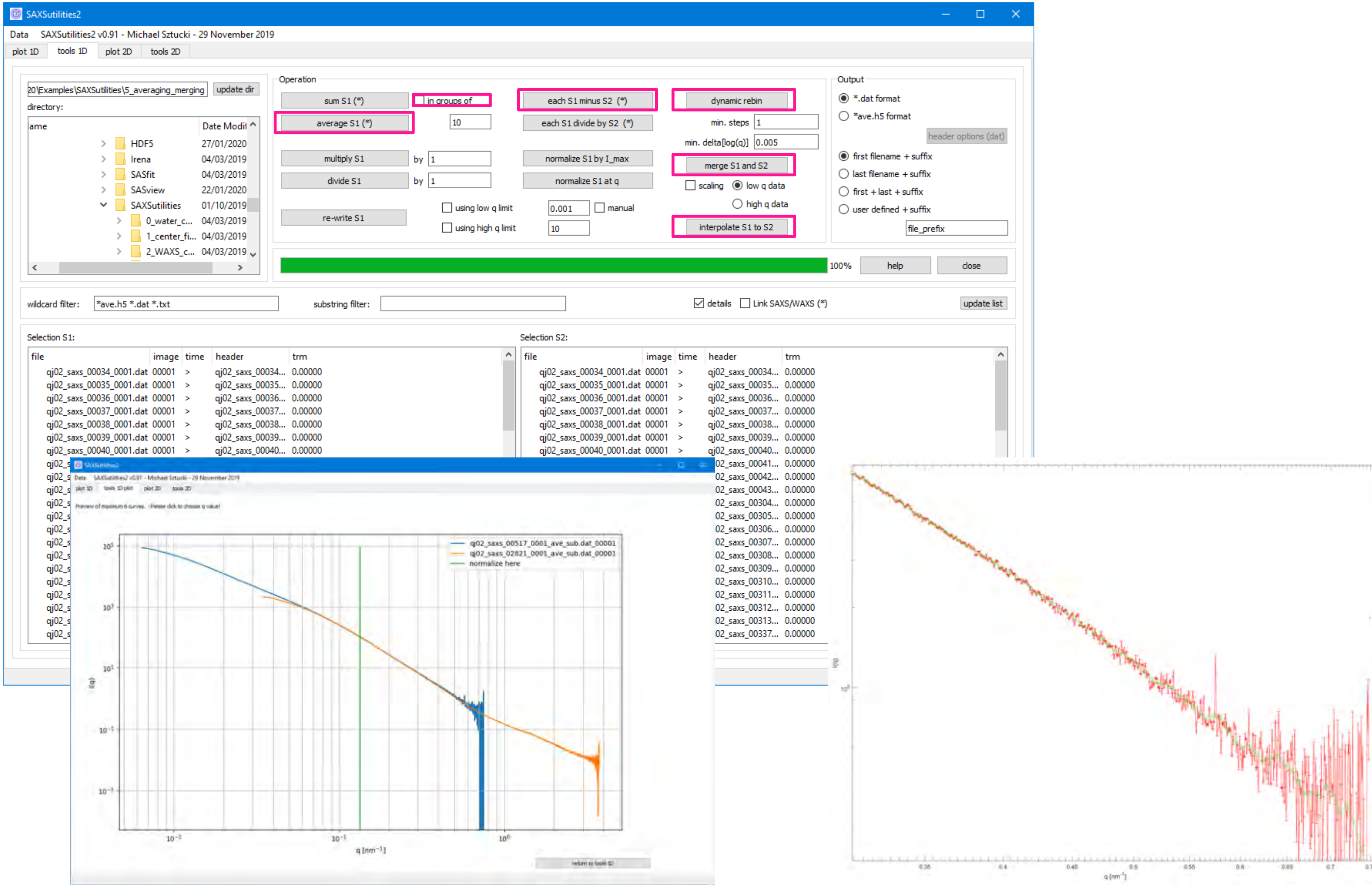




SAXSutilities(2) – 1D visualisation (BHplot / plot1D)



SAXSutilities(2) – 1D tools (DataTools / tools1D)



Outline

- SAXS instrumentation and theory
- SAXS data reduction and calibration
- Good practice for data recording
- SAXS data formats
- Tools for (on-line) data reduction and visualization:
  SPD, saxs programs, PyFAI, SAXSutilities

- Data Interpretation / modelling
- Form factor, Guinier / Porod law, Unified fitting, size distributions, structure factor
- Programs: SAXSutilities, IRENA, SASview, SASfit

Form factor (dilute case)

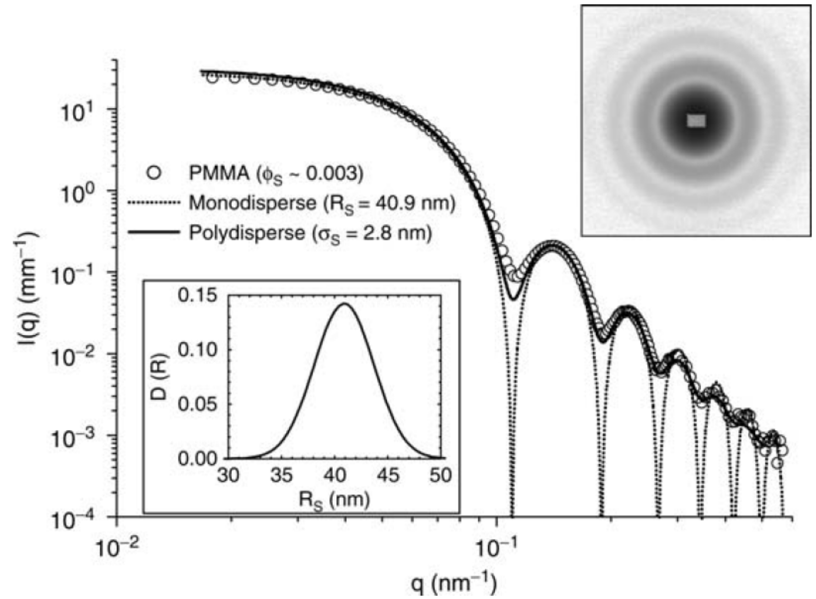
$$I(q) = N|F(q)|^2$$

scattering amplitude:

$$F(q) = \int_V \rho(r)\, e^{iqr}\, dV$$

in case of isotropic particles:

$$F(q) = 4\pi \int_0^\infty \Delta\rho(r) \frac{\sin(qr)}{qr} r^2 dr$$



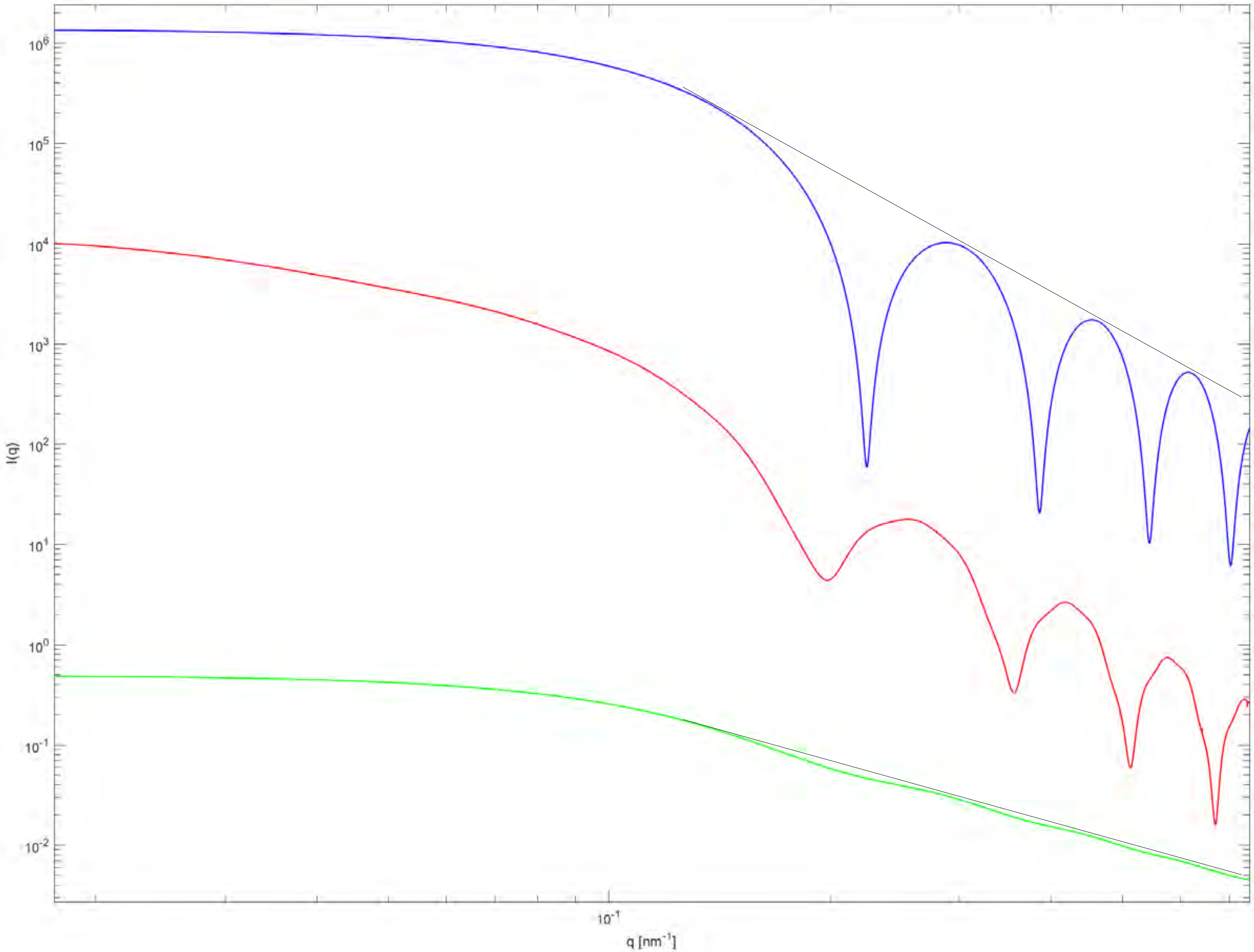
in case of isotropic sperical particles:

$$|F(q)|^2 = V_S^2 \Delta\rho^2 \left(\frac{3[\sin(qR_S) - qR_S \cos(qR_S)]}{(qR_S)^3} \right)^2 = V_S^2 \Delta\rho^2 P(q, R_S)$$

Form factor (dilute case)

Uniform sphere of radius, R_S	$P(q,R_S)=\left(\frac{3[\sin(qR_S)-qR_S\cos(qR_S)]}{(qR_S)^3}\right)^2=F_0^2(qR_S)$
Randomly oriented cylinder of radius R_C and height H	$P(q,R_c,H)=\int_0^{\pi/2}\left\{\left[\frac{2J_1(qR_C\sin\varphi)}{qR_C\sin\varphi}\right]\left[\frac{\sin((qH/2)\cos\varphi)}{(qH/2)\cos\varphi}\right]\right\}^2\sin\varphi\,d\varphi$ J_1 – first order Bessel function and φ – orientation angle.
Spherical shell of inner and outer radii R_1 and R_2	$V^2P(q,R_1,R_2)=\frac{16\pi^2}{9}\left[R_2^3F_0(qR_2)-R_1^3F_0(qR_1)\right]^2$ $F_0(q,R)$ – sphere function given above.
Spherical core-shell of core and shell radii R_1 and R_2	$F^2(q,R_1,R_2)=[V_2\Delta\rho_2F_0(qR_2)-V_1\Delta\rho_1F_0(qR_1)]^2$ V_1 and V_2 are volumes of inner and outer spheres, $\Delta\rho_1$ and $\Delta\rho_2$ are contrast between shell and core, and shell and medium, respectively.

Form factor (dilute case)



Limiting form of I(q): Guinier and Porod law

Guinier plot:

$$I(q) = N\, V^2 \Delta\rho^2 \,\exp\left(\frac{-q^2 R_G^2}{3}\right)$$

valid at low concentration and small values of q $qR_g < 1$

plot of $\ln(I)$ against q^2 has slope $-R_g^2/3$

radius of Gyration depends on particle shape

R_g^2 is the average squared distance of the scatterers from the centre of the object

Sphere $R_g^2 = \frac{3}{5} R^2$

Ellipse $R_g^2 = \frac{a^2 + b^2}{4}$

Cylinder $R_g^2 = \frac{R^2}{2} + \frac{h}{12}$

analysis based on limiting form of I(q):

Guinier and Porod plot

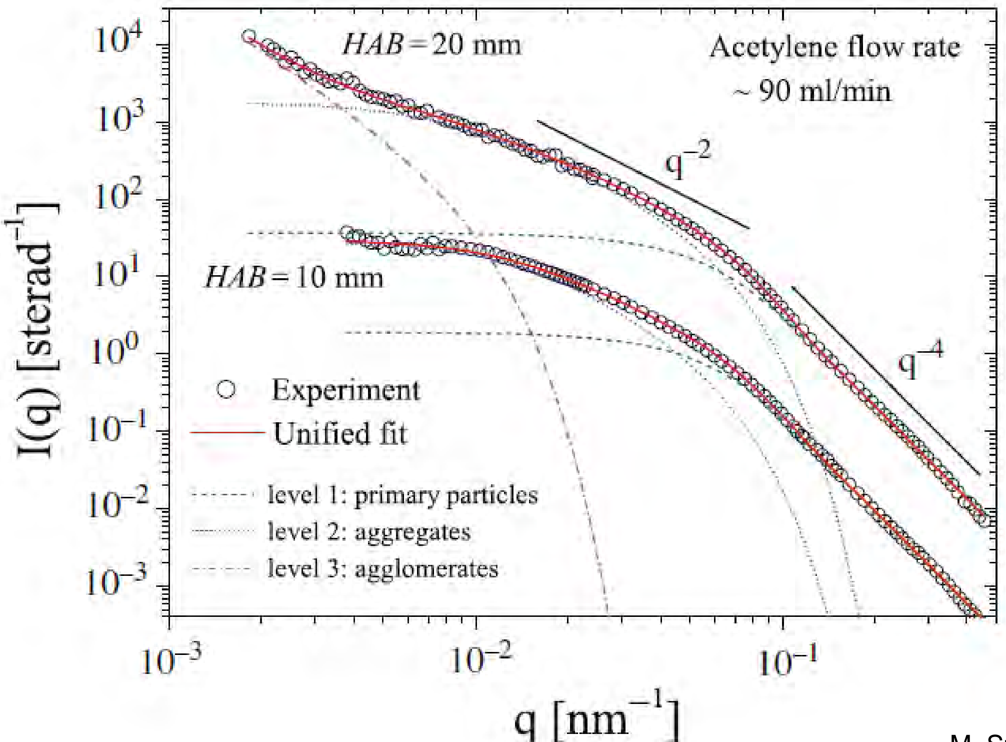
Porord law:

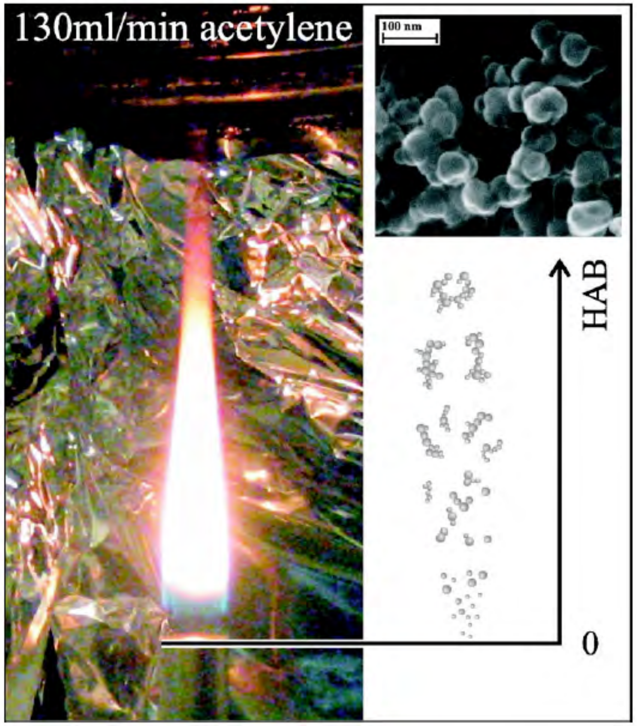
for $qR_g >> 1$

$$I(q) = 2\pi\, N\, \Delta\rho^2\, S\, q^{-4}$$

$$I(q) \propto q^{-p} \begin{cases} p = 4 & \Rightarrow \text{ sharp interface} \\ 3 \le p < 4 & \Rightarrow \text{ surface fractal} \\ p < 3 & \Rightarrow \text{ mass fractal} \\ p \approx 2 & \Rightarrow \text{ gaussian polymer chain} \end{cases}$$

Unified fitting (G. Beaucage)





M. Sztucki, T. Narayanan, G. Beaucage, J. Appl. Phys. 101, 114304 (2007)

$$I(q) = G \exp\left(-\frac{q^2 R_G^2}{3}\right) + B\left\{\frac{\left[erf\left(q\, R_G/\sqrt{6}\right)\right]^3}{q}\right\}^p$$

$$G = N \Delta\rho^2 V^2, \; B = 2\pi N \Delta\rho^2 S$$

for polydisperse systems consisting of multiple structural levels

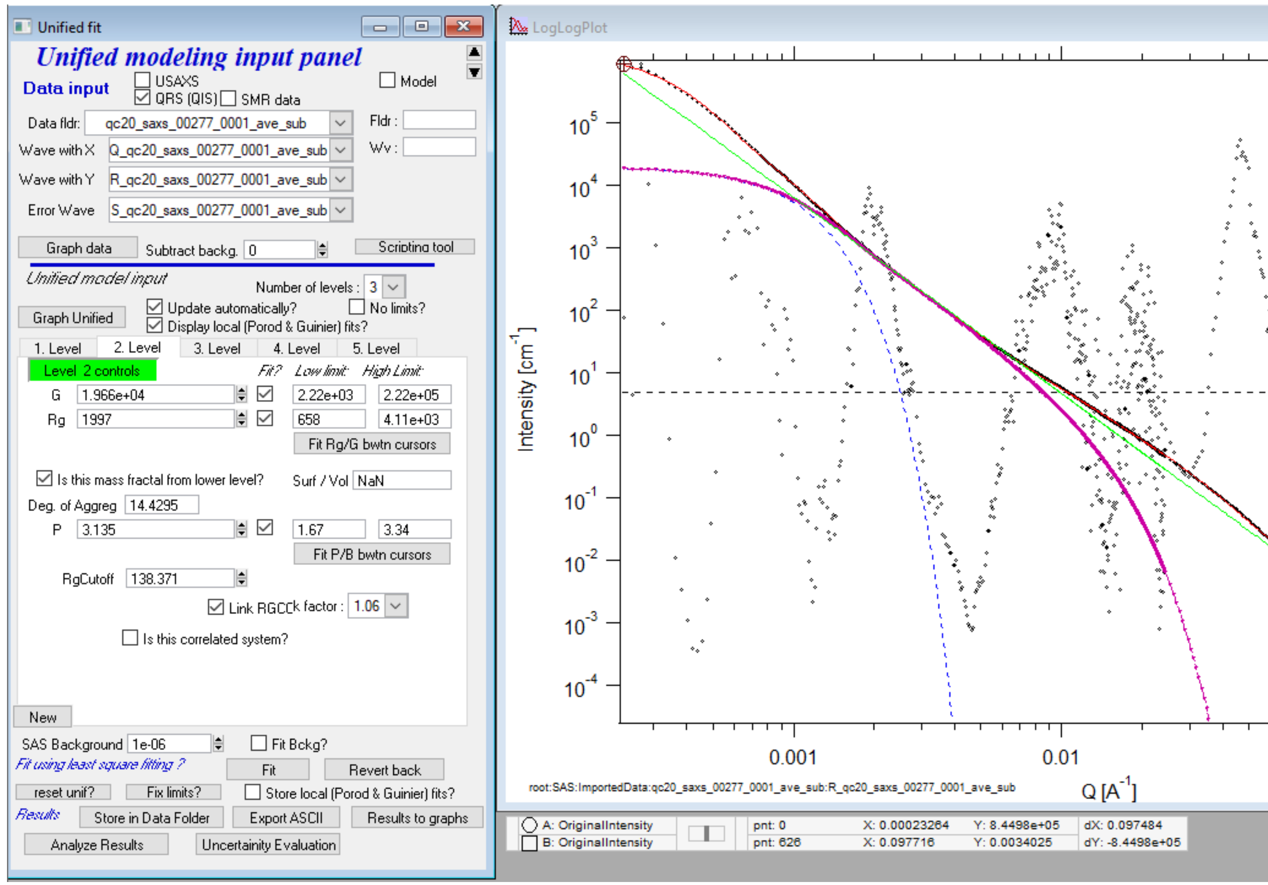
$BR_G^{\,4}/1.62G$ = polydispersity index

Unified fitting (G. Beaucage)

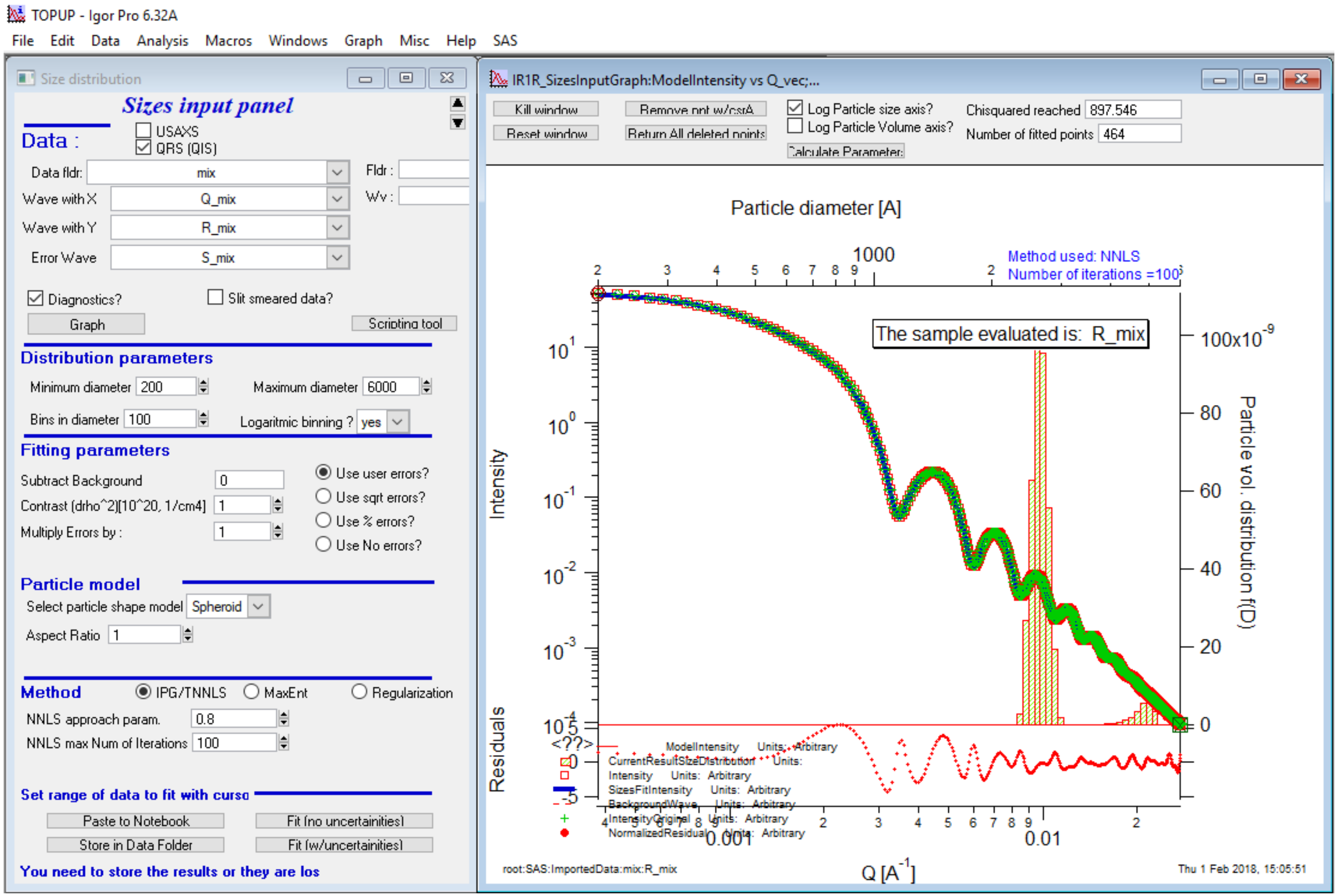
Beaucage G (2012) Combined Small-Angle Scattering for Characterization of Hierarchically Structured Polymer Systems over Nano-to-Micron Meter: Part II Theory.
In: Matyjaszewski K and Möller M (eds.) Polymer Science: A Comprehensive Reference, Vol 2, pp. 399–409. Amsterdam: Elsevier BV.

using Irena package by Jan Ilavsky in Igor Pro: https://usaxs.xray.aps.anl.gov/software/irena

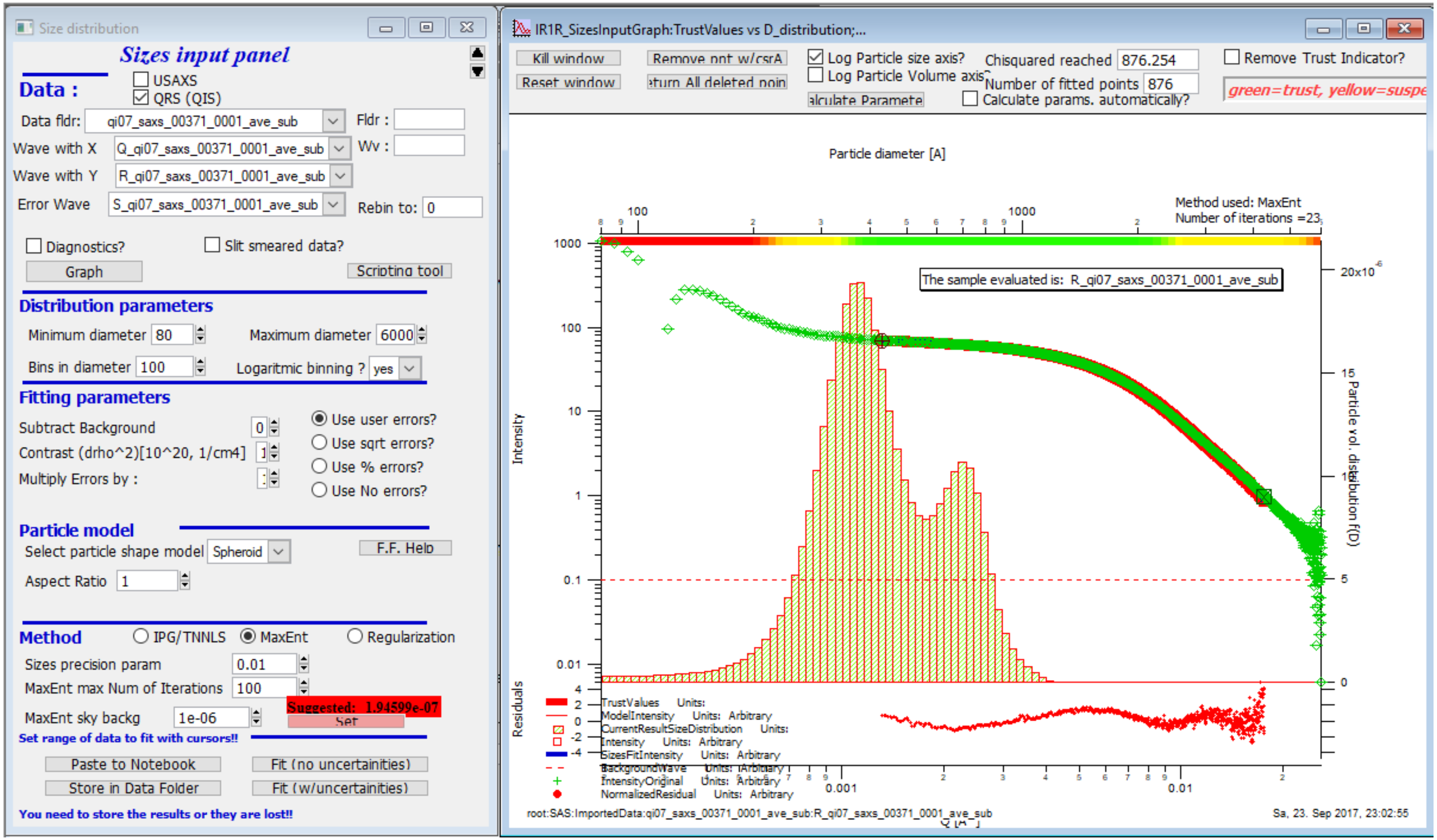
- **Unified fit**
- Modeling
- **Size distribution**
- Guinier-Porod model
- Fractal model
- Reflectivity
- PDDF
- Peak fitting tool
- ...



Size distribution – using Maximum Entropy, Total Non-negative least square (TNNLS) & Regularization methods for evaluation of small-angle scattering from scatterers represented by number of different form factors.



Size distributions



Interaction → Structure factor

Form Factor = scattering from within same particle
⇒ depends on particle shape

Structure Factor = scattering from different particles
⇒ depends on interactions between particles

$$I(q) = N\,V^2 \Delta\rho^2 P(q)\; S(q)$$

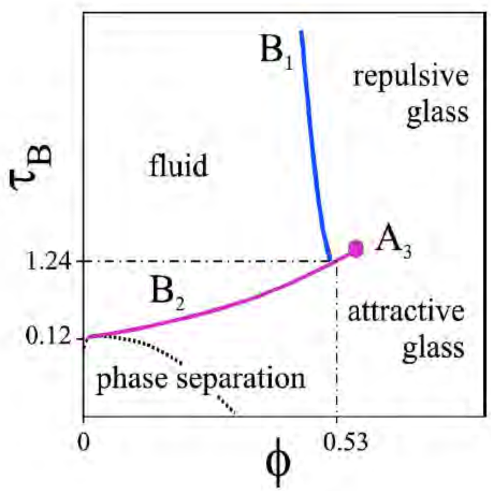
$S(q)$ relates scattered intensity to the microstructure through the pair correlation function, $g(r)$ which is related to the probability of finding a particle at a distance r from another particle

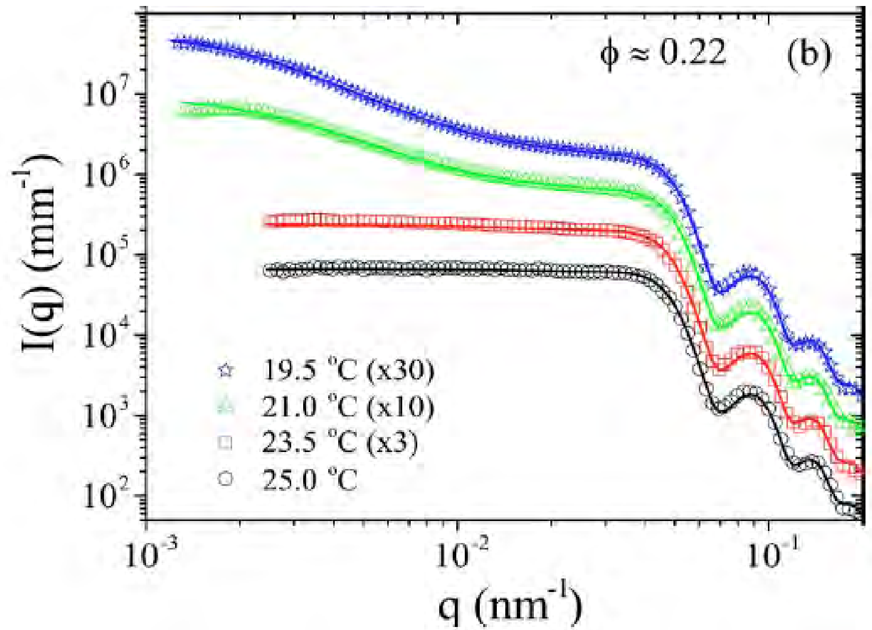
$$S(q) = 1 + 4\pi N \int_0^\infty (g(r) - 1)\frac{\sin(qr)}{qr} r^2 dr$$

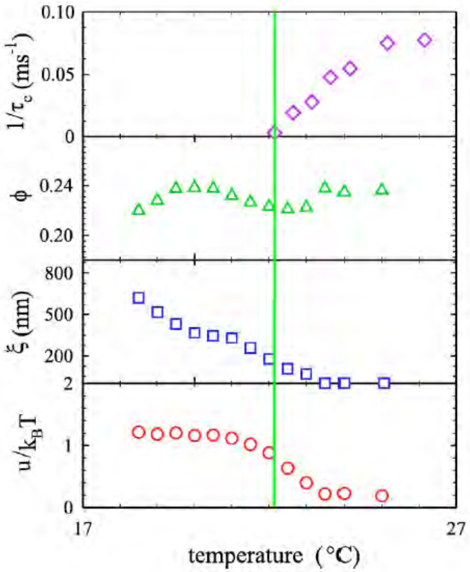
>> structure factors for monodisperse systems

+ hard sphere repulsive potential,
+ short range attractive square-well potential
+ 2Youkawa potential

Form (and structure) factor fitting







PHYSICAL REVIEW E **74**, 051504 (2006)

Kinetic arrest and glass-glass transition in short-ranged attractive colloids

M. Sztucki, T. Narayanan,* G. Belina, and A. Moussaïd
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F. Pignon
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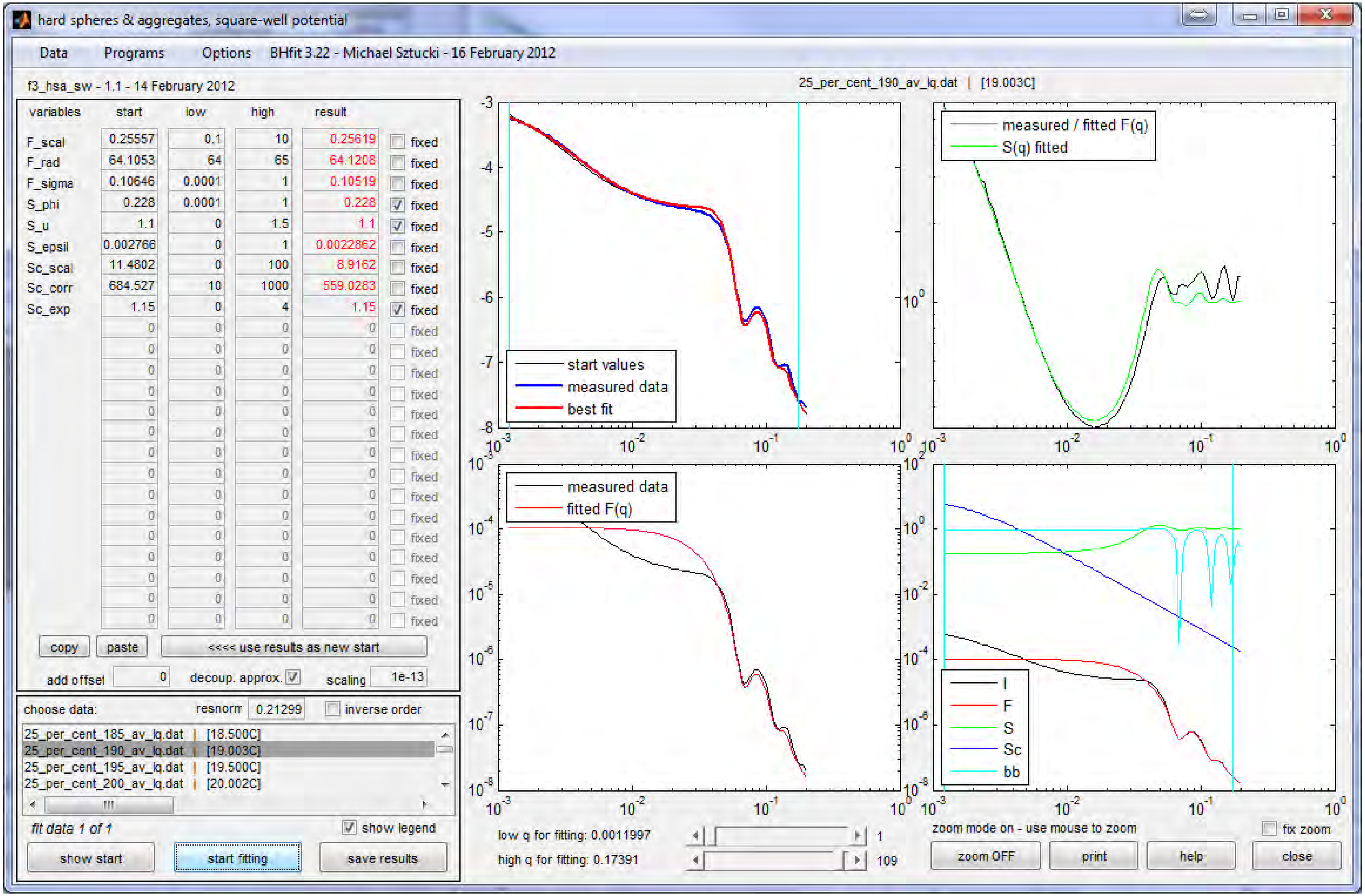
Katholieke Universiteit Leuven, W. de Croylaan 46, 3001 Leuven, Belgium

(Received 6 July 2006; published 17 November 2006)

A thermally reversible repulsive hard-sphere to sticky-sphere transition was studied in a model colloidal system over a wide volume fraction range. The static microstructure was obtained from high resolution small angle x-ray scattering, the colloid dynamics was probed by dynamic x-ray and light scattering, and supplementary mechanical properties were derived from bulk rheology. At low concentration, the system shows features of gas-liquid type phase separation. The bulk phase separation is presumably interrupted by a gelation transition at the intermediate volume fraction range. At high volume fractions, fluid-attractive glass and repul-

SAXSutilities - modelling

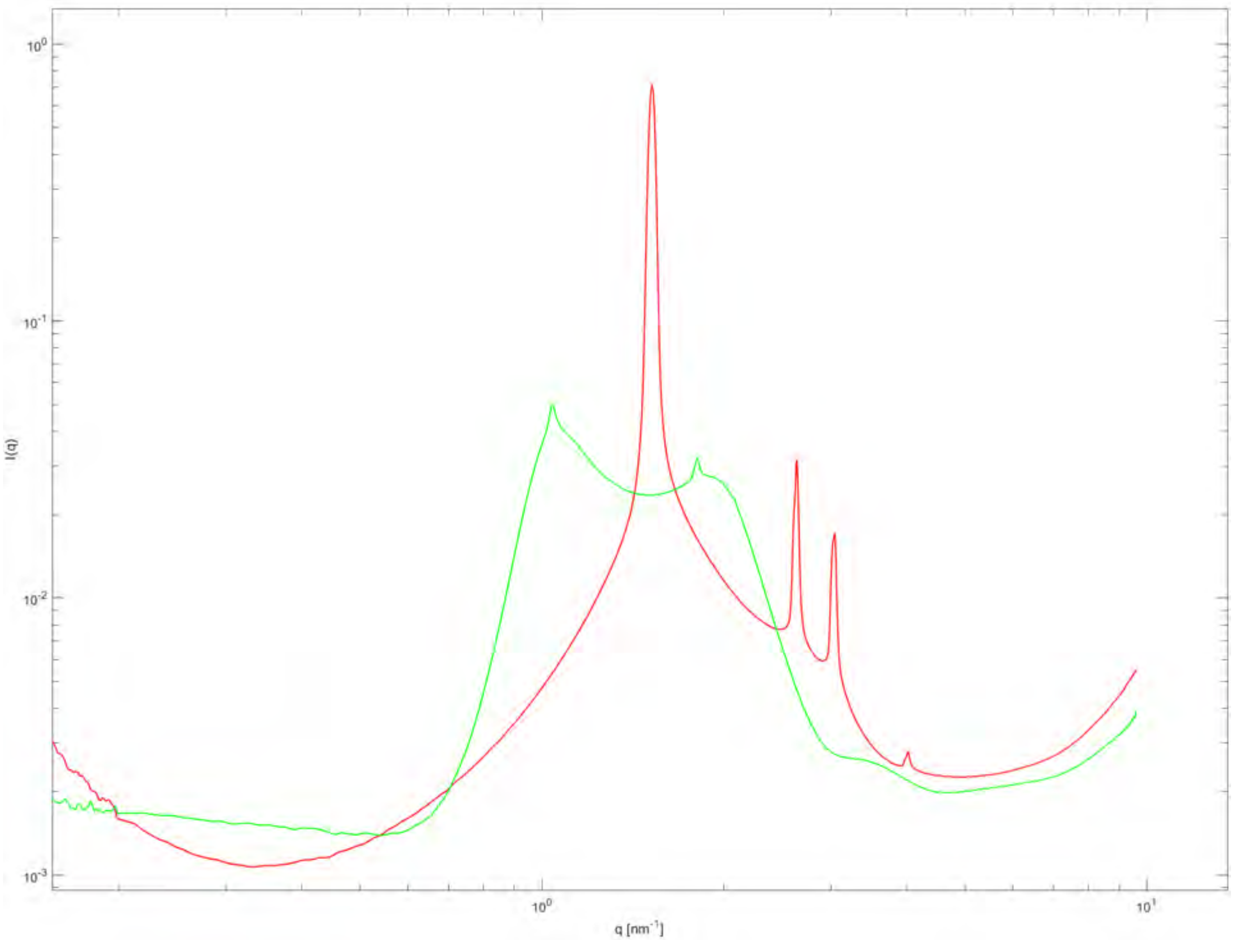


SAXSutilities – contrast calculation

Crystal structures

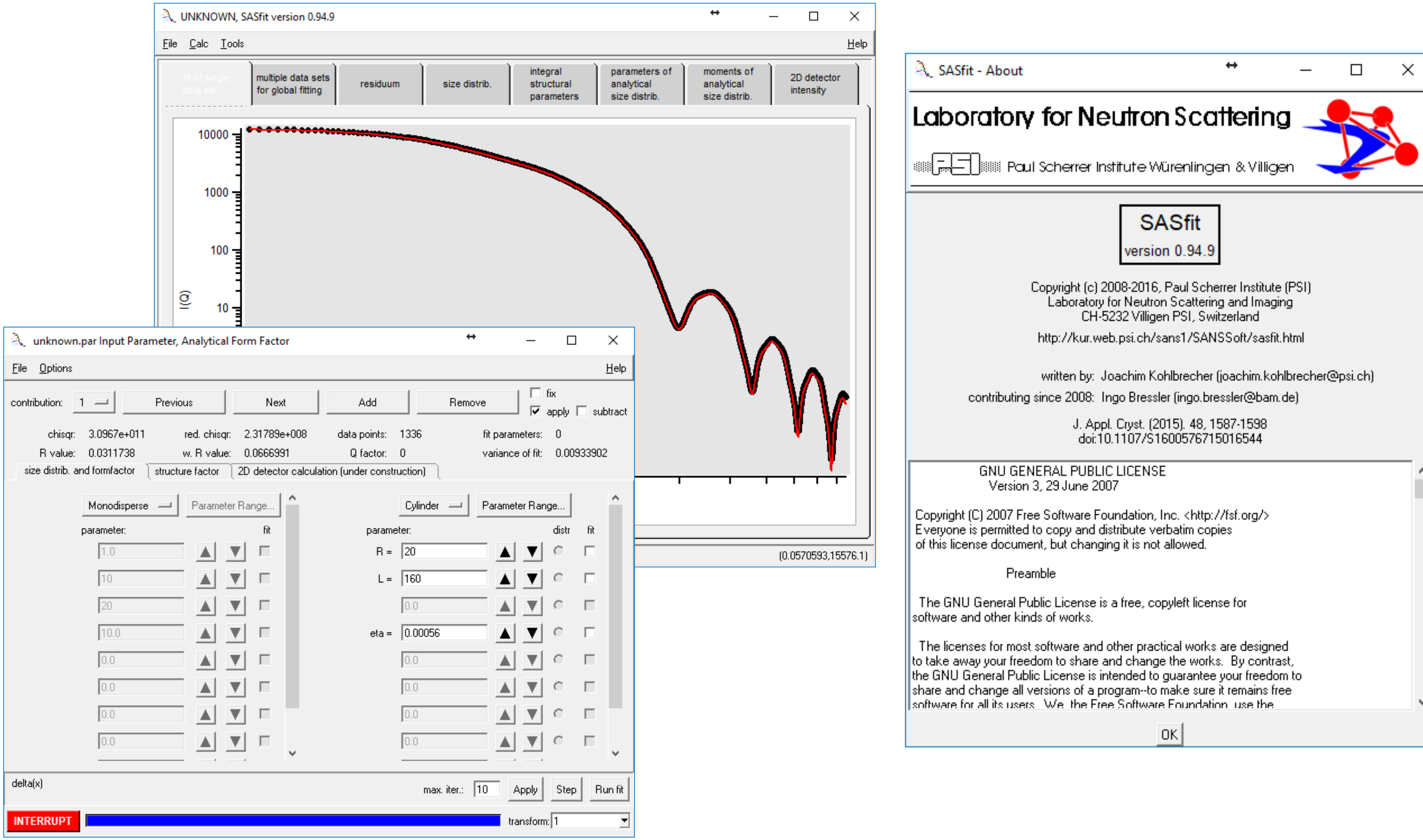
indexing and identifying different crystal structures

LAM	$1:2:3:4:5:6:7$
HCPC	$1:\sqrt{3}:2:\sqrt{7}:3:\sqrt{12}:\sqrt{13}:4$
PC	$1:\sqrt{2}:\sqrt{3}:2:\sqrt{5}:\sqrt{6}:\sqrt{8}:3$
BCC	$1:\sqrt{2}:\sqrt{3}:2:\sqrt{5}:\sqrt{6}:\sqrt{7}:\sqrt{8}:3$
FCC	$\sqrt{3}:2:\sqrt{8}:\sqrt{11}:\sqrt{12}:4:\sqrt{19}$
HCPS	$\sqrt{32}:6:\sqrt{41}:\sqrt{68}:\sqrt{96}:\sqrt{113}$
DD	$\sqrt{2}:\sqrt{3}:2:\sqrt{6}:\sqrt{8}:3:\sqrt{10}:\sqrt{11}$
$Ia\bar{3}d$	$\sqrt{3}:2:\sqrt{7}:\sqrt{8}:\sqrt{10}:\sqrt{11}:\sqrt{12}$
$Pm\bar{3}n$	$\sqrt{2}:2:\sqrt{5}:\sqrt{6}:\sqrt{8}:\sqrt{10}:\sqrt{12}$



SASfit

https://kur.web.psi.ch/sans1/SANSSoft/sasfit.html

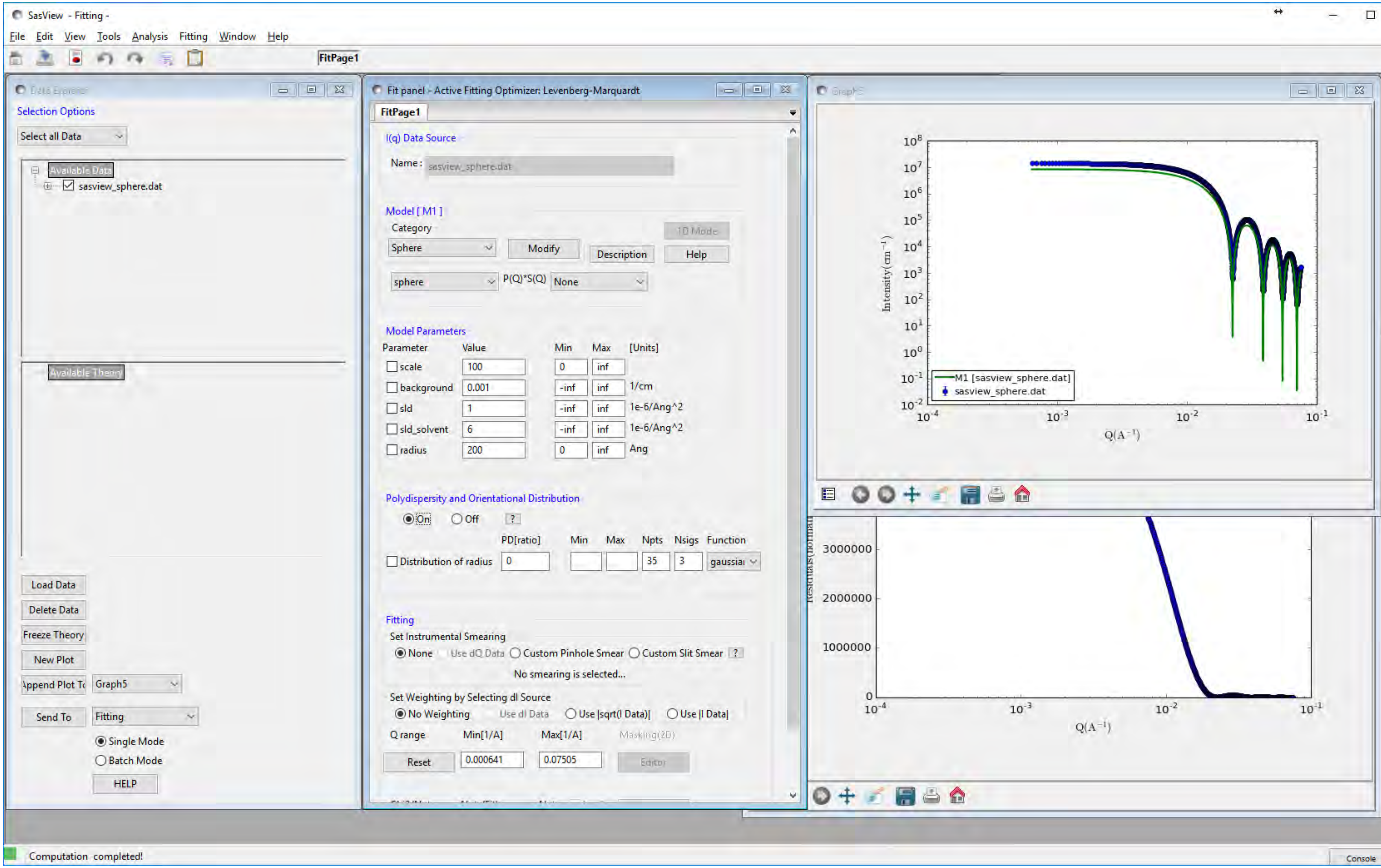


SASview

http://www.sasview.org/

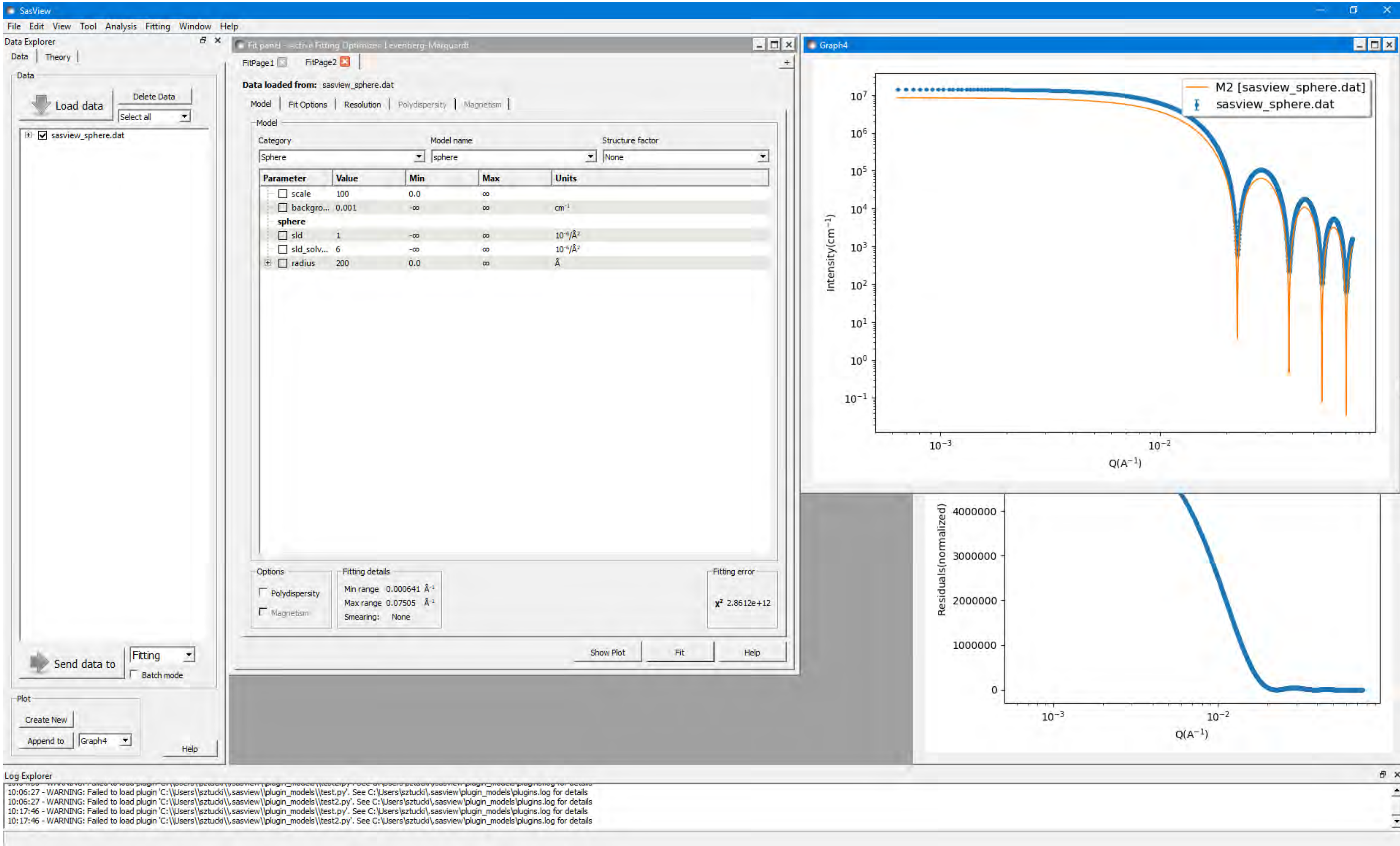
http://www.sasview.org/

SASview 4



SasView - Fitting -
File Edit View Tools Analysis Fitting Window Help
FitPage1
Selection Options
Select all Data
Available Data
sasview_sphere.dat
Available Theory
Load Data
Delete Data
Freeze Theory
New Plot
Append Plot To
Graph5
Send To
Fitting
Single Mode
Batch Mode
HELP
Fit panel - Active Fitting Optimizer: Levenberg-Marquardt
I(q) Data Source
Name: sasview_sphere.dat
Model [M1]
Category
Sphere
Modify
Description
Help
sphere
P(Q)*S(Q)
None
Model Parameters
Parameter Value Min Max [Units]
scale 100 0 inf
background 0.001 -inf inf 1/cm
sld 1 -inf inf 1e-6/Ang^2
sld_solvent 6 -inf inf 1e-6/Ang^2
radius 200 0 inf Ang
Polydispersity and Orientational Distribution
On Off
PD[ratio] Min Max Npts Nsigs Function
Distribution of radius 0 35 3 gaussian
Fitting
Set Instrumental Smearing
None Use dQ Data Custom Pinhole Smear Custom Slit Smear
No smearing is selected...
Set Weighting by Selecting dI Source
No Weighting Use dI Data Use |sqrt(I Data)| Use |I Data|
Q range Min[1/A] Max[1/A] Masking(2D)
Reset 0.000641 0.07505 Editor
Intensity(cm⁻¹)
M1 [sasview_sphere.dat]
sasview_sphere.dat
Q(A⁻¹)
3000000
2000000
1000000
0
Computation completed!
Console

SASview 5



SasView
File Edit View Tool Analysis Fitting Window Help
Data Explorer
Data
Theory
Load data
Delete Data
Select all
sasview_sphere.dat
Send data to
Fitting
Batch mode
Plot
Create New
Append to
Graph4
Help
FitPage1
FitPage2
Data loaded from: sasview_sphere.dat
Model
Fit Options
Resolution
Polydispersity
Magnetism
Category
Sphere
Model name
sphere
Structure factor
None
Parameter
Value
Min
Max
Units
scale 100 0.0 ∞
backgro... 0.001 -∞ ∞ cm⁻¹
sphere
sld 1 -∞ ∞
sld_solv... 6 -∞ ∞
radius 200 0.0 ∞ Å
Options
Polydispersity
Magnetism
Fitting details
Min range 0.000641
Max range 0.07505
Smearing: None
Fitting error
χ² 2.8612e+12
Show Plot
Fit
Help
Graph4
M2 [sasview_sphere.dat]
sasview_sphere.dat
Intensity(cm⁻¹)
Q(A⁻¹)
Residuals(normalized)
4000000
3000000
2000000
1000000
0
Log Explorer

Conclusions

Saxs Programs:
http://www.esrf.eu/home/UsersAndScience/Experiments/CBS/ID02/available_software.html
→ SAXS programs
Or directly: http://www.esrf.eu/Instrumentation/software/data-analysis/OurSoftware/SAXS

SAXSutilities:
http://www.saxsutilities.eu
--- there you will find soon this presentation ---

Irena:
https://usaxs.xray.aps.anl.gov/software/irena

SASfit:
https://kur.web.psi.ch/sans1/SANSSoft/sasfit.html

SASview:
http://www.sasview.org

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