SAXS at the ESRF
Beamlines ID01 and ID02

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• Online/Offline Treatment
  (SAXS package/SPD program)
1 History

before 1994: Discussion of a common ESRF data format for all beam lines based on existing solutions, e.g. hdf (->:not handy), ORACLE (->too expensive)

=> implementation of a home made “ESRF Data Format” (edf), allowing storage of metadata

1994: ID02 went into operation using a 2D gas-filled detector (1024x1024 pixels) using an ad hoc hardware format ("hm") using two files for data and SAXS metadata, but no easy way of data processing.

=> “ESRF Data Format” implemented + some simple programs

=> Offline conversion of “hm”-files to edf-files (including SAXS metadata)

1995: First version of “SAXS” data treatment programs for edf-files + SAXS metadata

1995 onwards: Ongoing discussions about metadata, improvements of the format.

~1999: To facilitate programming the edf-format is generally introduced at the ESRF, for automatic data processing the SAXS metadata becomes a standard at ID02.

since 1999: development of automatic offline/online data processing tools (spd, “SAXS”-programs)
2 Current Situation

ESRF SAXS Beamlines

- **ID01** SAXS, WAXS, ASAXS, GISAXS, GID, XD, micro focusing, diffuse scattering, coherent scattering, imaging, reciprocal space mapping, (hard + soft matter)
- **ID02** time-resolved SAXS/WAXS, ASAXS, USAXS (soft matter + biologic materials)
- **BM02** anomalous SAXS, WAXS, XD (hard + soft matter)
- **ID09B** ps-time resolved protein crystallography (PX) (biologic materials)
- **ID10** SAXS, WAXS, GISAXS, XD, coherent scattering, XPCS (soft matter)
- **ID11** high energy time-resolved XD, WAXS (material science)
- **ID13** micro focus, scanning diffractometry, SAXS, WAXS, GISAXS, PX (soft matter + biologic materials)
- **ID14/EH3** prospected SAXS station for biologic materials
- **BM16** SAXS, WAXS, PX (soft matter + biologic materials)
- **BM26** time-resolved SAXS/WAXS, GID, EXAFS, PX, ...

The list of beamlines and their experimental methods are not complete. There are more beamlines performing SAXS or WAXS experiments from time to time.
- The **productivity** of the beamline (#publications) increases when the data is processed immediately.

- Most of the users need **corrected data on-line** during acquisition to judge data quality.

- There is currently **no strong demand** by external users for a common data format.

- After the first experiment most of the users have found a way to analyze the data.

- The strongest demand for a common data format seems to come from **software developers**. Currently, most of the users seem to be happy with specific solutions.

A homogenization of data formats can be triggered by standard programs, e.g. for online correction, visualization etc.
3 Online/Offline Treatment

Expected Result of Online Correction (Absolute Units)

No Pol. Corr.: Pixel intensities $I$ normalized to:

$$I = \frac{1}{A} \frac{\partial \sigma}{\partial \Omega} = \frac{1}{T} \frac{\text{#scattered_photons}}{\text{sterad}}$$

scattering intensity per scattering cross section [1/sterad]
(normalized to $T=1$)

$$\frac{1}{V} \frac{\partial \Sigma}{\partial \Omega} = \frac{1}{t} \left( \frac{1}{A} \frac{\partial \sigma}{\partial \Omega} \right) = \frac{I}{t}$$

(T and $t$ can only be measured easily if sample is a flat plate)

scattering intensity per scattering volume [1/sterad/m]

$I$: pixel intensity, $A$: sample cross section, $t$: sample thickness, $V$: scattering volume, $\Omega$: spherical angle, $T$: sample transmission, $\sigma$: absolute scattering cross section, $\Sigma$: specific scattering cross section

With Pol. Corr.: Pixel intensities $I$ normalized to:

$$\frac{1}{t} \left( \frac{1}{A} \frac{\partial \sigma}{\partial \Omega} \right) = \frac{\text{#number_of_electrons}}{\text{scattering_volume}}$$

number of electrons per sample volume [#e-/nm³]
(normalized to $T=1$)
3 Online/Offline Treatment

General SAXS/WAXS Scattering Geometry

monochromatic beam

SAXS pinhole camera
Peter Boesecke: SAXS at the ESRF

3 Online/Offline Treatment
General SAXS/WAXS Scattering Geometry

SAXS pinhole camera

monochromatic beam
The axes of the averaged pattern are given in reciprocal units in the SAXS reference system:

$$q = 2\pi s$$
Peter Boesecke: SAXS at the ESRF

3 Online/Offline Treatment

General SAXS/WAXS Scattering Geometry

A, B, C: X-ray detectors

additional detectors
(e.g. microscopes, fluorescence detectors, thermocouples, strain gauges, spectrometer etc.)

SAXS

WAXS

A at large distance

sample

frame number

experiment control (SPEC)

name_0_0001.edf (SAXS)
name_1_0001.edf (WAXS)
...
name_0_0999.edf
name_1_0999.edf

beam stop

monochromatic X-ray beam

I1-monitor

I0-monitor

name_0_0999.edf
name_1_0999.edf
3 Online/Offline Treatment

SAXS/WAXS Scattering Geometry (General Considerations)

- Time resolved 2d data from SAXS and WAXS detectors
- Peak data rates -> 40 Megabytes/s
- Increasing amount of data (GB -> TB)

- Detector corrections are only obvious to specialists
- Data quality can only be estimated after basic corrections
- Data must be reduced before it can be used

- Raw data is saved with all experimental information
- Data is automatically reduced after an exposure
- History of data treatment is saved
- Corrected data is given in absolute units (1/sterad)
3 Online/Offline Treatment
Detector Orientations and Geometries

Orientations

Geometries

a) full unbinned detector  b) region of interest  c) binned
Corrections

- **dark-image**: subtraction of zero level
- **flat-field**: normalization of quantum efficiency of each pixel
- **spatial distortion**: correction

Each corrected pixel contains the number of incident photons (+statistical error)

-> all steps done online during data acquisition (SPD)
3 Online/Offline Treatment

SAXS/WAXS Scattering Geometries

a) (A) SAXS/WAXS/WAXD
detector perpendicular to the incident beam

b) (A) WAXS/WAXD
detector (strongly) inclined with respect to the incident beam

c) (A) GISAXS

d) (A) GID
3 Online/Offline Treatment
SAXS/WAXS Scattering Geometry (General Parametrization)

\[ C = \text{Center} \equiv \text{PointOfNormalIncidence, } L = \text{SampleDistance} \]

### 3 Online/Offline Treatment

**SAXS/WAXS Scattering Geometry (General Keywords)**

<table>
<thead>
<tr>
<th>Keyword</th>
<th>Unit</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dim_1, Dim_2</td>
<td>pixel</td>
<td>Array dimension [0] [1]</td>
</tr>
<tr>
<td>RasterOrientation</td>
<td>-</td>
<td>Raster orientation [1]</td>
</tr>
<tr>
<td>Offset_1, Offset_2</td>
<td>pixel</td>
<td>Spatial array offsets [0]</td>
</tr>
<tr>
<td>BSize_1, BSize_2</td>
<td>pixel</td>
<td>Pixel size relative to</td>
</tr>
<tr>
<td></td>
<td></td>
<td>size of unbinned pixel [1]</td>
</tr>
<tr>
<td>Center_1, Center_2</td>
<td>pixel</td>
<td>Point of normal incidence (PoNI)</td>
</tr>
<tr>
<td>PSize_1, PSize_2</td>
<td>m</td>
<td>Pixel size in meters</td>
</tr>
<tr>
<td>SampleDistance</td>
<td>m</td>
<td>Distance PoNI to sample</td>
</tr>
<tr>
<td>WaveLength</td>
<td>m</td>
<td>X-ray wavelength</td>
</tr>
<tr>
<td>DetectorRotation_1,</td>
<td>rad</td>
<td>Rotations of the detector</td>
</tr>
<tr>
<td>DetectorRotation_2,</td>
<td></td>
<td>plane in the laboratory</td>
</tr>
<tr>
<td>DetectorRotation_3</td>
<td></td>
<td>system [0]</td>
</tr>
<tr>
<td>ProjectionType</td>
<td>-</td>
<td>&quot;Saxs&quot; or &quot;Waxs&quot;</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Keyword</th>
<th>Unit</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intensity0</td>
<td>(*)</td>
<td>Integrated beam intensity before the sample during the exposure time</td>
</tr>
<tr>
<td>Intensity1</td>
<td>(*)</td>
<td>Integrated beam intensity after the sample during the exposure time</td>
</tr>
<tr>
<td>ExposureTime</td>
<td>s</td>
<td>exposure time</td>
</tr>
</tbody>
</table>

(*) Ideally, the intensities should be measured in number of photons integrated during the exposure time.
The SAXS Reference system is not appropriate for large scattering angles. To compare different scattering patterns taken at large scattering angles, non-affine transformations are necessary. The parameter ProjectionType=Waxs indicates that the data is represented in the Waxs projection (default: ProjectionType=Saxs).
3 Online/Offline Treatment

SAXS/WAXS Scattering Geometry (Data Header)

[ByteOrder = LowByteFirst ;
  DataType = UnsignedShort ;
  Dim_1 = 1242 ;
  Dim_2 = 1152 ;
  Title = test ( nu=0 mu=0 chi=90 phi=0 del=0.0124 energy=5.0002 ) (R1F1) ;
  Intensity0 = 1.23937e+12 photons (Mon5) ;
  Intensity1 = 9.27289e+11 photons (saxs1) ;
  ExposureTime = 1 s (Seconds) ;
  Dummy = 0 ;
  DDummy = 0.1 ;
  Offset_1 = 0 pixel ;
  Offset_2 = 0 pixel ;
  Center_1 = 597.019 pixel ;
  Center_2 = 1214.3 pixel ;
  BSize_1 = 1 ;
  BSize_2 = 1 ;
  PSize_1 = 5.5e-05 m ;
  PSize_2 = 5.55e-05 m ;
  SampleDistance = 3.13572 m ;
  WaveLength = 2.47963e-10 m ;
  RasterOrientation = 1 ;]
3 Online/Offline Treatment
SAXS/WAXS Scattering Geometry (Tools)

SAXS program package
Peter Boesecke (http://www.esrf.eu/computing/scientific/SAXS)
- SAXS Package Manual
- SAXS Format Manual
- SAXS package download

SAXSutilities
Michael Sztucki (http://www.sztucki.de/physik/physik.php)
- BHplot (online treating and fitting of 1D SAXS data)
- DataTools (1D SAXS data analysis)
- EDFplot (processing of 2D SAXS images)
3 Online/Offline Treatment

General SAXS/WAXS Scattering Geometry (Reference Systems)

SAXS L=1 m

SAXS L=3 m

combined L=1 m & L=3 m

SAXS reference system (affine transformation of detector coordinates):

\[ S = \frac{\text{Normal}/\text{SampleDistance}/(\text{WaveLength/nm})}{(\text{Offset-Center} + A) \times \text{PSize}/\text{SampleDistance}/(\text{WaveLength/nm})} \]

```
saxs_ave -rsys saxs lupolen_1m.msk lupolen_3m.msk lupolen_1m.ave
```

In the same way saxes and waxes images can be combined
3 Online/Offline Treatment
SAXS/WAXS Scattering Geometry (SAXS/WAXS Example)

WAXS
SAXS
combined

saxs_ave -rsys saxs lupolen.wax lupolen_3m.msk lupolen.ave
3 Online/Offline Treatment
SAXS/WAXS Scattering Geometry (EDFplot)

MatLab based GUI
by Michael Sztucki
www.sztucki.de/Physik
3 Online/Offline Treatment
SAXS/WAXS Scattering Geometry (BHplot)

MatLab based GUI
by Michael Sztucki
www.sztucki.de/Physik
3 Online/Offline Treatment

SAXS/WAXS Scattering Geometry (SPEC interface)
Spatial Distortion Correction Program

(credits: Joerg Klora, Andy Hammersley, Rainer Wilcke, Armando Sole, Claudio Ferrero, Andy Goetz, Jerome Kieffer, ...)

The program SPD exists in several versions:
- offline program (command line driven)
- data pipe version (spec data pipe driven)
- server version (spd is running as a server) (A. Goetz, under test)

SPD is used online for basic detector corrections (dark image, flat field, distortion) and absolute intensity normalization. The speed of azimuthal regrouping is going to be optimized. The calculation time is typically 1 s per image. Azimuthal regrouping can be longer, depending on the chosen integration range.
4 Summary

Parametrization (if necessary, extendable to higher dimensions)

Data Specific
- DATA ARRAY, VARIANCE ARRAY (optional),
- ByteOrder, DataType, Dim_1, Dim_2, DataRasterOrientation,
- Dummy, DDummy (to mark invalid pixels)

Detector Specific
- Offset_1, Offset_2, RasterOrientation, BSize_1, BSize_2

Geometry Specific
- PSize_1, PSize_2, SampleDistance, Center_1, Center_2,
- DetectorRotation_1, DetectorRotation_2, DetectorRotation_3

Scattering Specific
- WaveLength

Projection Specific
- Projection Type

Intensity Specific
- Intensity0, Intensity1, ExposureTime

Time Specific
- Time

Informational
- Title, History

2D NEXUS SAS

2D Plugin (Soleil)
4 Summary
SAXS/WAXS Scattering Geometry (General Keywords)

What is the meaning of the parameters in NEXUS/SAS or at Soleil/SAS?

Parameters are not obvious, even if they are as simple as detector distance!

A strict definition is needed!!!