The Future of SAXS

Brian R. Pauw

BAM
Bundesanstalt für
Materialforschung
und -prüfung

STANDARDIZATION

To convincingly show that our small-angle X-ray scattering data is reliable, it needs to be compared against the data from other instruments. This implies (inter-)calibration and standardisation.

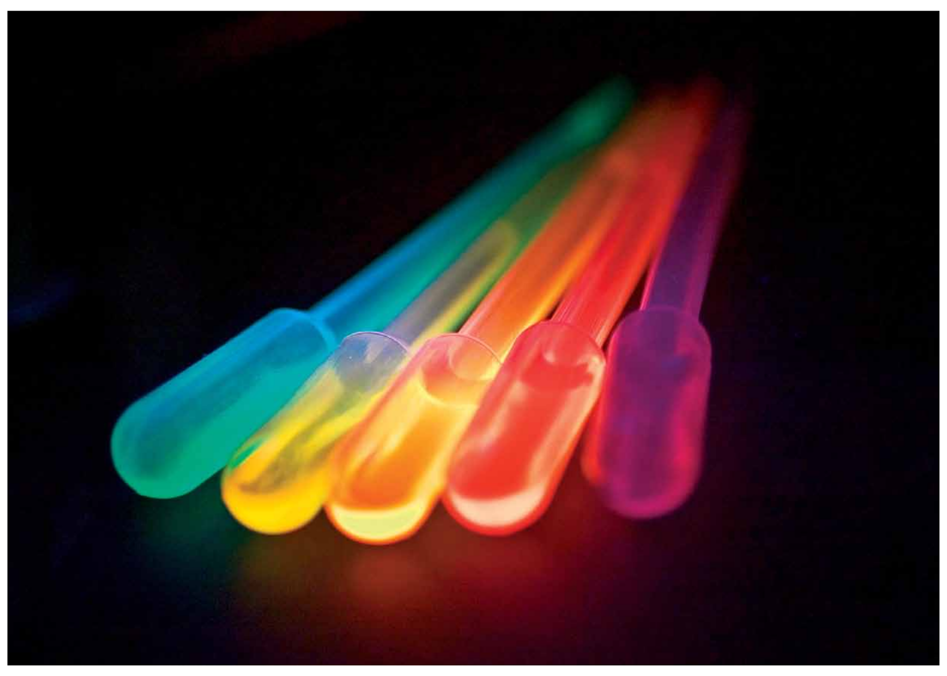
There are already some materials avialable for calibration. The glassy carbon standard currently being developed at NIST will be suited for intercalibration of absolute scattering intensity. Furthermore, silver behenate is the de facto standard for calibrating sample-to-detector distances. For validation of measurement capabilities, a bimodal silica dispersion (ERM-FD-102) is available. Efforts are underway (e.g. at CanSAS and various institutes) to find more such materials. Over time, these will become available and shared between laboratories for improved consistency.

In order to compare these datasets, a standardization effort also needs to be established with regards to the data correction regimen: if participants apply their own subset of corrections, differences in the data may not be traceable to the instrument, but merely to the (lack of) corrections. Agreeing on, and exact documentation of the necessary correction steps will improve intercomparability.

To fully utilize such data, however, improved standards for data storage will also need to be developed. The current efforts to define a CanSAS data set as part of the NeXus format are very promising in this direction, and should be the future standard for storage of corrected, uni- and multidimensional data.

Lastly, good advances are being made in the standardization of data analysis, with the first ISO definition (ISO 17867) for the analysis of scattering patterns of polydisperse systems already availble.

Despite their (often glacial pace, these standardization efforts are key to the future of SAXS..



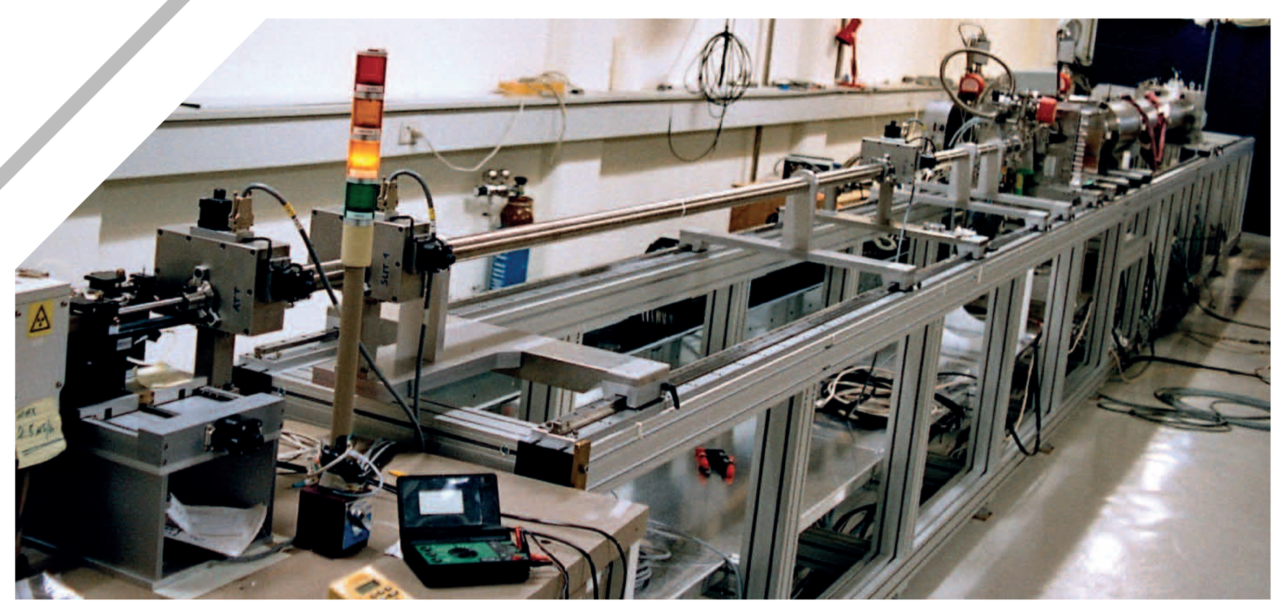
INSTRUMENTATION

Interestingly, with the availability of syncrotron SAXS instrumentation, laboratory instruments did not disappear. Instead, they now coexist symbiotically: synchrotron instruments are used for exceptional samples demanding its high flux: e.g. those that are temporally sensitive or require extreme conditions. For the remaining measurements, however, the laboratory instrument is more than capable of collecting beautiful data. Its high availability and short lead time furthermore allows for good integration in academic workflows.

Indeed, during a recent tour of institutes, it was clear that many had access to their own, often in-house designed instruments. The trade-off between buying a commercially available instrument and building an instrument depends much on the group focus and availability of time and manpower. While acquiring a commercially available instrument is tempting, a beautiful cowling and simplified or simplistic user interface can easily obscure the underpinnings of the technique. Understanding this foundation thoroughly is essential to correct application of the technique, and can be gained when designing instrumentation (i.e.: when you spend time in-depth investigating your components one by one, you will learn much).

The current accessibility of high-end components enables the design of unparalleled instrumentation. Simultaneously, standard design instruments are becoming more affordable. The modern instrument may now benefit from:

- A microfocus source for excellent temporal stability and low running costs
- Parallelisation optics for improved comparability over the Q-range
- Scatterless collimation for a cleaner background and shorter collimation section
- Sample change robots and scriptability
- An in-vacuum, mobile detector, preferably a direct-detection, photon counting detector.
- Inexpensive, open, and easily integrated hardware and software for added flexibility.



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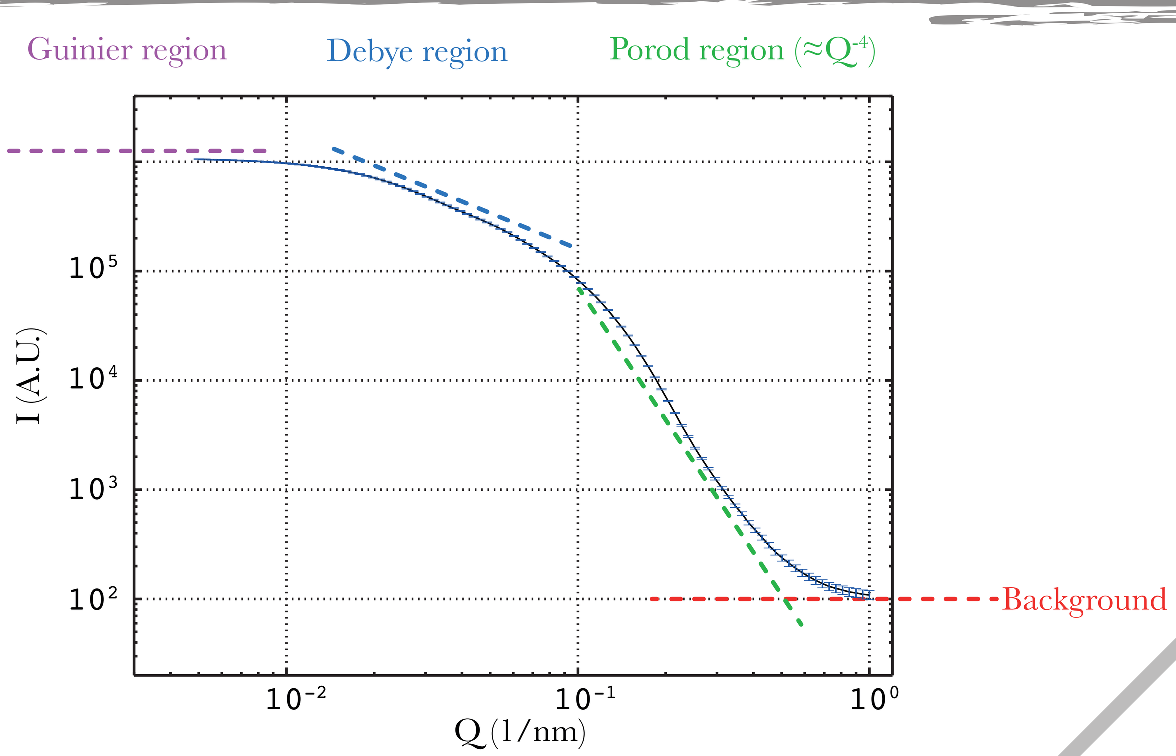


TEACHING

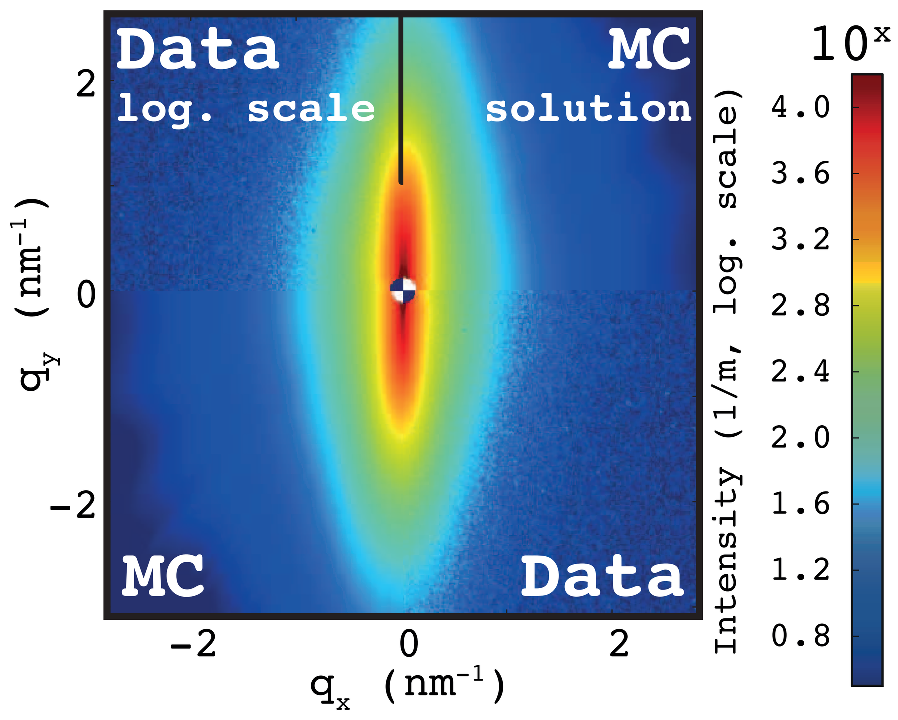
Regardless of how good one's understanding is of the technique, communication of this knowledge to future generations is critical for further development. Such communications should be intelligible, concise and strictly correct. Efforts to develop such teaching material should be weighted: the majority of effort should be spent towards explaining the basics to a large number of people, a little further effort goes into explaining the specifics.

Fortunately, the internet allows such teaching materials to be shared to a wide audience, making the most out of the efforts. For example, some of the explanatory videos created for the LookingAtNothing weblog have been viewed more than 10000 times over the last five years. Indexing and ordering the available videos will be a need for the immediate future.

However, there is also a need for development of practical demonstrations, as these bring theory to life. Examples of such demonstrations include the observation of laser light scattering from a single strand of hair (and the subsequent calculation of its diameter), and "Live FT"-software which shows the magnitude of the Fourier transform given a camera image. Demonstrations of SAXS data fitting, however, very quickly devolve into "click here"-exercises, and are in dire need of renovation.

Lastly, there is a need for instrument building practicals, which would allow the construction of an elementary SAXS instrument from available components. Such hands-on experience will convey a lot of information on the need and purpose of the components in a given instrument. Such demonstrations will form a cornerstone of understanding of data corrections.

Based on feedback received, understanding scattering remains a tough topic for many nonspecialists, with little material available to resolve this. This needs improving soon.



ANALYSIS

The analysis of scattering patterns has long revolved around linearisations or transformations of subsets of data. While this works for simple cases, ubiquitous computing means we no longer need such "voodoo", or "tea-leaf reading" (with the latter term attributed to Dr. Stribeck). Linearisations do not provide insight or understanding, and tend to fail in nonobvious ways for many practical samples.

The appropriate way to analyse data, then, is by fitting a complete dataset. This can be done by least-squares model fitting or by fitting using less restricting methods such as Monte Carlo approaches or inverse Fourier transforms. However, for these (or any) approaches to deliver reliable information, the data uncertainty is to be taken into account. At the moment, there are only a limited number of software packages available that can exploit this information.

In the last few years, the flexibility and power of the new Monte Carlo approach for the analysis of scattering patterns from size-disperse systems has been demonstrated. As an example of one of the modern approaches, it demonstrates that advances in analysis methods will still be significant in the near future. It also, however, unveils the limited information content inherent in SAXS data.

The future of analysis, therefore, lies in the combination of methods, both internally as well as externally. An "internal combination of methods" implies that multiple fitting approaches are used to provide information on the sample. An "external combination" implies that symbiotic measurement *techniques* are employed to gain a more comprehensive picture of the morphology. As small-angle scattering data analysis cannot inherently distinguish between a range of physically relevant solutions for most practical samples, such information or restrictions need to be supported or supplied by symbiotic techniques in any case.