uf-TS/PDF EuXFEL Processing/Analysis Meeting

diamond

Agenda

1. uf-TS/PDF processing requirements (Dean)
2. EuXFEL processing capabilities (Luca)
3. Discussion of best processing route
4. Downstream analysis
5. AOB

uf-TS/PDF Processing Requirements

Dean Keeble

Senior Software Scientist, Diamond Light Source

12 April 2023

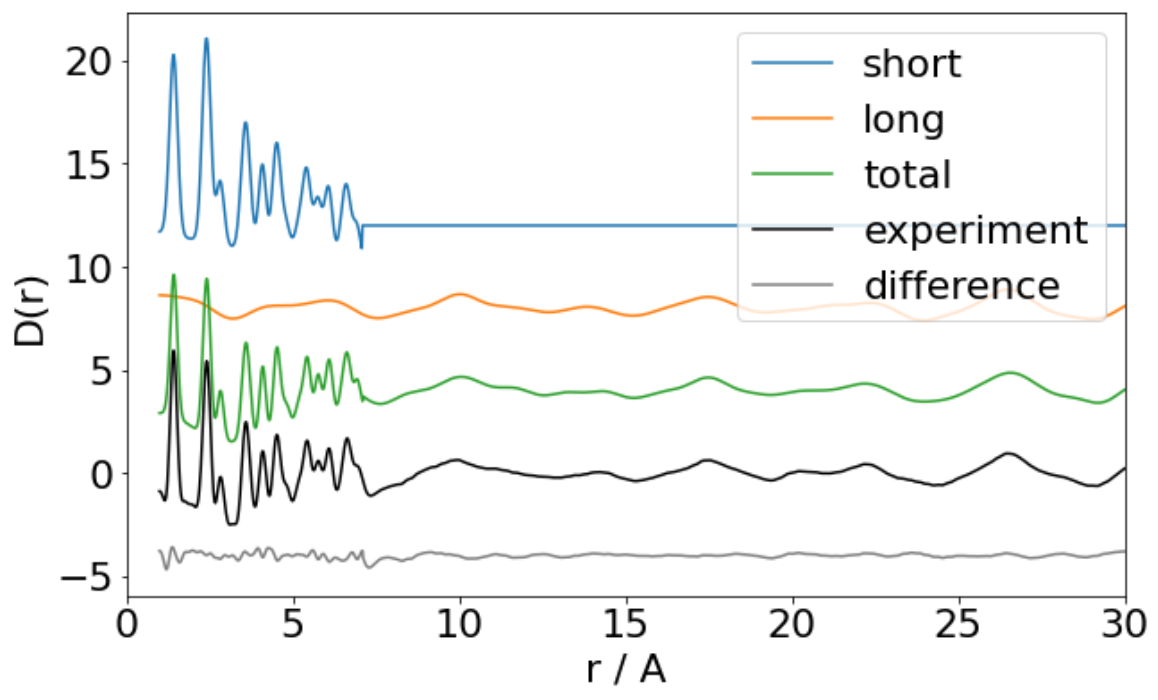
diamond

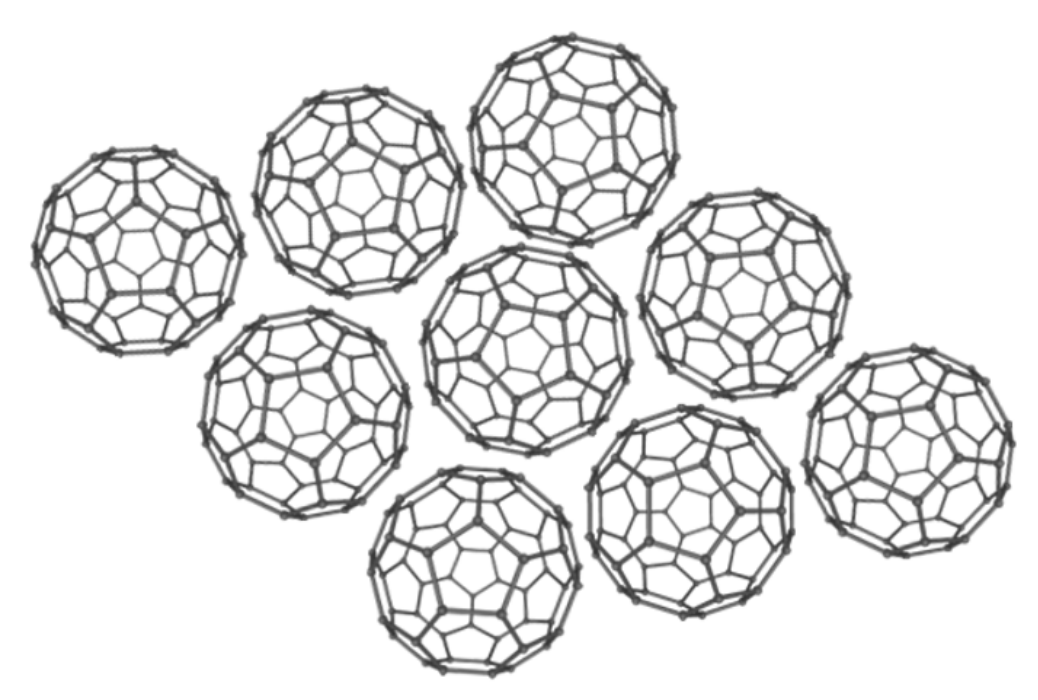
Contents

- What is TS/PDF
- What is different to "normal" scattering experiments
- What is required to process the data
- One possible solution
- Processing vs Analysis

diamond

What is a PDF?

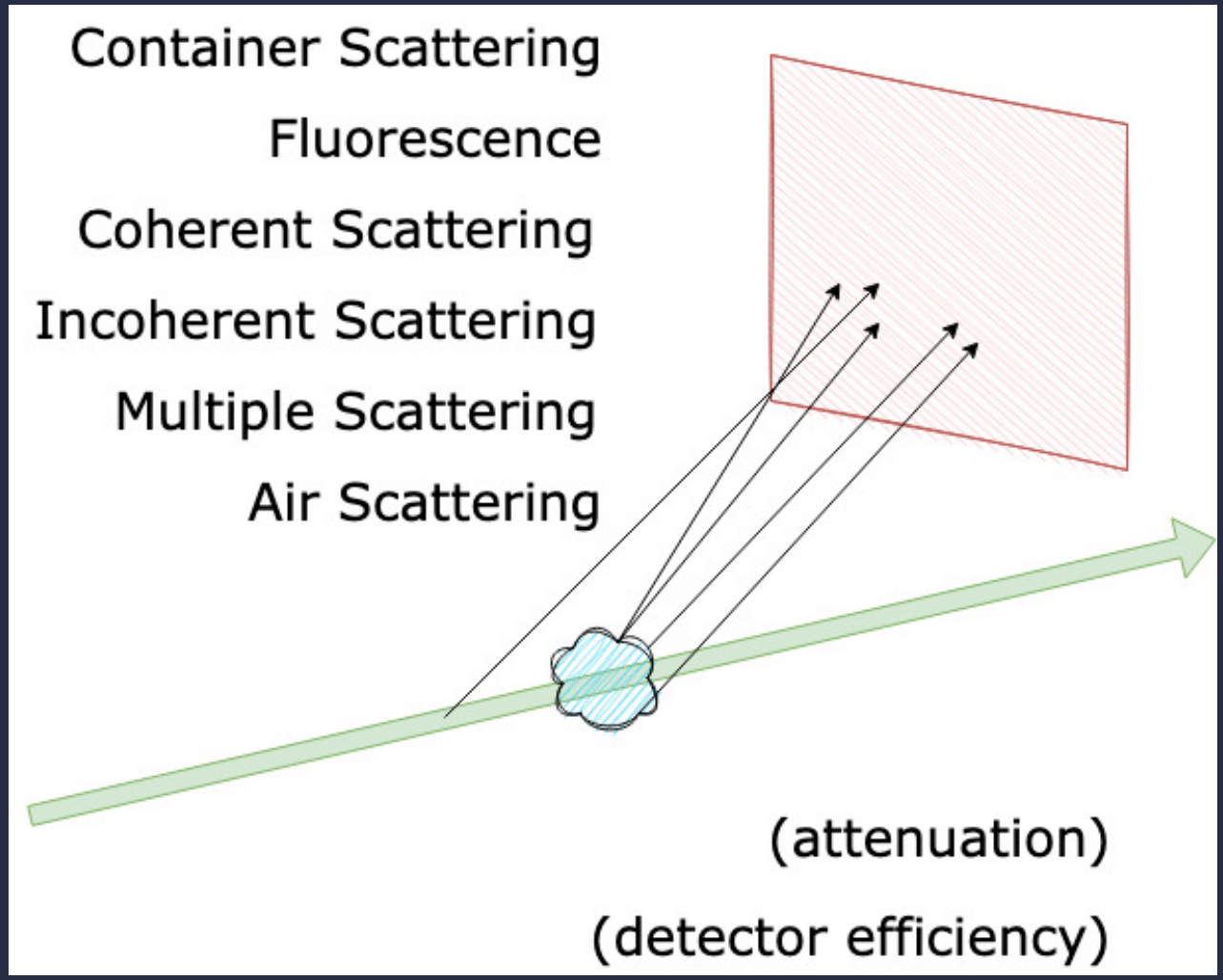

short
long
total
experiment
difference
D(r)
r / A
20
15
10
5
0
−5
0
5
10
15
20
25
30



What is TS/PDF?

We want to get to $F(Q)$, the total scattering structure factor

$$F(Q) = \sum_{i,j=1}^{n} c_i c_j f_i(Q) f_j(Q)[A_{ij}(Q) - 1]$$



diamond

How to get a PDF?

If you've successfully extracted your $F(Q)$, it's straightforward$^{\text{TM}}$ to convert it to the pair distribution function

$$G(r) = \frac{1}{8\pi^3 \rho_0} \int_0^\infty 4\pi Q^2 F(Q) \frac{\sin Qr}{Qr} \, \mathrm{d}r$$

diamond

Differences to "normal" diffraction

In order to extract the TS from a "normal" powder diffraction pattern, we need to:

1. Correctly subract the scattering from anything which isn't the sample
2. Correctly subtract everything which isn't coherent scattering
3. Normalise our data to arrive at the differential scattering cross section
4. Normalise to the sample's form factors

diamond

A reminder of the proposed detector geometry on HED

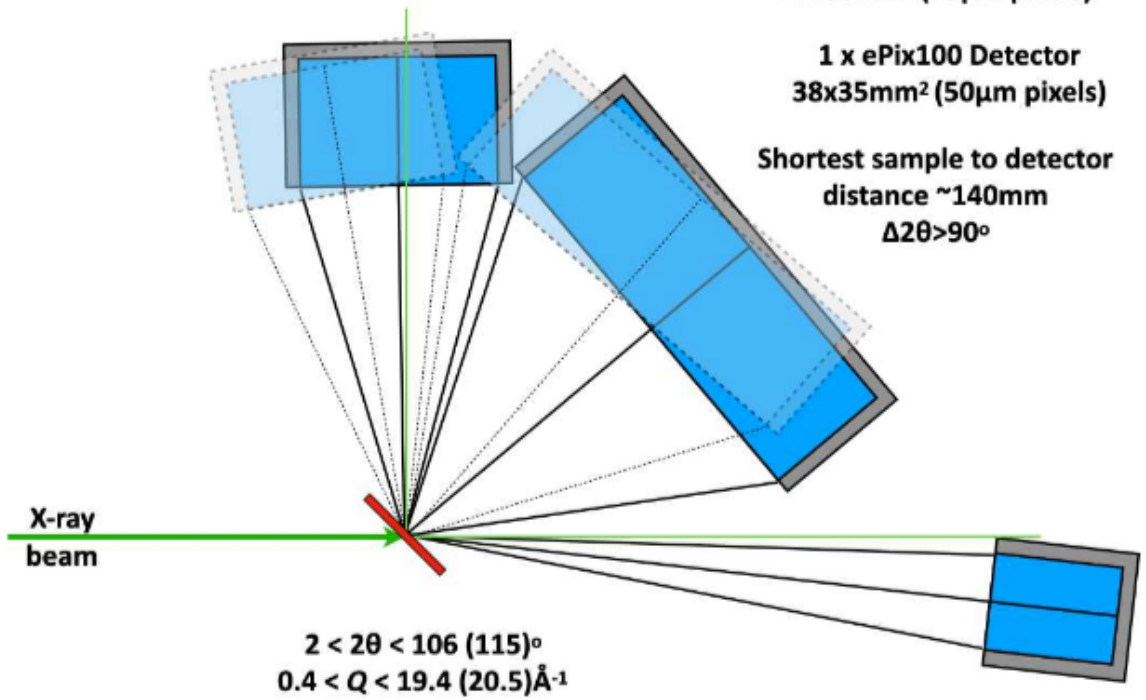


Figure 1. *Arrangement for uf-TS /PDF measurements in HED IC1. The Jungfrau detectors are mounted within existing housings onto a single wagon on the inner vertical arc and can rotate to different scattering angles. The ePix100 detector is placed below the X-ray beam to collect the lowest-Q data. Further details, including Q-ranges (for 24 keV X-rays), are given within the figure*

Fundamental Requirements

- Data that are *reproducible*
- Data that are *calibratable*
- Data that are *mergeable*
- A way to record and retrieve backgrounds/substrates/containers
- A way to record and retrieve sample metadata
- A way to link data from different 2θ positions

diamond

The two approaches

Fully correct everything	The "*ad hoc* method"
relies on exactly known experimental conditions	leverages known behaviour of various functions as $\{Q, r\} \to \{0, \infty\}$
delivers correctly scaled TS/PDF	delivers TS/PDF with arbitrary scale factor
as used in gudrun, PDFgetX2, vaxadium	as used in PDFgetX3

diamond

One possible solution

- we populate a small sample database beforehand
- access this metadata at the point of data collection
- trigger one (or more) jupyter notebooks
    - use pyFAI to integrate data to 1D
    - use PDFgetX3 to subtract container, normalise, FT
- … analysis?

diamond

Processing vs Analysis

- Everything up to this point is "processing"
- Some analyses need no further data (peak fitting etc.)
- Some require further linking (cluster analysis, NMF etc.)
- Some require further sample information (structural fitting)

diamond