

uf-TS/PDF EuXFEL Processing/Analysis Meeting

Agenda

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

Dean, have you pressed
record?

uf-TS/PDF Processing Requirements

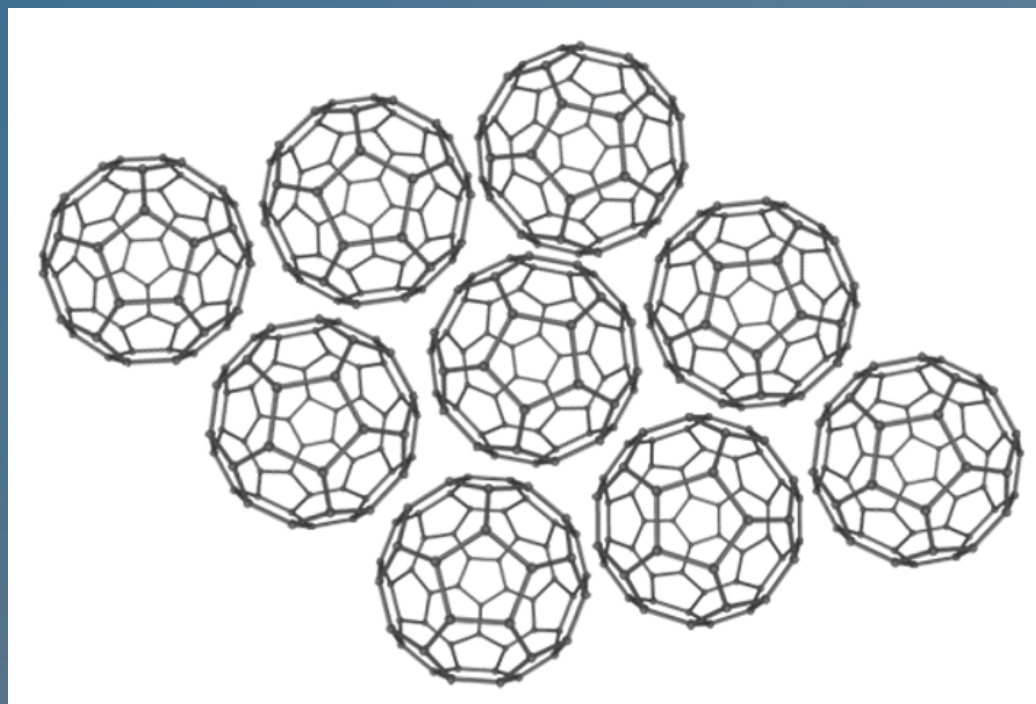
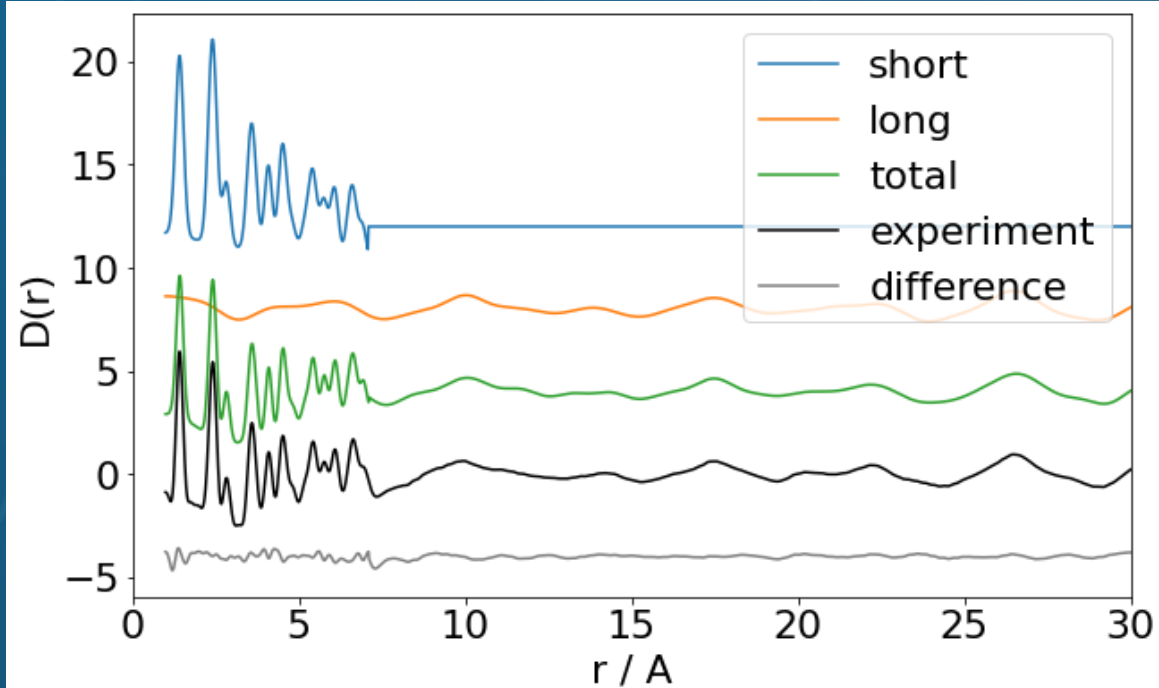
Dean Keeble

12 April 2023

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

What is a PDF?

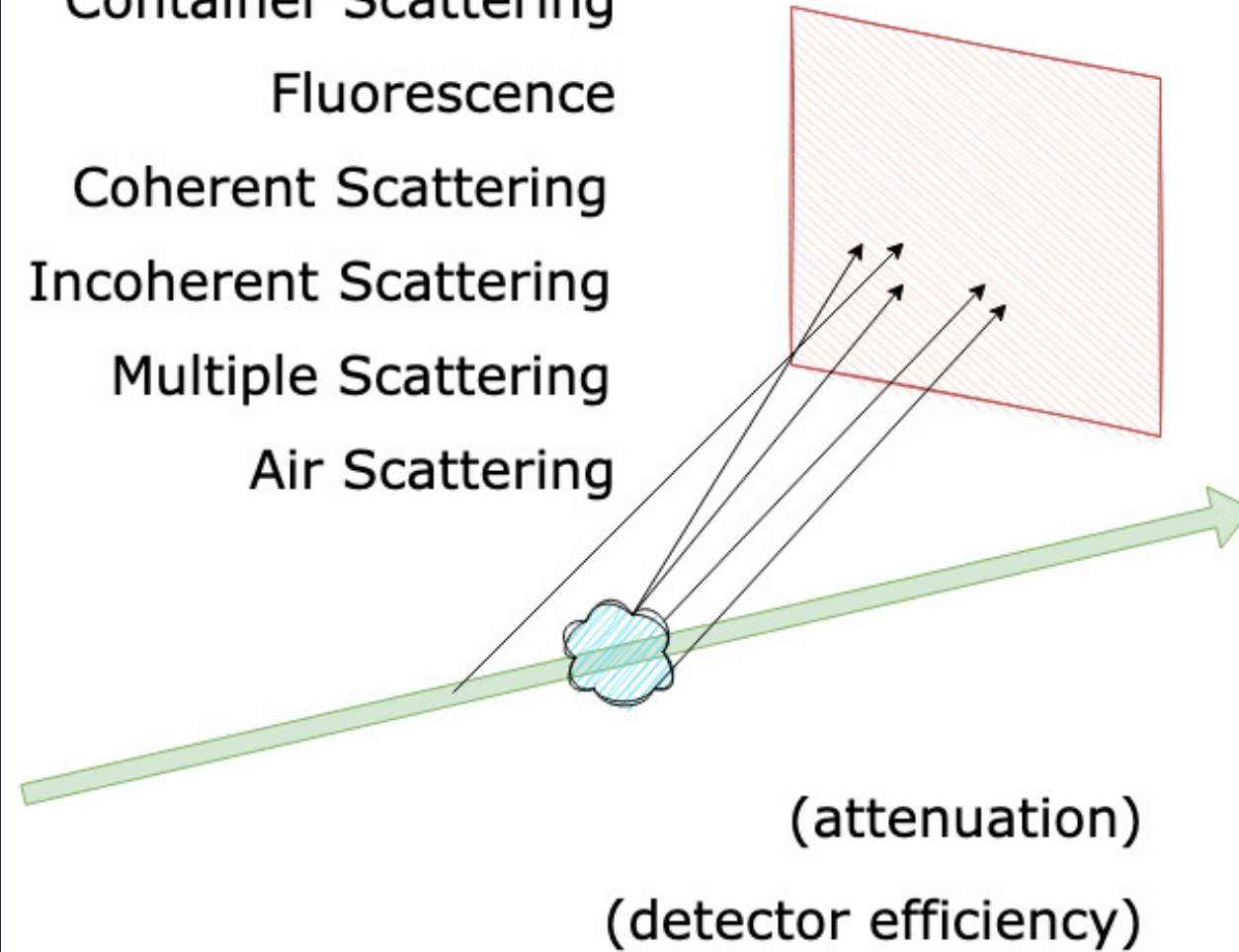


What is TS/PDF?

TS = Total Scattering
i.e. we want to get to
 $F(Q)$, the total
scattering structure
factor

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

Container Scattering
Fluorescence
Coherent Scattering
Incoherent Scattering
Multiple Scattering
Air Scattering



How to get a PDF?

If you've successfully extracted your $F(Q)$, it's straightforwardTM to convert it to the pair distribution function

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

Differences to "normal" diffraction

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

1. Correctly subtract 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

A reminder of the proposed detector geometry on HED

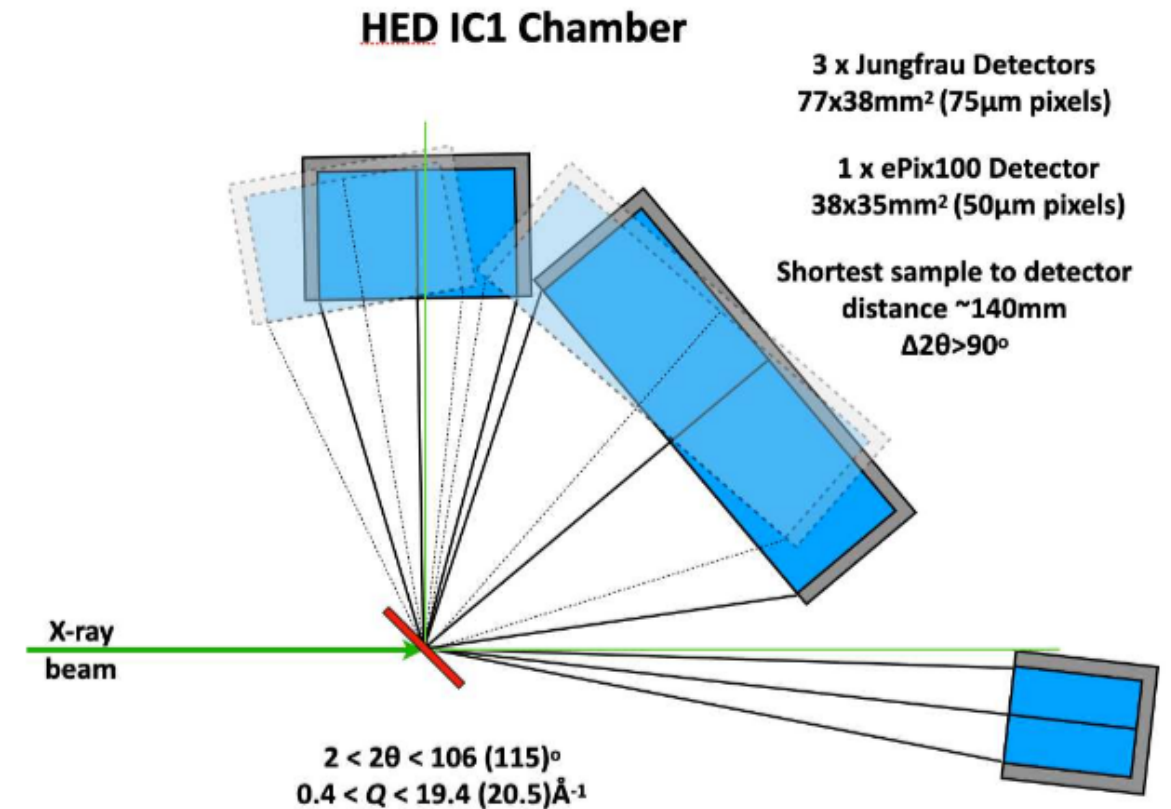


Figure 1. Arrangement for *uf*-TS /PDF measurements in HED IC1. The Jungfrau detectors are mounted within existing housings onto a single wagon on the inner vertical arc and can rotate to different scattering angles. The ePix100 detector is placed below the X-ray beam to collect the lowest-*Q* data.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

The two approaches

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

One possible solution

- we populate a small sample database beforehand
- (somehow) get this metadata at the point of data collection
- use pyFAI to integrate data to 1D
- use PDFgetX3 to subtract container, normalise, FT
tenuous example

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)