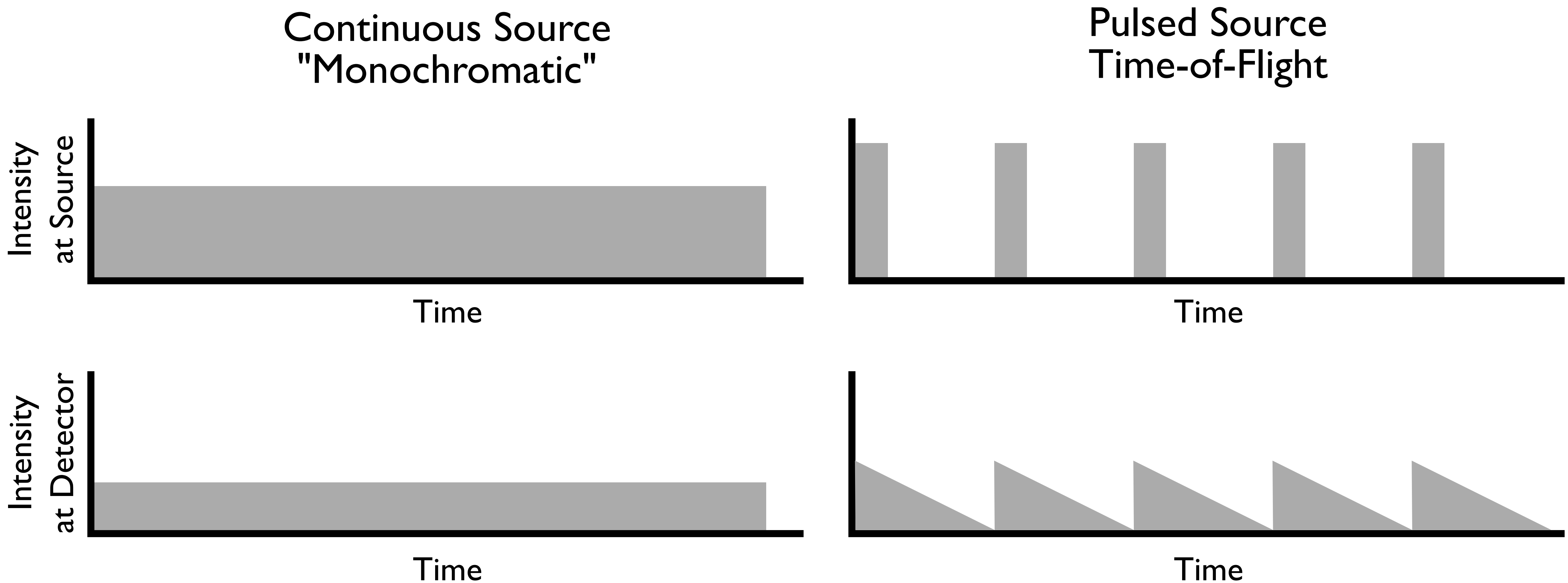
Time-of-flight SANS

Blessing or Curse?

Andrew Jackson (ESS) & Richard Heenan (ISIS)

Fixed Wavelength vs TOF

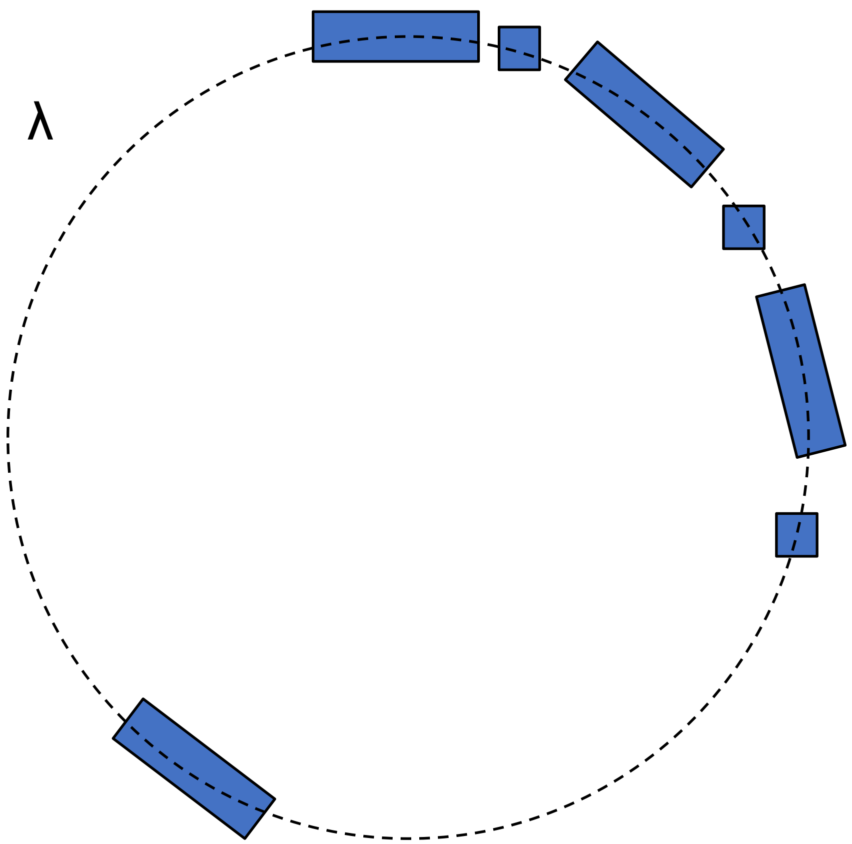


- High time-average beam flux
- Straightforward data processing – detector image more meaningful!

- Wide simultaneous Q range
- Good $d\lambda/\lambda$ resolution:
    - short-pulse source
    - constant $d\lambda/\lambda$ choppers at continuous source

Averaging

Fixed wavelength

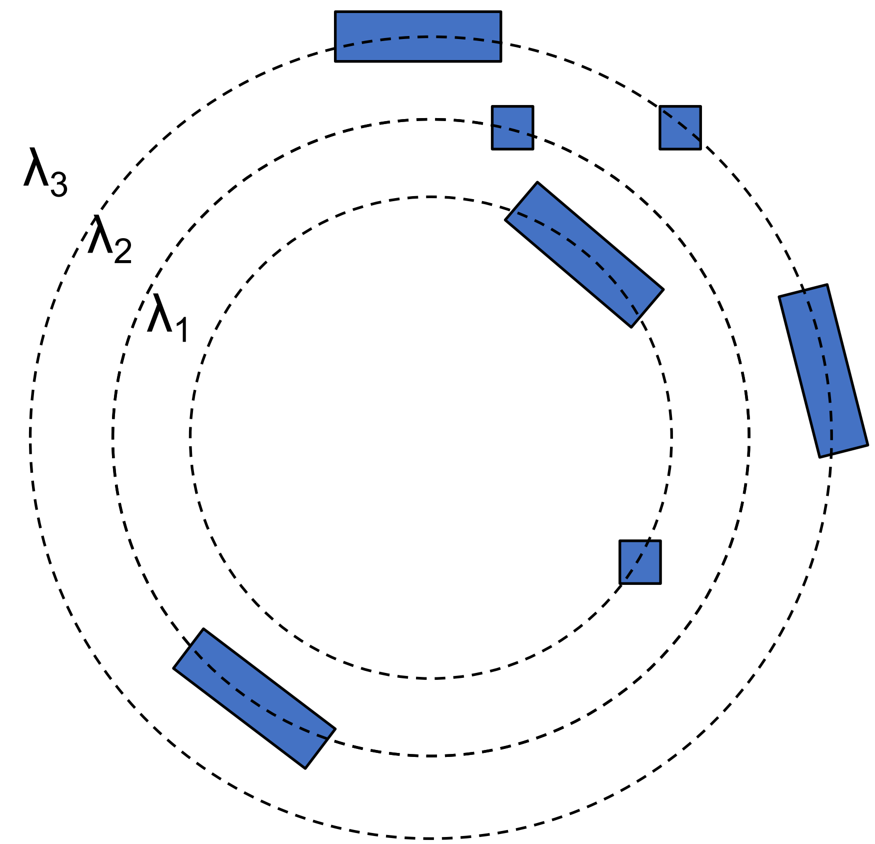


$$I(Q) \propto \frac{\sum_{R,\lambda \subset Q} C(R)}{\sum_{R,\lambda \subset Q} \Omega(R)}$$

At fixed wavelength we happily merge pixels at the same radius, summing the counts, summing the solid angles.

Note that C(R)/Ω(R) is expected to be the same for all pixels, so the best average has a sum in the numerator and a sum in the denominator.

Time of flight



$$I(Q) \propto \frac{\sum_{R,\lambda \subset Q} C(R,\lambda)}{\sum_{R,\lambda \subset Q} M(\lambda) T(\lambda) D(\lambda) \Omega(R)}$$

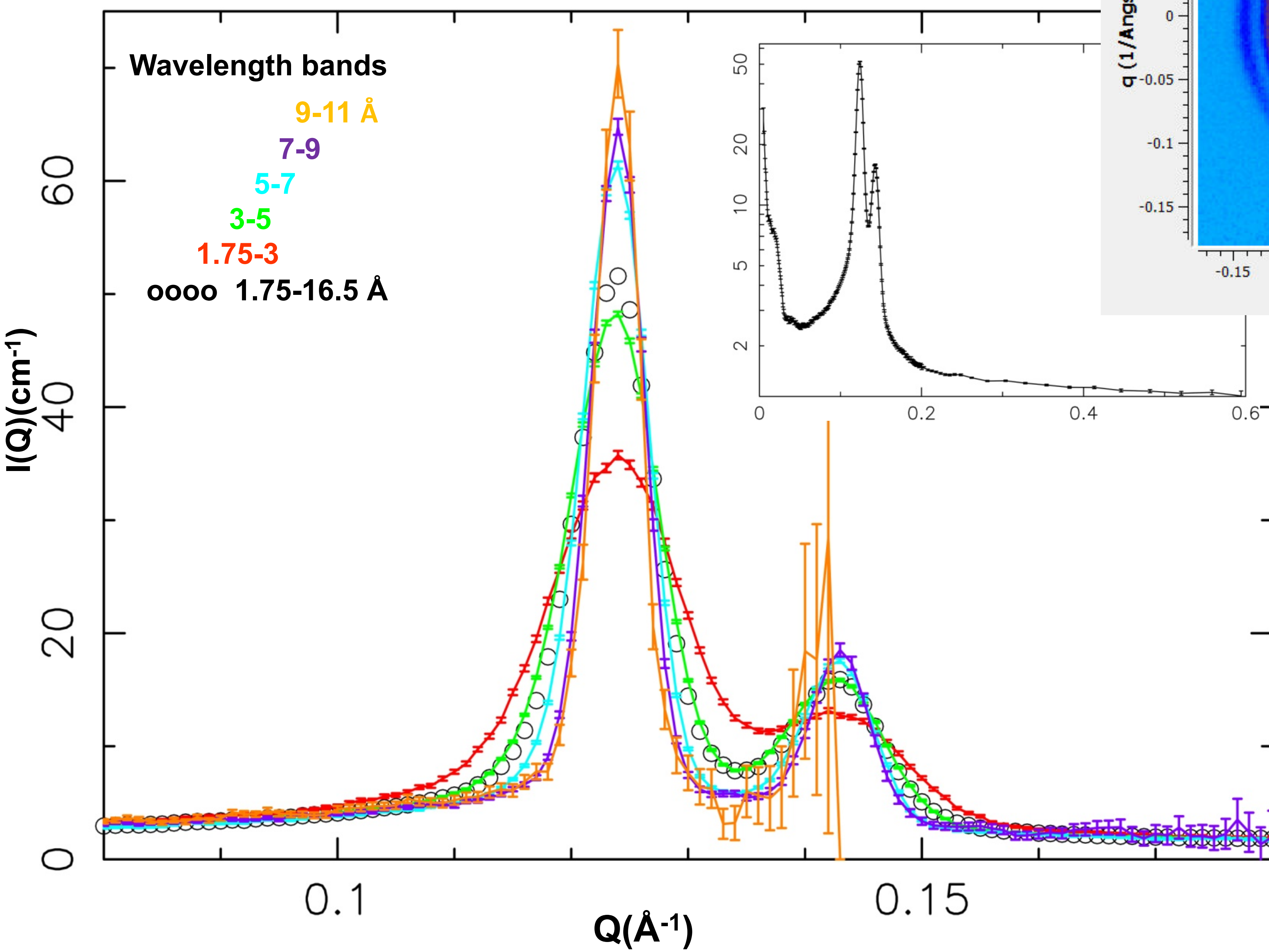
In TOF we equivalently merge data "pixels" from radius & wavelength combinations at same Q, but now have to allow for wavelength dependence!

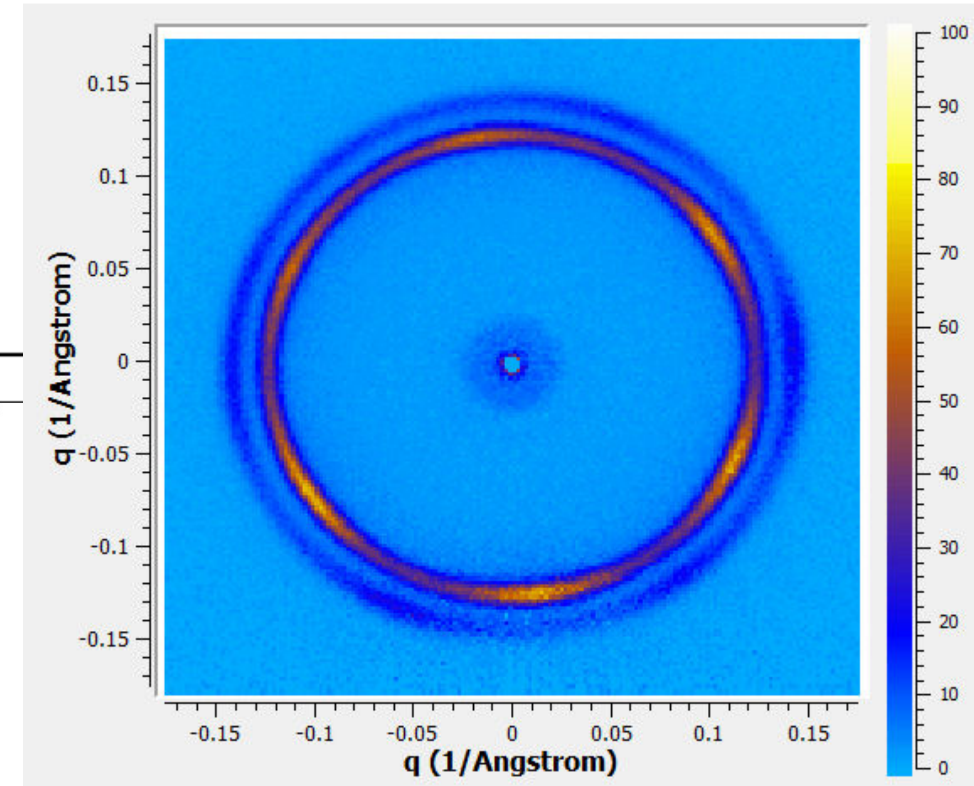
[NB : there is some ongoing debate about the correct way to do the above calculation, but it is not just "adding monochromatic curves"]

Resolution

Q resolution varies inversely with λ - sharper peak with broader tails from shorter wavelengths, which may be removed to improve resolution at expense of statistics.

[Cubic phase silica particles on SANS2d, W.Briscoe (Bristol), Short pulse ISIS source, ESS long pulse will be worse!]



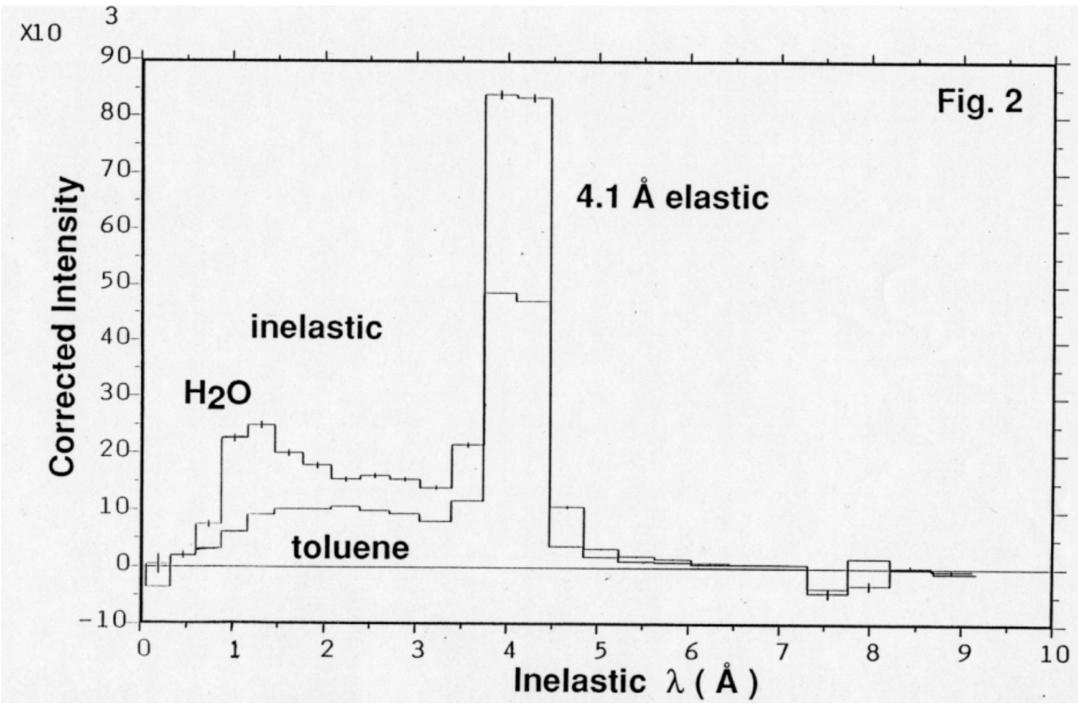


As shown by Dewhurst, Nelson, Heenan (and likely others), the traditional Mildner & Carpenter gaussian resolution approximation is often not adequate for TOF-SANS ...

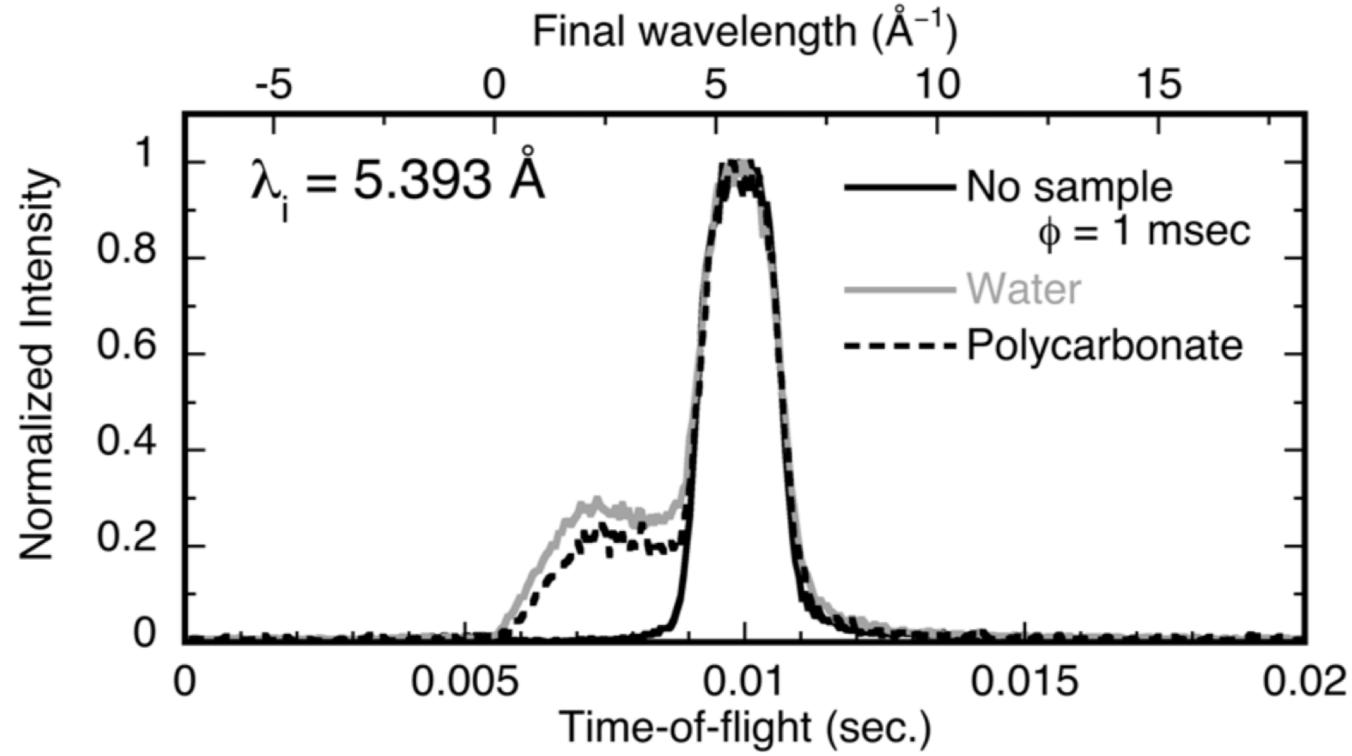
... we can calculate the correct resolution kernel ...

... but need data formats and software to use it!

Inelastic Effects



R.K.Heenan & A.R.Rennie, ICANS XII (1993) RAL Report 94-025, i241-i247.



Wildes Eur. Phys. J. Plus (2012) 127: 10 DOI 10.1140/epjp/i2012-12010-6

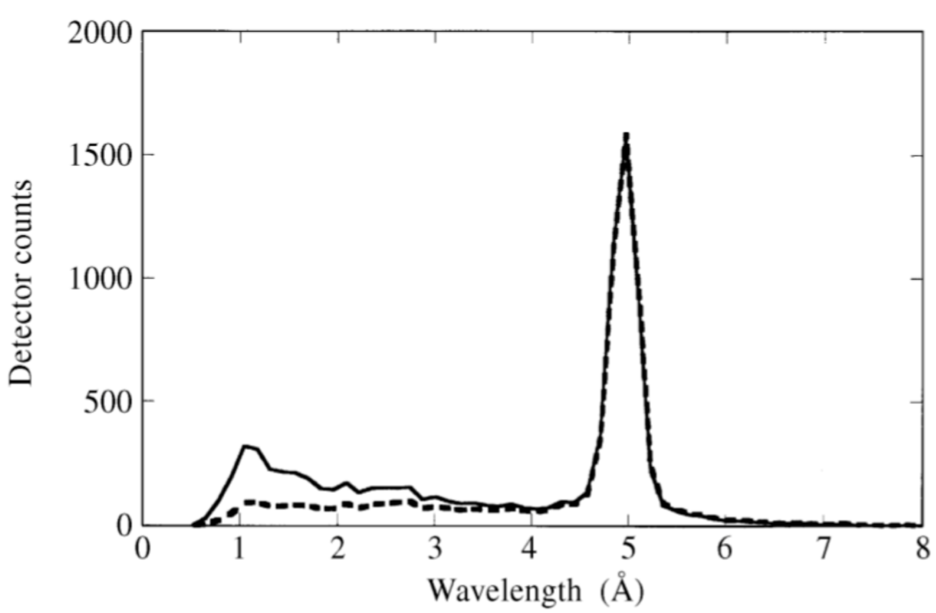
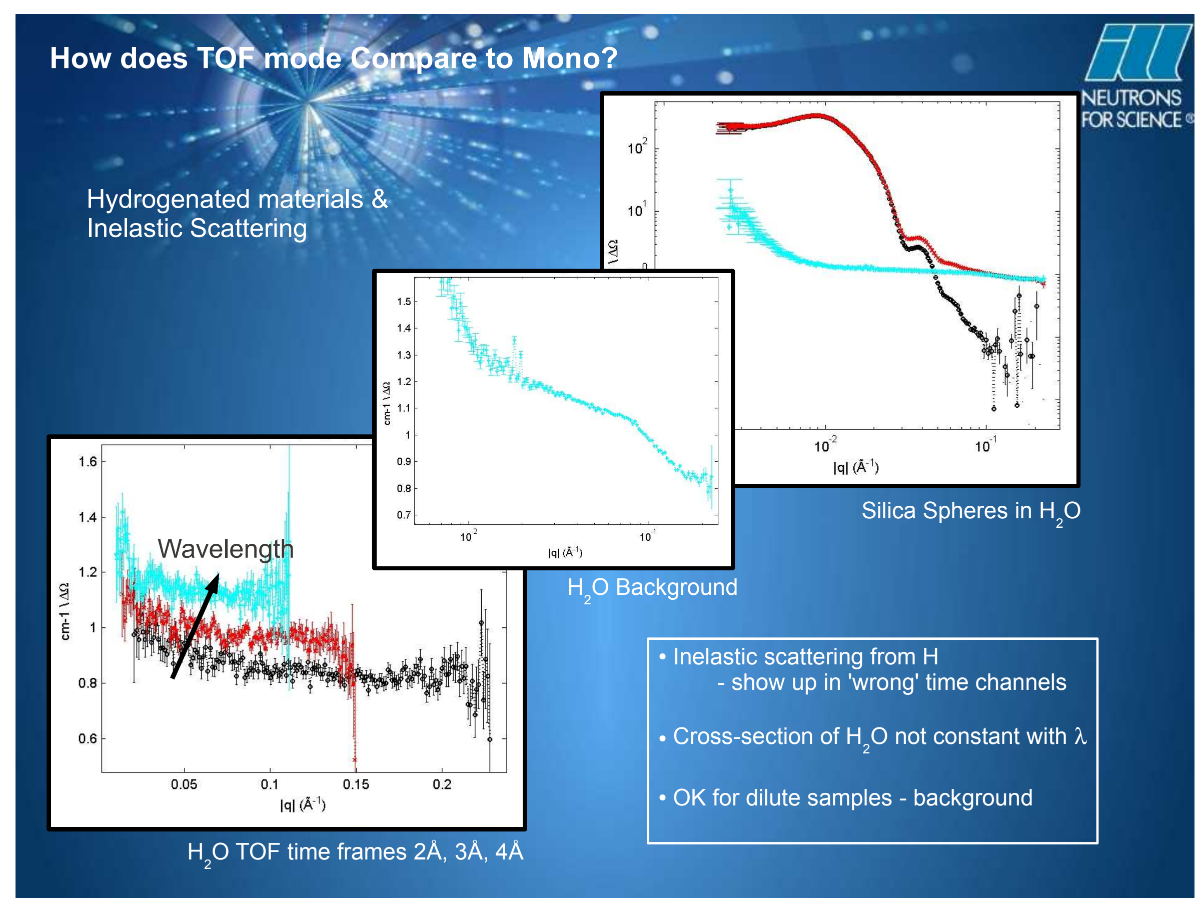


Fig. 1. Spectrum of scattered neutrons for water at 4 ± 0.5°, indicating the difference between data uncorrected (dashed line) and corrected (continuous line) for detector efficiency. The incident wavelength was 5 Å.

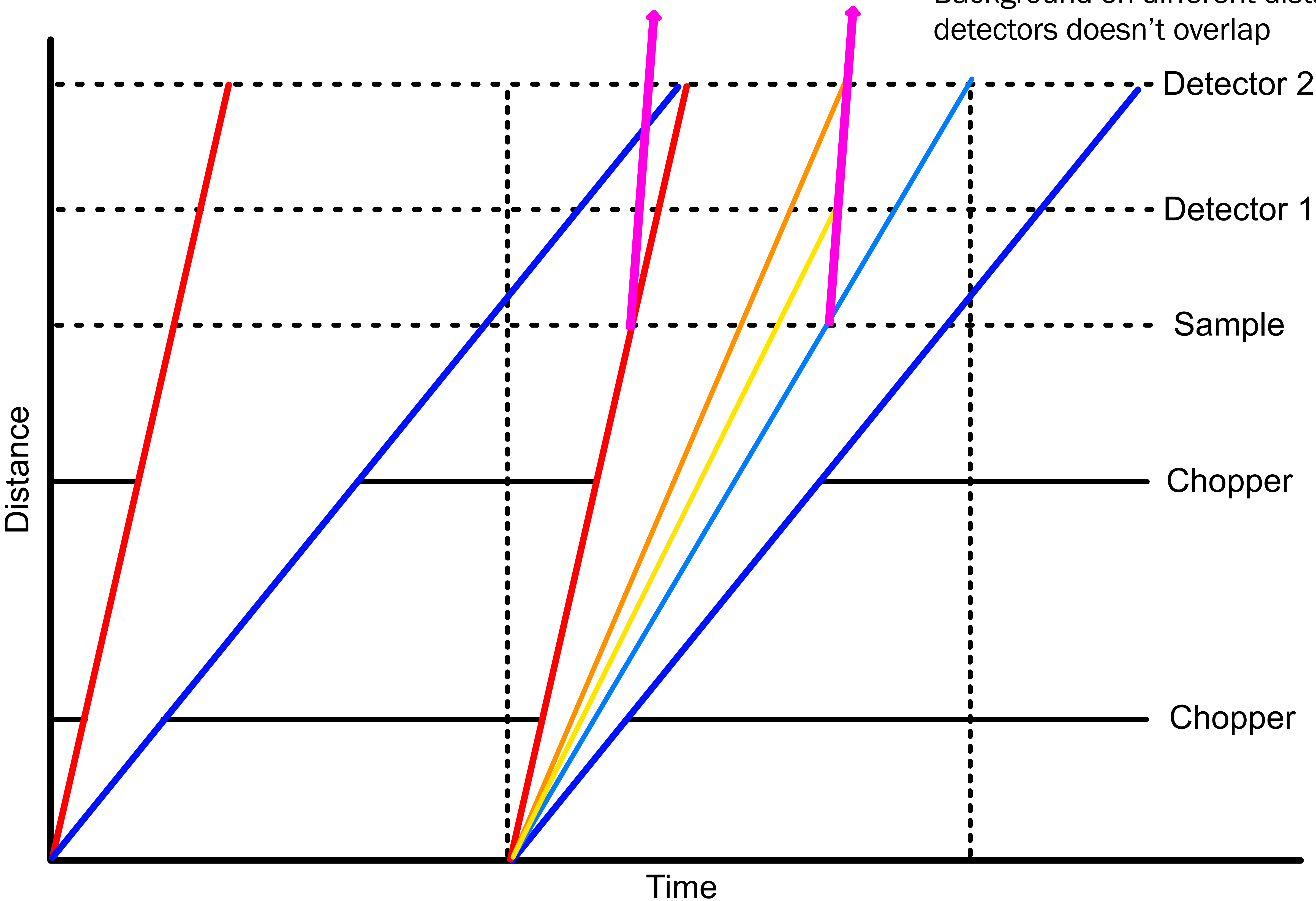
Ghosh and Rennie J. Appl. Cryst. (1999). 32, 1157±1163



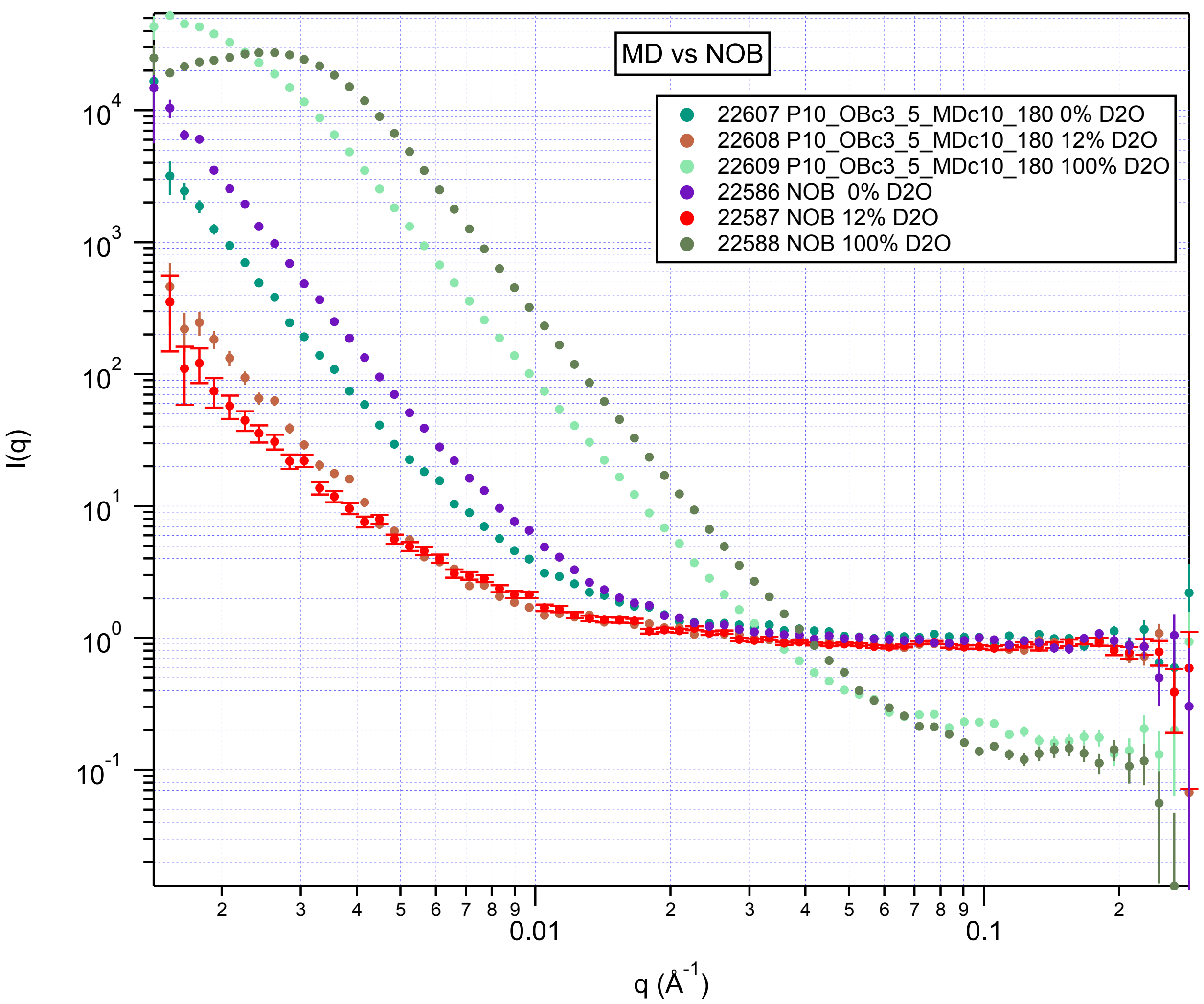
Dewhurst, canSAS-VIII presentation

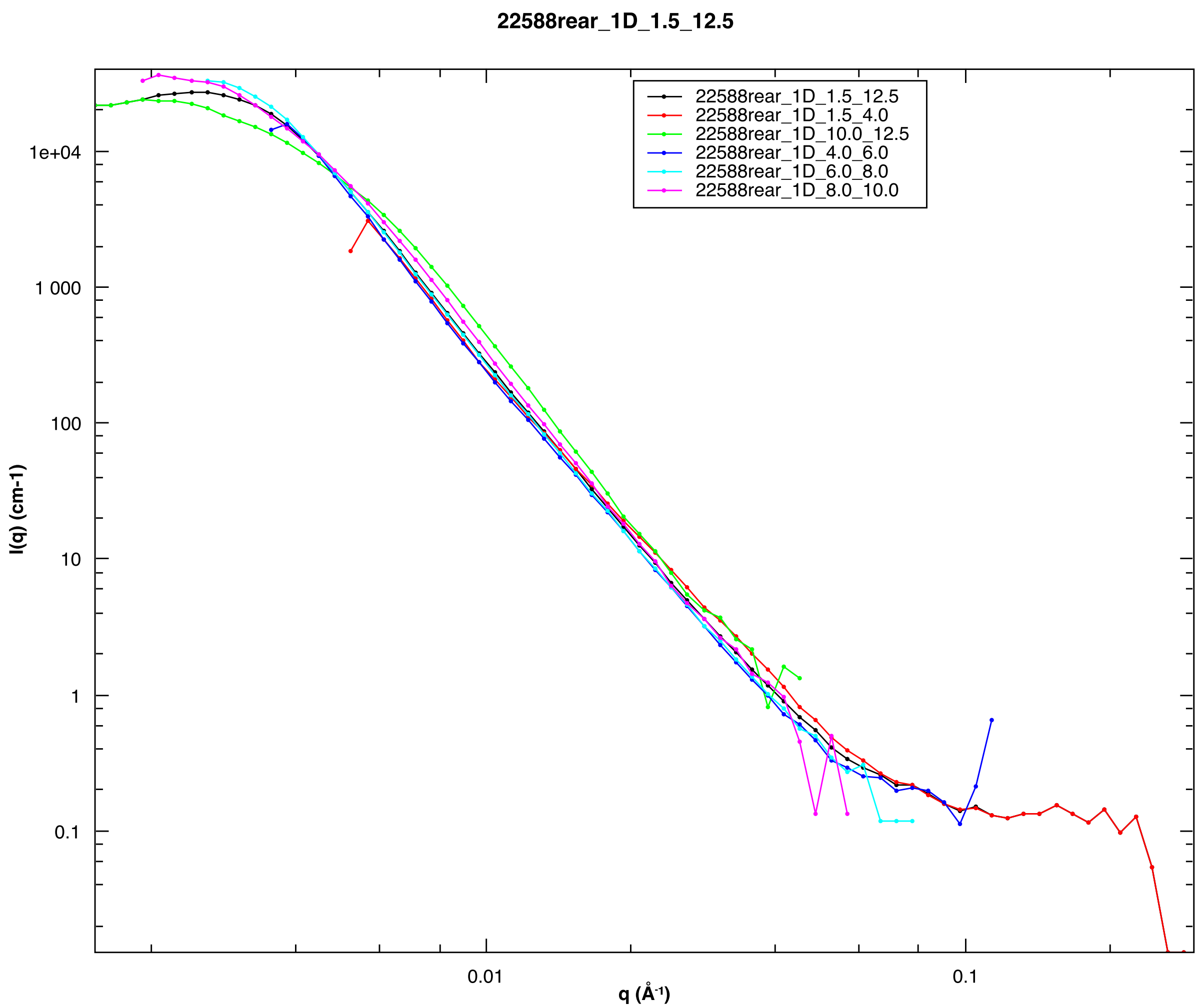
Inelastic Effects

- Unexpected frame overlap
- Non-flat solvent backgrounds
- Background on different distance detectors doesn't overlap

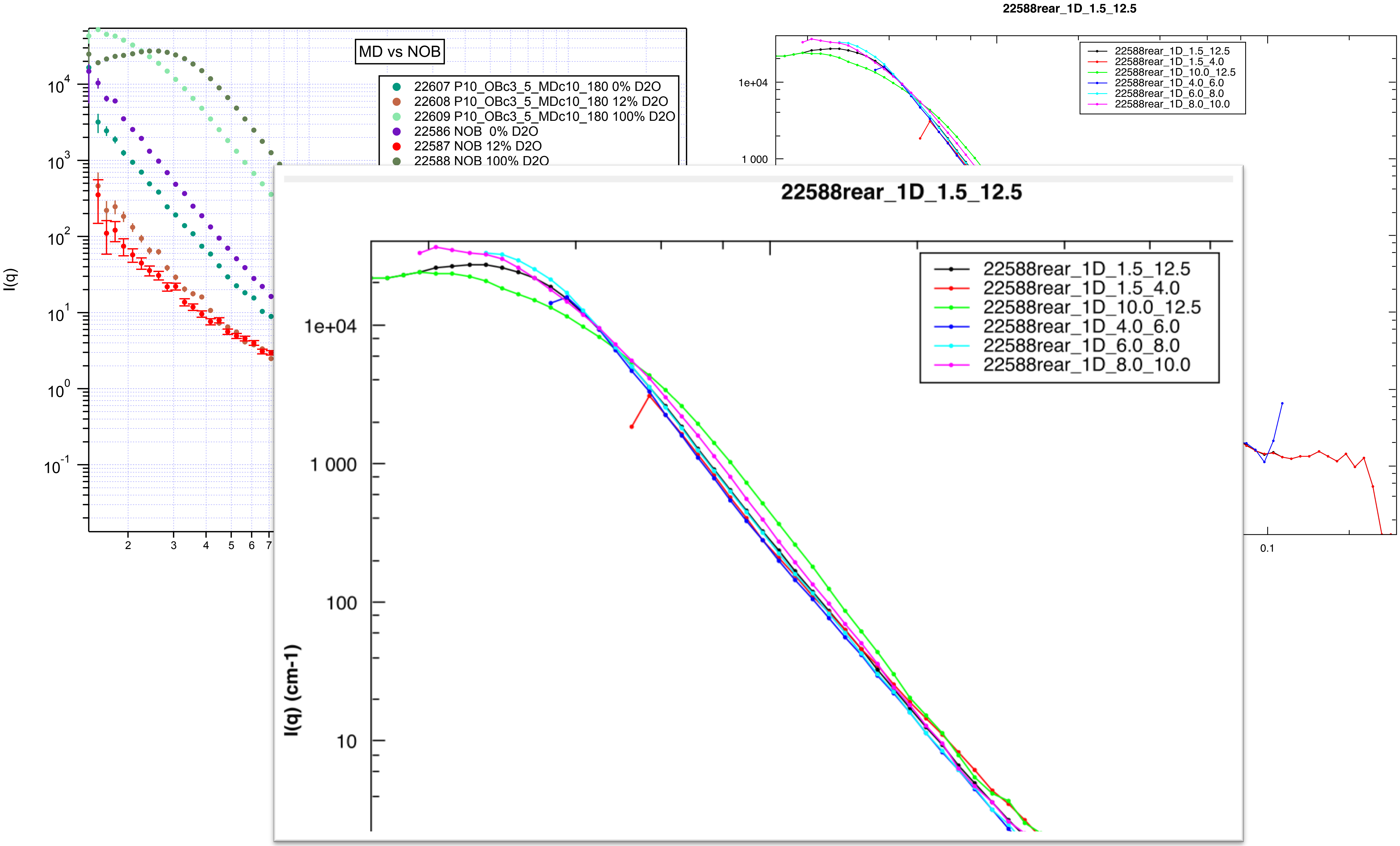


Multiple Scattering





Multiple Scattering



Challenges

- Calibration standards for Q and I that work for a wide Q range and have no inelastic scattering (and preferably are purely coherent)
- ”Flood pattern” samples that impart no wavelength dependence (probably impossible!?!)
- Support for better resolution descriptions
- How to handle multiple scattering properly with TOF
- Multiple detector banks - overlap, visualisation, 2D data analysis [data formats]

TOF Session …

- Complex detector geometries and TOF
  - Judith Houston (ESS)

- TOF calibration ideas
  - Sebastian Jaksch (JCNS)

- Experiences from commissioning and running Bilby
  - Anna Sokolova (ANSTO)