Data

Acquisition, analysis, visualisation, modelling and simulation

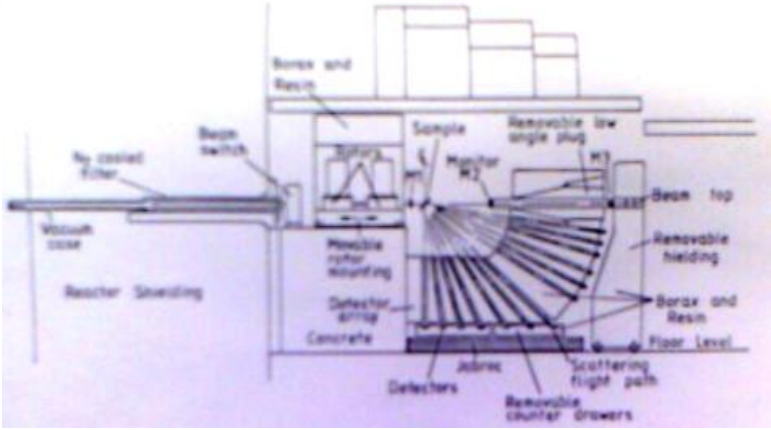
Robert McGreevy

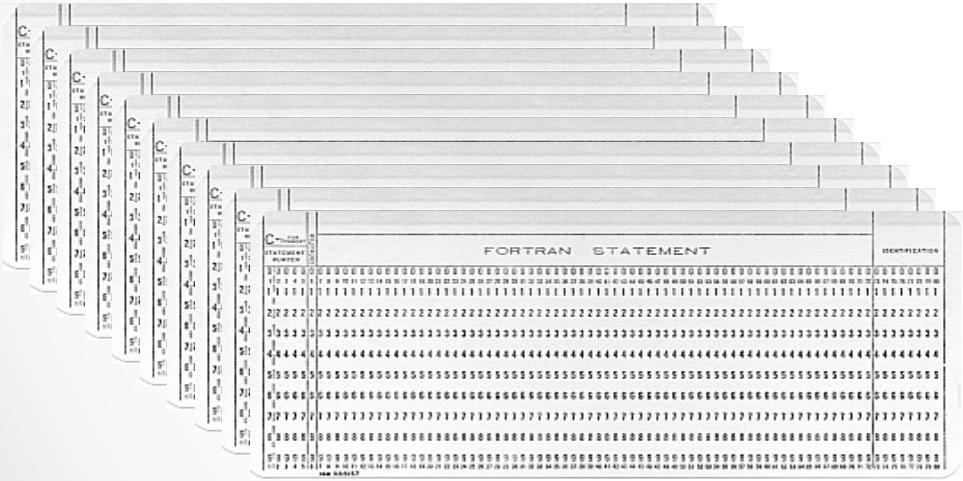
The world has changed …

The world has changed …

If you bought a premium-class automobile recently, ”it probably contains close to 100 million lines of software code,” says Manfred Broy, a professor of informatics at Technical University, Munich, and a leading expert on software in cars.

The world has changed …





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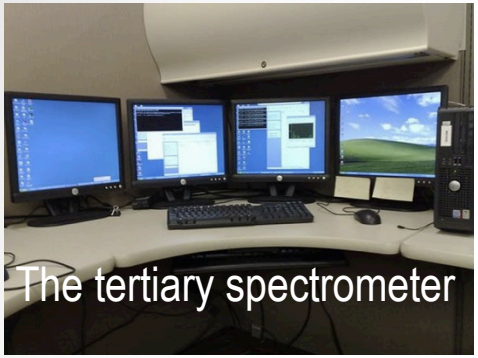
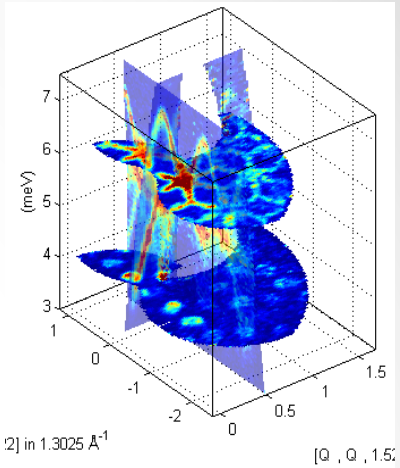
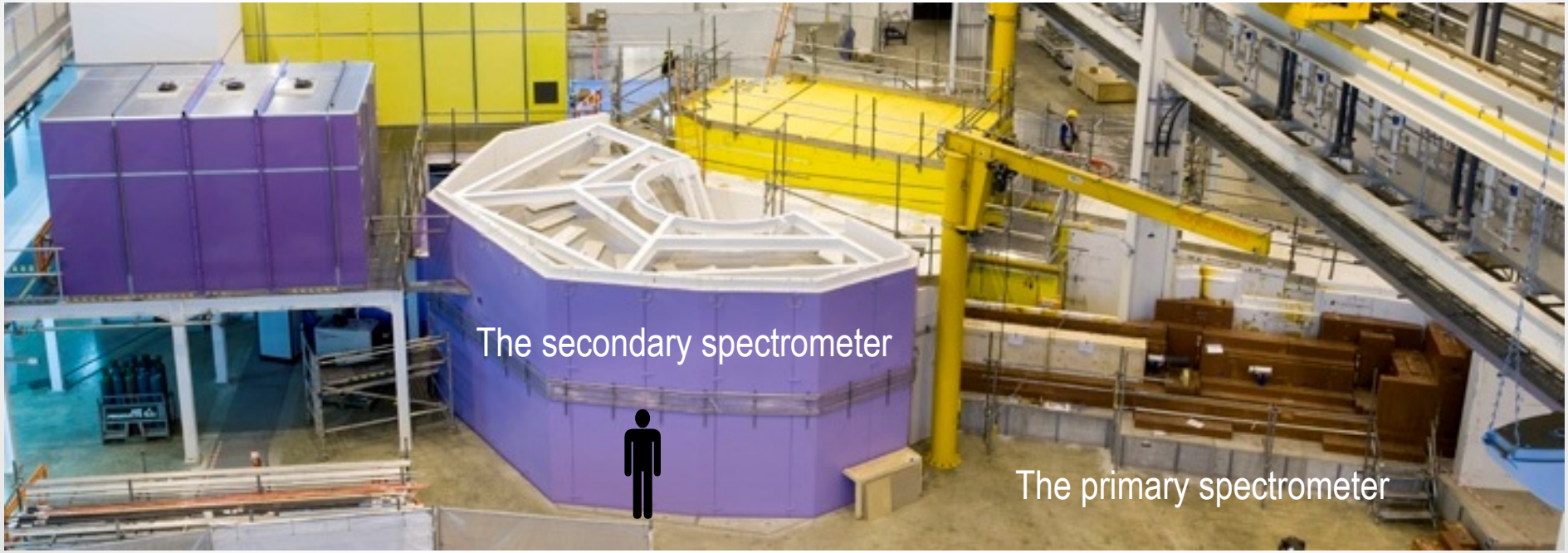
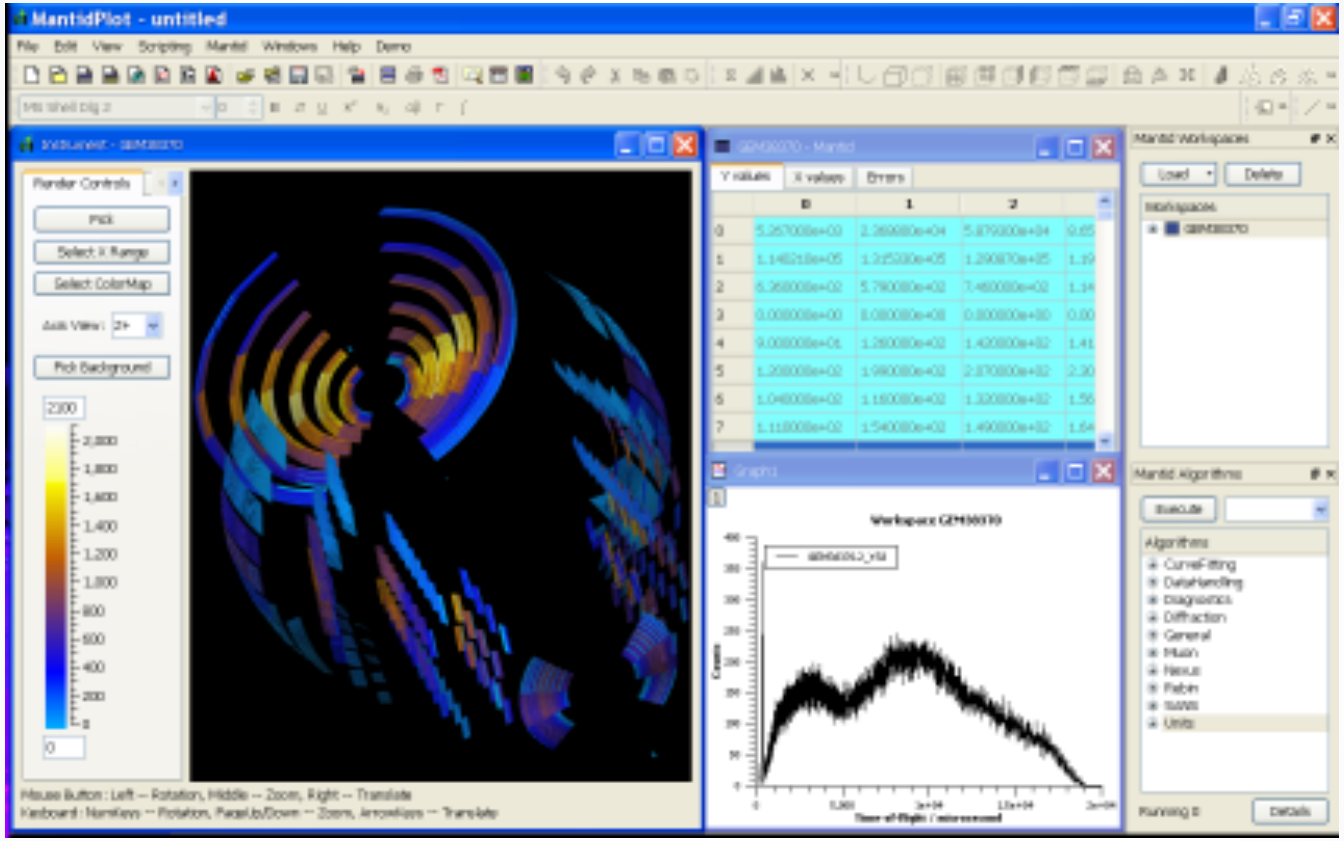






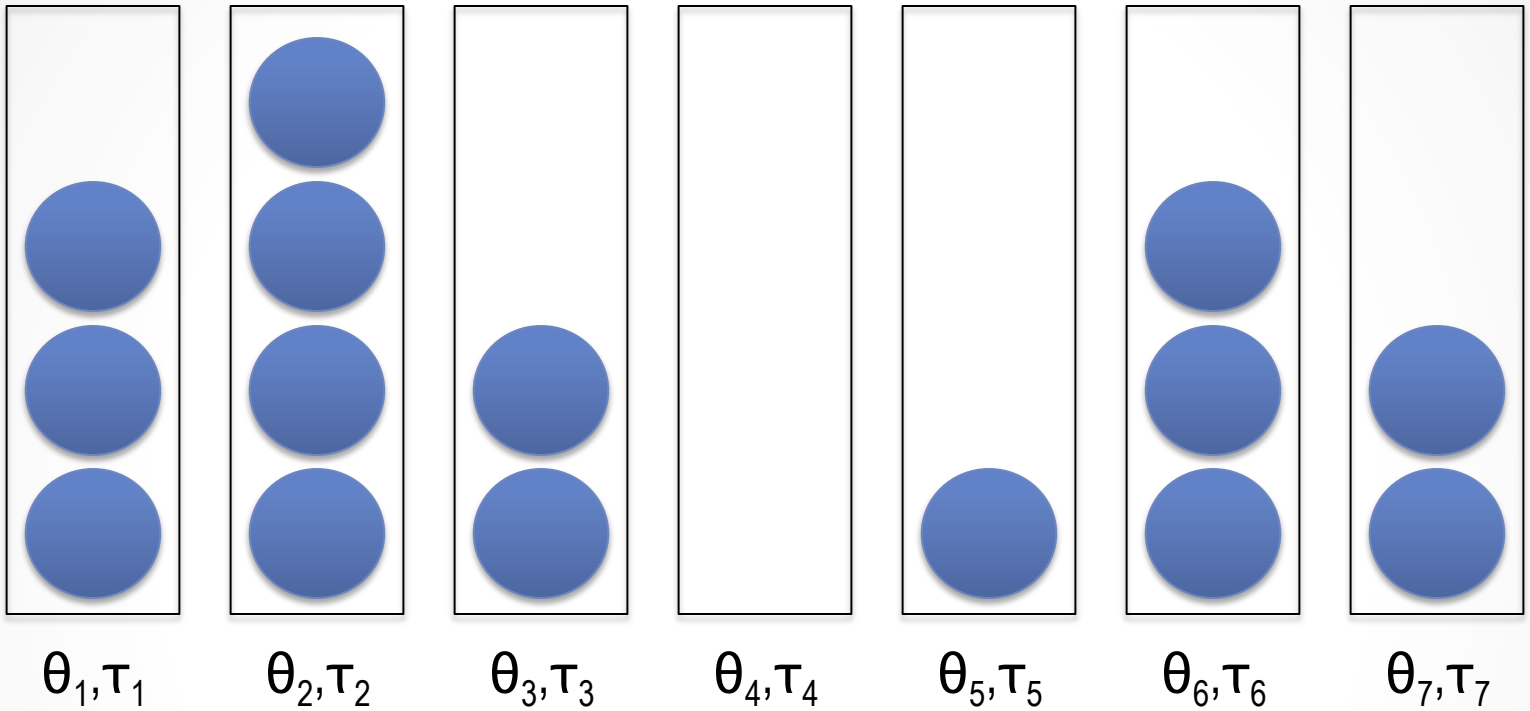
Data acquisition



First turn analog detector signal into digital (week 2)

Turn position (θ) and time (t) on a detector into (Q,w)

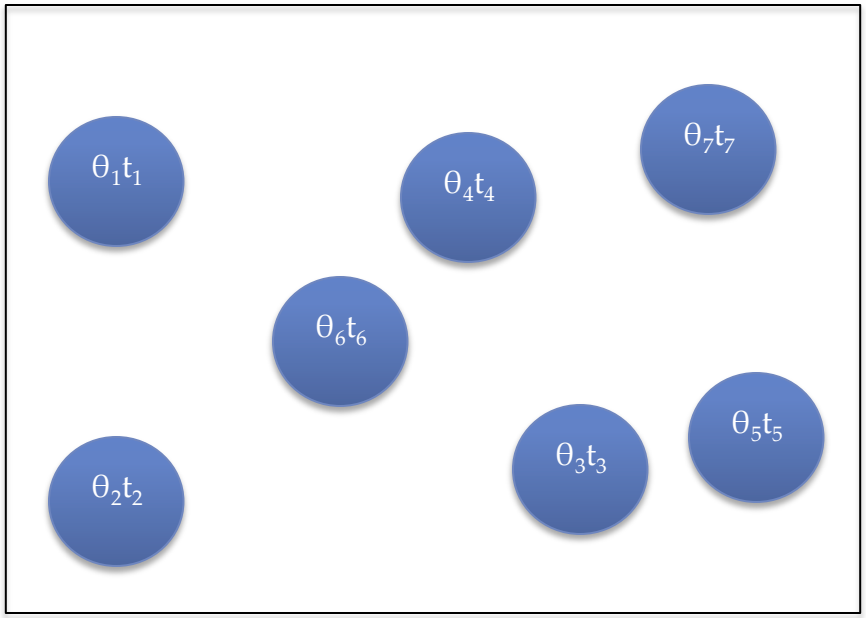
Data acquisition



Histograms and events

Convert (θ,τ) to (Q,ω)

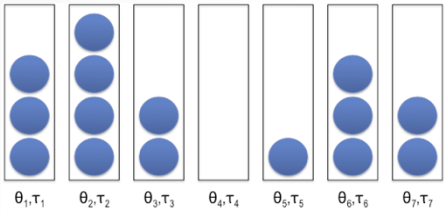
Data acquisition

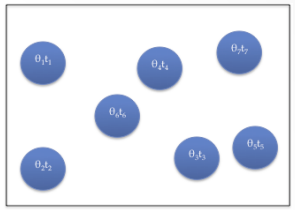


Histograms and <u>events</u>

Convert (θ,t) to (Q,ω)

Data acquisition

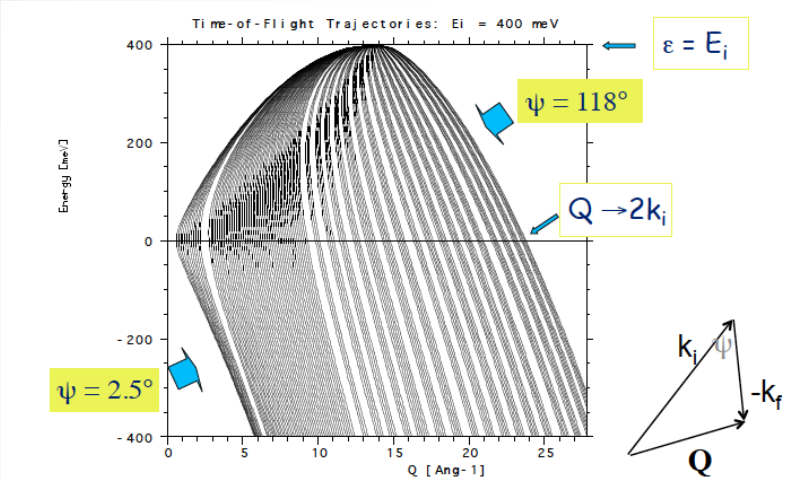


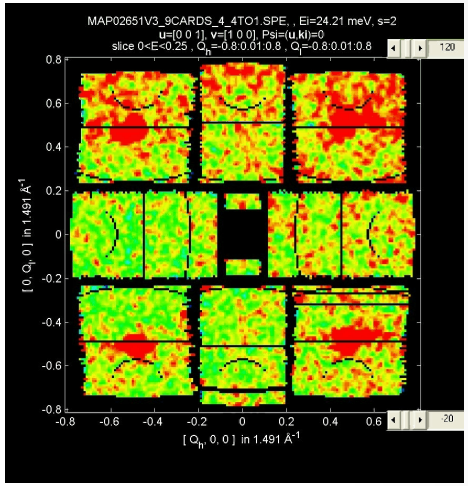


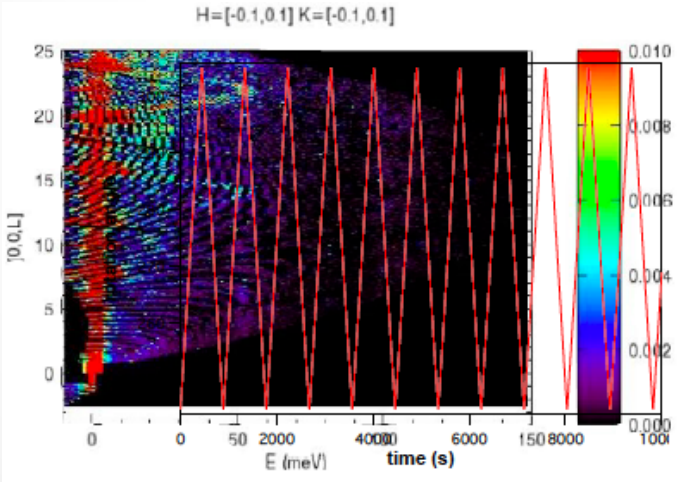
Histograms or events?

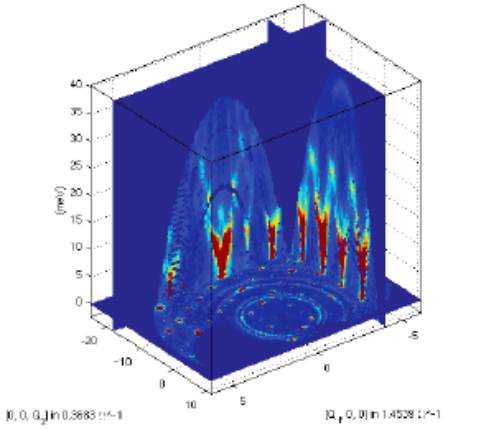
- Histogram data sets for large area inelastic detectors can be very large (lots of zeroes!)
- Event data sets for large area diffraction detectors can be very large (when you only want a 1-D histogram)
- Events allow 'after the event' analysis, e.g. for kinetic or parametric experiments
- Events (will) allow novel uses of instruments, e.g. continuous sample rotation ((**Q**,ω) mapping) or resolution optimisation

Event mode – a game changer?

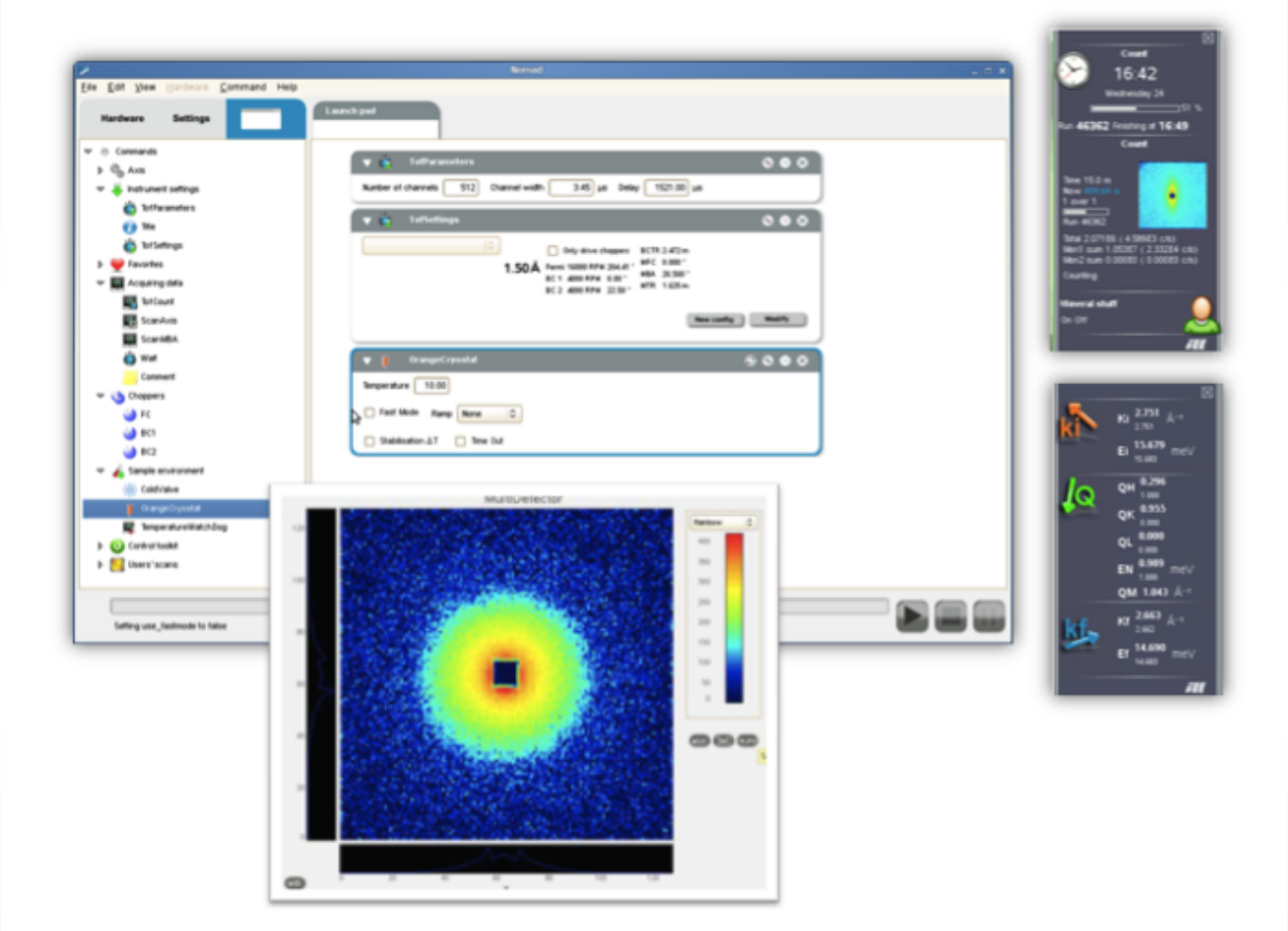








Instrument control



Metadata: user, sample, sample environment …

Data reduction

Contributions to the measured intensity:

- Sample (s), container (c), sample environment/background (b)
- Incident spectrum (monitor) – wavelength (time) dependent

Need to correct and normalise

- a_n – absorption coefficients (geometry dependent, energy dependent, calculated)

$$I = \frac{a_1 I_s - a_2 I_c - a_3 I_b}{a_4 I_v - a_5 I_b}$$

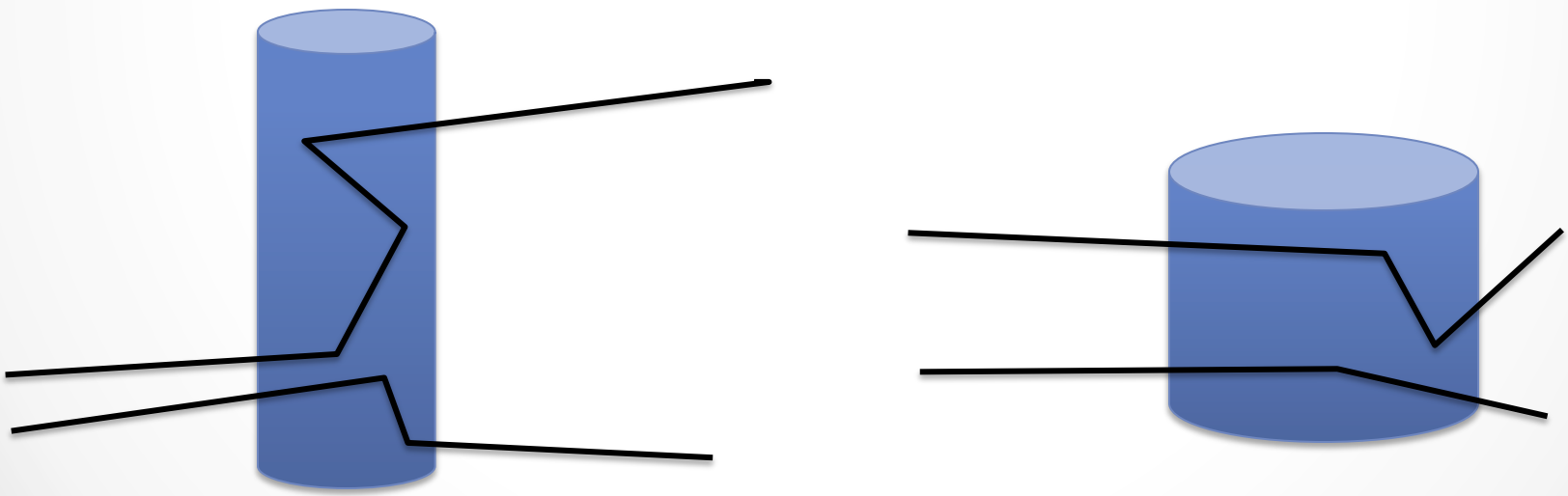
Data reduction

Multiple scattering – dependent on sample geometry, scattering and absorption

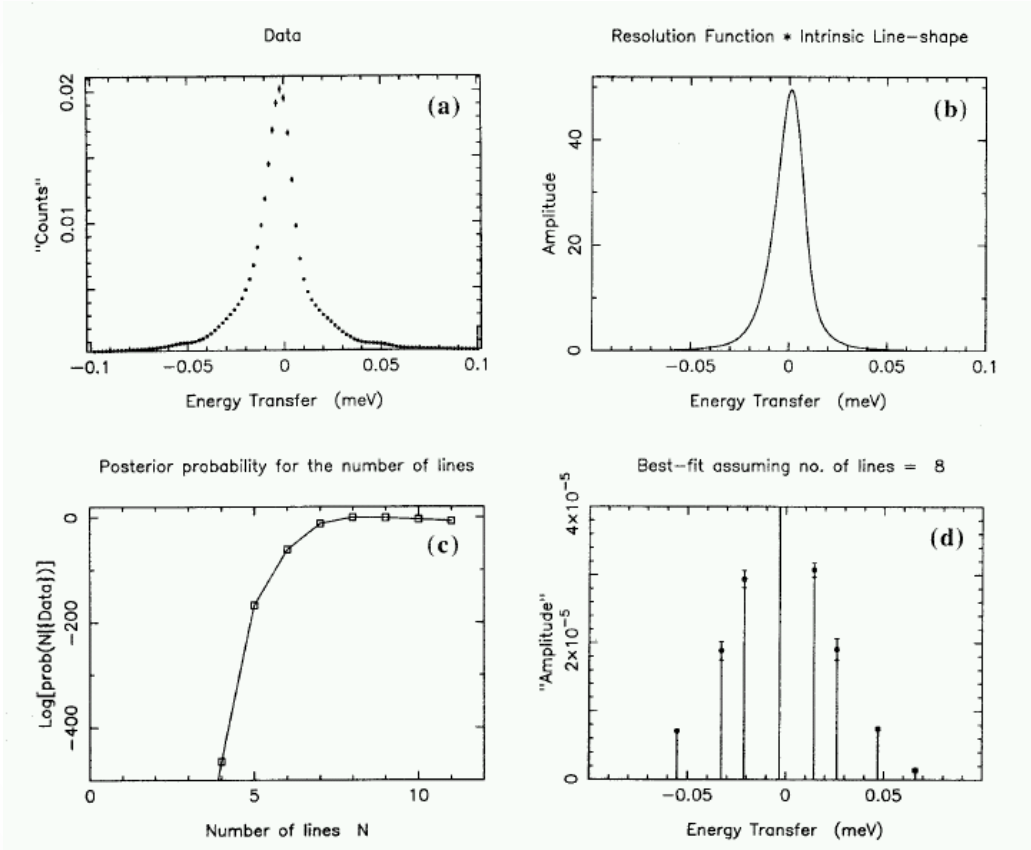
General rule is to keep the sample less than a 10% scatterer

$$I = I_1 + I_2 + I_3 + \ldots$$

Calculate analytically or via Monte Carlo

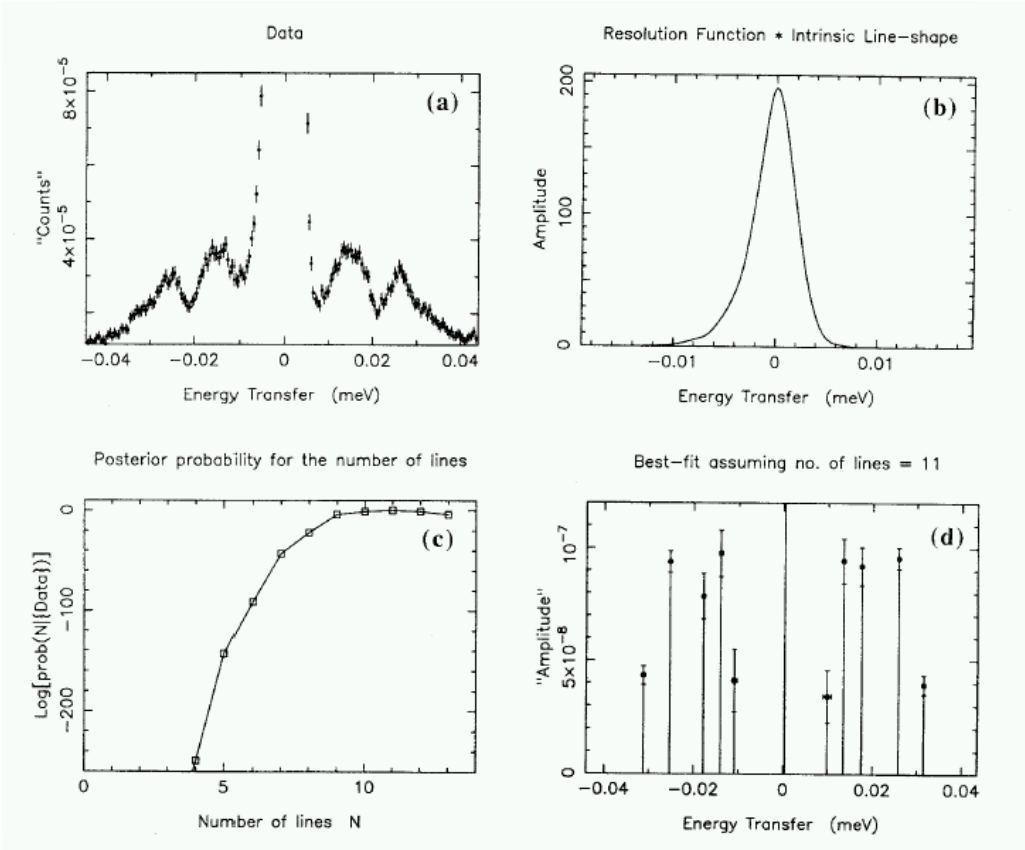


Dealing with instrument resolution



Convolute a model: Bayesian analysis

Dealing with instrument resolution



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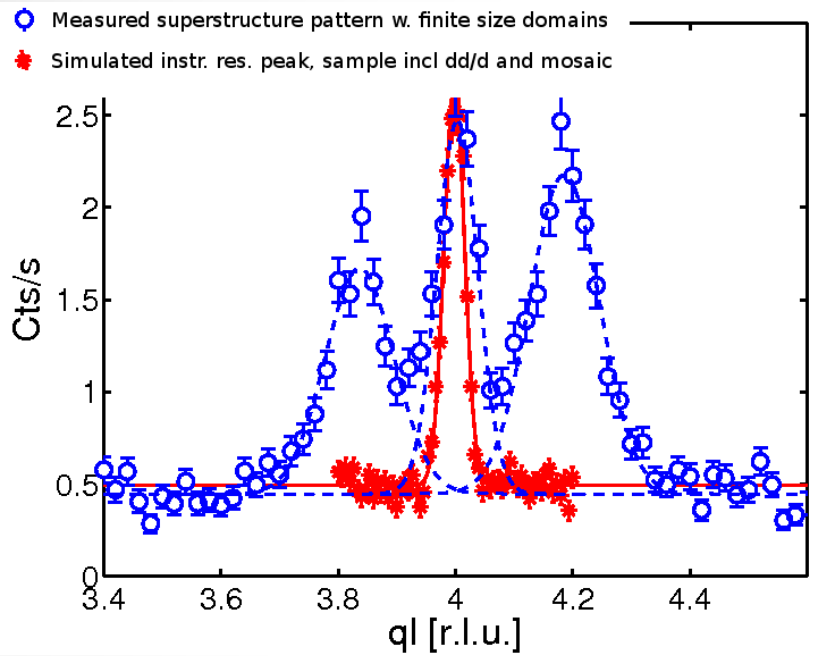
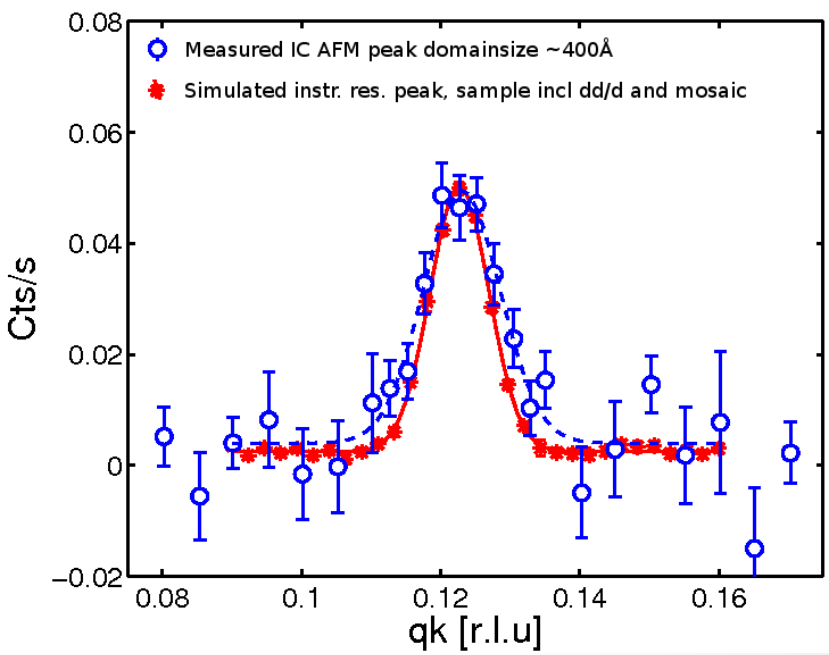




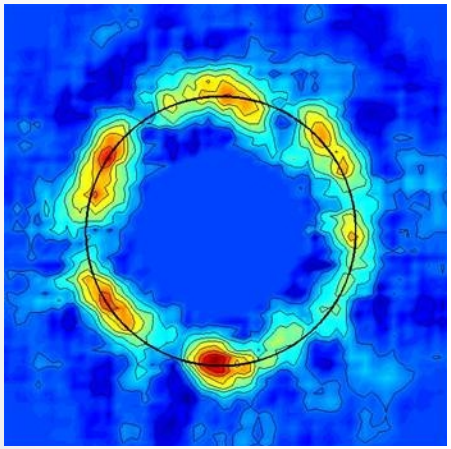
Convolute a model: Monte Carlo

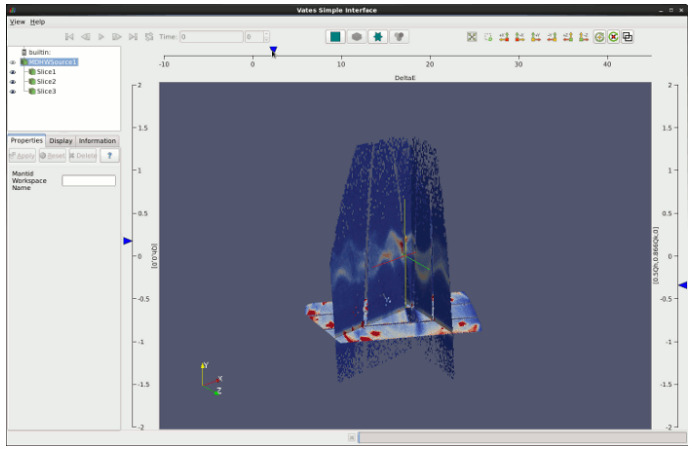
Data analysis

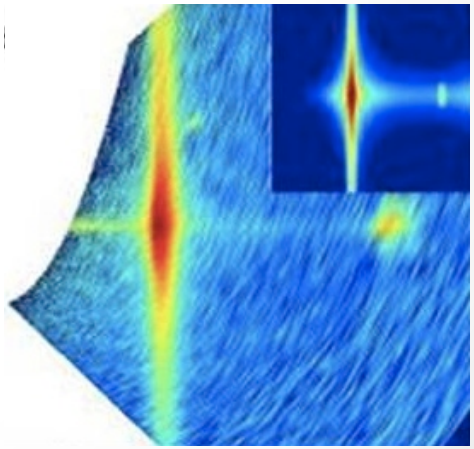
What do I do with S(Q) or S(Q,ω)?

Visualise it, model it

(Some) physicists think in reciprocal space







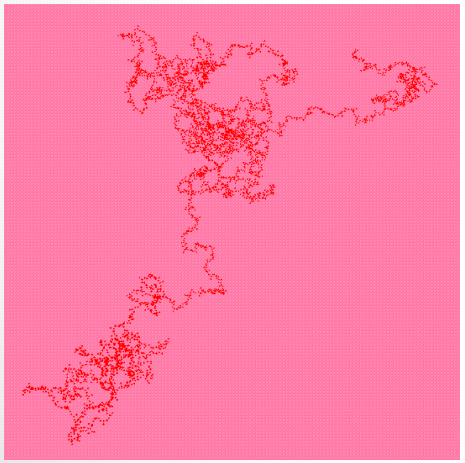
Data analysis

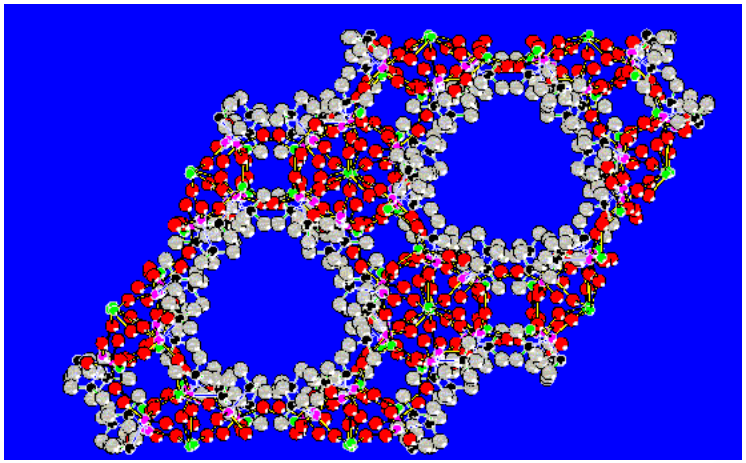
What do I do with S(Q) or S(Q,ω)?

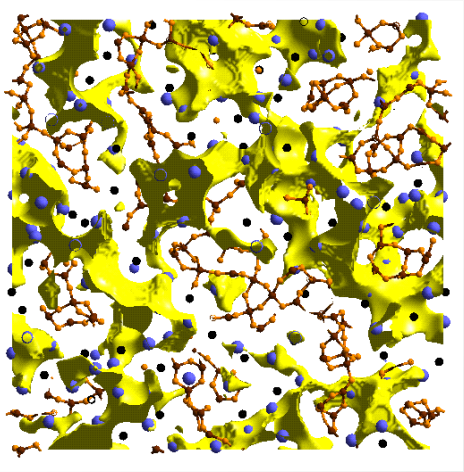
Visualise it, model it

(Some) physicists think in reciprocal space

Most users think in real space

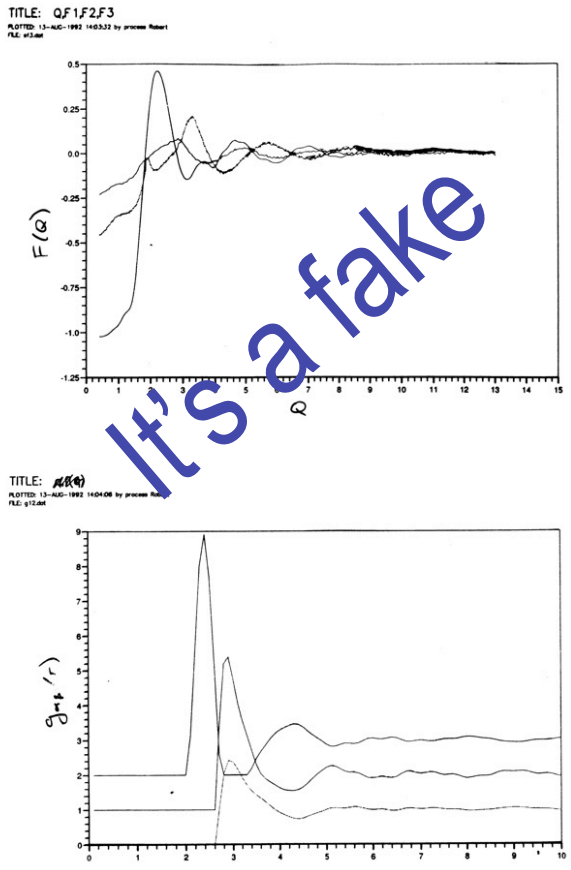




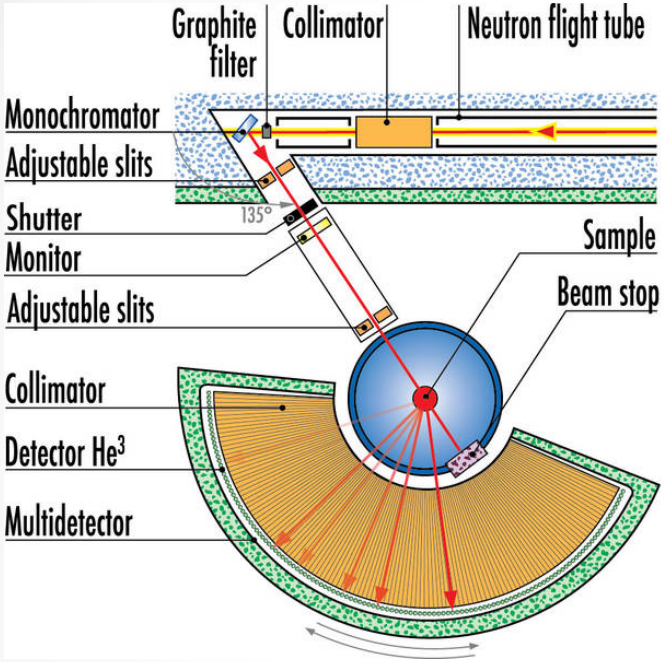


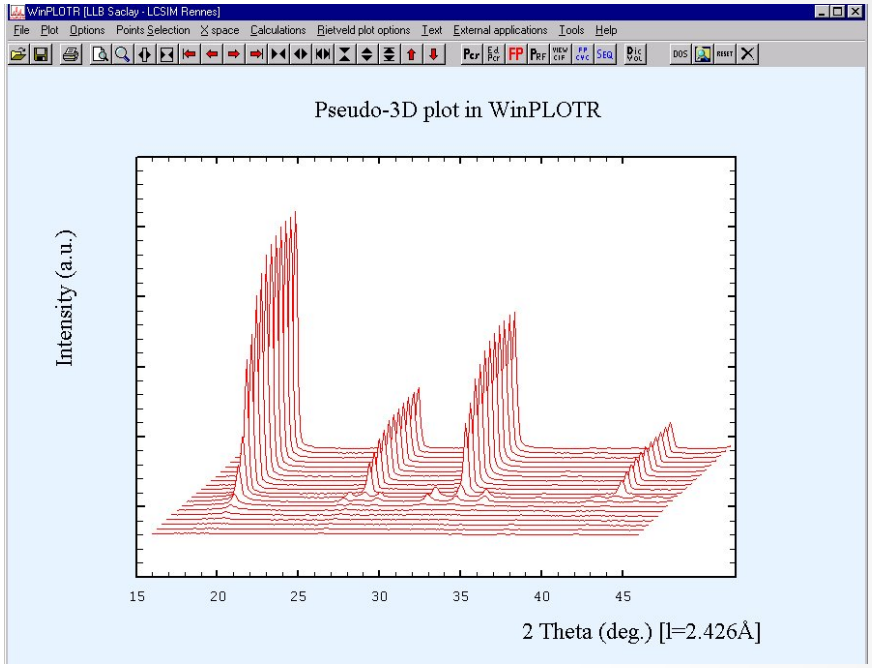
Data analysis

Be careful …



How does data analysis affect instrument design?





Rietveld refinement for powder diffraction data

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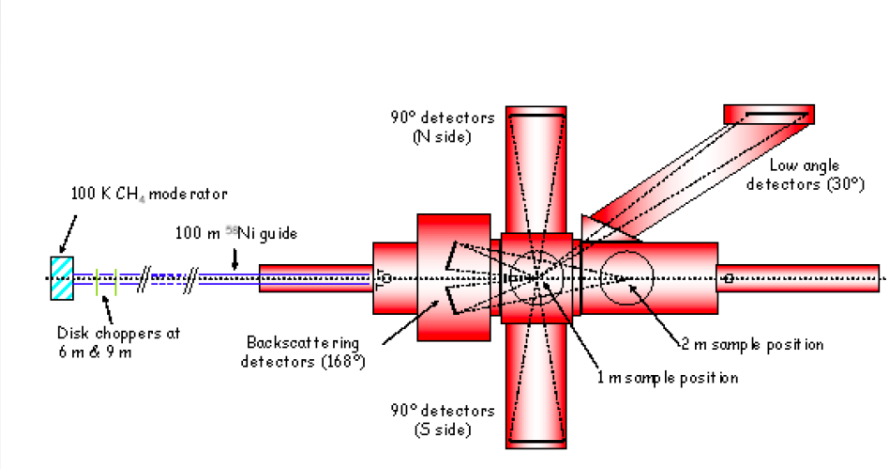

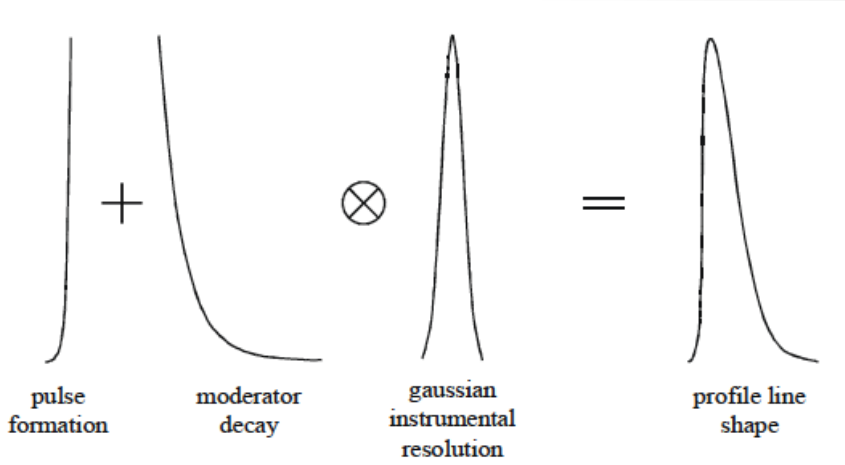

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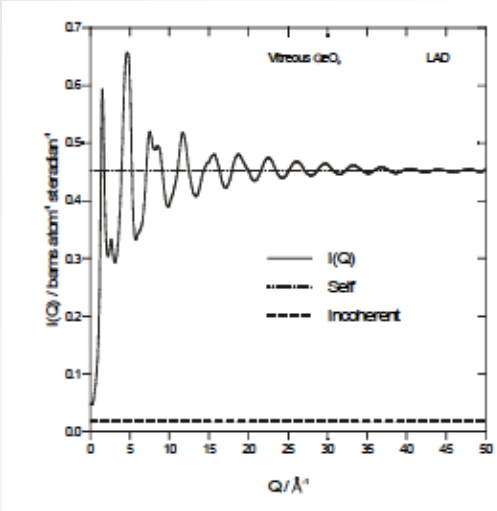
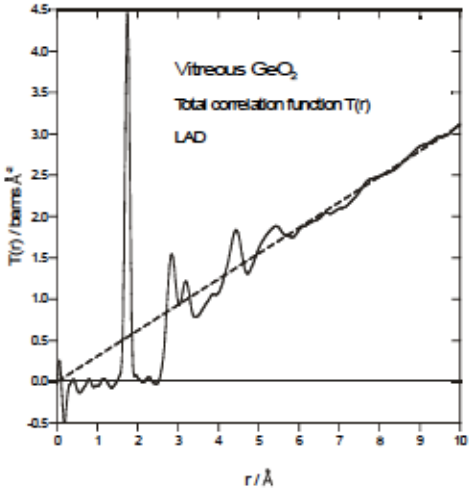
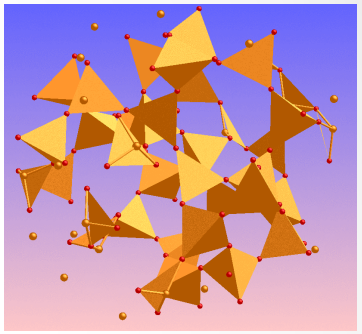


FT



model



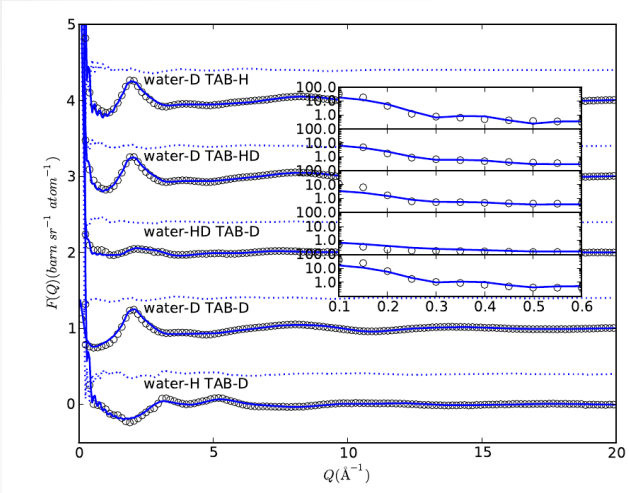
Disordered materials diffraction

Need high Q to avoid FT truncation ➔ short λ

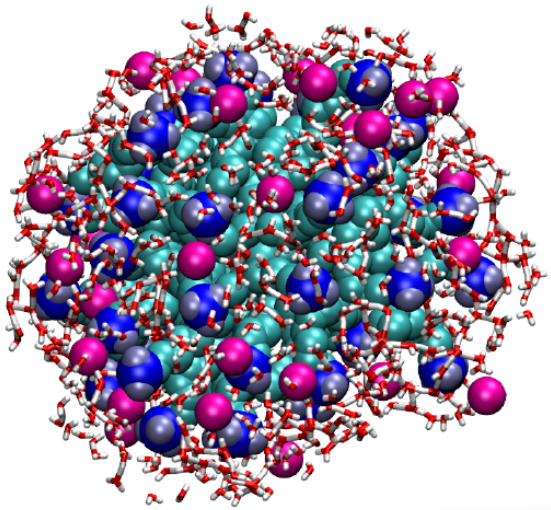
But – 'information content' of data decreases with Q

Instrumental effects lead to dephasing at high Q

How does data analysis affect instrument design?



FT



Disordered materials diffraction

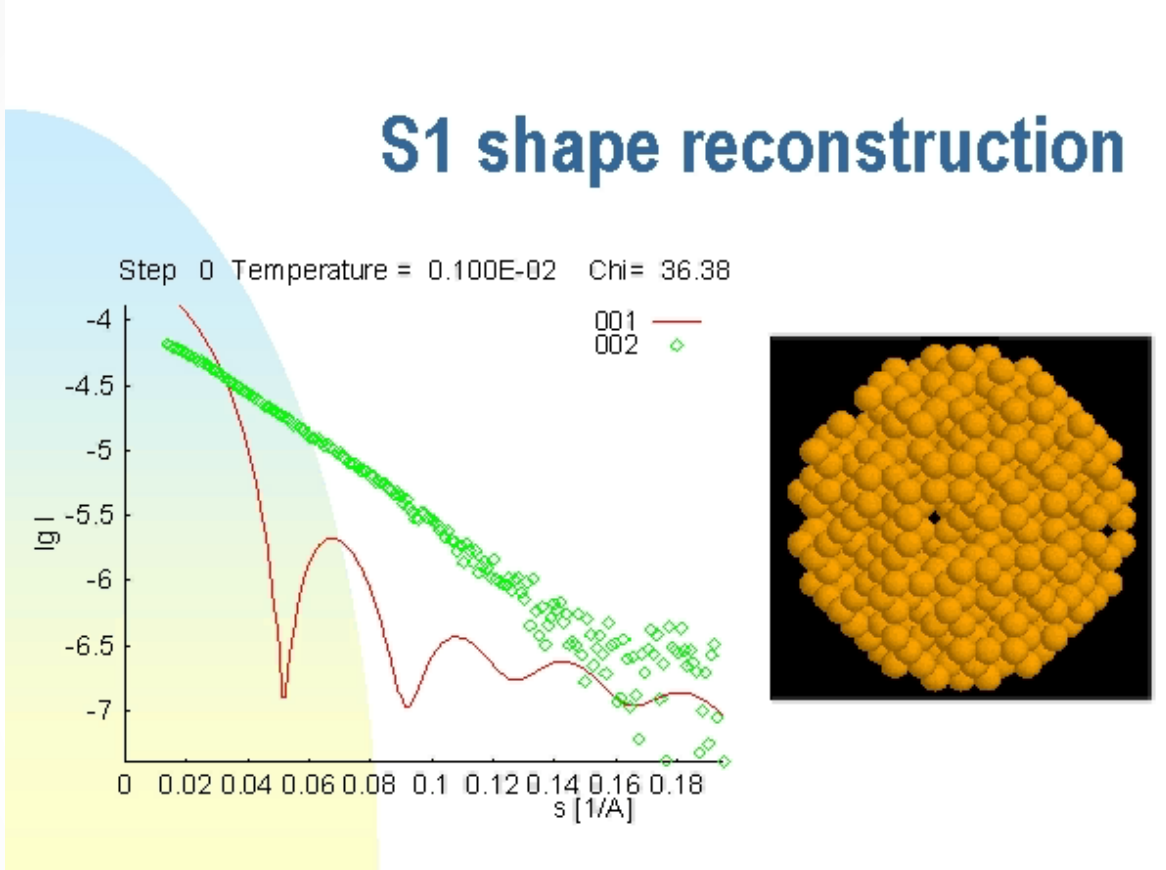
Inverse methods don't require high Q – can even cope with 'holes' in data

Can combine many data types

Resolution effects can be easily included

But – missing information is still missing information

The information content of data

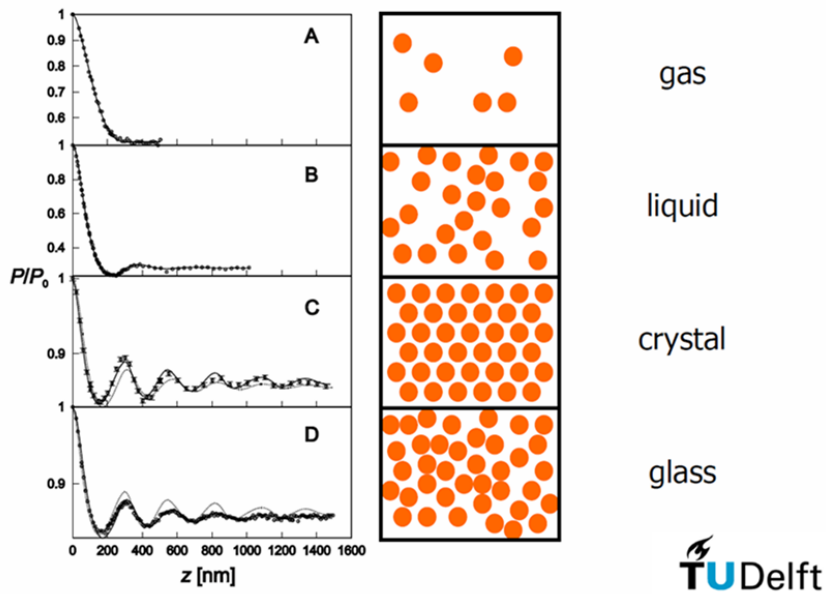


Neutron data is generally information poor – but can be precise and absolute

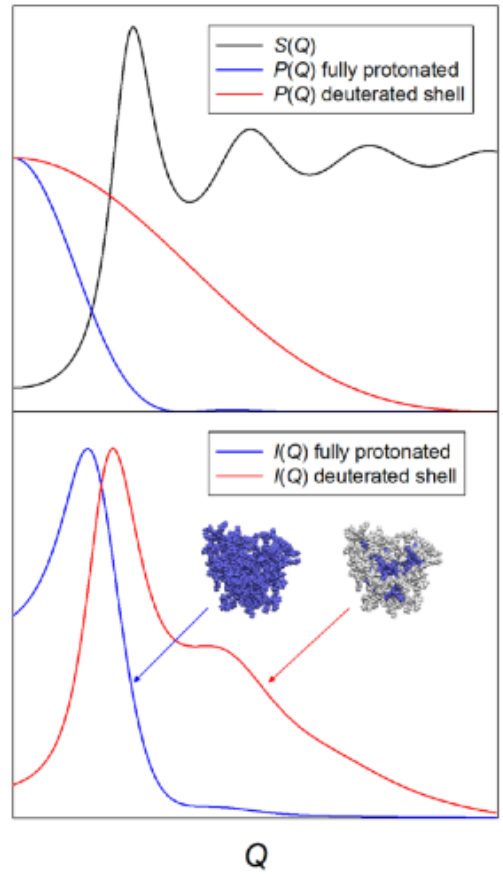
The information content of data

Wim Bouwman
http://www.tnw.tudelft.nl/en/about-faculty/departments/radiation-radionuclides-reactors/research/research-groups/npm2/research-projects/sesans/

Colloidal phase transitions as function of concentration



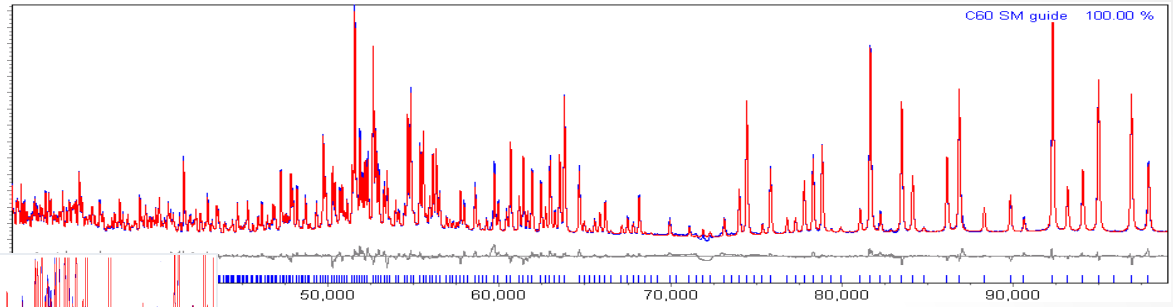
TU Delft

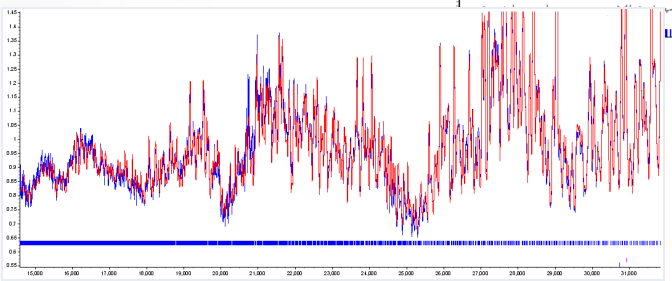


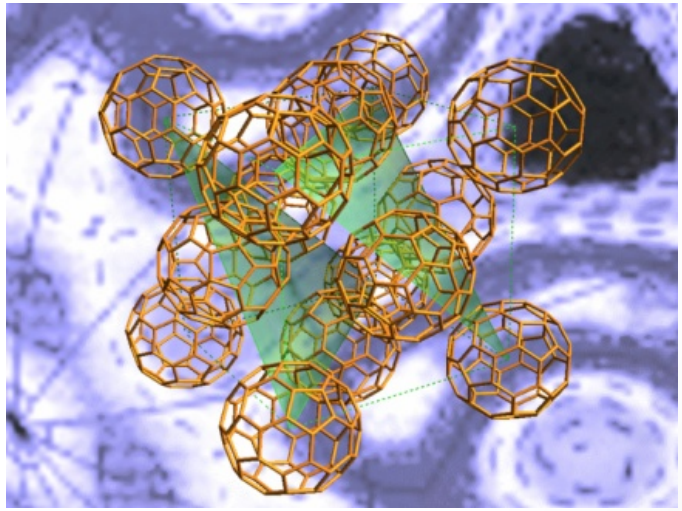
Neutron data is generally information poor – but can be precise and absolute

The information content of data

17,820 reflections to 0.3 Å







Neutron data is generally information poor – but can be precise and absolute

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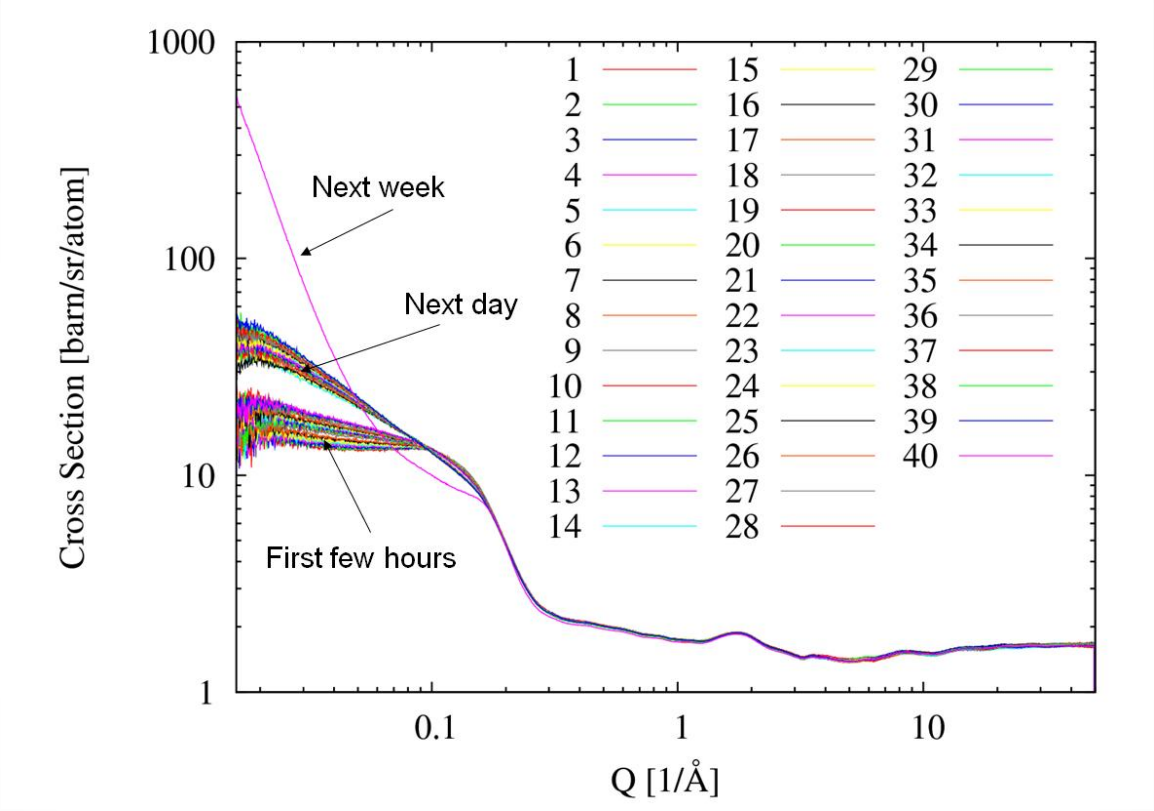
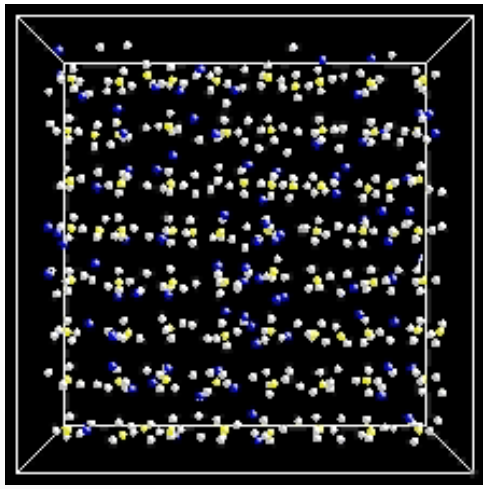
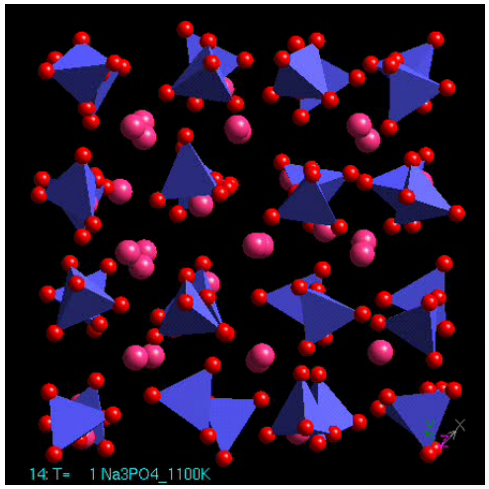


Neutron data is generally information poor – but can be precise and absolute

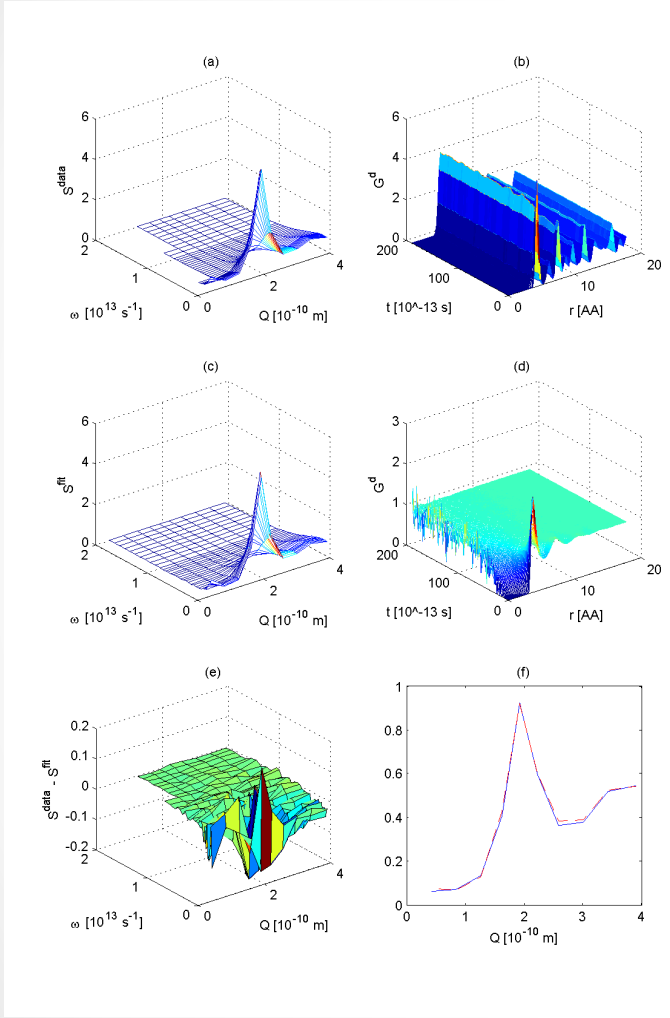
Modelling and simulation

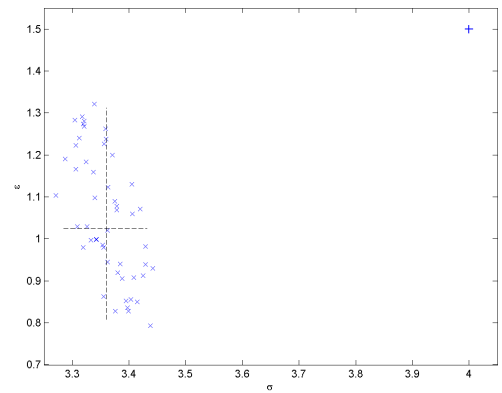
- Every neutron experiment will use some form of modelling or simulation (There is no such thing as a model free analysis)
- Models/simulations are becoming increasingly large/demanding. These virtual instruments' need to be 'supported' in the same way as a real instrument.
- We have not yet provided the ability to routinely calculate 'neutron data' from models/simulations

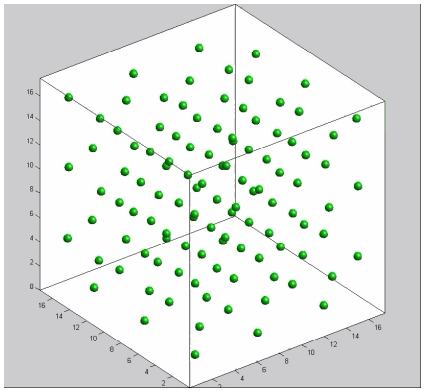


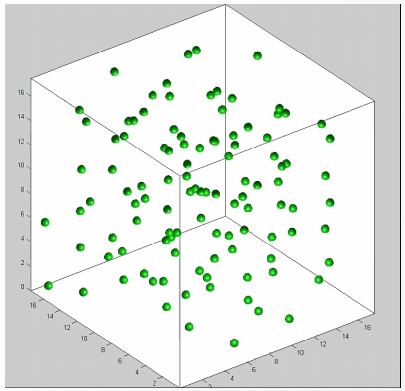


Modelling and simulation









Fully automated reduction, analysis and modelling

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ADAA: new software for intelligent instrument control

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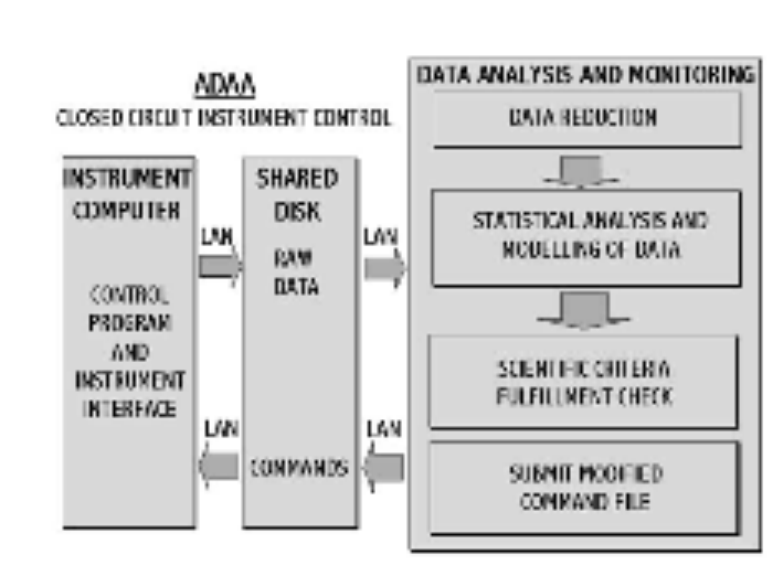
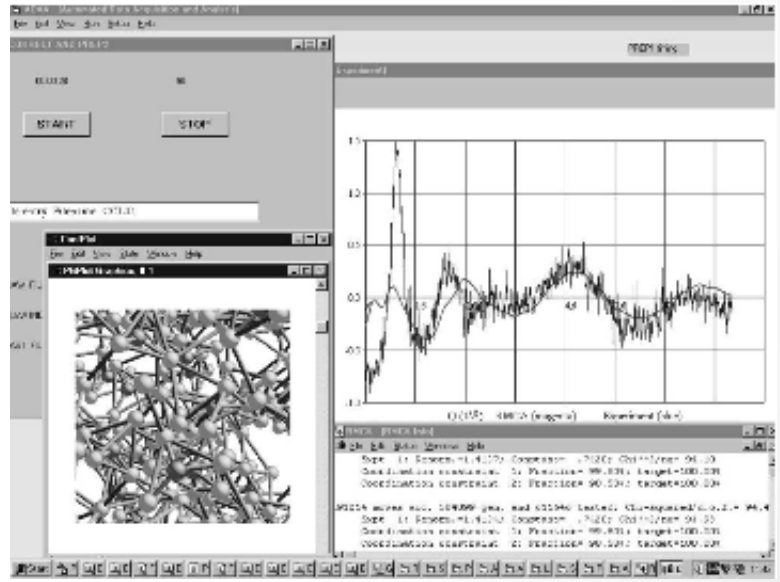
[b] ISIS Facility, CCLRC Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire OX11 0QX, UK

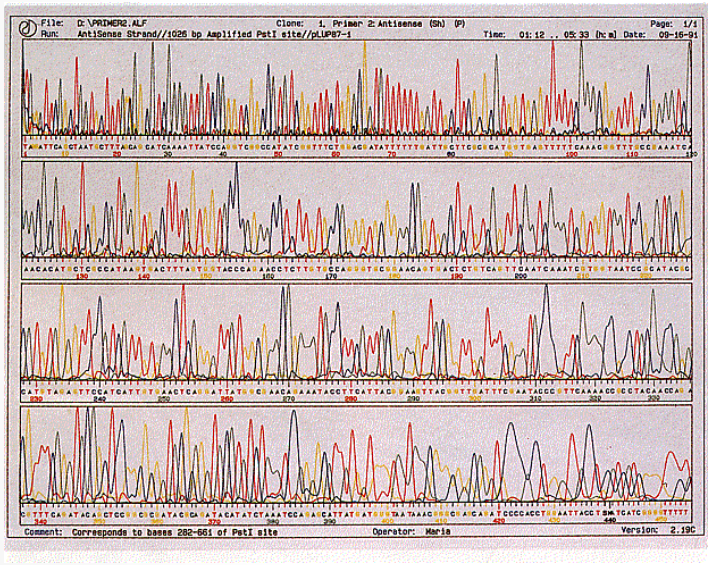


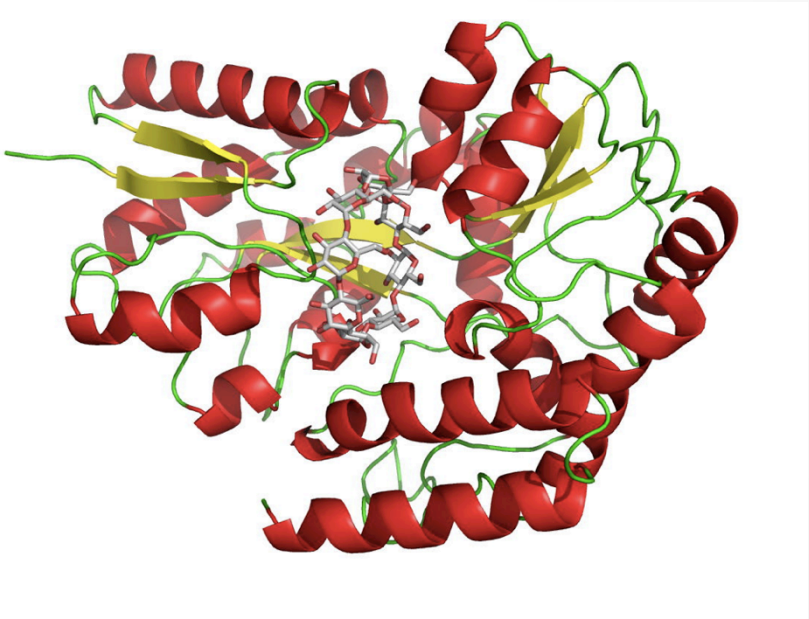


Data management: adding value to data

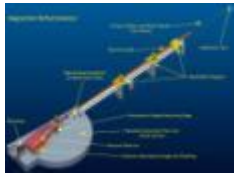
Most neutron data is only ever seen by one or two people …

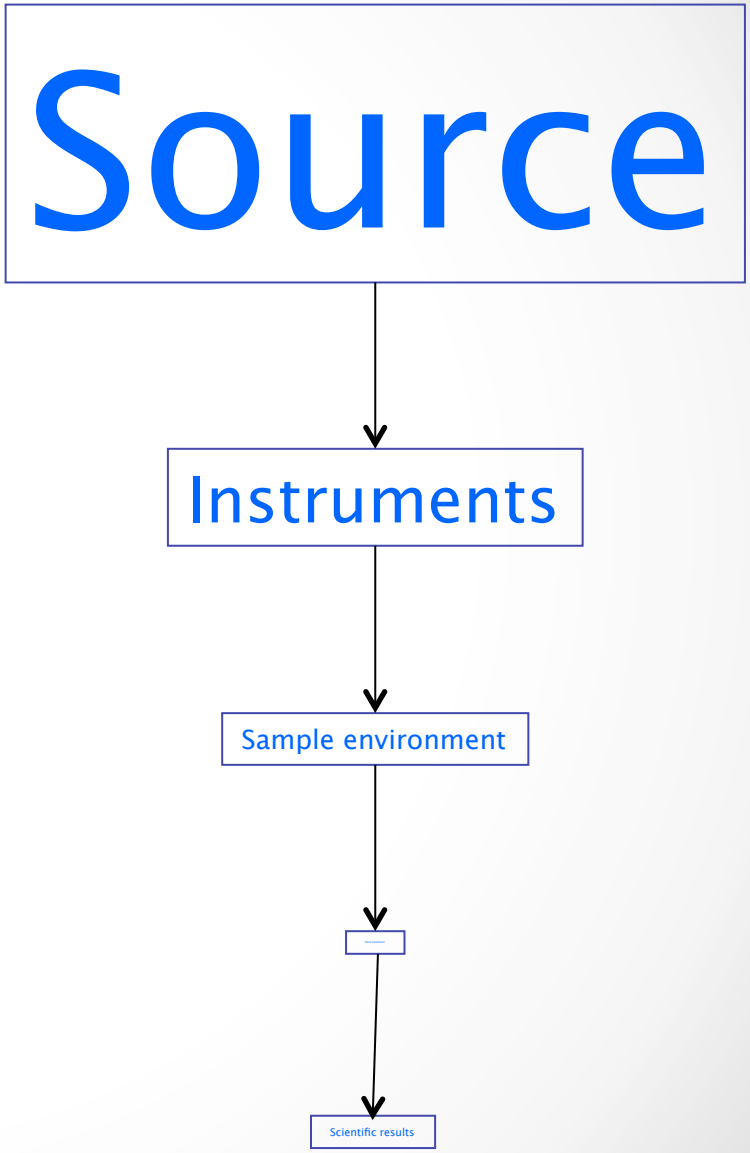
… so why do we try so hard to count every neutron?





How we spend money …





Conclusions

- There are more efficiency gains to be made in neutron scattering through improved software than through improved sources and instruments
- We don't invest enough in the 'tertiary spectrometer'
- Instrument design should consider the data - information content and analysis
- Most users are from the iPad/Youtube generation …