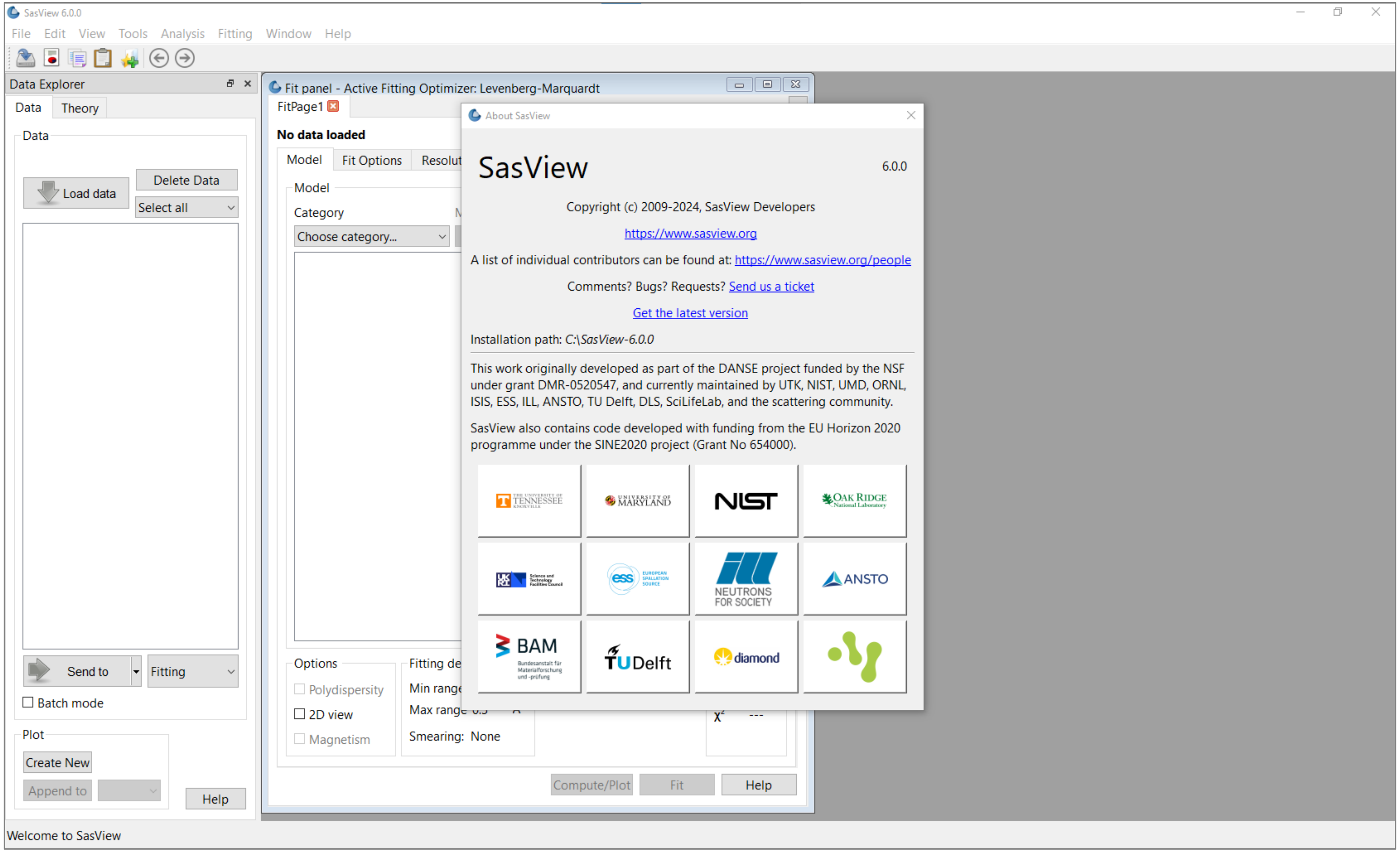
A Toolkit for Small-Angle Scattering Data Analysis

Before we start…



The plan…

Paul Butler	**Overview**	(15 min)
Steve King	**Basic Features**	(45 min)

- 1D Fitting
  - P(Q)
  - P(Q)$\times$S(Q)
  - with polydispersity
  - with resolution smearing
- Correlation Functions
- Distance Distributions

Annika Stellhorn	**Magnetic Analysis**	(10 min)
Elizabeth Kelley	**Using the Command Line**	(10 min)
Paul Butler	**Model Writing**	(35 min)

Model-Fitting

$$'\boldsymbol{I}(\boldsymbol{q})' = (\partial\Sigma/\partial\Omega)(q) = I_{q=0}\, P(q)\, S(q) + B(q)$$
$$= \Lambda\, N\, V^2\, (\rho - \rho_{matrix})^2\, P(q)\, S(q) + B(q)$$
$$= \Lambda\, \phi\, V\, (\rho - \rho_{matrix})^2\, P(q)\, S(q) + B(q)$$

SasView offers:

Form Factor

$$P(q,R)_{sphere} = 9\left[\frac{\sin(qR) - (qR)\cos(qR)}{(qR)^3}\right]^2, \quad P(q,R_g)_{debyecoil} = \frac{2\left[exp\left(-(qR_g)^2\right) + (qR_g)^2 - 1\right]}{\left[(qR_g)^2\right]^2}$$

, etc… ~90 *P(q)*

Structure Factor

$$S(q) = 1 + 4\pi N \int_0^\infty \left[(g(r) - 1)r^2 \frac{\sin(qr)}{(qr)}\right] dr; \quad where\ g(r) \propto U(r)$$

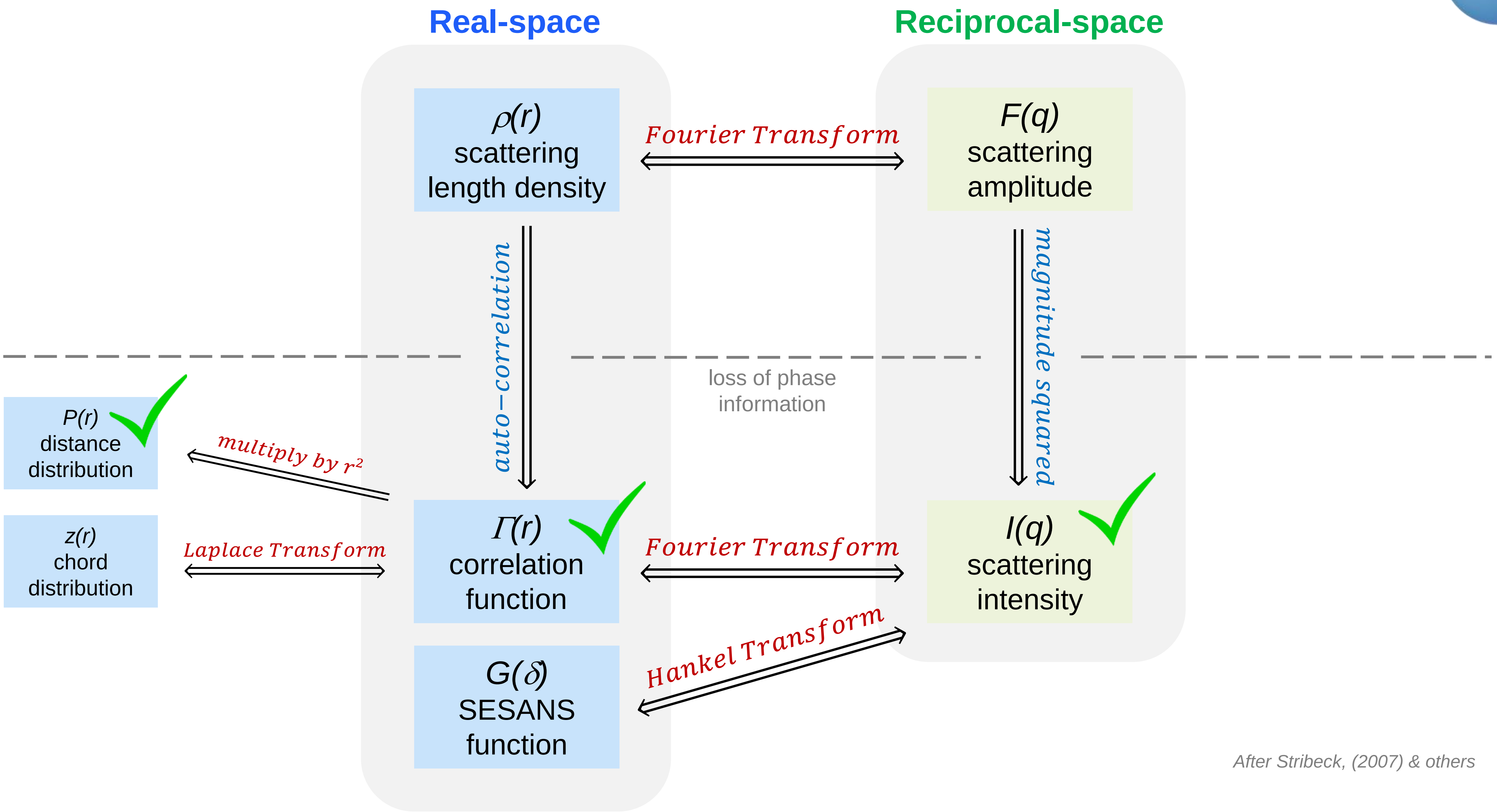
4 *S(q)*

But you can add more!

Method:

- choose a *P(q)* & *S(q)* if required
- choose a set of starting parameters
- compute *I(q)*
- compare the model calculation (theory) with the experimental data
- adjust some parameters
- iterate until an acceptable solution is found (hopefully…)

The 'Magic Square'



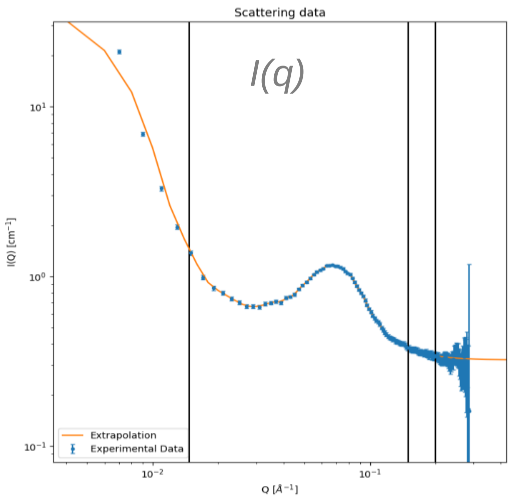
After Stribeck, (2007) & others

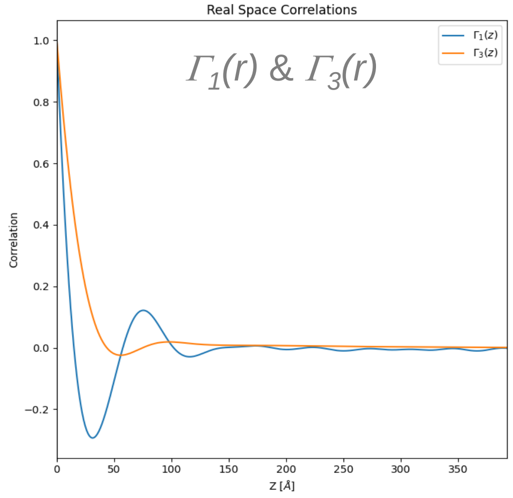
Real-Space Methods (1)

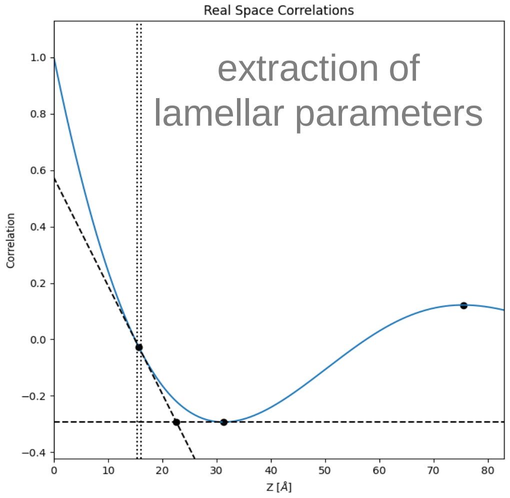
Correlation Function, $\Gamma(r)$

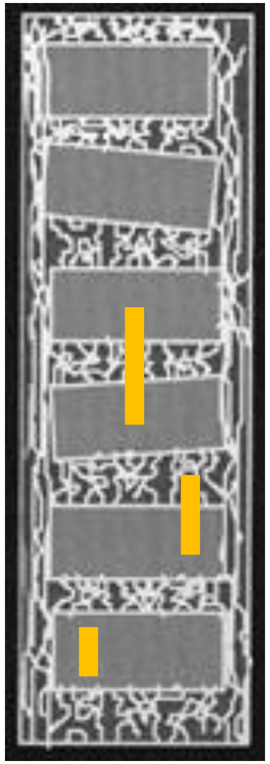
- **describes spatial inhomogeneity in SLD in the sample**
  - in essence, the probability that rods of different lengths moving through the sample have equal SLD at either end

1D: $\Gamma_1(r) = \frac{2}{Q^*}\int_0^{\infty} I(q)\cos(2\pi q r)\,dq$ 3D: $\Gamma_3(r) = \int_0^{r_{max}} \frac{\Gamma_1(r)}{r}\,dr$









Rieger, (2002)

***SasView* computes $\Gamma_1(r)$ & $\Gamma_3(r)$ + IDF**

Real-Space Methods (2)

- **few analytical expressions for *Γ(r)***
  - homogeneous sphere: (radius, *R*)

$$\Gamma(r) = 1 + \frac{3}{4}\frac{r}{R} + \frac{1}{16}\left(\frac{r}{R}\right)^3$$

where $0 \le (r/R) \le 2$
see Glatter & Kratky, (1982)

  - **randomly-distributed 2-phase system**: (*single* correlation length, ξ)

$$\Gamma(r) = exp\left(-\frac{r}{\xi}\right)$$

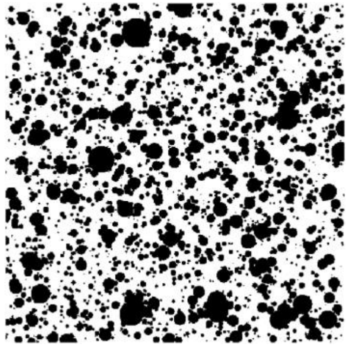
Debye & Bueche, (1949)
Debye, Anderson & Brumberger (1957)

$$I(q) = 8\pi\phi(1-\phi)(\Delta\rho)^2 \frac{\xi^3}{[1+(q\xi)^2]^2}$$

  - randomly-distributed 2-phase system: (*dual* correlation lengths, ξ & Ξ)

$$\Gamma(r) = f\ exp\left(-\frac{r}{\xi}\right) + (1-f)\ exp\left(-\frac{r^2}{\Xi^2}\right)$$

Debye, Anderson & Brumberger (1957)



$$I(q) = f\ K_1 \frac{\xi^3}{[1+(q\xi)^2]^2} + (1-f)\ K_2\, \Xi^3\ exp\left[-\frac{(q\Xi)^2}{4}\right]$$

$$K_1 = 8\pi\phi(1-\phi)(\Delta\rho)^2$$
$$K_2 = \pi^{3/2}\phi(1-\phi)(\Delta\rho)^2$$

Moritani *et al*, (1970)

Real-Space Methods (3)

(Pair) Distance Distribution Function, *P(r)*

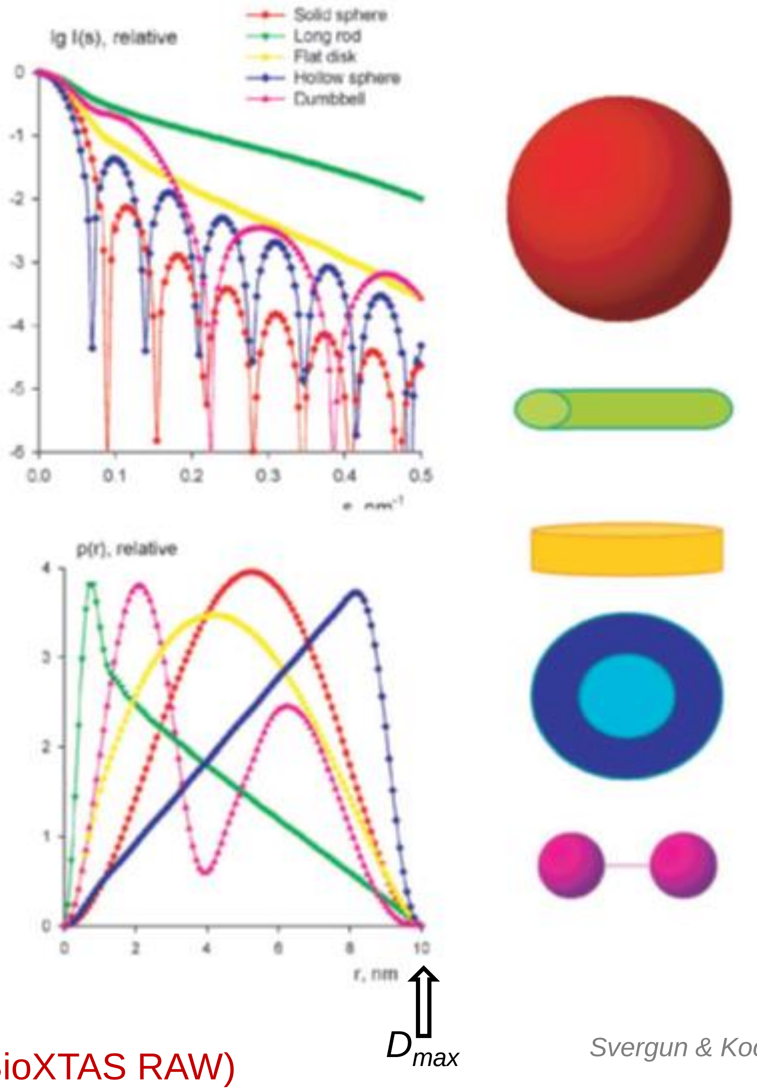
- in essence, a **histogram of pair-wise distances** between atoms in the scatterer

$$P(r) = \frac{r^2}{2\pi^2}\int_0^\infty q^2 I(q)\frac{sin(qr)}{qr}dq$$

- solve set of basis functions by *Indirect* Fourier Transformation (IFT)
- Glatter, (1977); Moore, (1980); Hansen & Pedersen, (1991)

- ***SasView* implements the Moore method**

$$I_{q=0} = 4\pi\int_0^{D_{max}} P(r)dr \ \propto \ M_z \qquad R_g^2 = \frac{\int_0^{D_{max}} r^2 P(r)dr}{2\int_0^{D_{max}} P(r)dr}$$



Svergun & Koch, (2003)

Other implementations:
GIFT (from Glatter); *GNOM* (in ATSAS Suite); *BIFT* (in BioXTAS RAW)

The master plan…

- Overview of features and new in 6.0 (10-15 min) **PAUL**
  - Slides general overview of layout and where to find things … ethos of project? Points of contact at facilities, contributor list, contacts at SAS2024. Put stickers on “badges”
  - Maybe preview of future features to come (beyond 6.0)
  - Where to find help
- Overview of using basic features (45 min) **STEVE**
  - 1d fit simple (polymer Gaussian coil)
  - 1d with structure factor (SDS data)
  - Fit with polydispersity
  - Impact of resolution smearing
  - Correlation function
  - P(R) of protein – Apoferritin .. and maybe sphere and rod?
  - BONUS if time permits
    - add/multiply used in response to question
- 10 min coffee
- Note on magnetic/pol beam stuff 10 min **ANNIKA**
- Brief look at CLI (quick demo of Caitlyn Wolf stuff?) (10 min) **LIZ**
- Model writing (35 min) **PAUL**
  - Different API (add/multiply and reparam)
  - Use sphere and have equations ready on on board – also in back .. how about a handout. Could point to tutorials and send pdf handout
  - Step through
    - Easy editor and “hand write” all equations including bessel NO polydisperse parameters
    - Use scipy functions
    - Use library functions
    - Make polydisperse → point out the need to move 1/V out of the equation and use form_volume. Difference between z average (volume average) and number average
    - Make possible to use structure factor
    - Move to C
    - Add beta approximation (have_fq=true)
    - What if it IS a structure factor?