Incorporation of the Beta Approximation in SasView

August 8, 2018

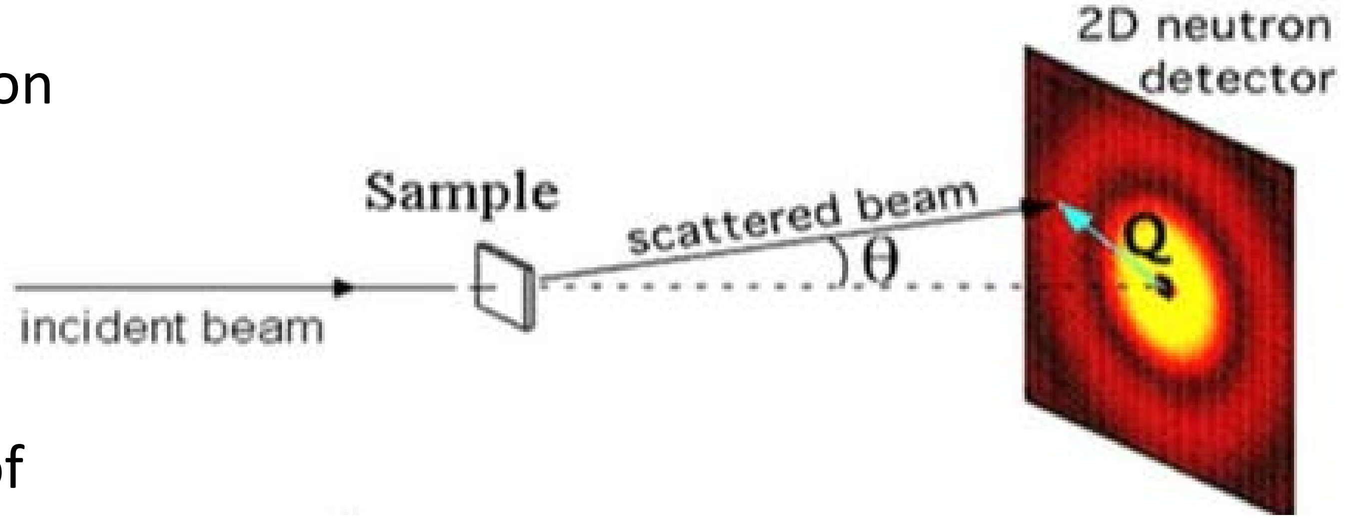
Greg Suczewski
Summer Undergraduate Research Fellowship (SURF)
Middlebury College Class of 2020

Paul Kienzle and Yun Liu
National Institute of Standards and Technology (NIST)
NIST Center for Neutron Research (NCNR)

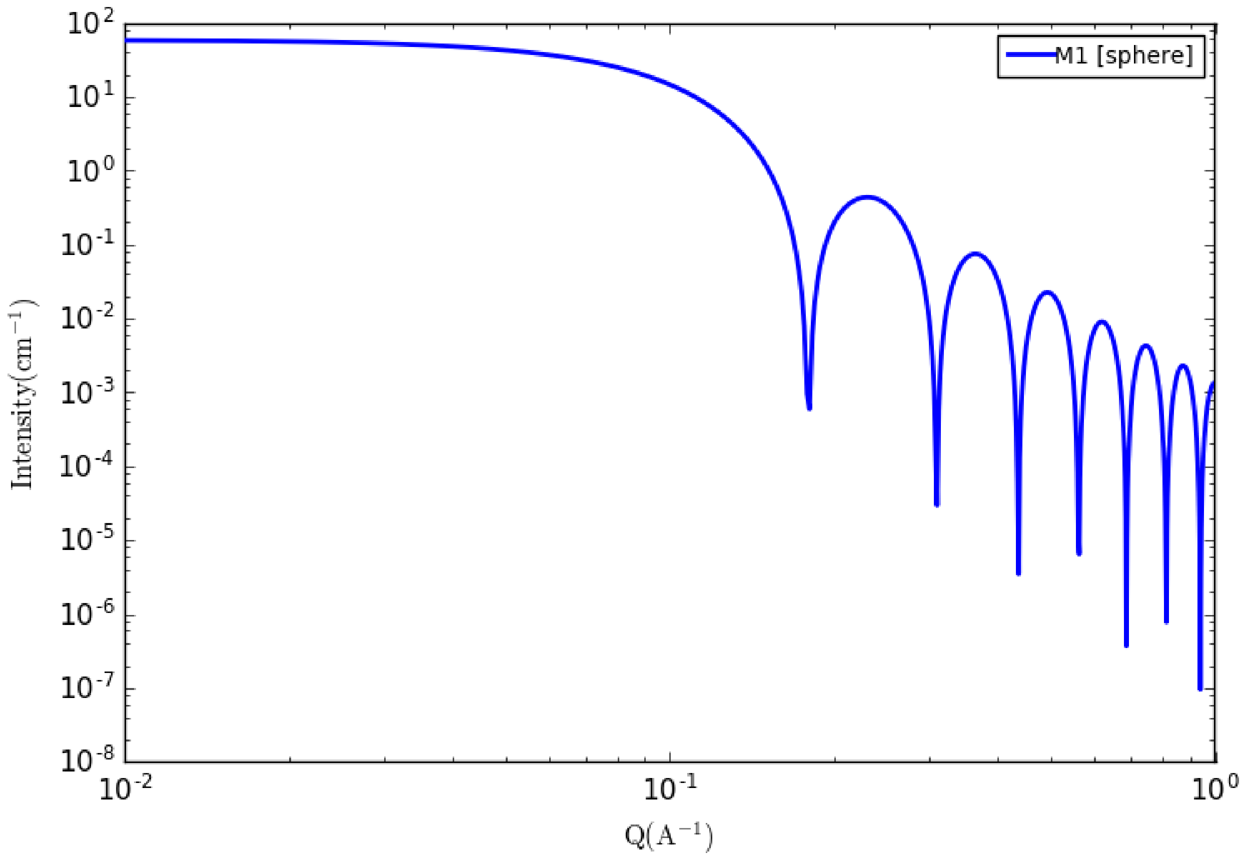
What is Small Angle Neutron Scattering?

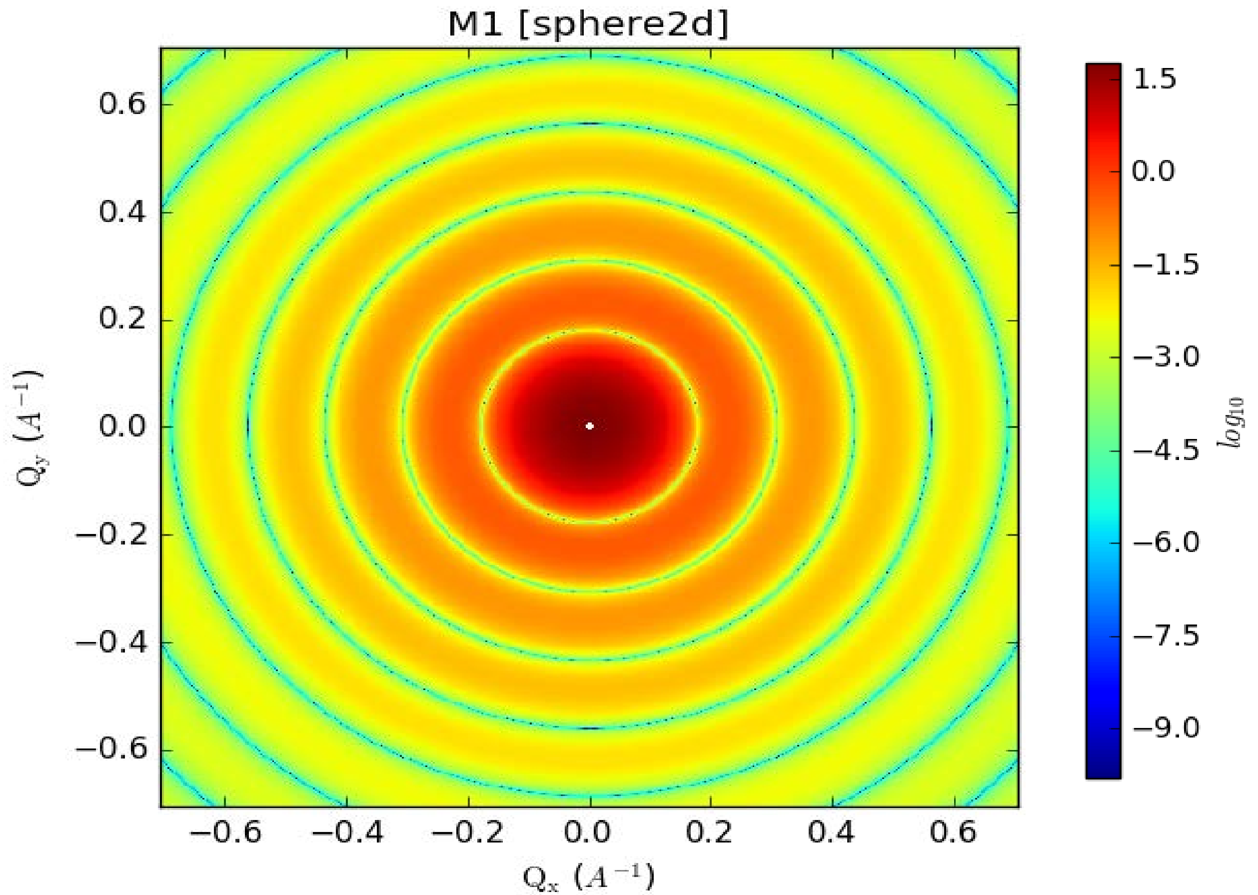
Steps:

1. Produce free neutrons (nuclear fission with ^{235}U)
2. Select speed of neutrons and direct beam towards sample
3. Neutrons diffract through sample
   - Interactions are with the nuclei of sample
   - Scatters neutrons at different angles
4. Neutrons are recorded by a detector

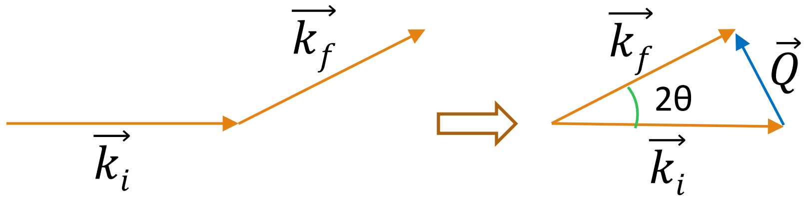


Gallego, Nidia & Burchell, Timothy & He, Lilin & Kirkham, Melanie & Contescu, Cristian. (2016). Neutron Irradiation Effects on the Structure of Highly Oriented Graphite: A XRD and SANS Study.





Elastic (no energy loss):



$\overrightarrow{k_i}$: incident wavevector

$\overrightarrow{k_f}$: scattered wavevector

$\vec{Q}$: scattering vector

$$\vec{Q} = \overrightarrow{k_f} - \overrightarrow{k_i}\ , \quad |\overrightarrow{k_f}| = |\overrightarrow{k_i}| = \mathrm{k} = \frac{2\pi}{\lambda}, \quad 1 - \cos 2\theta = 2\sin^2\theta$$

$$=> \ Q = \sqrt{(\overrightarrow{k_f} - \overrightarrow{k_i}) \cdot (\overrightarrow{k_f} - \overrightarrow{k_i})}$$

$$= \sqrt{k_f{}^2 + k_i{}^2 - 2k_i k_f \cos 2\theta}$$

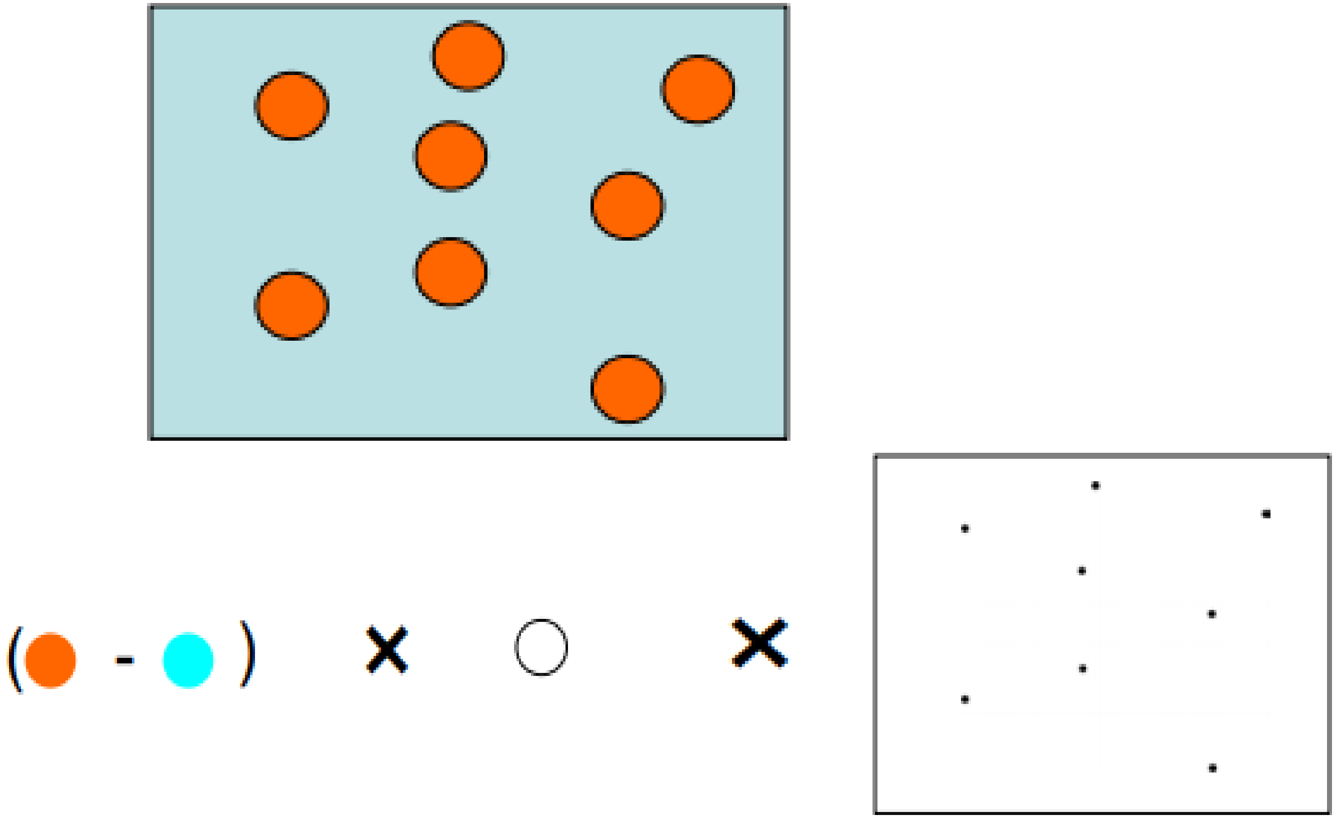
$$= k\sqrt{2(1 - \cos 2\theta)} = \boxed{\frac{4\pi}{\lambda}\sin\theta}$$

SasView is a program used worldwide that simulates intensity patterns and fits experimental data

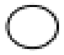
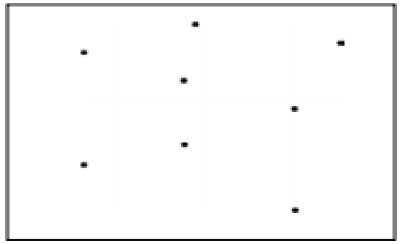
http://freesongs.us

The scattering patterns are determined by the properties and characteristics of the sample

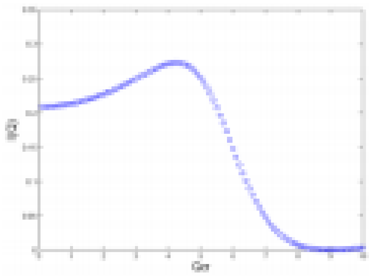
I(Q) :

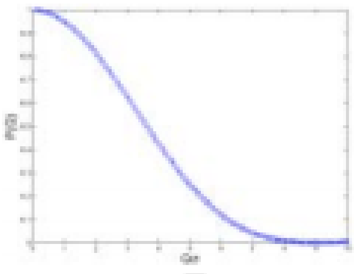


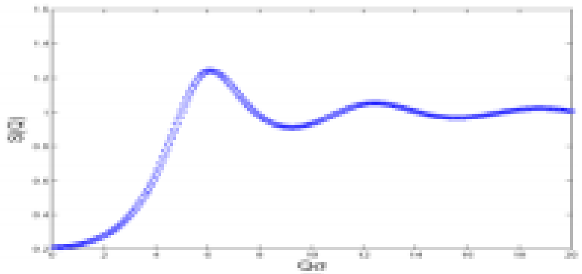
Liu, Yun. Static scattering techniques (SLS, SAXS, and SANS) – theories and applications.

I(Q) : () ×  × 

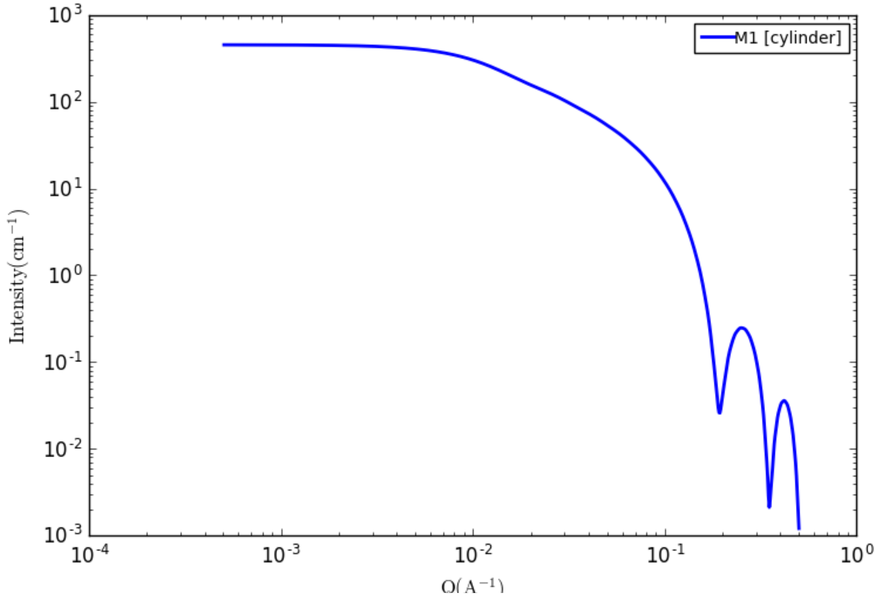
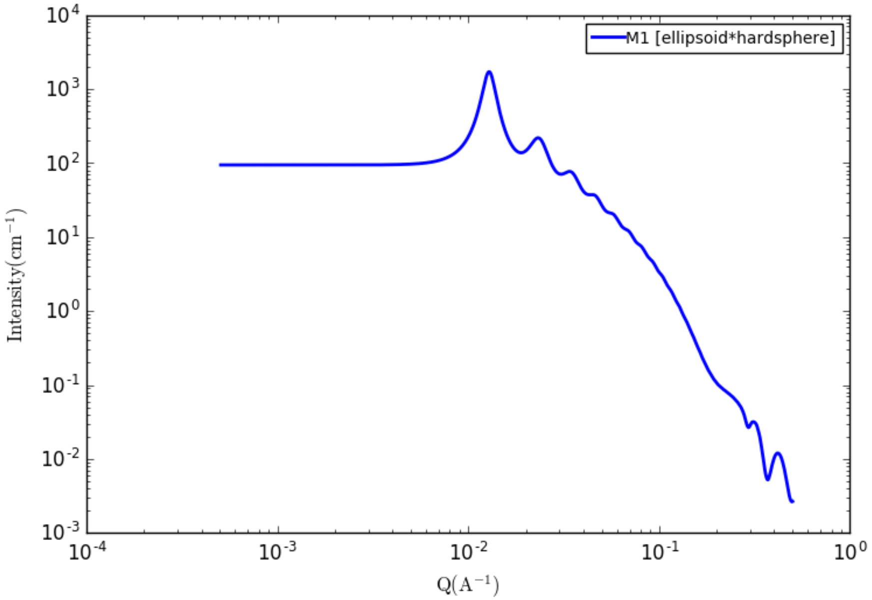
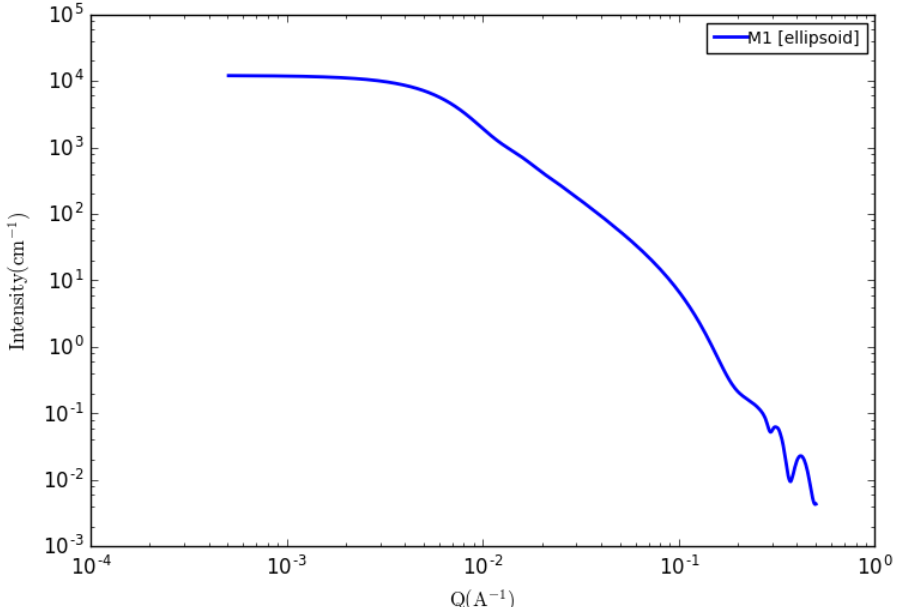
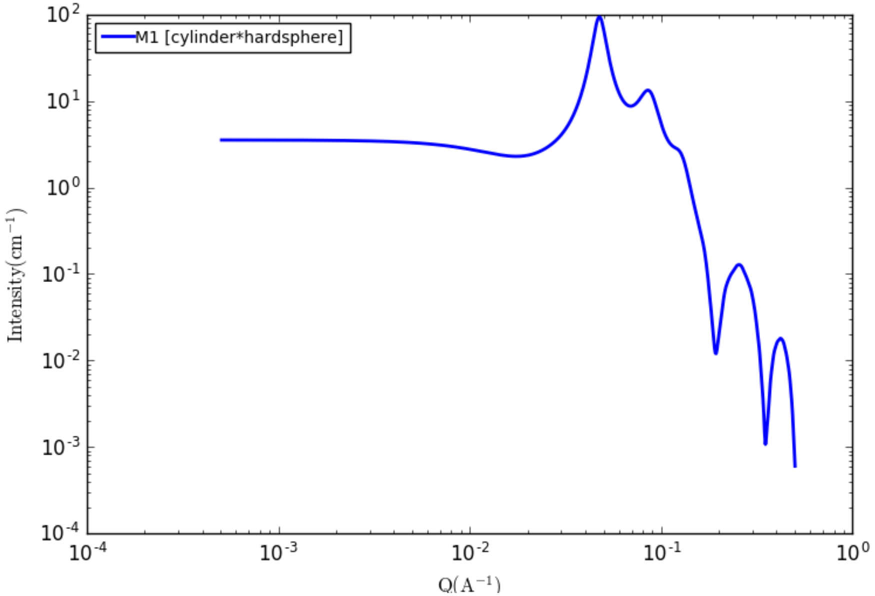
I(Q) = A × P(Q) × S(Q)







Liu, Yun. Static scattering techniques (SLS, SAXS, and SANS) – theories and applications.

	S(Q) = 1	S(Q) = Hardsphere
Cylinder:		
Ellipsoid:		

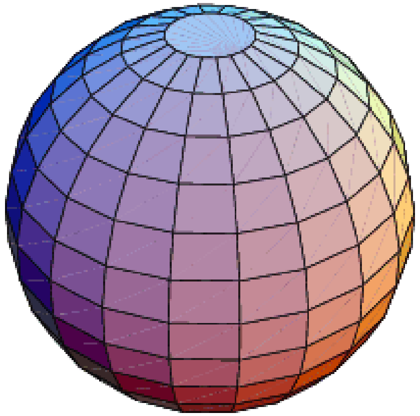
Simulating Intensity Patterns

Dilute Case (without structure factor):

$$\mathrm{I(Q)} = \mathrm{P(Q)}$$

P(Q) = F^2(Q) where F(Q) is dependent on the shape of the constituents

ex. Sphere: $$\mathrm{F(Q)} = \left[V\Delta\rho\, 3\,\frac{\sin(qr) - qrcos(qr)}{(qr)^3}\right]$$



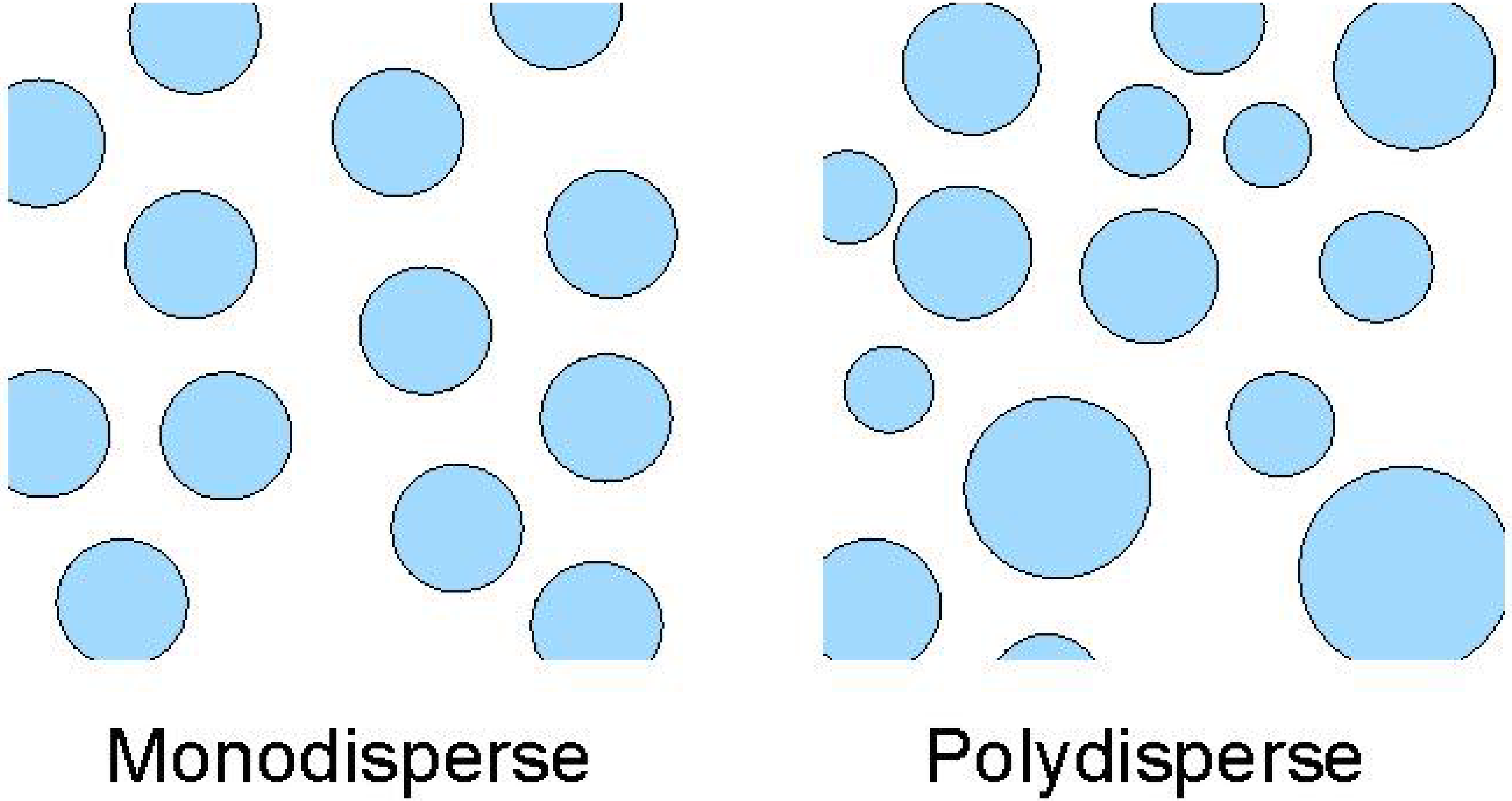
http://mathworld.wolfram.com/Sphere.html

Not Dilute (with structure factor):

$$\mathrm{I(Q)} = \mathrm{P(Q)S(Q)}$$

ex. Hardsphere, sticky hardsphere, hayter-penfold model

WHAT IF THERE IS POLYDISPERSITY?

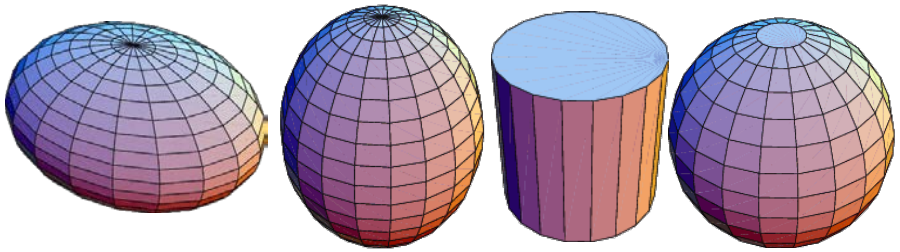


Existing code

VS.

Dense colloids

-

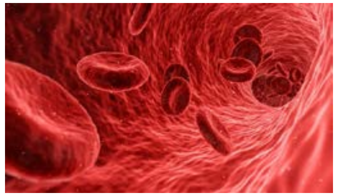


mathworld.wolfram.com

- DILUTE samples with POLYDISPERSE particle size and orientation
  - i.e. $I(Q) = \langle P(Q) \rangle$

- DENSE samples with MONODISPERSE particle size and orientation
  - i.e. $I(Q) = P(Q)\, S(Q)$

-



scienceabc.com

https://en.wikipedia.org/wiki/Milk

Nymag.com

adamkempfitness.com

-DENSE colloids with POLYDISPERSE particle size and shape

How can we study these materials more accurately?

BETA APPROXIMATION

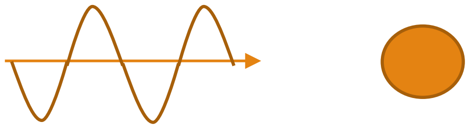
(Not currently implemented in SasView)

$$I(Q) = \langle P(Q) \rangle S_{eff}(Q)$$

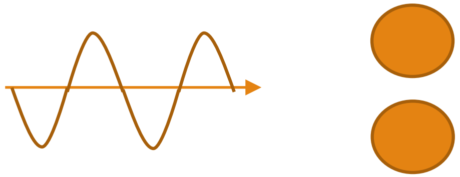
$$= \langle F^2 \rangle \left[1 + \frac{\langle F \rangle^2}{\langle F^2 \rangle} (S(Q) - 1) \right]$$

$$= \langle F^2 \rangle + \langle F \rangle^2 (S(Q) - 1)$$

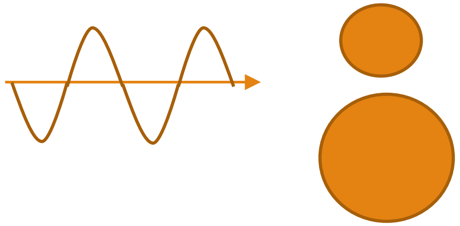
$$I(Q) = P(Q)$$



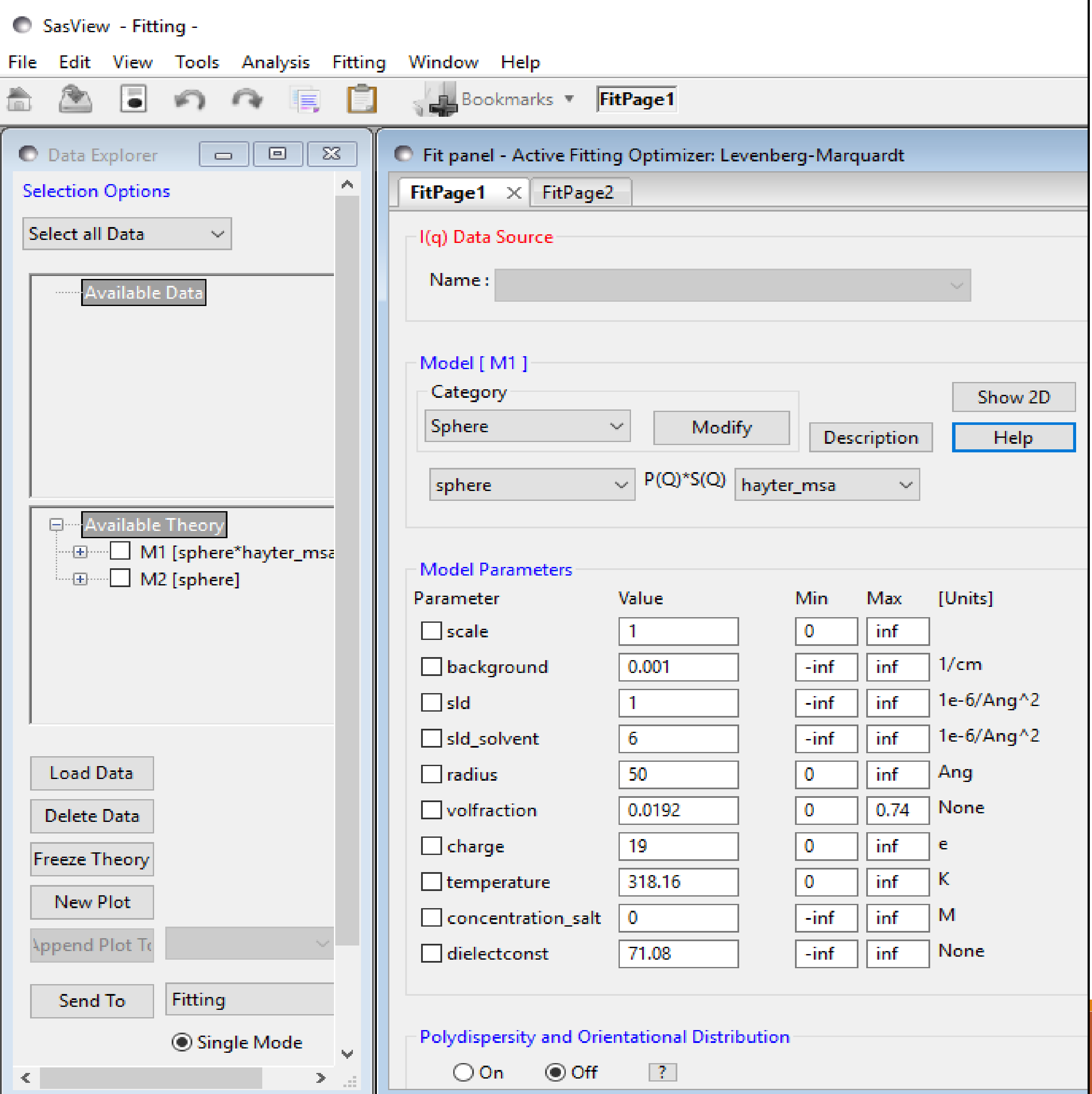
$$I(Q) = P(Q)S(Q)$$



$$I(Q) = \langle P(Q) \rangle S_{eff}(Q)$$

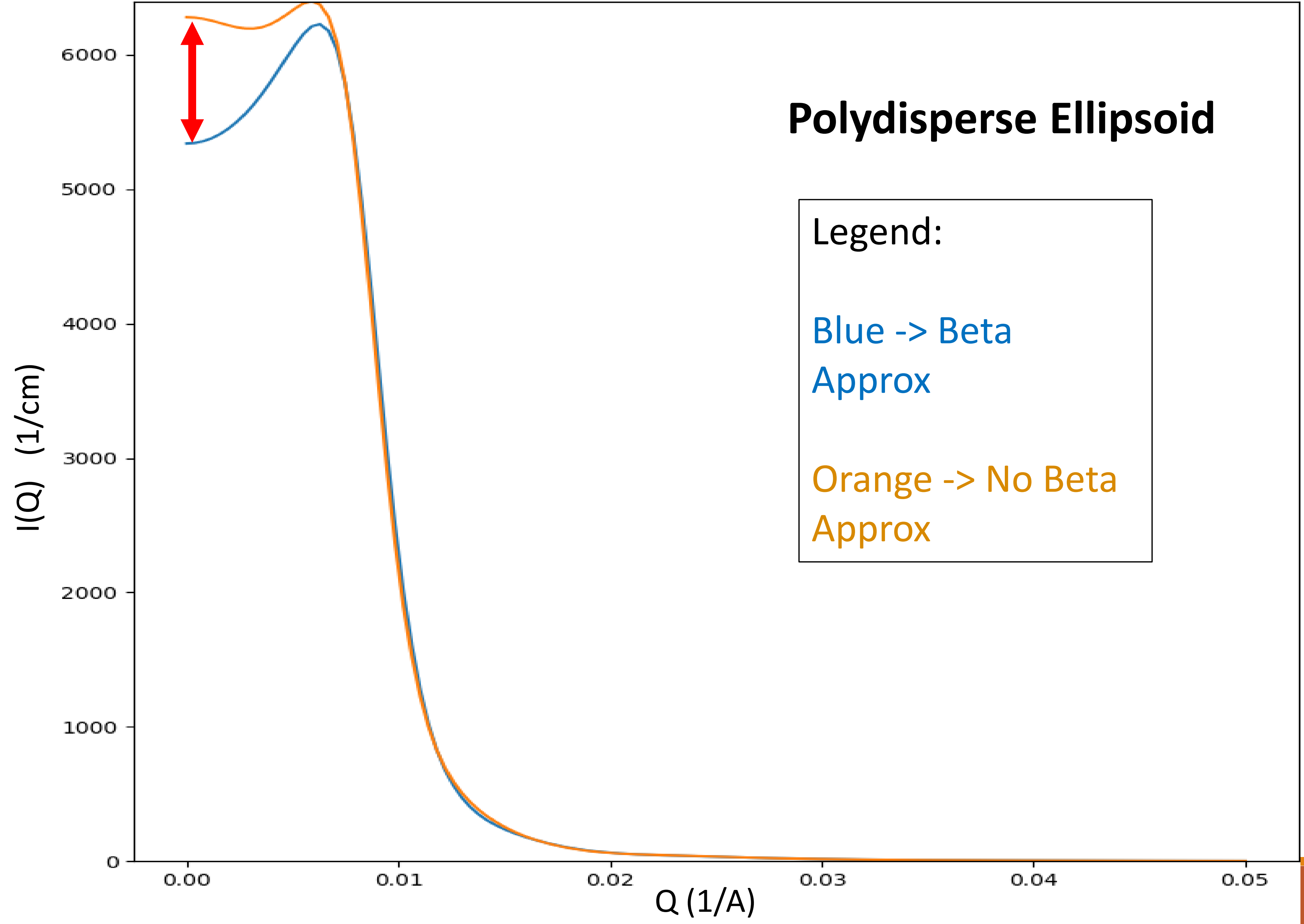


Graphical User Interface

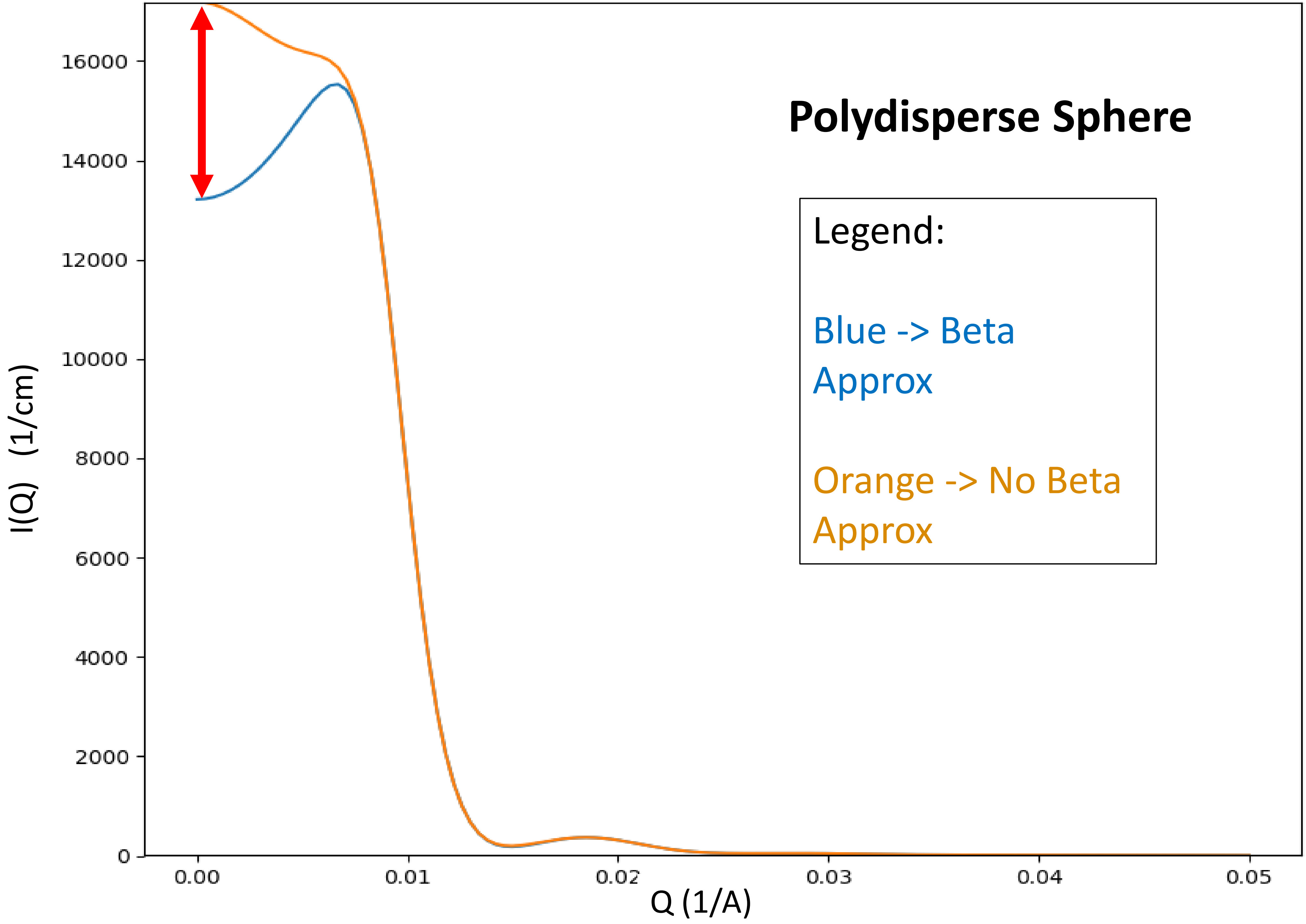


Simulating Engine

- Build mathematical tools
- Introduce additional parameters
  - Effective radius
  - Beta vs. non-beta
- Easily expandable
- 3 computational engines
  - GPU
  - DLL
  - Pure python
- Update individual models
- Crosschecking

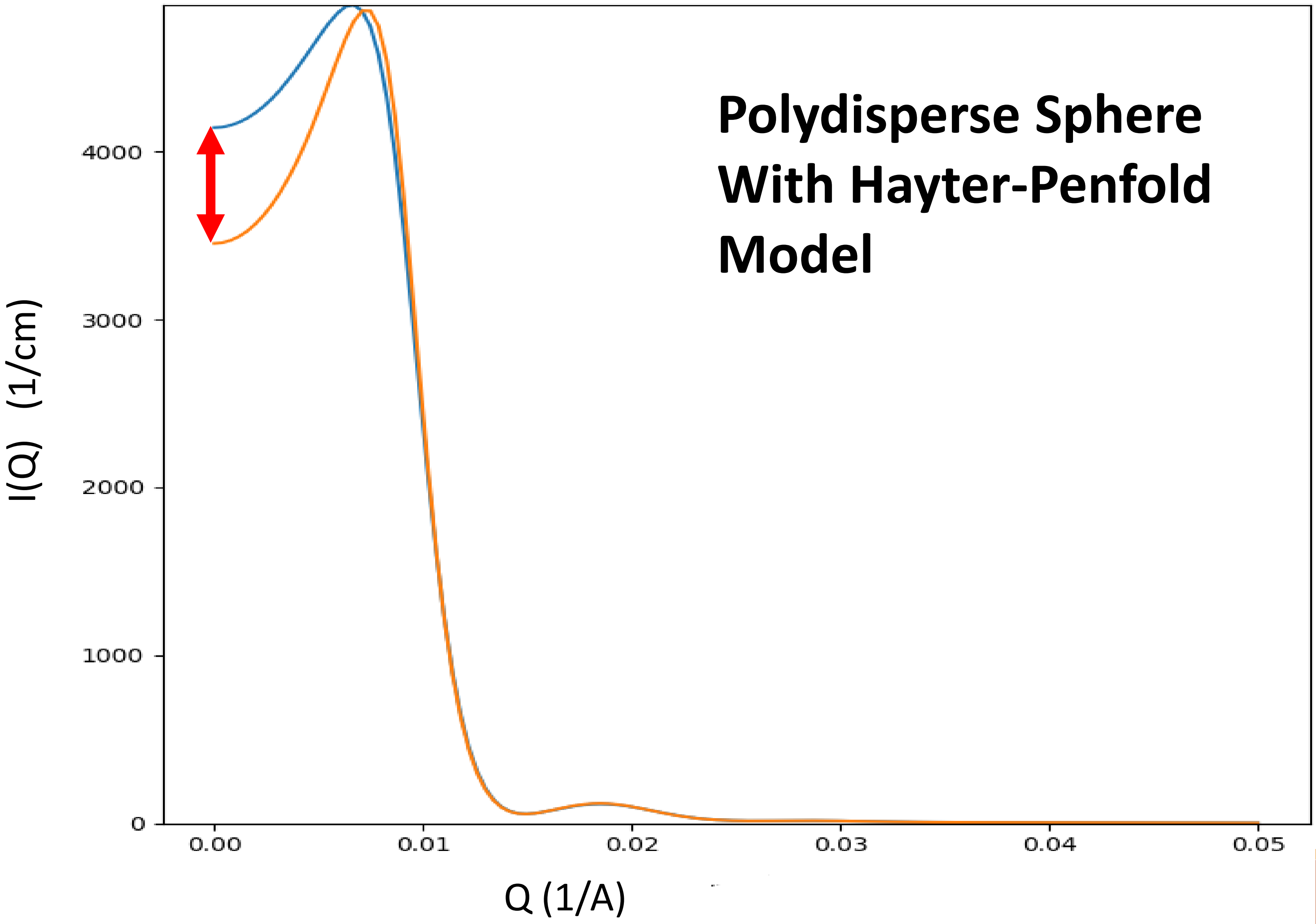


Max Relative Difference: 15%



Max Relative Difference: 23.1%

To see the importance of these differences, we can look at how much intensity patterns change as we adjust their parameters.

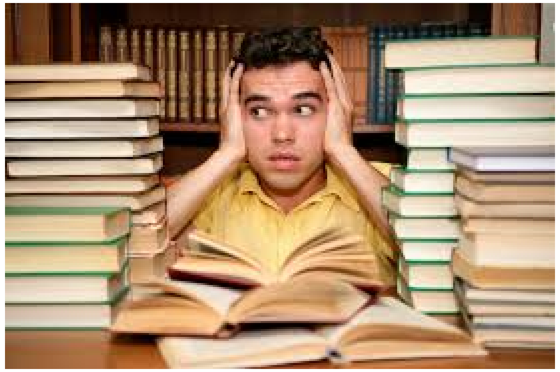


Max Relative Difference: 20%

Legend:
Blue -> charge = 10 e
Orange -> charge = 200 e

CHALLENGES

ec.europa.eu



https://www.theodysseyonline.com/30-thoughts-college-students-have-while-studying

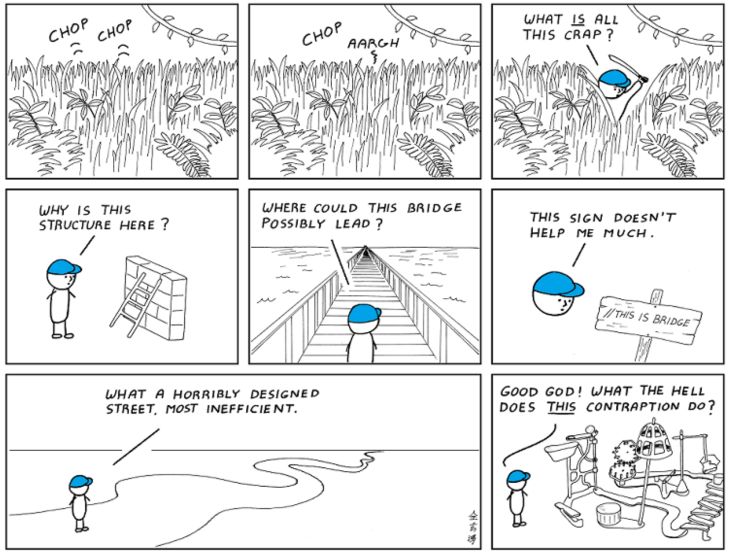
C

Programming

http://www.circuitbasics.com/how-to-write-and-run-a-c-program-on-the-raspberry-pi/

python™

http://blog.klocwork.com/general-coding/python-coding-tips-1-with-statements/



I hate reading other people's code.

https://twitter.com/mariofusco/status/603894311177035776

Future work

NUMERICAL INTEGRATION

-improving Legendre-Gaussian quadrature

-implementing Romberg integration

ADDING STRUCTURE FACTORS

- local monodisperse approximation

- partial structure factor

-scaling approximation of partial structure factor

Acknowledgements

- Paul Kienzle
- Yun Liu
- Paul Butler
- Torin Cooper, Steve King, Richard Heenan (ISIS)
- Julie Borchers, Joe Dura, and Brandi Toliver
- NIST/NCNR
- SURFers
- Center for High Resolution Neutron Scattering