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Live Neutron Data Analysis
LiNDA

Sine2020

PSI meeting April 4th and 5th 2016

Static data analysis

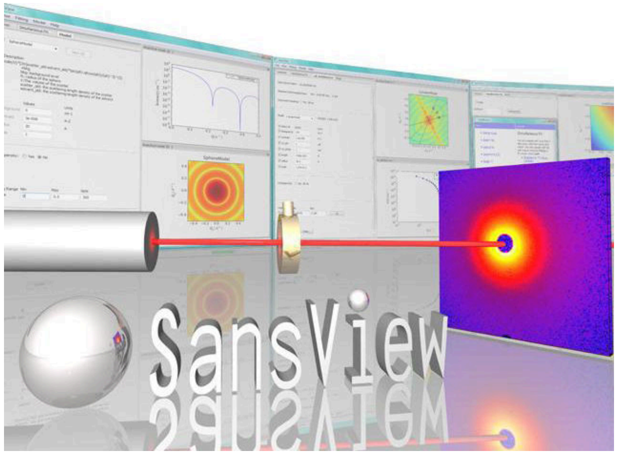
- Data analysis often performed after the experimental run

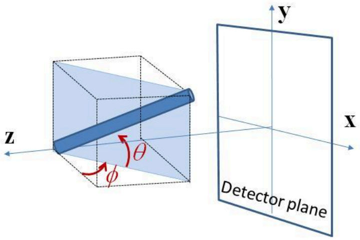
- Could it be possible to do a full data analysis during an experimental run ?

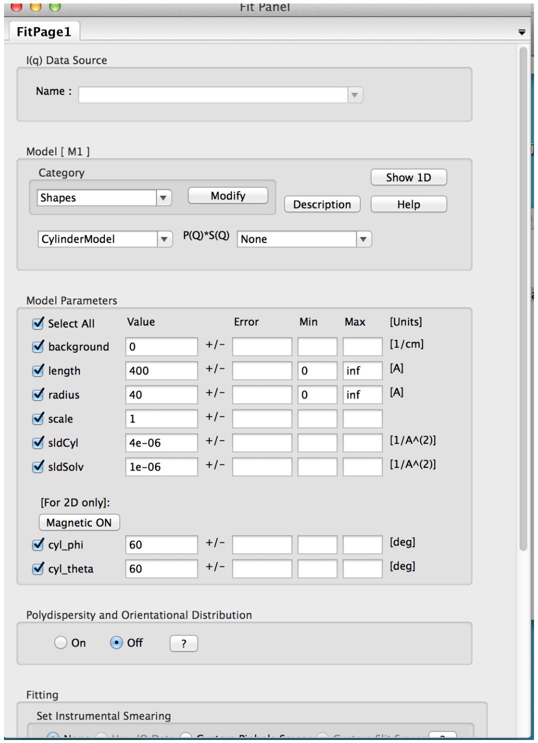
- Test case for Live Neutron Data Analysis: SANS

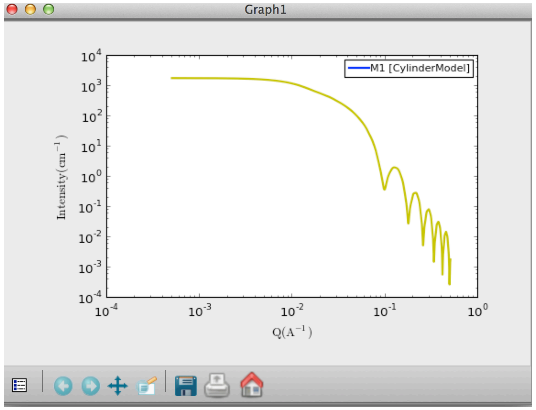
SANS data analysis

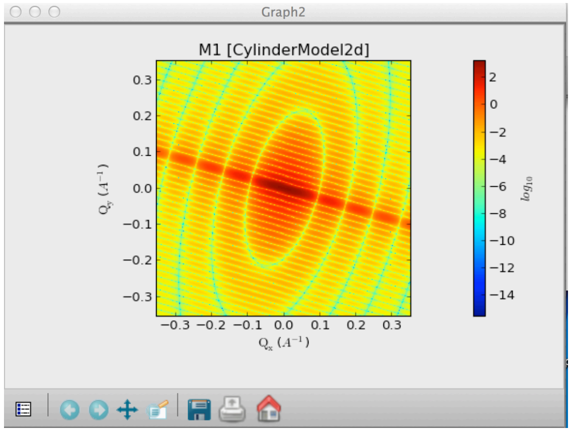
- Can this be done Live ?











SasView scattering kernel: Orientated cylinder

Live Data workflow

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- x,y,z,t

- Experiment data
- Simulated data
- E.g. McStas

- qx, qy, qx, hw

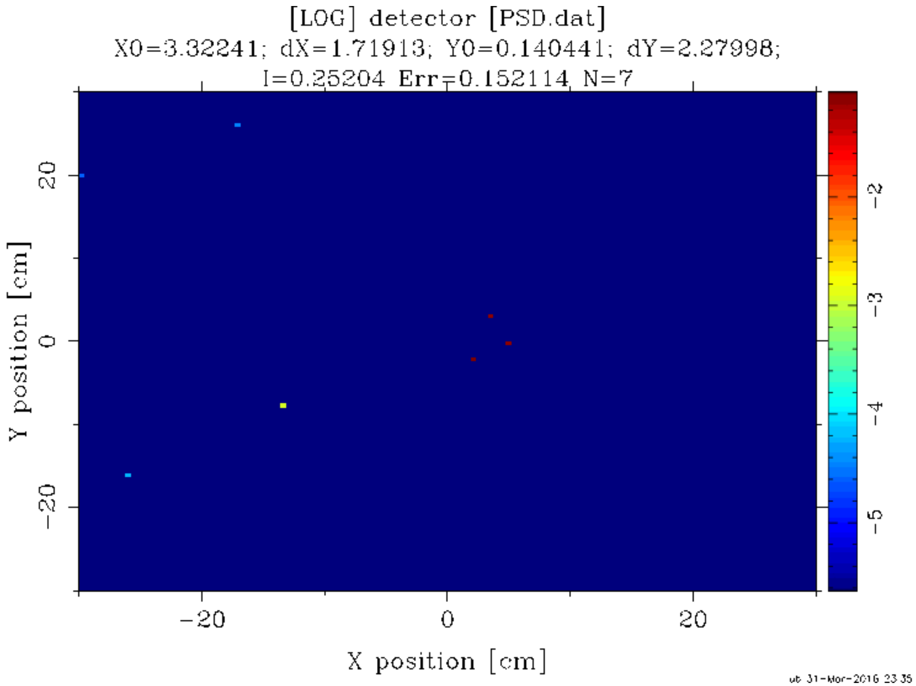
- Reduction method
- E.g. Mantid

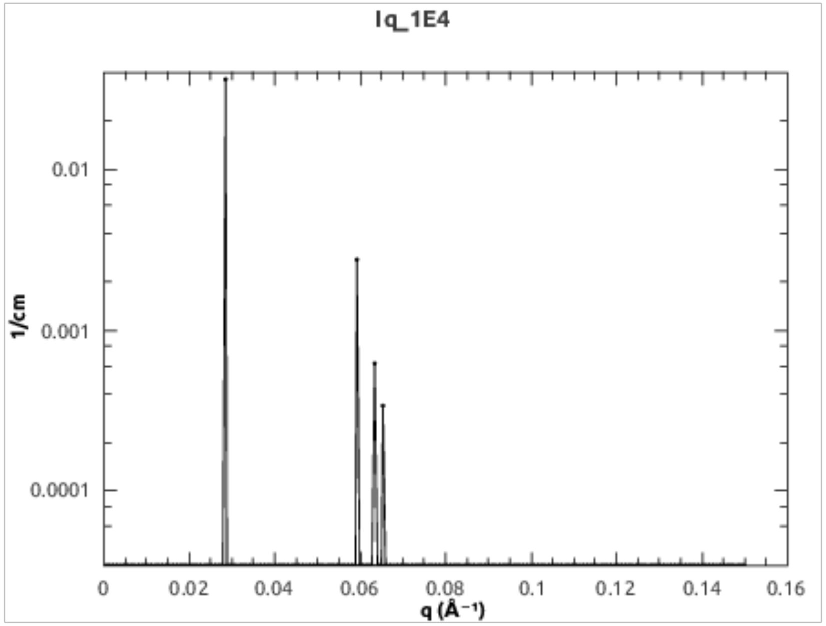
- Determine experimental parameters

- SasView

- Fullprof

“Live” SANS McStas data – Mantid reduction





McStas SANS scattering kernel: spheres

Curve fitting

- Obtaining a good fit depends foremost on having the correct model to fit.

- In general there is a trade-off between convergence rate and robustness, with the fastest algorithms most likely to find a local minimum rather than a global minimum.

From: bumps.readthedocs.org

Curve fitting - Interoperability

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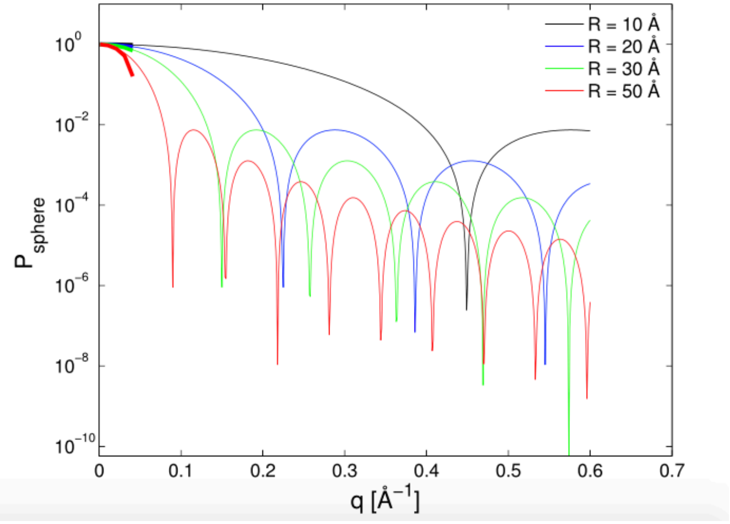
Fit engine	Fit package	Fit method	Fit parameters
	• scipy • lmfit • bumps • etc …	• Levenberg-Marquardt • Differential evolution • dream	• parameter range • max iterations • number of repetitions • etc …

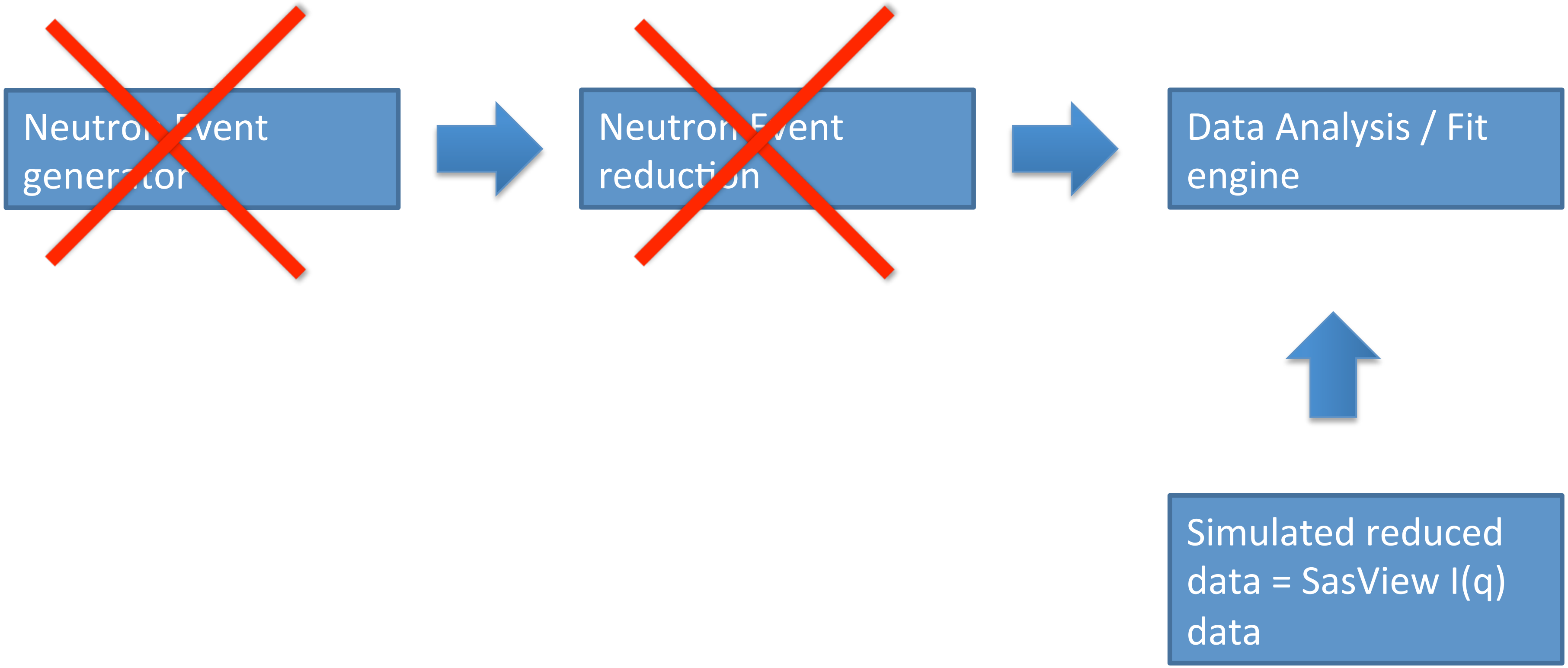
Fit model - SANS – Spherical nanoparticles

$$\left.\frac{d\Sigma}{d\Omega}\right|_{\mathrm{SANS,\,simple}} \equiv \phi \Delta\rho^2 V S(\mathbf{q}) P(\mathbf{q})$$

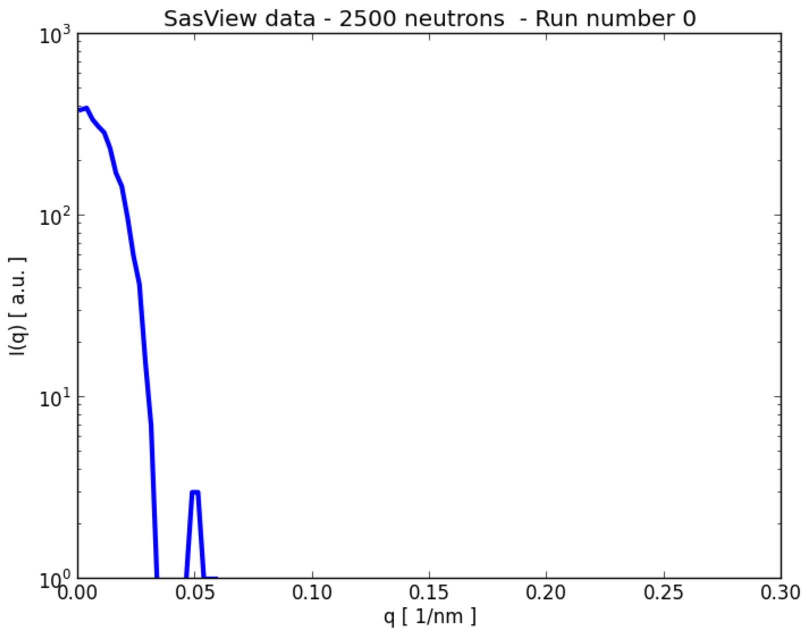
$$P_{\mathrm{sphere}}(q) = \left(3\,\frac{\sin(qR) - qR\cos(qR)}{(qR)^3}\right)^2$$

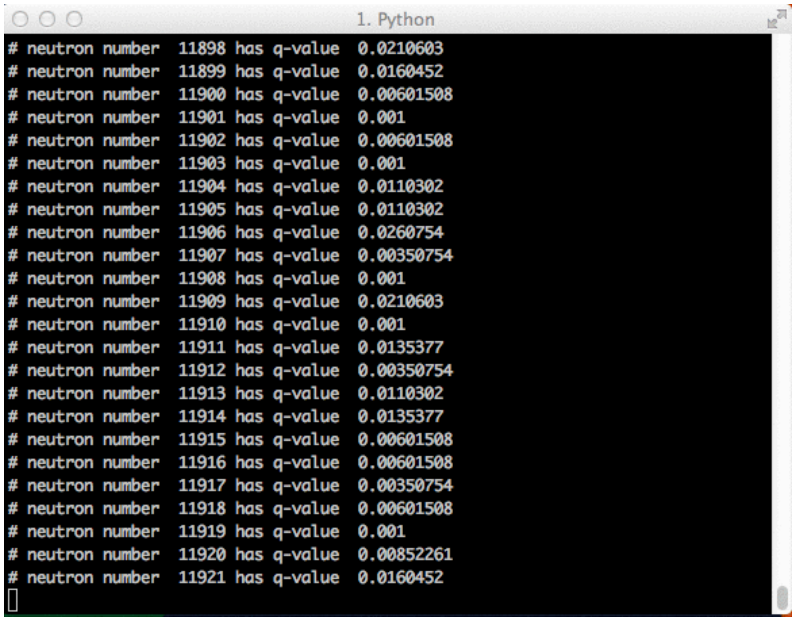


Data workflow – Simulated reduced data



Streamed – SANS data – radius = 120 Å



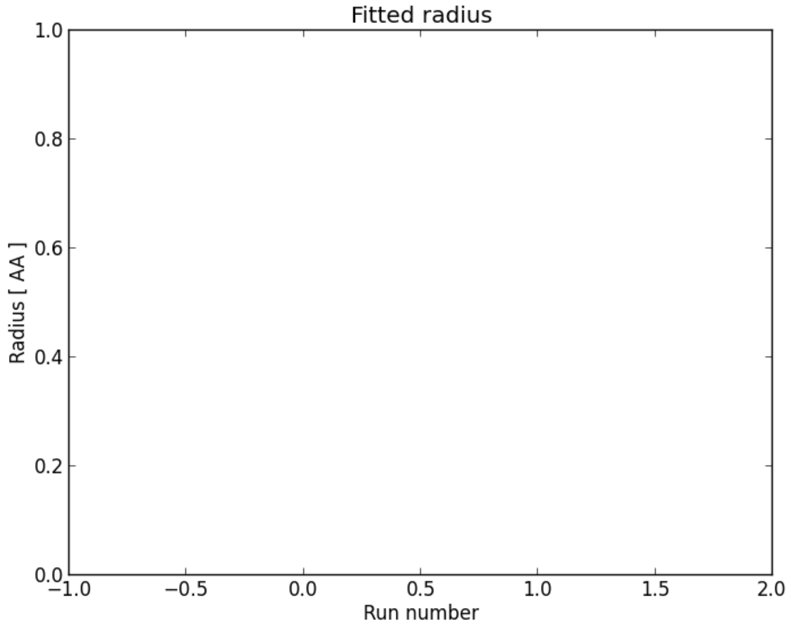


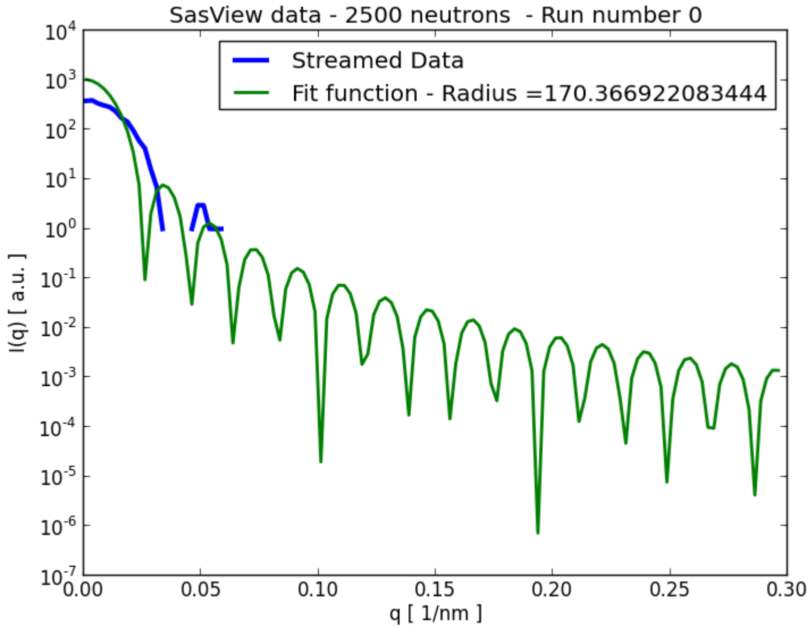
- Data are streamed

- Each neutron event carries a q value
- Histogram data for intensity

SANS: Spherical nanoparticels – radius = 120 Å

- Initial guess for radius = 120 Å





Fitted radius & 65% CI

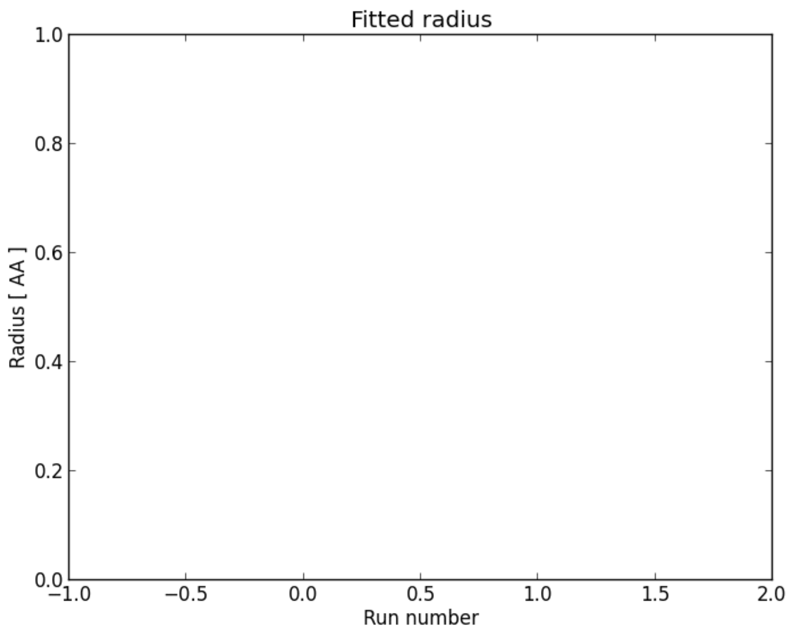
- Data streamed
- Fitted model

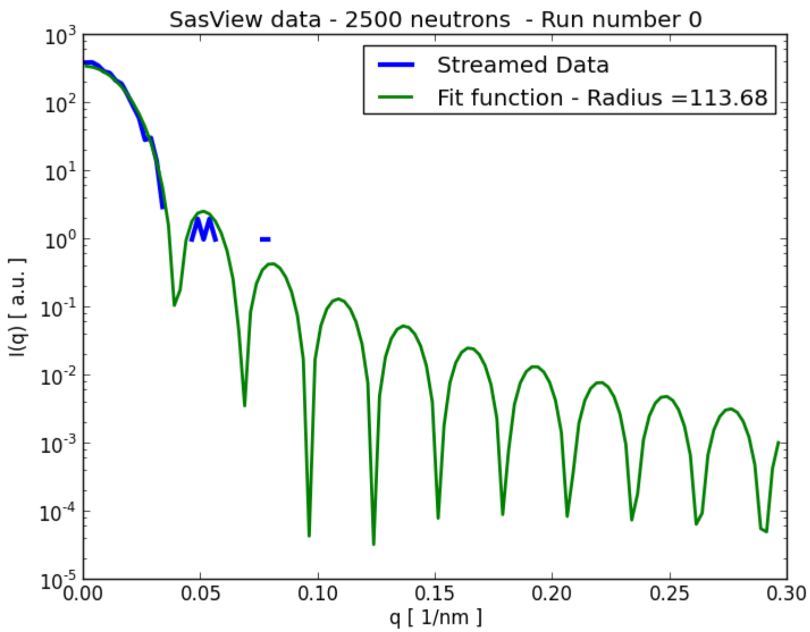
Discussion items

- Agree on a standard for fitting method ?
- How to benchmark different fitting methods ?
- Practical viewpoint – Need a sustainable solution
  - List what is currently being used
  - How much manpower is available ?

SANS: Spherical nanoparticels – radius = 120 Å

- Initial guess for radius = 100 Å





Fitted radius & 95% CI

- Data streamed
- Fitted model