

Live Neutron Data Analysis

LiNDA

Sine2020

PSI meeting April 4th and 5th 2016

www.europeanspallationsource.se

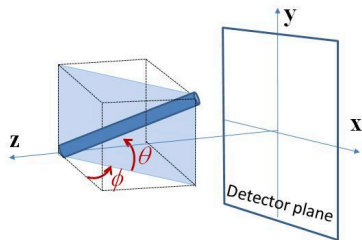
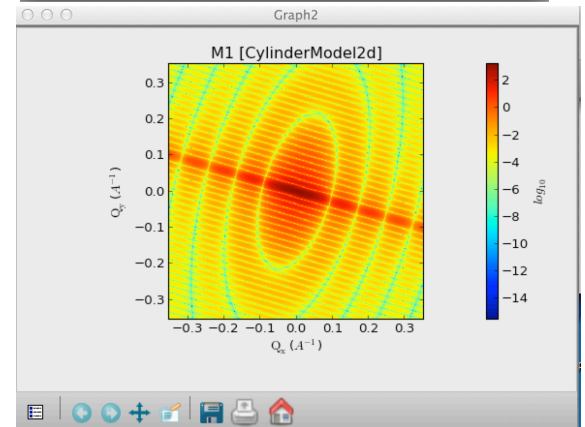
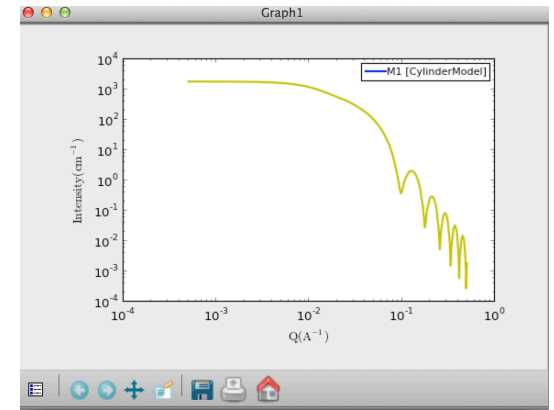
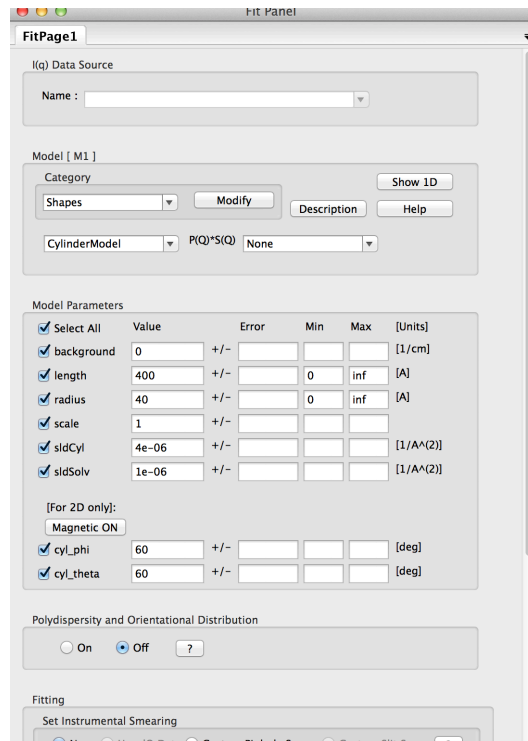
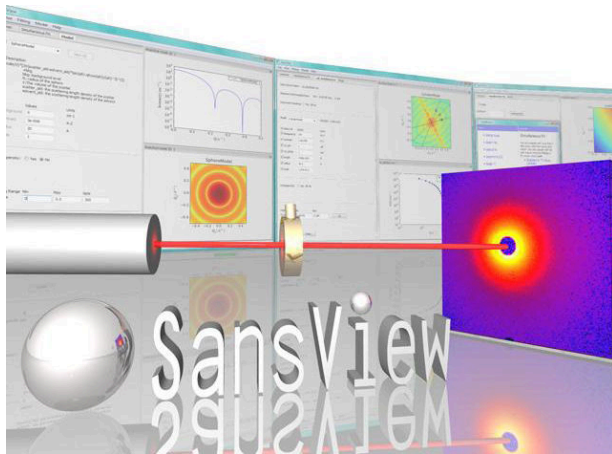
5th april 2016

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**

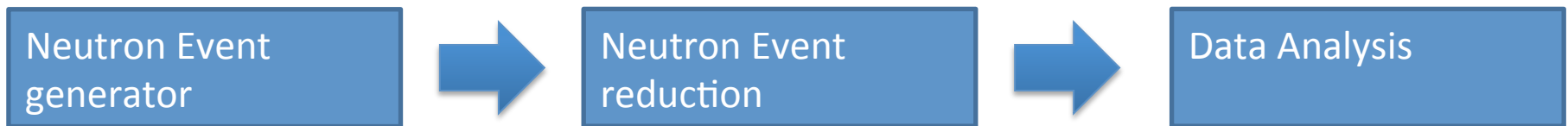
SANS data analysis

- Can this be done Live ?



SasView scattering kernel: Orientated cylinder

Live Data workflow

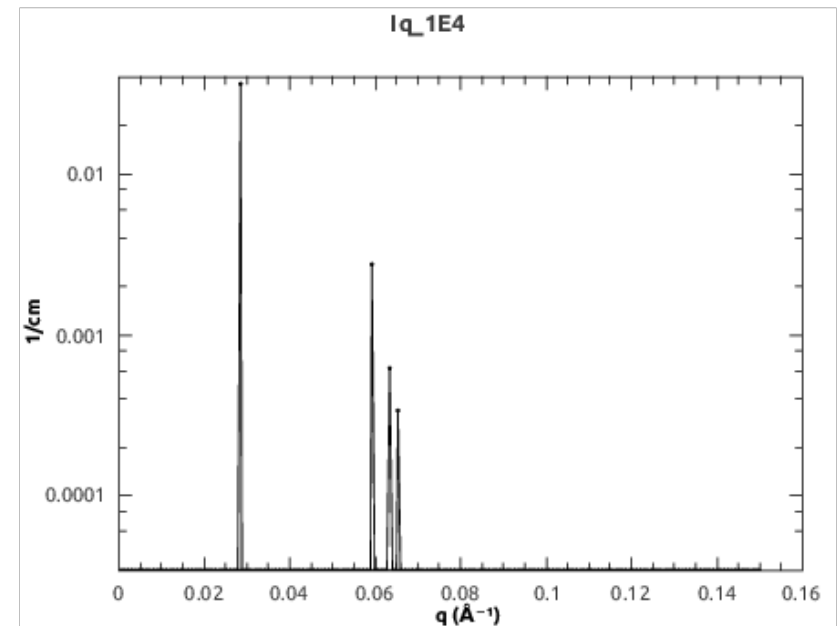
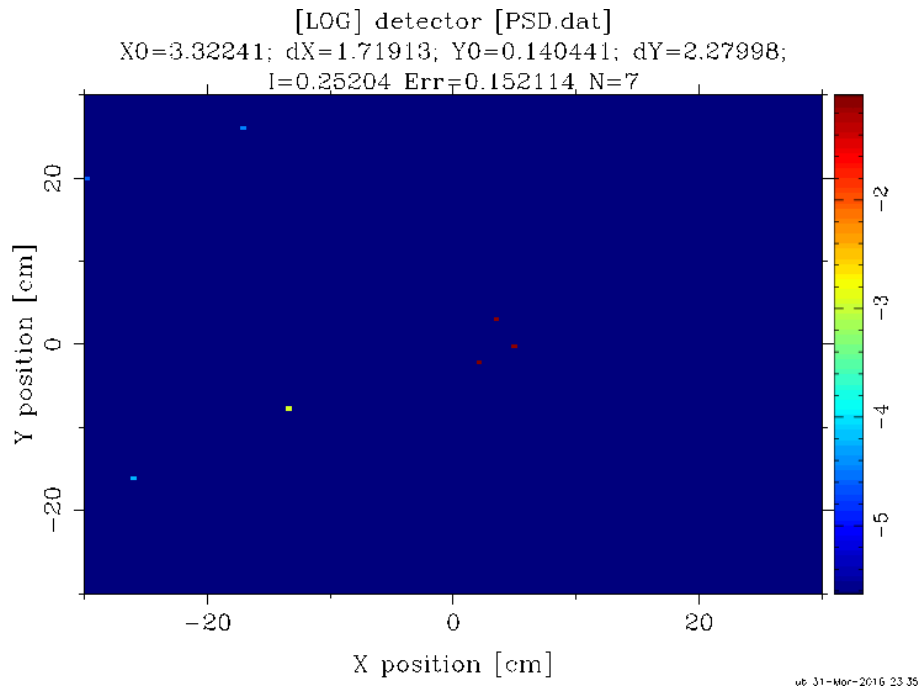


- x, y, z, t
- Experiment data
- Simulated data
- E.g. McStas

- qx, qy, qx, hw
- Reduction method
- E.g. Mantid

- Determine experimental parameters
- SasView
- Fullprof

“Live” SANS McStas data – Mantid reduction



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.

Curve fitting - Interoperability

Fit engine

Fit package

- scipy
- lmfit
- bumps
- etc ...

Fit method

- Levenberg-Marquardt
- Differential evolution
- dream

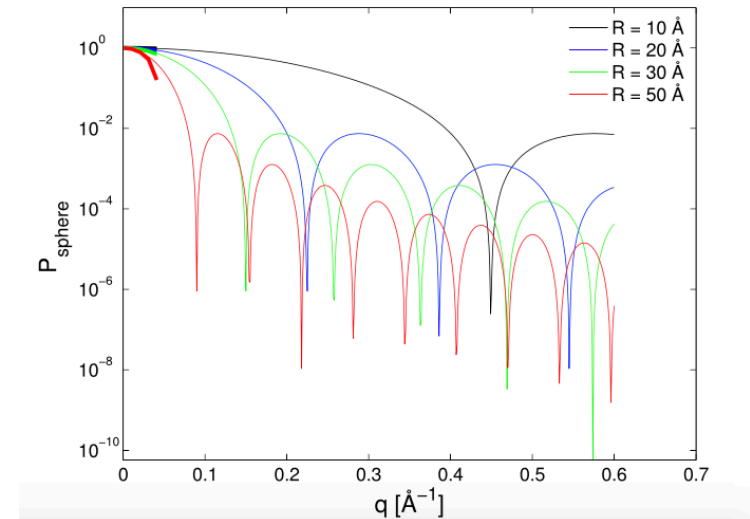
Fit parameters

- parameter range
- max iterations
- number of repetitions
- etc ...

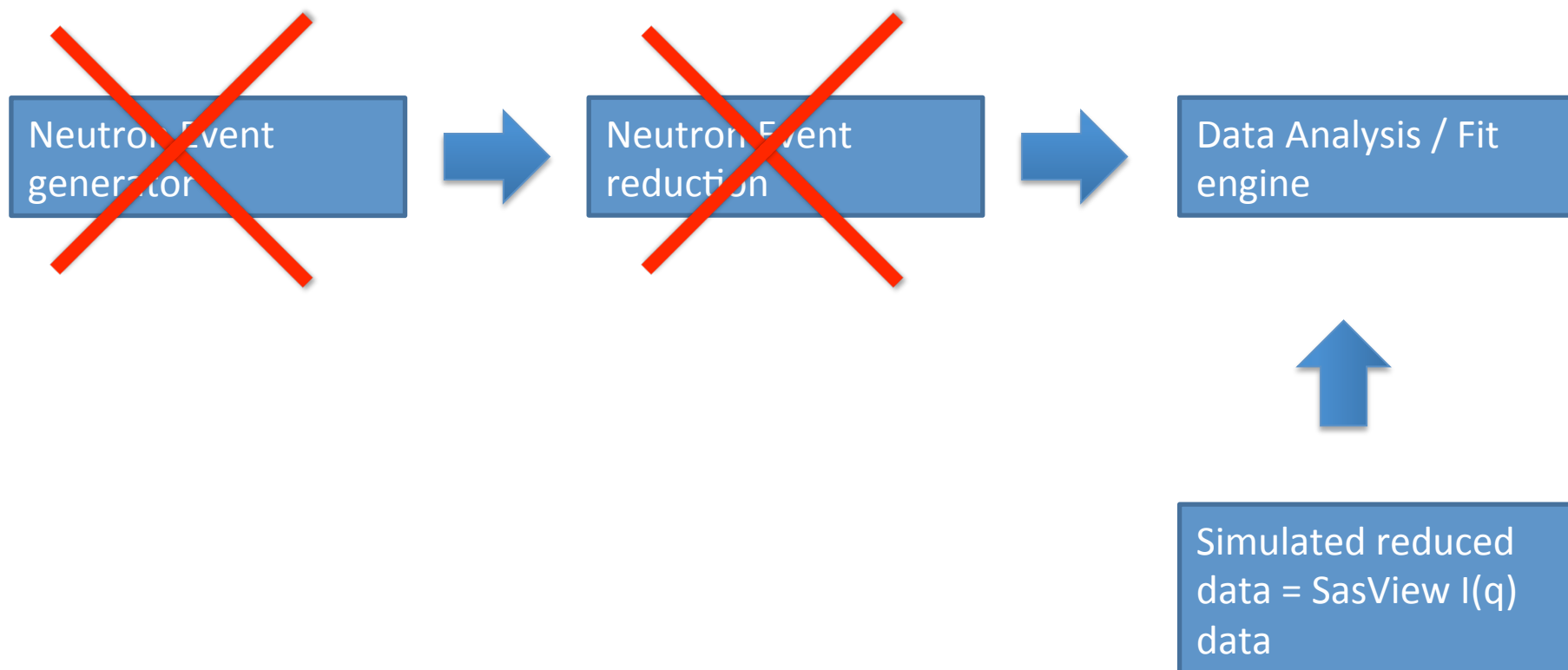
Fit model - SANS – Spherical nanoparticles

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

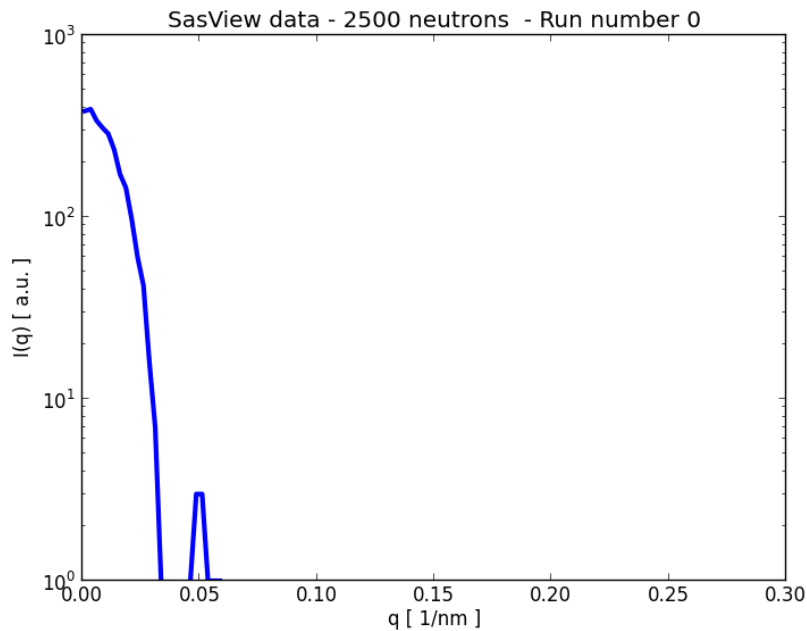
$$P_{\text{sphere}}(q) = \left(3 \frac{\sin(qR) - qR \cos(qR)}{(qR)^3} \right)^2$$



Data workflow – Simulated reduced data



Streamed – SANS data – radius = 120 Å



```

1. Python
# neutron number 11898 has q-value 0.0210603
# neutron number 11899 has q-value 0.0160452
# neutron number 11900 has q-value 0.00601508
# neutron number 11901 has q-value 0.001
# neutron number 11902 has q-value 0.00601508
# neutron number 11903 has q-value 0.001
# neutron number 11904 has q-value 0.0110302
# neutron number 11905 has q-value 0.0110302
# neutron number 11906 has q-value 0.0260754
# neutron number 11907 has q-value 0.00350754
# neutron number 11908 has q-value 0.001
# neutron number 11909 has q-value 0.0210603
# neutron number 11910 has q-value 0.001
# neutron number 11911 has q-value 0.0135377
# neutron number 11912 has q-value 0.00350754
# neutron number 11913 has q-value 0.0110302
# neutron number 11914 has q-value 0.0135377
# neutron number 11915 has q-value 0.00601508
# neutron number 11916 has q-value 0.00601508
# neutron number 11917 has q-value 0.00350754
# neutron number 11918 has q-value 0.00601508
# neutron number 11919 has q-value 0.001
# neutron number 11920 has q-value 0.00852261
# neutron number 11921 has q-value 0.0160452

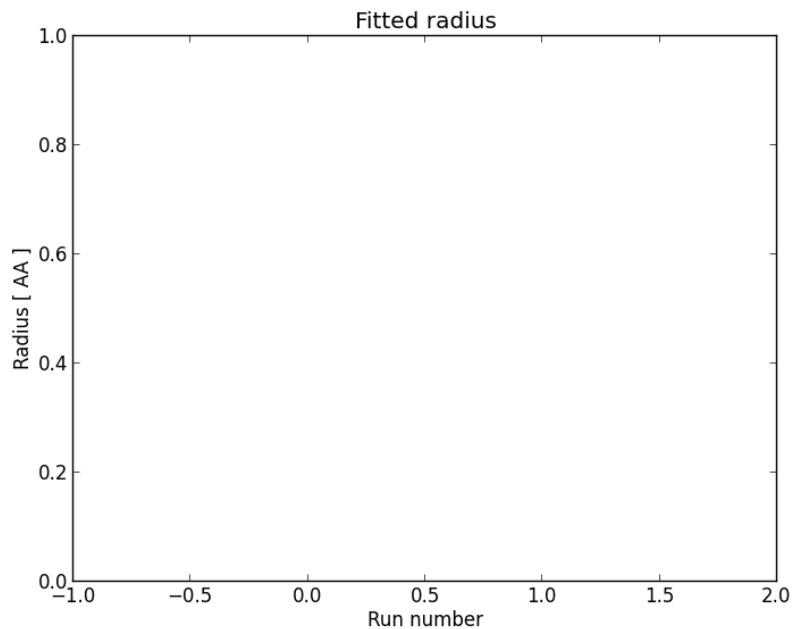
```

- Data are streamed

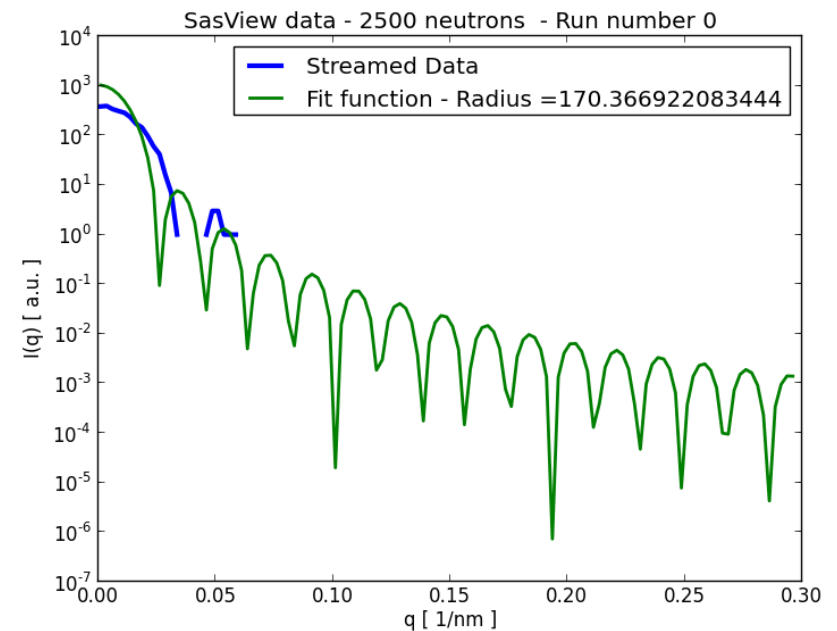
- Each neutron event carries a q value
- Histogram data for intensity

SANS: Spherical nanoparticles – radius = 120 Å

- Initial guess for radius = 120 Å



Fitted radius & 65% CI



- Data streamed
- Fitted model

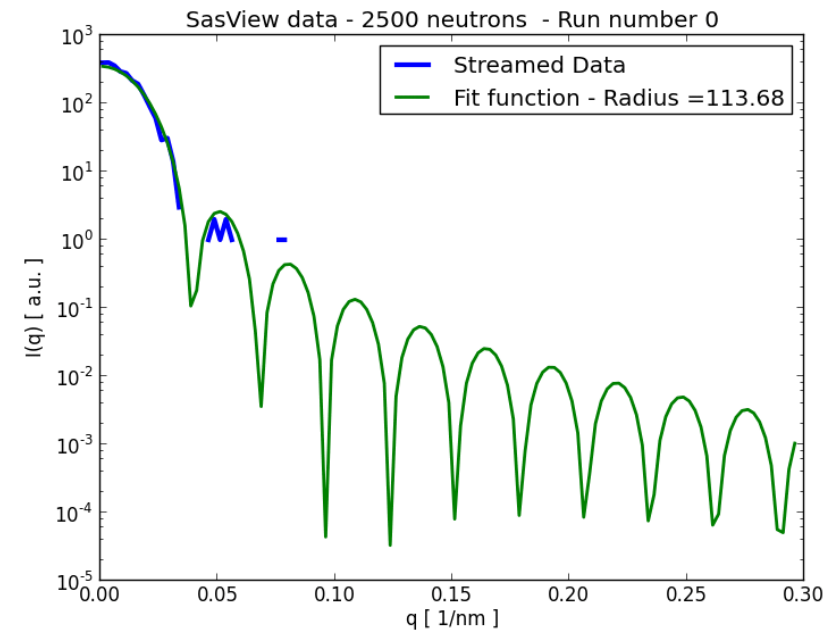
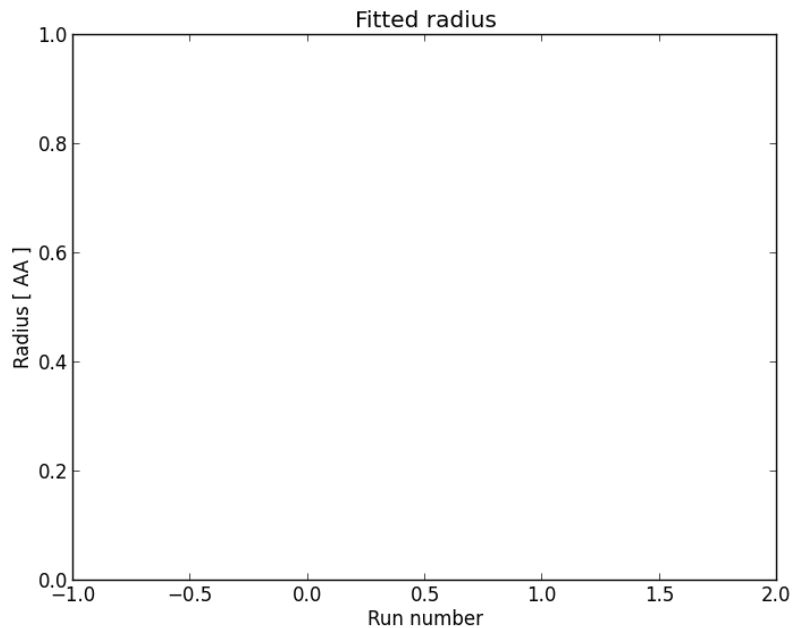
Discussion items

- 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 nanoparticles – radius = 120 Å

- Initial guess for radius = 100 Å



Fitted radius & 95% CI

- Data streamed
- Fitted model