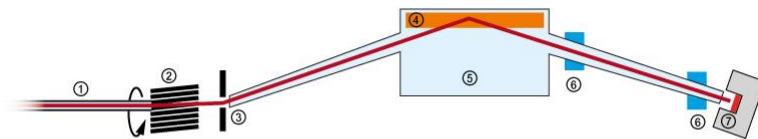
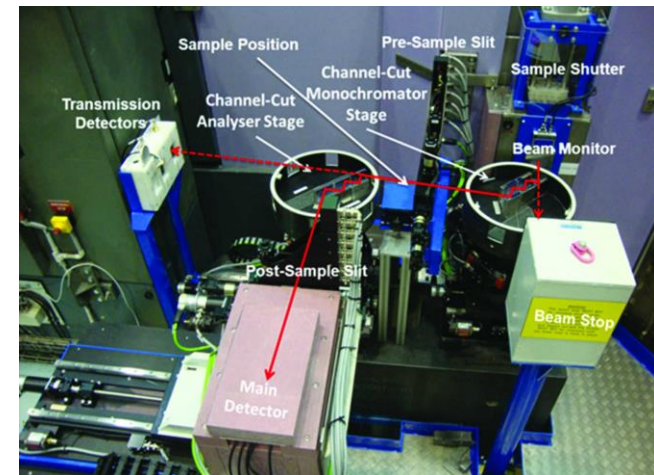
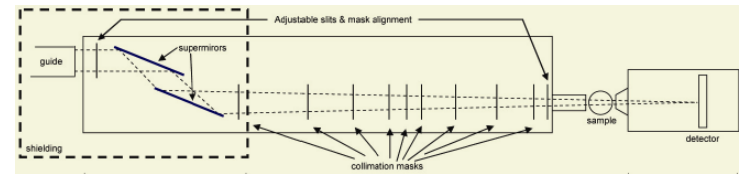


Extended Q -range



- ① Neutron guide NL3a
- ② Velocity selector
- ③ Entrance aperture
- ④ Toroidal mirror
- ⑤ Mirror chamber
- ⑥ Sample positions
- ⑦ Detector

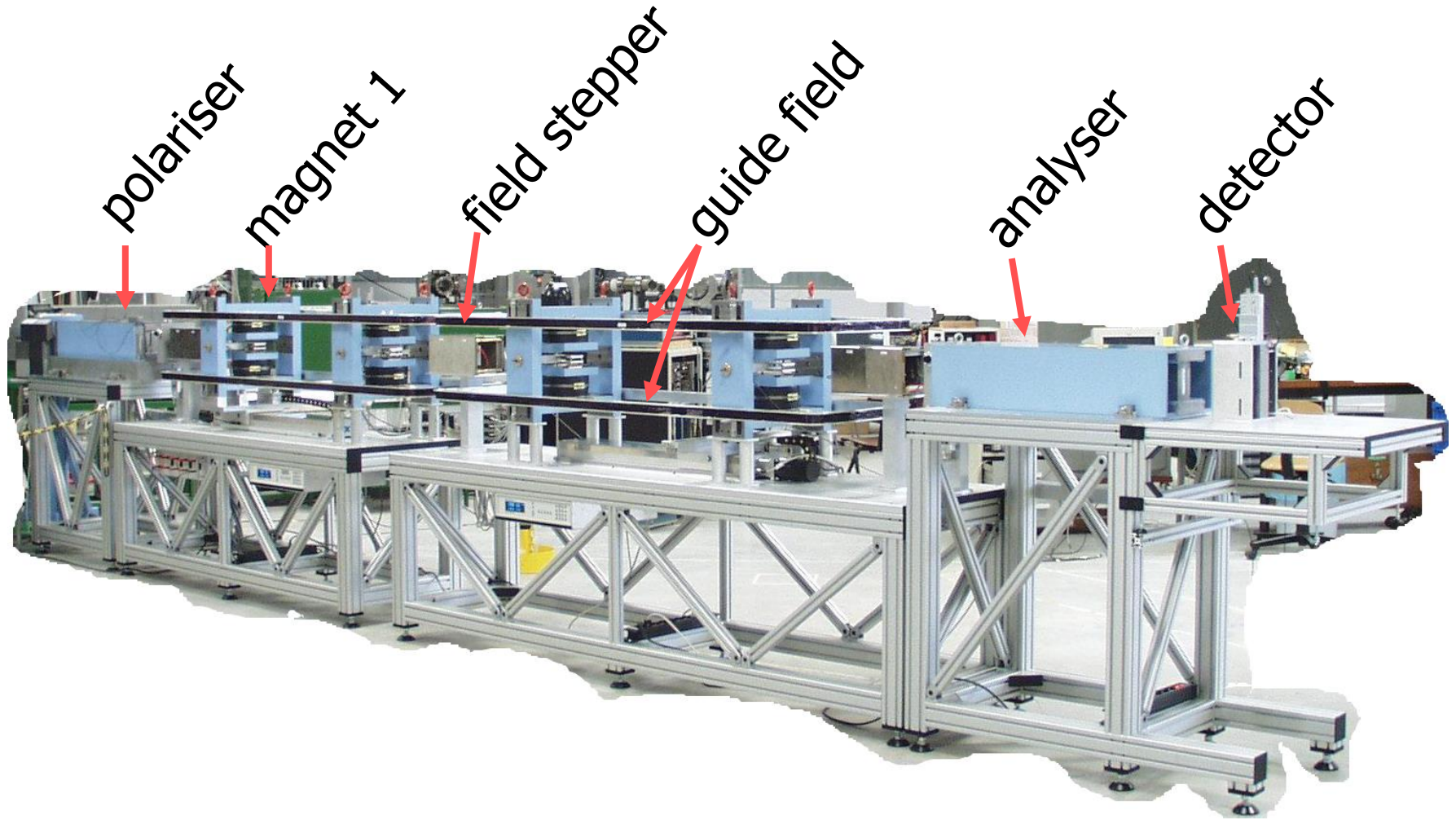


Possible discussion topics extended Q -range

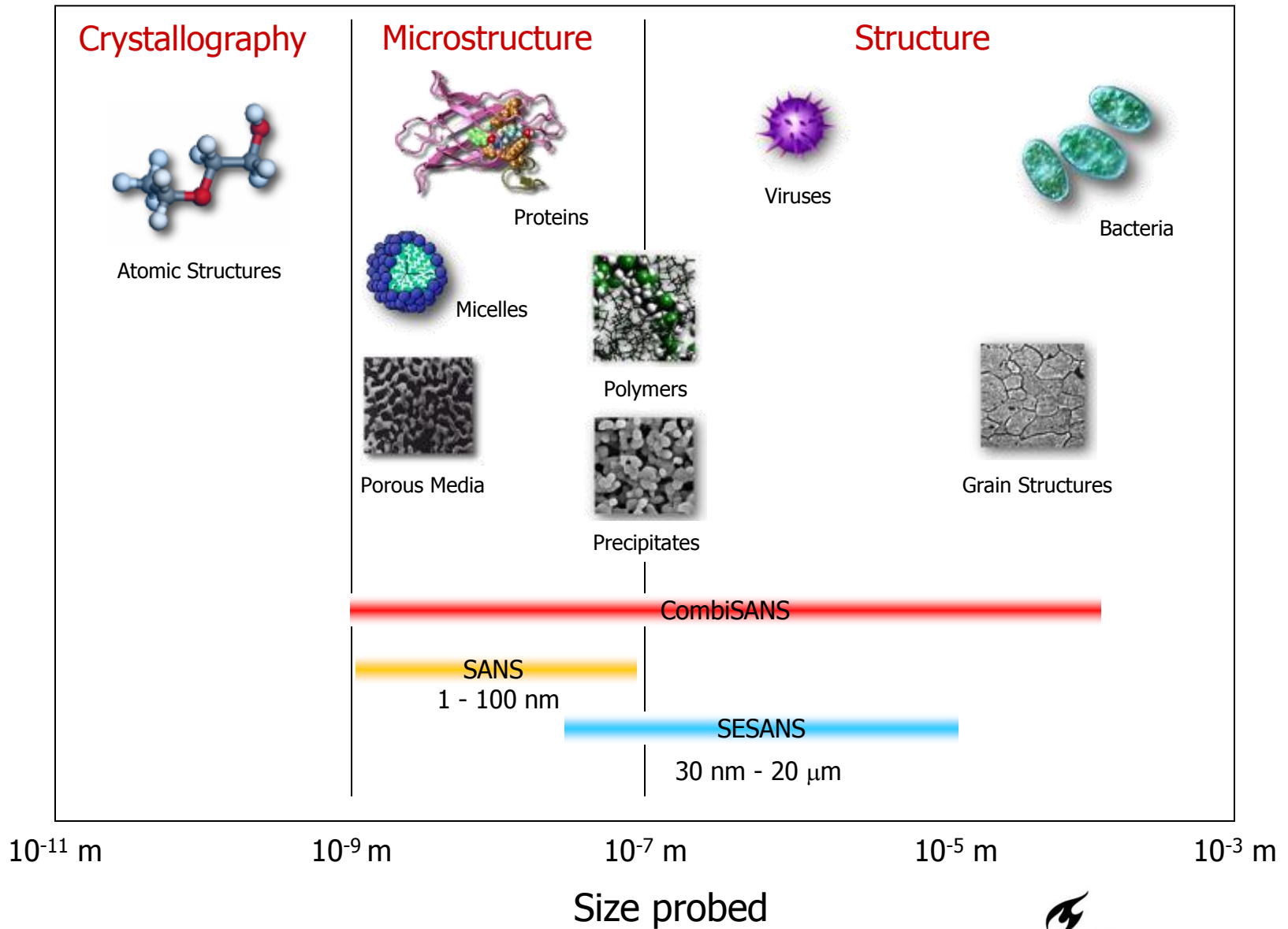
- Software for data-analysis
- Multiple scattering
- Anisotropic scattering in USANS and SESANS
- Combined analysis with imaging/tomography
- Combined analysis with conventional SAS
- Calibration samples

SESANS

spin-echo small-angle neutron scattering



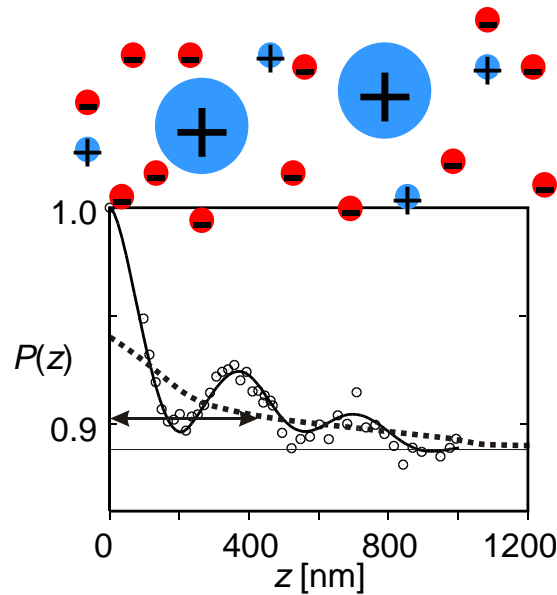
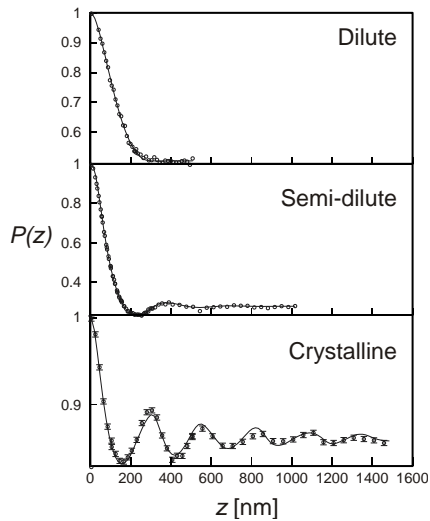
Length scales accessible



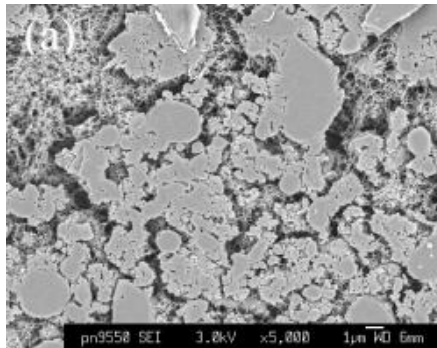
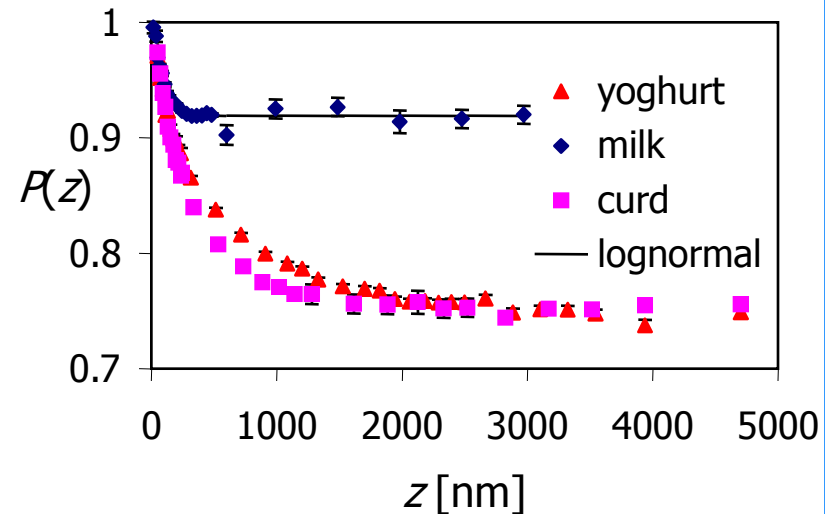
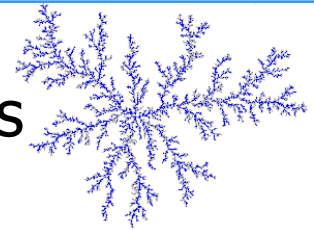
Applications of SESANS

real space, range 30 nm – 18 μm , no collimation

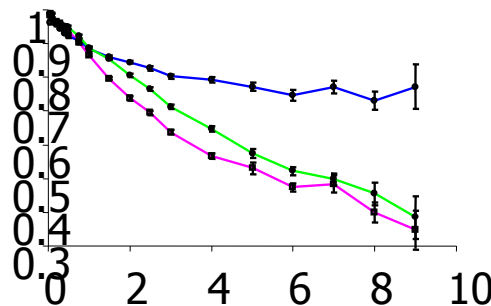
Colloidal interaction



Dairy products

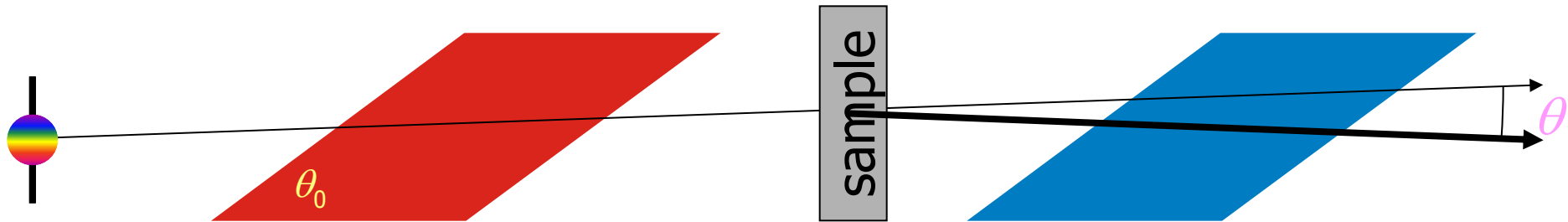


μ -emulsions



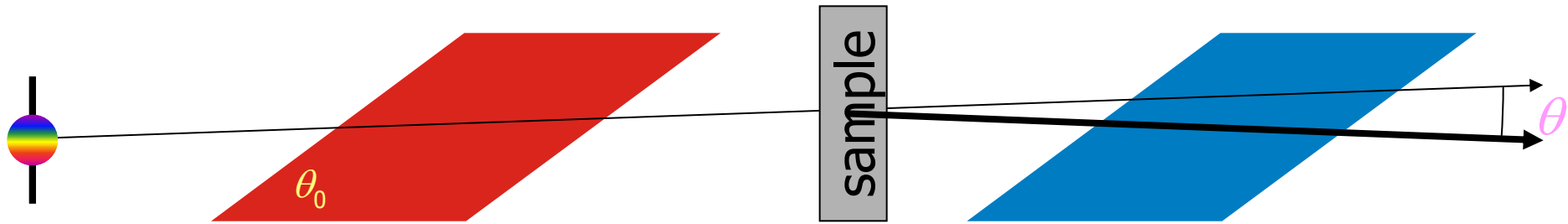
- Granular materials
- Drug delivery systems

Larmor encoding of scattering angle spin-echo small angle neutron scattering

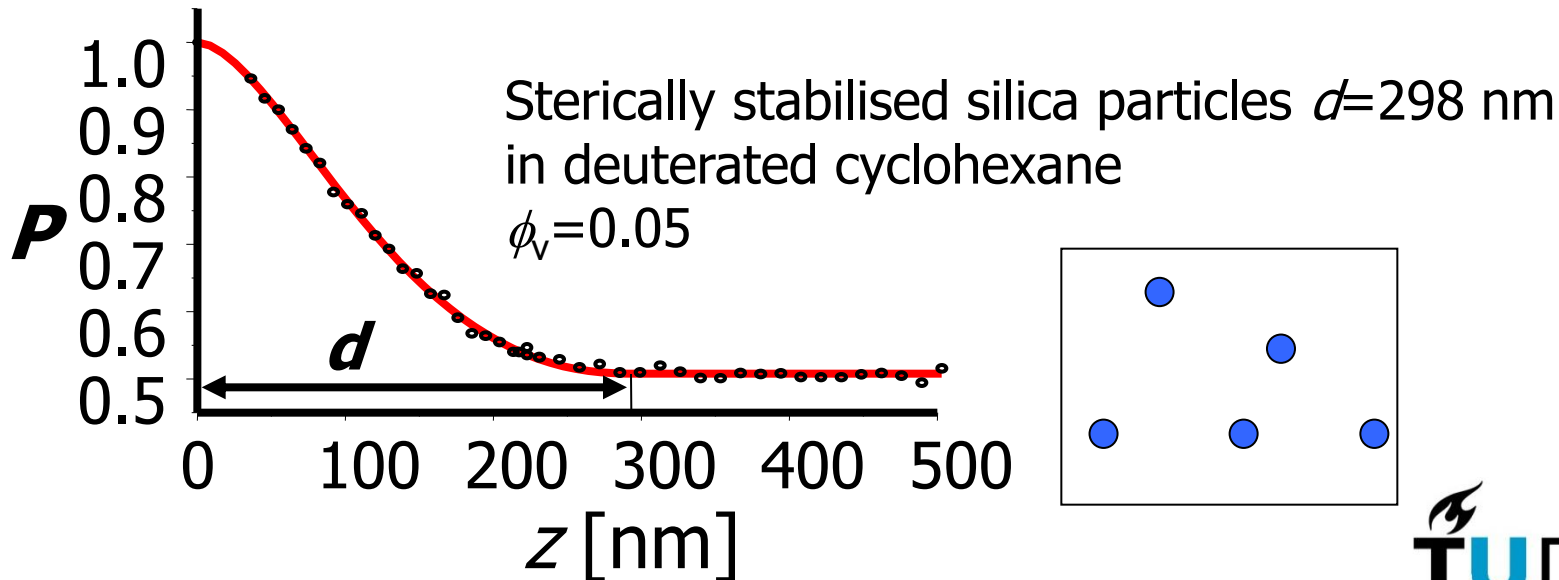


- Unscattered beam gives spin echo $\phi = 0$
independent of height and angle
- Scattering by sample → no complete spin echo
→ net precession angle
- Measure precession angle (or neutron polarization)
as a function of magnetic field → correlation function $G(\delta)$

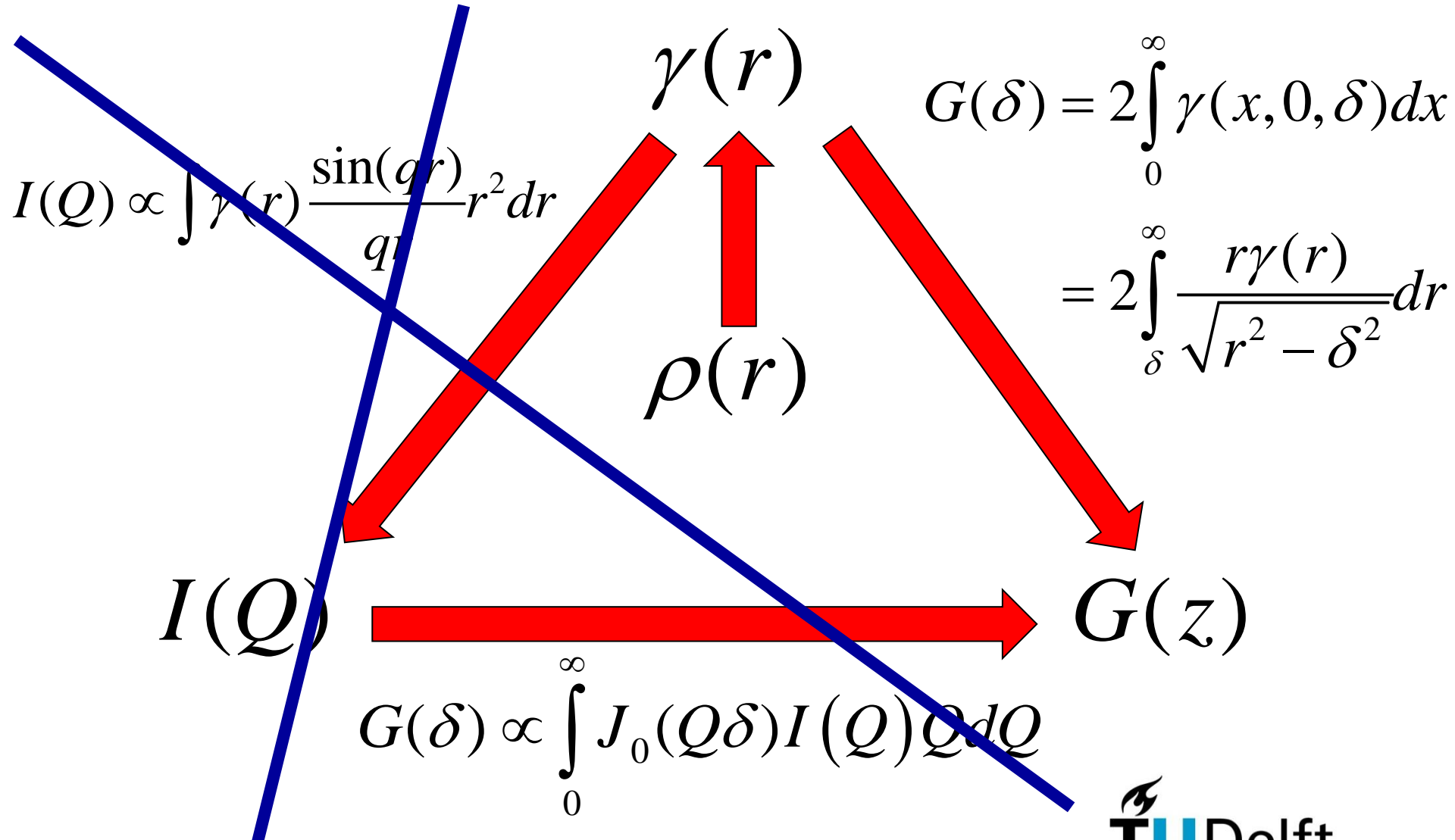
SESANS = density correlation functions



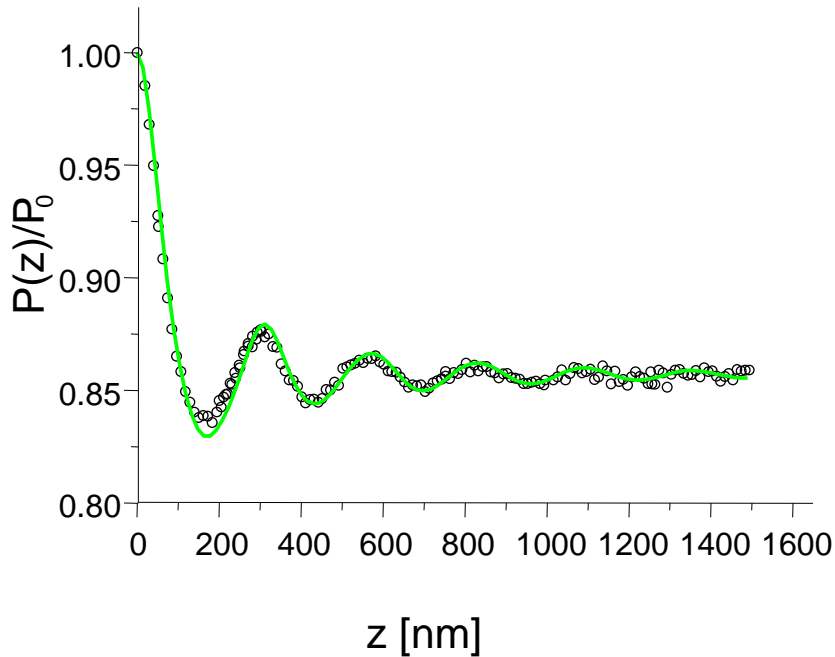
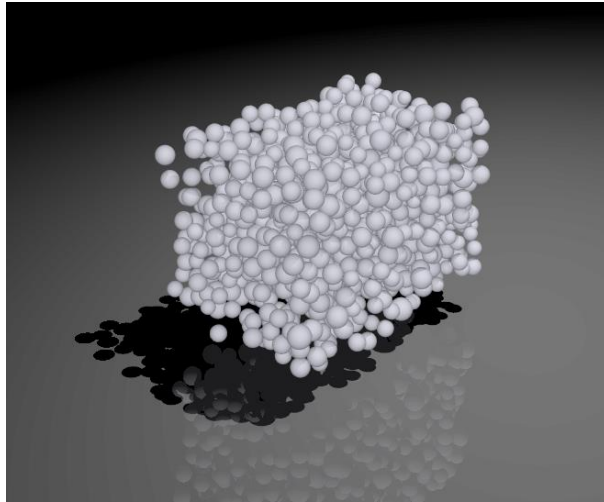
- Polarisation as function spin-echo length = scattering length density correlation function



Density, correlation, SANS, SESANS



From structure to polarisation



structure

$$\gamma(\mathbf{r}) = \int_V \rho(\mathbf{r}') \rho(\mathbf{r} + \mathbf{r}') d\mathbf{r}'$$

density correlation function

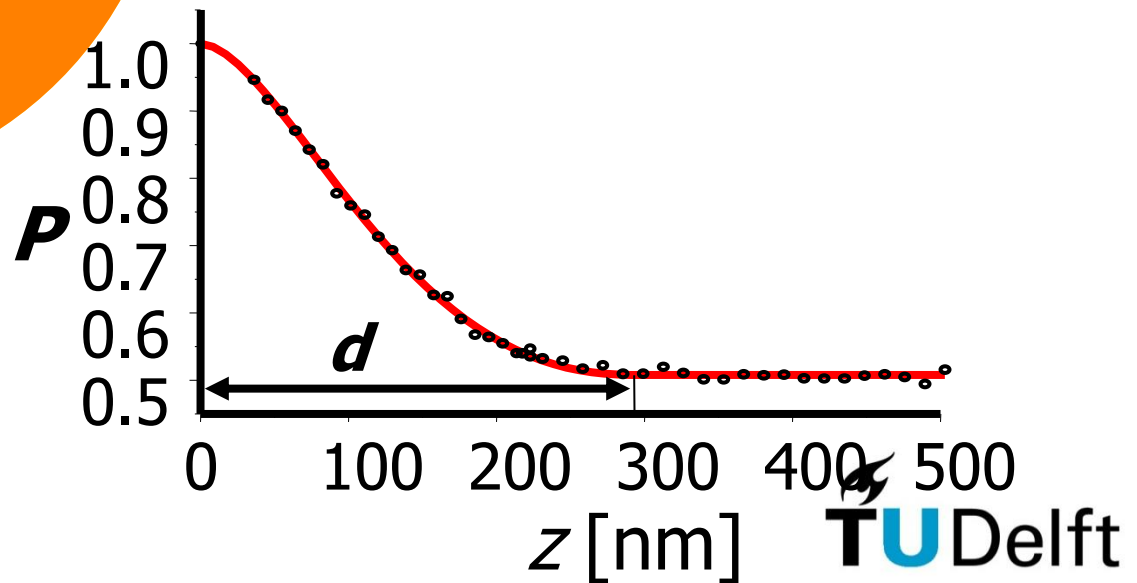
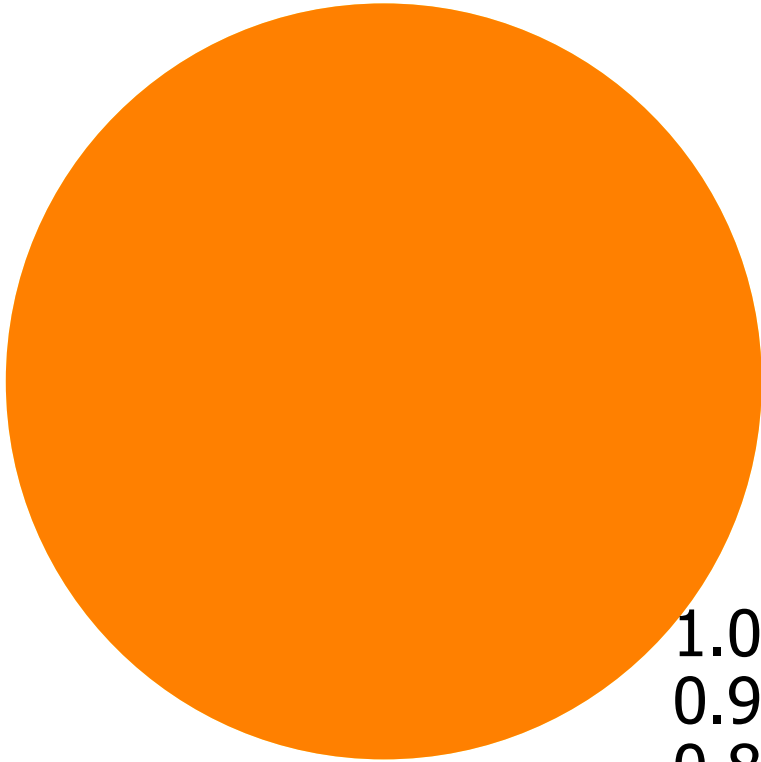
$$G(z) = 2 \int_0^{\infty} \gamma(x, 0, z) dx$$

SESANS correlation function

$$P(z) = e^{(G(z) - G(0))}$$

polarisation

Reciprocal space is redundant



Data analysis until 2014

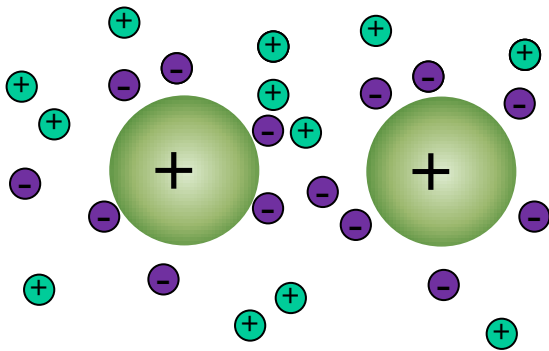
- Mostly ad hoc Matlab written real space models
- Loads of work allready for the few users

Need for user friendly SESANS analysis software

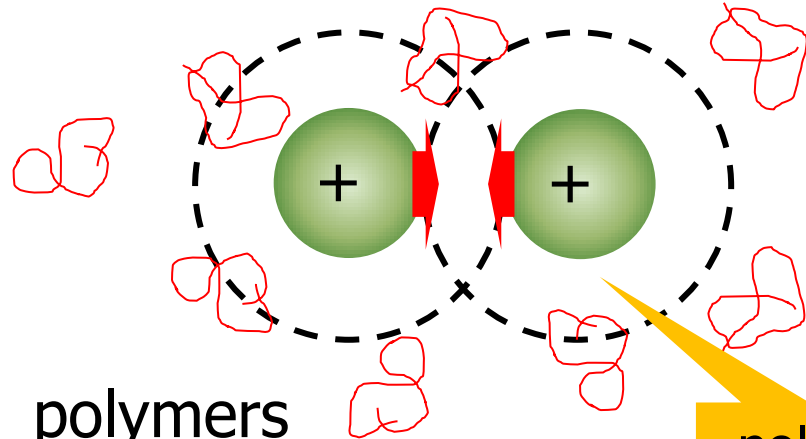
- Collaboration with ISIS: OFFSPEC & Larmor
- Users in Delft
- LENS and ad hoc at Oak Ridge
- Gatchina

- SKADI: SANS with SESANS add on

Depletion interactions in charged, aqueous colloid-polymer mixtures (model for e.g. milk)



salt
reduces
repulsion



polymers
give
attraction

polymer
depletion
zone



Kitty van Gruijthuisen



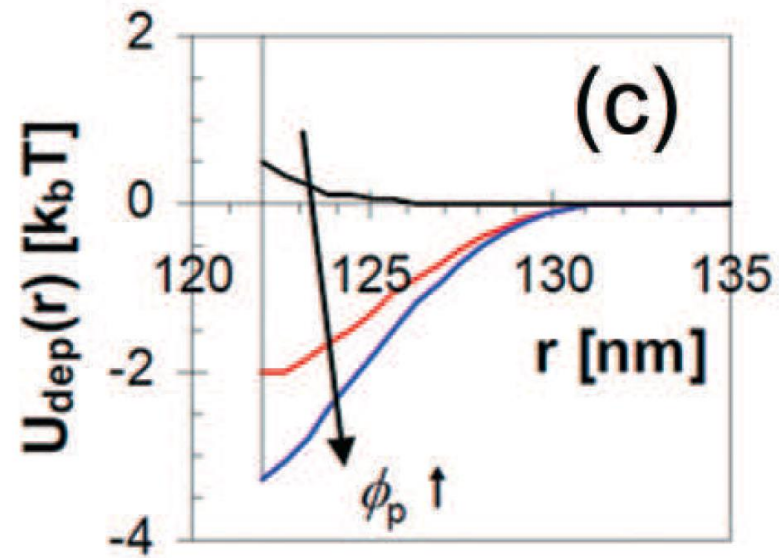
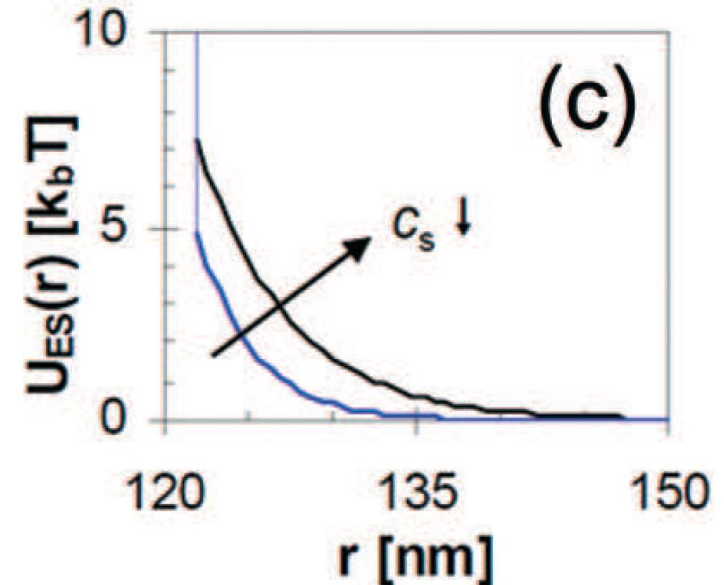
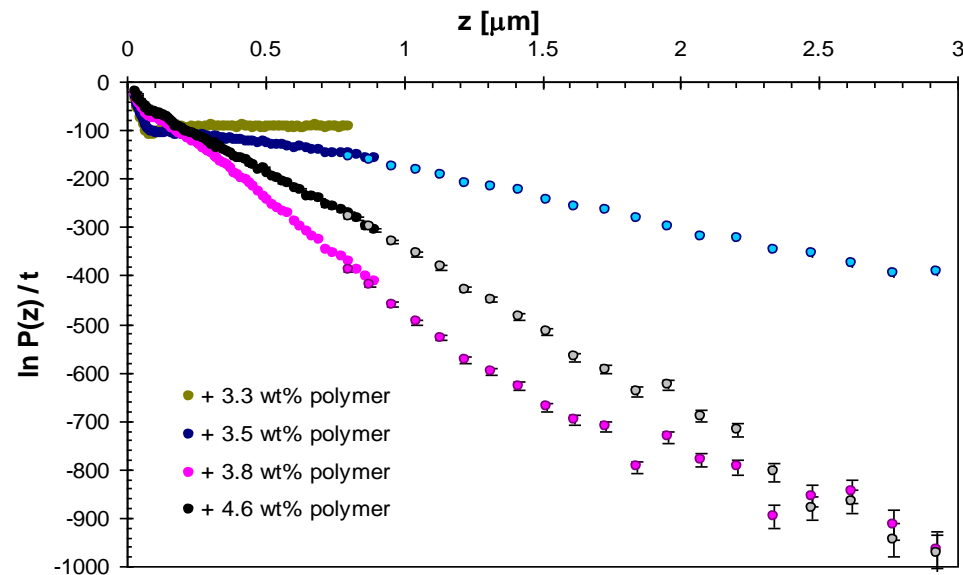
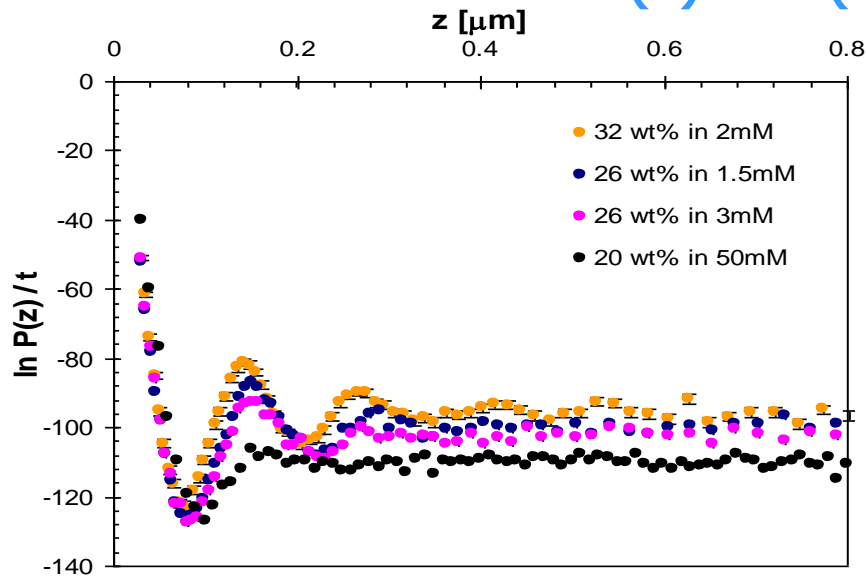
Peter Schurtenberger, Anna Stradner - Lund University



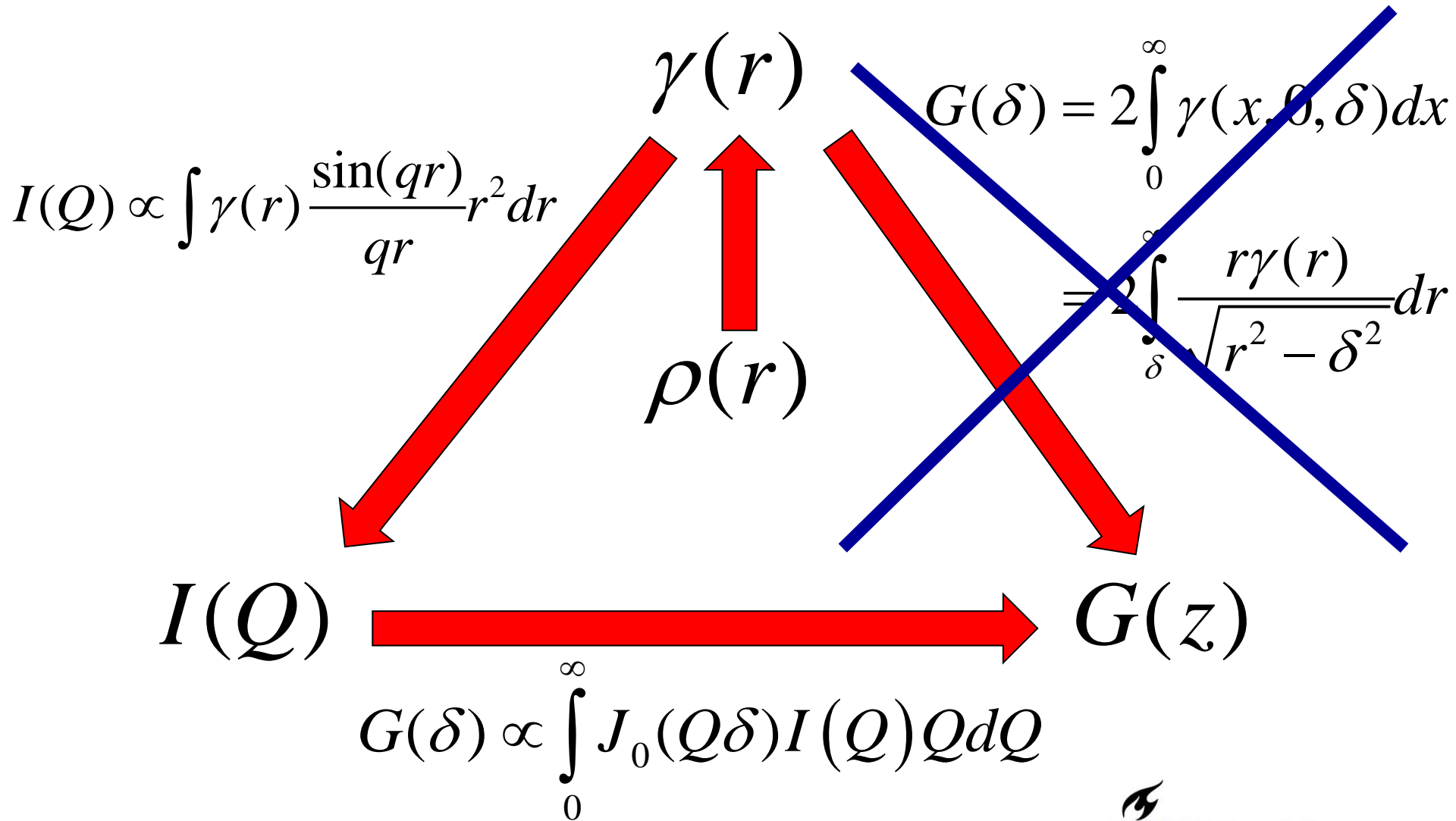
Adolphe Merkle Institute, Université de Fribourg

Fit SESANS with interaction potential:

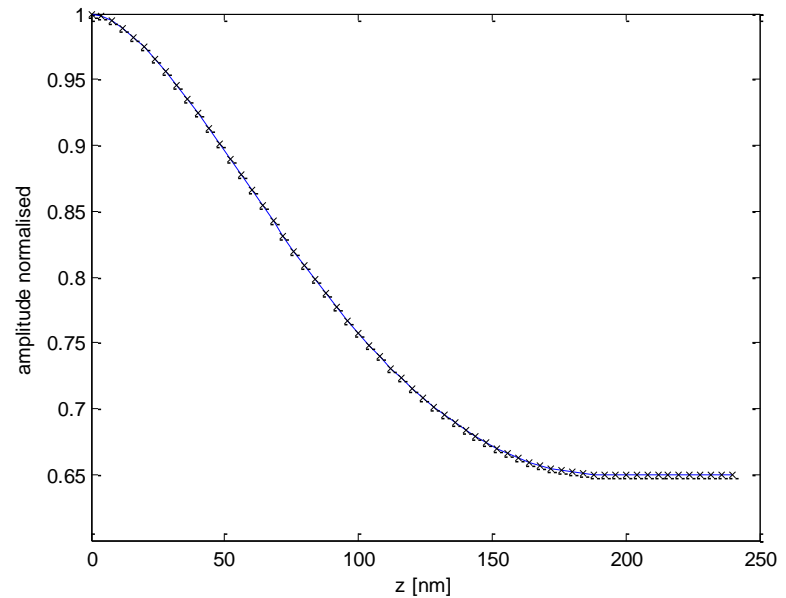
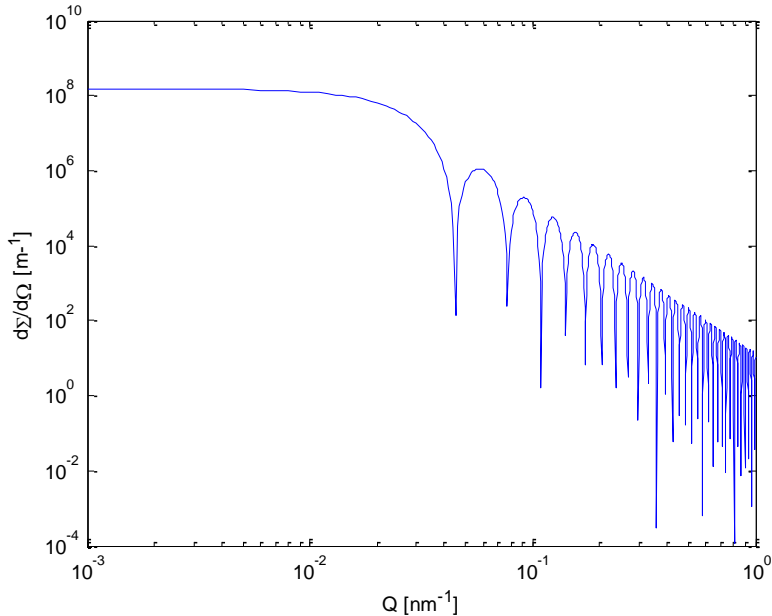
$$U(r) - I(q) - G(z)$$



Density, correlation, SANS, SESANS



Need SANS into SESANS conversion spheres R=100 nm



$$\tilde{G}(z) = \int_0^{\infty} J_0(Qz) \frac{d\Sigma}{d\Omega}(Q) Q dQ \quad P(z) = e^{\frac{t\lambda^2}{2\pi}(\tilde{G}(z) - \tilde{G}(0))}$$

4 code camps with SasView team

Jurrian Bakker



Full functionality and all models from SasView

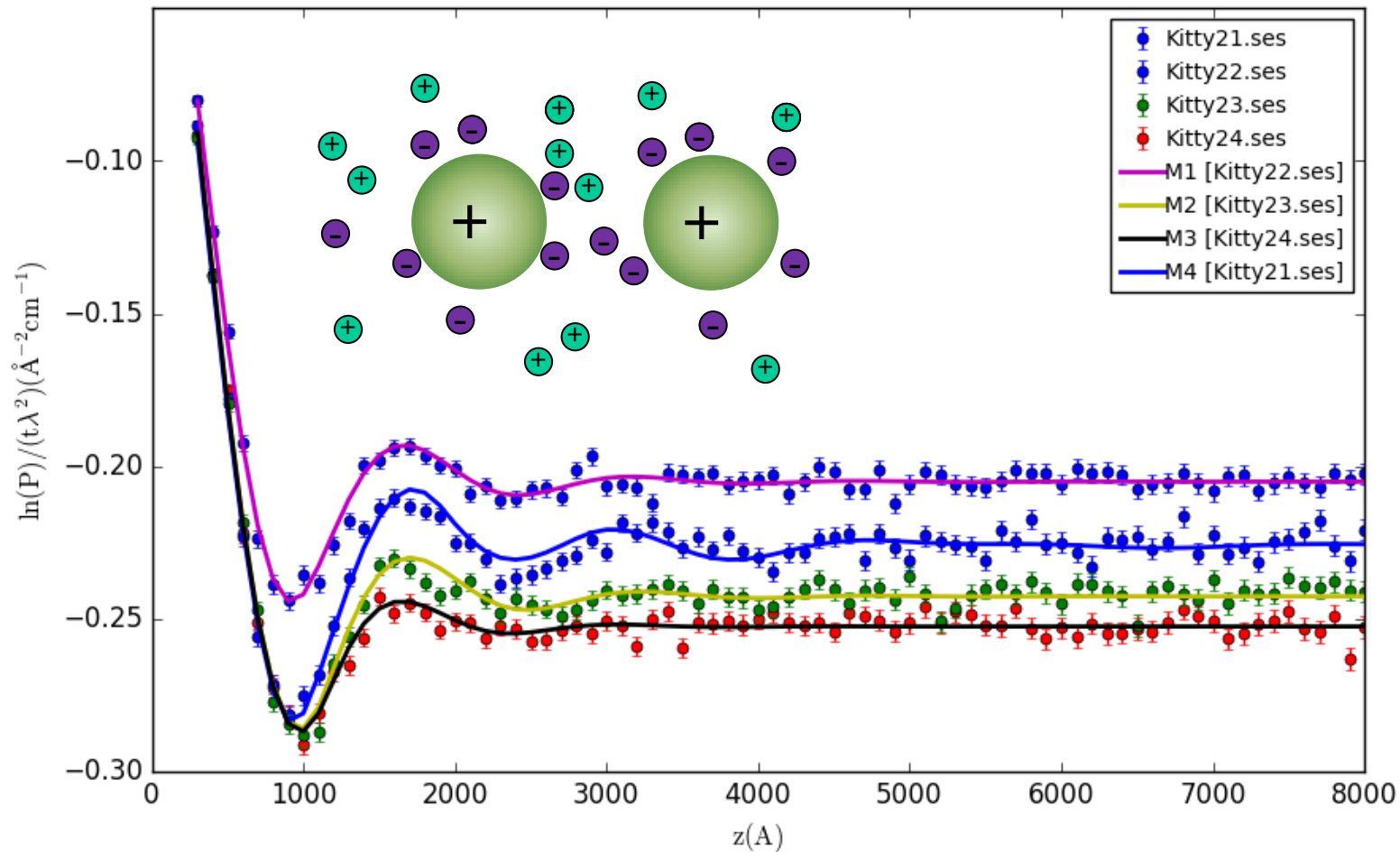
The screenshot displays the SasView software interface, which is used for fitting experimental data. The main window is titled "FitPage1" and contains several panels:

- Data Explorer:** Shows the available data file "se011953_01.ses".
- Fit panel - Active Fitting Optimizer: Levenberg-Marquardt:** Contains the "FitPage1" sub-panel with the following settings:
 - Model: sphere (P(Q)*S(Q) hardsphere)
 - Model Parameters table:

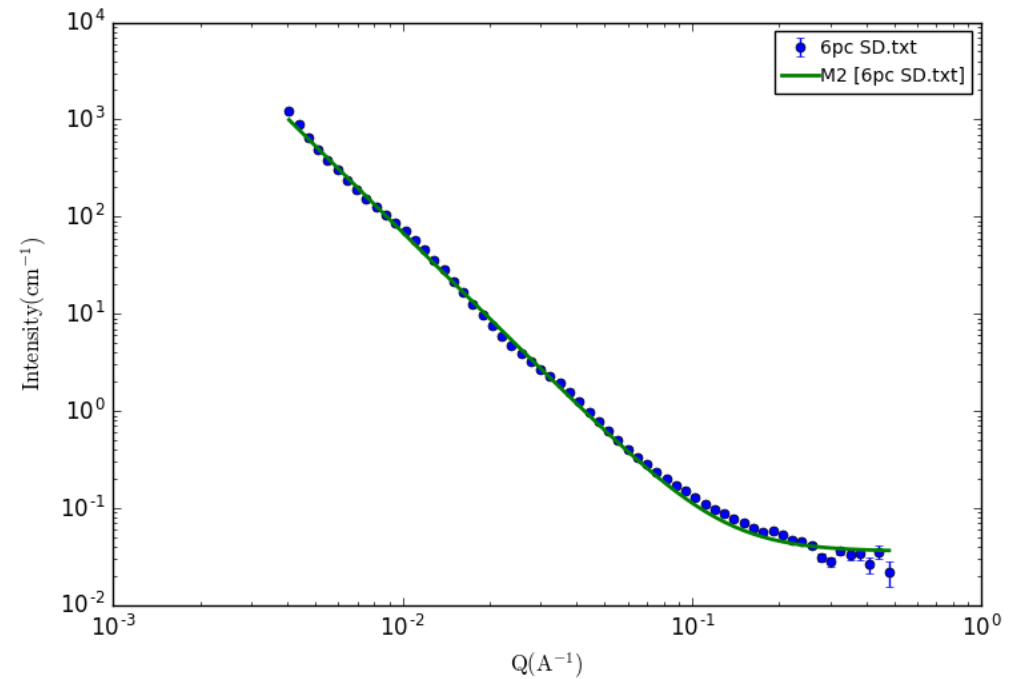
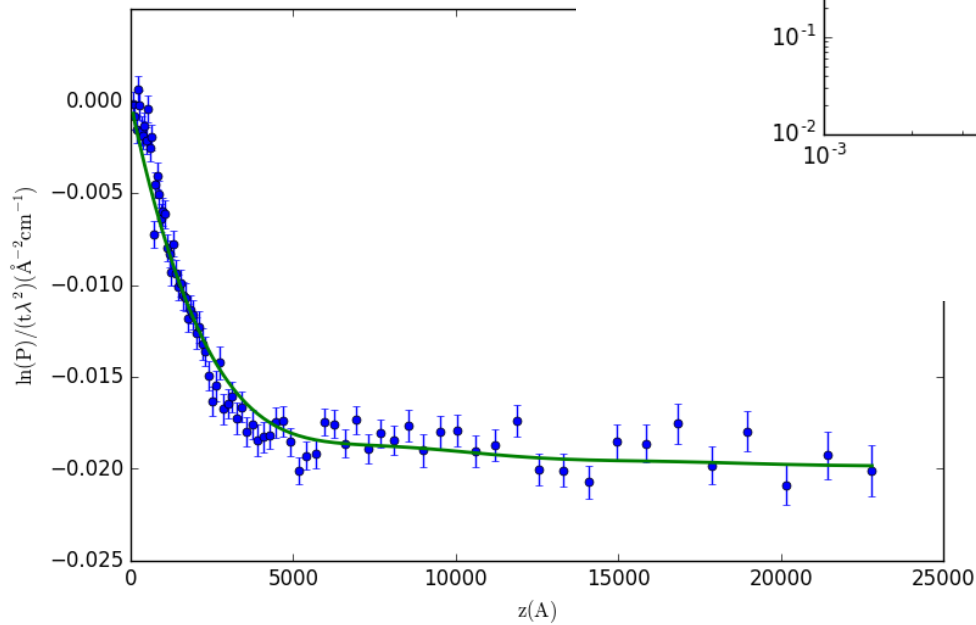
Parameter	Value	Error	Min	Max	[Units]
<input checked="" type="checkbox"/> scale	1.1915	+/- 0.00914	0	inf	
<input type="checkbox"/> background	0		-inf	inf	1/cm
<input type="checkbox"/> sld	0		-inf	inf	1e-6/Ang^2
<input type="checkbox"/> sld_solvent	6		-inf	inf	1e-6/Ang^2
<input checked="" type="checkbox"/> radius	2598.2	+/- 20.749	0	inf	Ang
<input type="checkbox"/> volfraction	0.1		0	0.74	
 - Polydispersity and Orientational Distribution: On, Off
 - Fitting: None, Use dQ Data, Custom Pinhole Smear, Custom Slit Smear. The dQ data is being used for smearing... Type: Pinhole, 13.827, dQ[%]: 1721.2
 - Set Weighting by Selecting dI Source: No Weighting, Use dI Data, Use |sqrt(I Data)|, Use |I Data|
 - Q range: Min[1/A] = 276.54, Max[1/A] = 34425.0, Masking(2D) = Editor
 - Reduced Chi2 = 10.876, Npts(Fit) = 37, Npts = 37, Log? = . Buttons: Compute, Fit, Help.
- Graph1:** A plot of $\ln(P)/(\lambda^3)(\text{\AA}^{-2}\text{cm}^{-1})$ versus $z(\text{\AA})$. The data points (blue diamonds) show a sharp initial decay followed by a plateau. A green line represents the fit model "M1 [se011953_01.ses]".
- Graph2:** A plot of "Residuals (normalized)" versus $z(\text{\AA})$. The residuals (blue diamonds) fluctuate around zero, indicating a good fit. The legend shows "Residuals for M1[se011953_01.ses]".

At the bottom of the window, a status bar indicates "Computation completed!".

Batch fit



Simultaneous fit SESANS and SANS



Joachim Kohlbrecher included also SESANS in SasFit



research papers



JOURNAL OF
APPLIED
CRYSTALLOGRAPHY

ISSN 1600-5767

Transformation cycle between the spherically symmetric correlation function, projected correlation function and differential cross section as implemented in *SASfit*

J. Kohlbrecher^{a*} and A. Studer^b

Received 16 December 2016

Accepted 18 August 2017

^aLaboratory for Neutron Scattering and Imaging (LNS), Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland, and

^bScientific Computing, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland. *Correspondence e-mail: joachim.kohlbrecher@psi.ch

Possible discussion topics extended Q -range

- Software for data-analysis
- Multiple scattering
- Anisotropic scattering in USANS and SESANS
- Combined analysis with imaging/tomography
- Combined analysis with conventional SAS
- Calibration samples