Jülich Centre for Neutron Science

Heinz Maier-Leibnitz Zentrum

# GISAS Data Analysis with BornAgain

Céline Durniak, Marina Ganeva, Gennady Pospelov, Walter Van Herck, Joachim Wuttke

May 13, 2014

Jülich Centre for Neutron Science

Heinz Maier-Leibnitz Zentrum

# Outline

- MLZ Scientific Computing Group
- A user story
- Future development and support

# Outline

- MLZ Scientific Computing Group
- A user story
- Future development and support

# MLZ

- MLZ: joint group (TUM, FZJ, HZG, HZB)
- FRM-II neutron source in Garching (Munich)

# Scientific Computing Group

- Group was founded in July 2011
- Currently 6 members:






- Responsibilities:
  - Support instruments for questions at the interface of physics and IT
  - Enhance understanding of experimental results by providing simulations
- First big project: BornAgain

# BornAgain project

- Start community  project for data analysis and simulation
- Grazing incidence small angle scattering as a first task
  - different user experiments (neutron and x-rays)
  - more generally structured than existing software
  - IsGISAXS as reference software
- Apply acquired experience to other experiments

# Outline

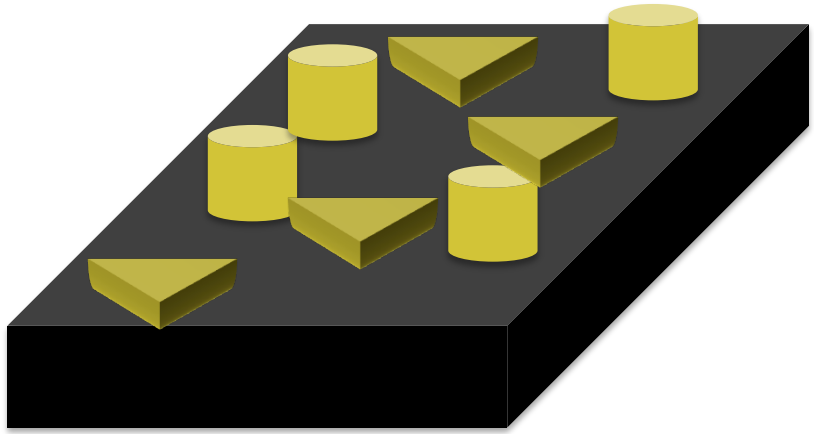
- MLZ Scientific Computing Group
- A user story
- Future development and support

# From sample to quantitative understanding

- Choice of experiment
- Theory of DWBA simulations
- Exploring the data (simulations and other techniques)
- Fitting the data

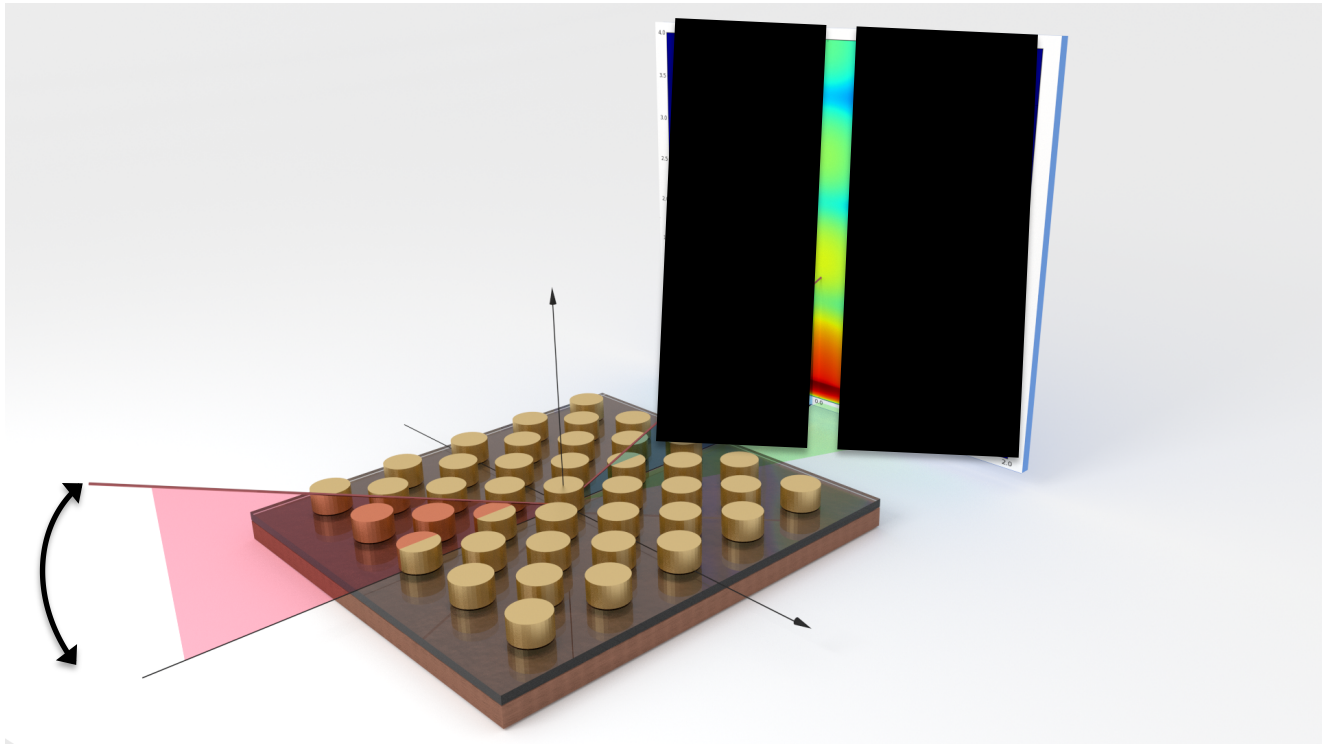
# Max' challenge

What are the dimensions of these nanoparticles?



# Choice of experiment

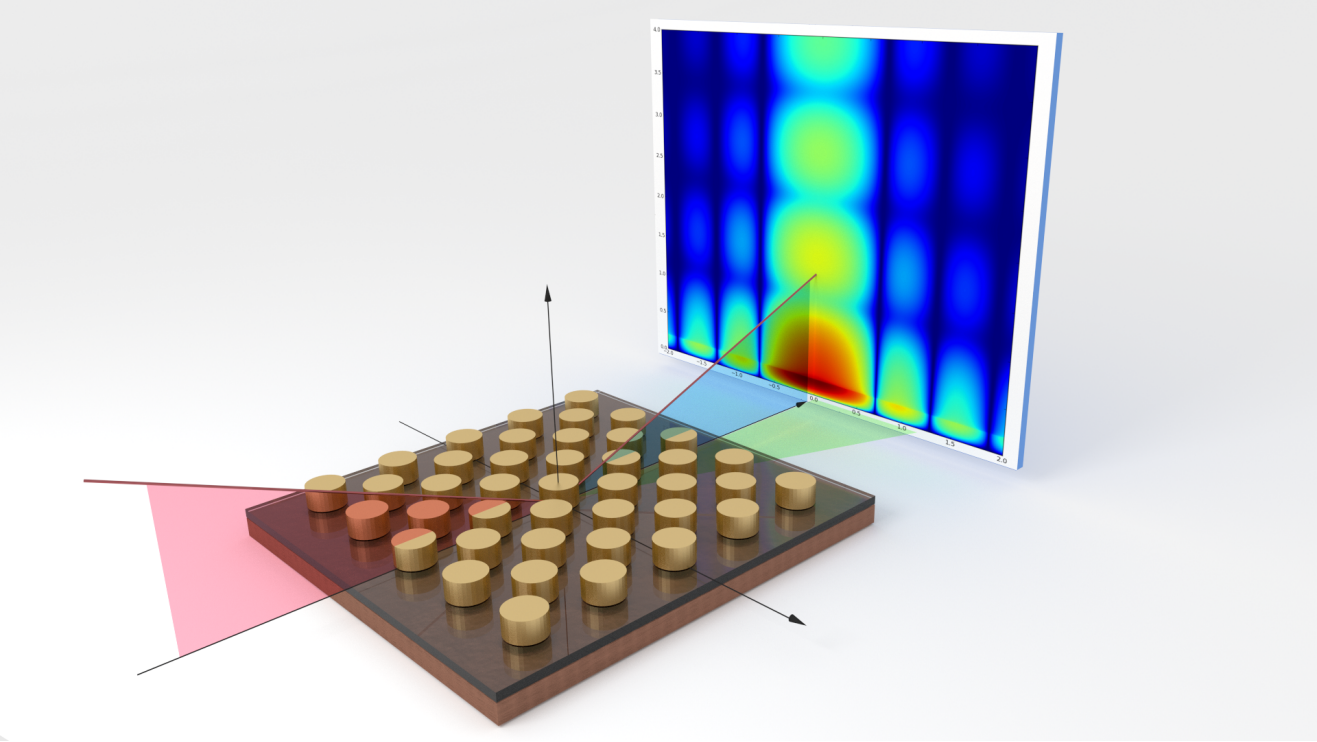
(off-specular) reflectivity GISAS



# Choice of experiment

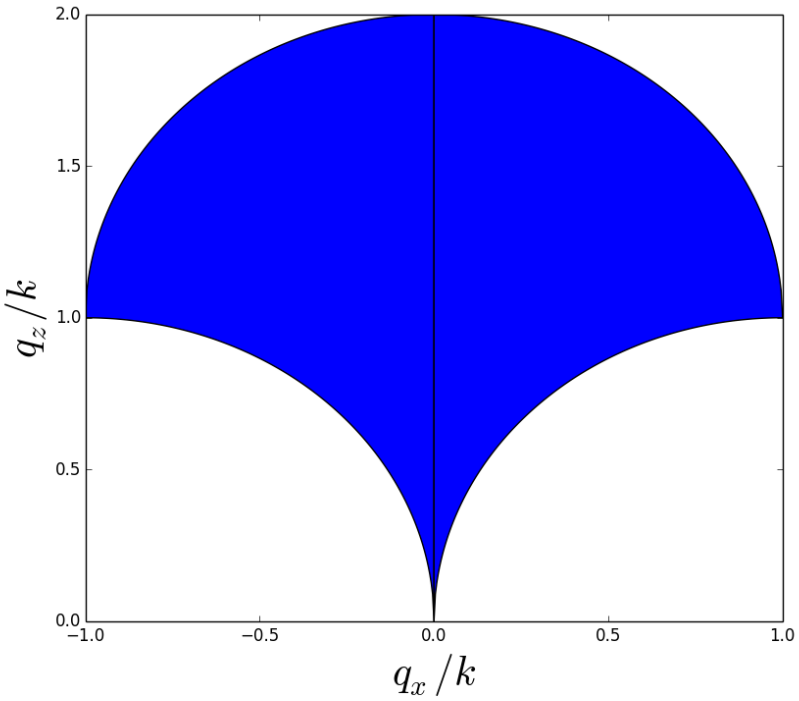
(off-specular) reflectivity

GISAS

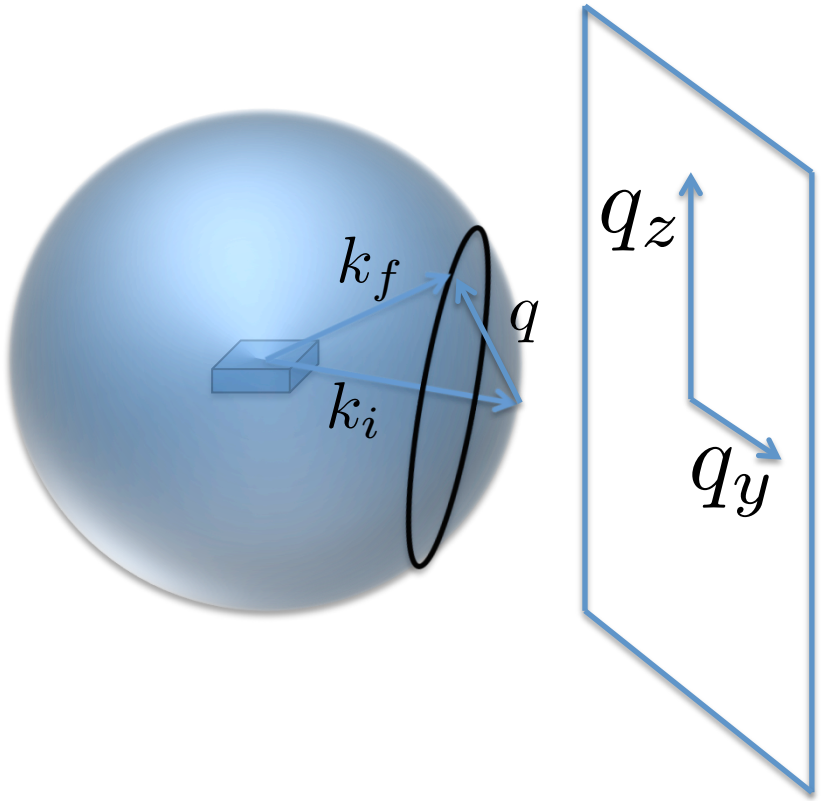


# Choice of experiment

(off-specular) reflectivity




GISAS

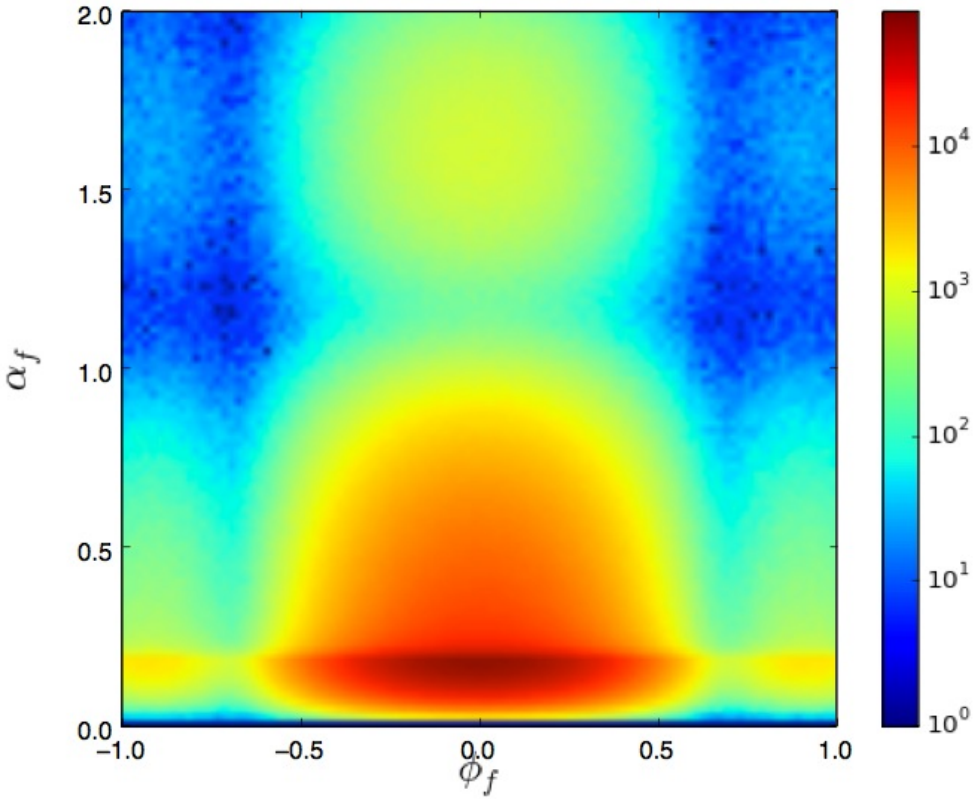


# Choice of experiment

Other choices to make:

- X-rays or neutrons
- Wavelength
- Required intensity
- Polarization
- Which instrument/facility

# GISAXS data




Remarks:

Gaussian noise

Rough estimate of particle sizes

# GISAXS data

From the workshop page:

…

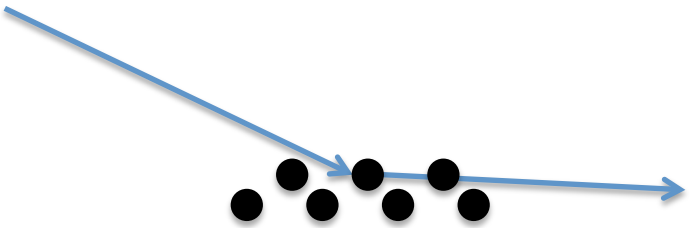
Presently, a major bottleneck preventing GISAXS from reaching its full potential persists in the availability of data analysis and modeling resources for interpreting the data. The problem arises mainly because reflections in GISAXS add to the complexity of the analysis and simulation. A common approach adopted for treating the reflection is the distorted wave Born approximation (DWBA). Several DWBA-based software packages have been developed.

…

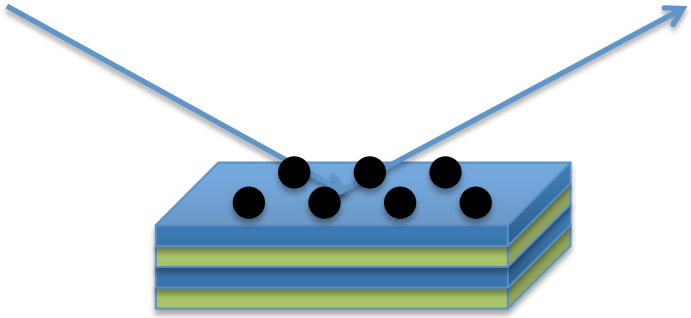
# DWBA

Perturbed Hamiltonian: $H = H_0 + V$

Born Approximation



Distorted Wave
Born Approximation



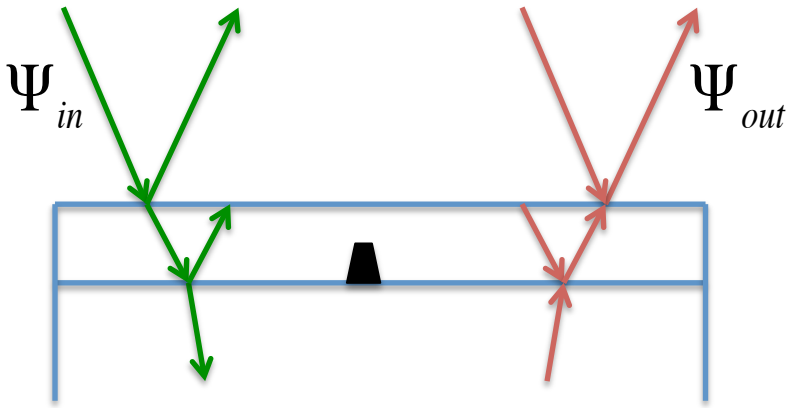
# DWBA

Scattering amplitude: $A\left(k_i, k_f\right) \approx \left\langle \Psi_{out} \middle| V(r) \middle| \Psi_{in} \right\rangle$

Born Approximation

$$\propto \int d^3r \, V(r) \exp\left[ i\left(k_i - k_f\right) \cdot r \right]$$

Distorted Wave
Born Approximation



# DWBA: interference between particles

The expectation value of the differential cross–section is:

$$\begin{aligned}\left\langle \frac{d\sigma}{d\Omega}(q) \right\rangle &= \sum_{\alpha} p_\alpha \left|F_\alpha(q)\right|^2 + \frac{\rho_V}{V} \sum_{\alpha,\beta} p_\alpha p_\beta F_\alpha(q) F_\beta^*(q) \\ &\times \iint_V d^3R_\alpha d^3R_\beta \mathcal{G}_{\alpha,\beta}\left(R_\alpha, R_\beta\right) \exp\left[iq\cdot\left(R_\alpha - R_\beta\right)\right] \\ &= I_d(q) + \left\langle F_\alpha(q) S_{\alpha\beta}(q) F_\beta^*(q) \right\rangle_{\alpha\beta}\end{aligned}$$

with:

$$I_d(q) \equiv \left\langle \left|F_\alpha(q)\right|^2 \right\rangle_\alpha - \left|\left\langle F_\alpha(q)\right\rangle_\alpha\right|^2$$

$$S_{\alpha\beta}(q) \equiv 1 + \rho_V \int_V d^3R_{\alpha\beta} \mathcal{G}_{\alpha\beta}\left(R_{\alpha\beta}\right) \exp\left[iq\cdot R_{\alpha\beta}\right]$$

# DWBA: interference between particles

Decoupling Approximation:

$$\left\langle \frac{d\sigma}{d\Omega}(q) \right\rangle = I_d(q) + \left|\langle F_\alpha(q)\rangle_\alpha\right|^2 \times S(q)$$

Local Monodisperse Approximation:

$$\left\langle \frac{d\sigma}{d\Omega}(q) \right\rangle = \left\langle \left|F_\alpha(q)\right|^2 S_\alpha(q) \right\rangle_\alpha$$

Size-Spacing Correlation Approximation:

$$D(\alpha_0, \alpha_1) = D_0 + \kappa\left[\Delta R(\alpha_0) + \Delta R(\alpha_1)\right]$$

# BornAgain features

As a start, functionality based on successful IsGISAXS software

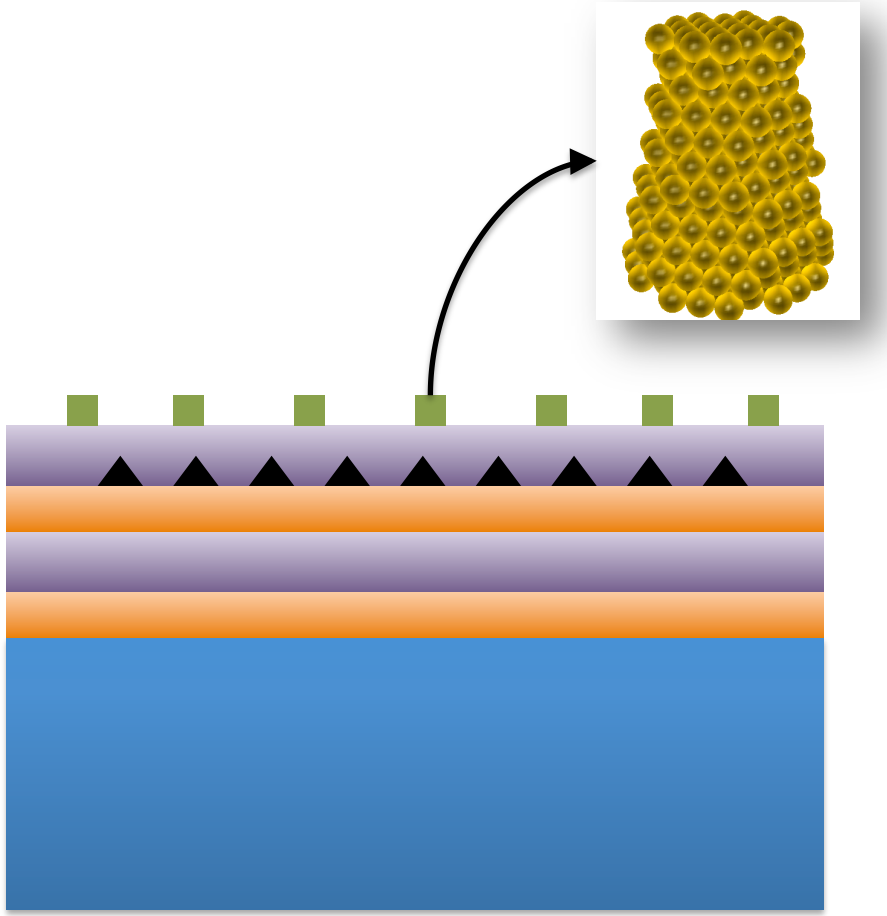
- Reproduce its functionality
- Also use DWBA
- Extend it (less restricted sample geometry, support for neutrons, usability)

Other requirements:

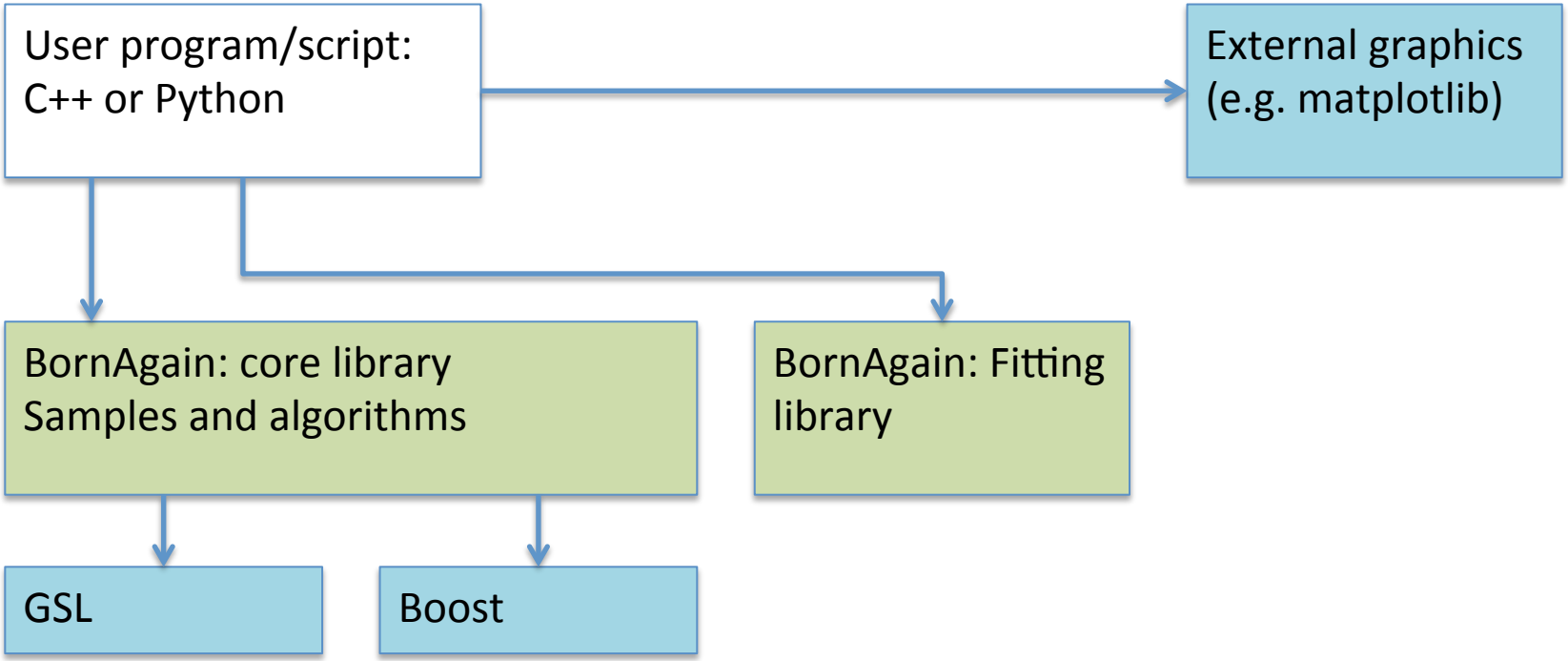
- Open source
- Multi platform (Linux, Mac OS, Windows)
- Performance

# BornAgain features

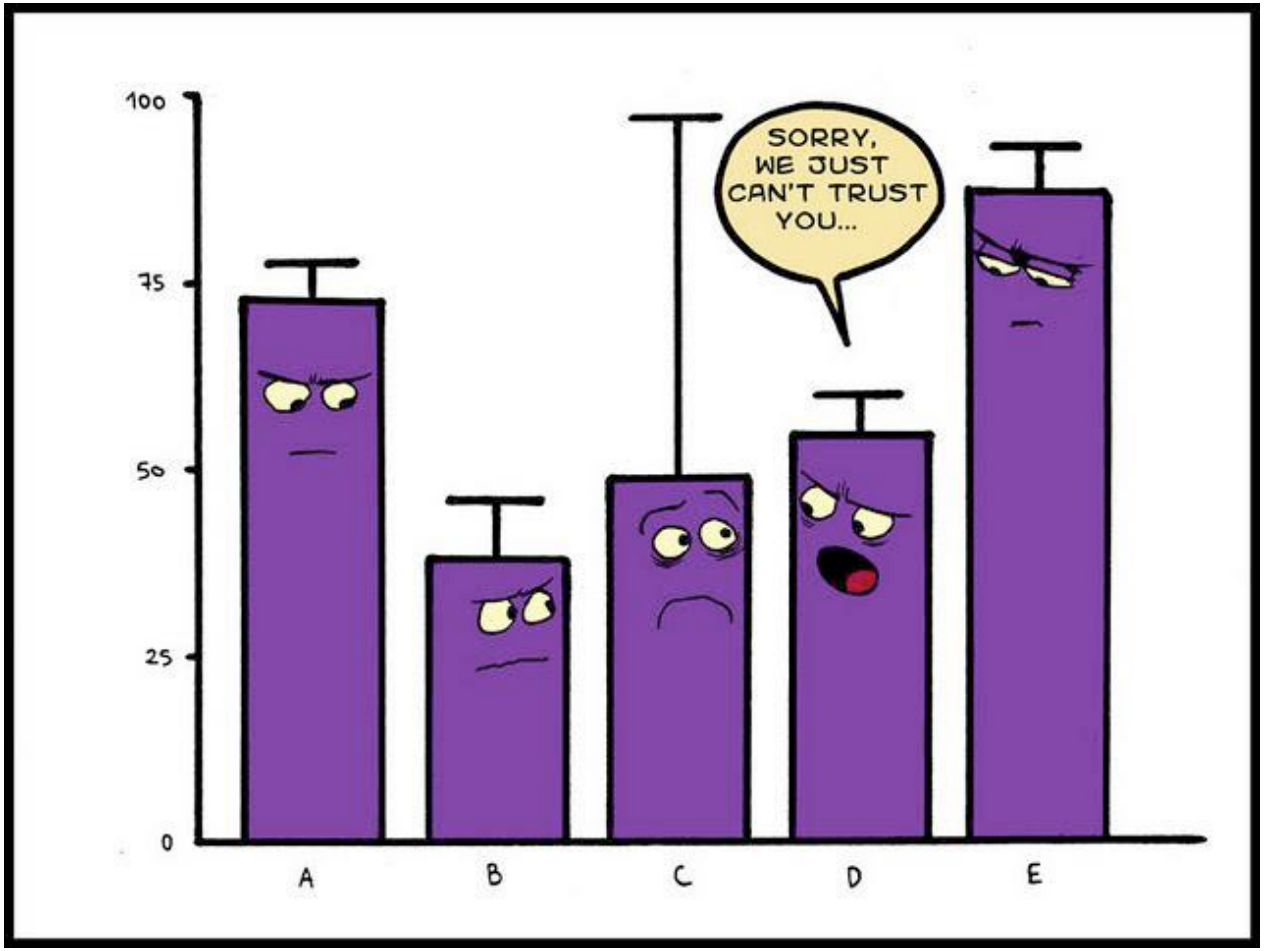
- Multilayer
- Interface roughness
- Multiple nanoparticles (shapes, densities)
- Interference functions
- Nanoparticles assemblies (mesocrystals)
- Polarized neutron scattering



# Exploring the data



# Fitting the data



# Fitting the data

I would smile now, if I wasn't a picture…

Jülich Centre for Neutron Science

Heinz Maier-Leibnitz Zentrum

# Outline

- MLZ Scientific Computing Group
- A user story
- Future development and support

# Future development

- GUI: beta release in September 2014

# Future development

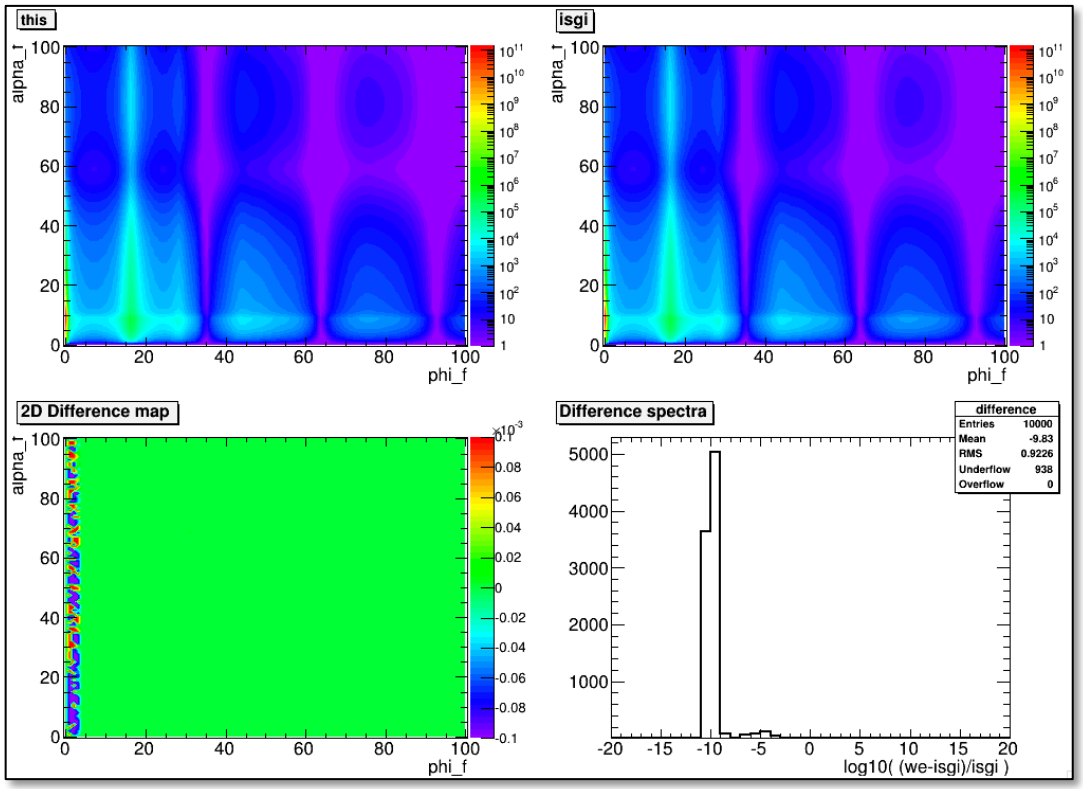
- GUI: beta release in September 2014
- Polarized GISANS: interface roughness, magnetic domains
- Performance: GPU, cluster
- More complex sample structures

# Support

Issue and bug tracker

Agile development model:

- Short release cycles
- Code quality
- Code stability: functional and unit tests



# Thank you !

For further information or questions:

http://www.bornagainproject.org

Or email me at:

w.van.herck@fz-juelich.de