GISAS Data Analysis with BornAgain

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Outline

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

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Choice of experiment

(off-specular) reflectivity

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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:

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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.

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DWBA

Perturbed Hamiltonian: $H = H_0 + V$

Born Approximation

Distorted Wave Born Approximation
**DWBA**

Scattering amplitude: \[ A(k_i, k_f) \approx \langle \Psi_{out} | V(r) | \Psi_{in} \rangle \]

**Born Approximation**

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

**Distorted Wave Born Approximation**

\[ \Psi_{in} \quad \text{and} \quad \Psi_{out} \]
DWBA: interference between particles

The expectation value of the differential cross-section is:

\[
\left\langle \frac{d\sigma}{d\Omega}(q) \right\rangle = \sum_{\alpha} p_{\alpha} |F_{\alpha}(q)|^2 + \frac{\rho V}{V} \sum_{\alpha,\beta} p_{\alpha} p_{\beta} F_{\alpha}(q) F_{\beta}^*(q)
\]

\[
\times \int_{V} \int_{V} d^3R_{\alpha} d^3R_{\beta} G_{\alpha,\beta}(R_{\alpha}, R_{\beta}) \exp [iq \cdot (R_{\alpha} - R_{\beta})] 
\]

\[
= I_d(q) + \left\langle F_{\alpha}(q) S_{\alpha\beta}(q) F_{\beta}^*(q) \right\rangle_{\alpha\beta}
\]

with:

\[
I_d(q) \equiv \left\langle |F_{\alpha}(q)|^2 \right\rangle_{\alpha} - \left| \left\langle F_{\alpha}(q) \right\rangle_{\alpha} \right|^2
\]

\[
S_{\alpha\beta}(q) \equiv 1 + \rho V \int_{V} d^3R_{\alpha\beta} G_{\alpha\beta}(R_{\alpha\beta}) \exp [iq \cdot R_{\alpha\beta}]
\]
DWBA: interference between particles

Decoupling Approximation:

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

Local Monodisperse Approximation:

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

Size-Spacing Correlation Approximation:

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

User program/script: C++ or Python

BornAgain: core library
Samples and algorithms

GSL

Boost

BornAgain: Fitting library

External graphics (e.g. matplotlib)
Fitting the data
Fitting the data

I would smile now, if I wasn’t a picture...
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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:
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