BornAgain

GISAS Data Analysis
BornAgain school & user meeting

- 19-21 December 2018, Garching bei München
Our group

- Heinz Maier-Leibnitz Zentrum (MLZ) in Garching

- Scientific Computing Group: develop and maintain software for data reduction and analysis
- BornAgain: GISAS simulation and fitting software:
  - For both expert and novice users
  - Support for polarized neutrons
  - Extensible: reflectivity, off-specular scans, ...
Simulation of GISAS experiment

During planning, execution and analysis
Architecture

- open-source
- multi-platform
- C++/Python

User

script.py

Python bindings

C++ kernel

External dependencies:
Eigen, fftw3, GSL

Standalone
GUI

External dependencies:
Qt5
Lines of code
Sample model

Object tree of sample components
Functionality

• X-rays, non-polarized and polarized neutrons
• Arbitrary number of layers
• Rough layer interfaces
• Around 20 basic particle shapes
• Complex particle shapes (mesocrystal, composition, core-shell)
• Correlated particle positions
• Off-specular geometry, reflectivity, beam divergence, noise background, ...
Development

• **Development organization:**
  • Source control: github
  • Code review: github
  • Issue tracking: Redmine
  • Management of release cycles: Redmine

• **Code stability:**
  • Continuous integration: github, buildbot
  • Unit testing: googletest
  • Functional tests: ad hoc

• **Documentation:**
  • Website: Hugo
  • Theory manual
  • API documentation: Doxygen
Exercise 1

- Gold spheres halfway buried in silicon substrate
- Radius: 5nm
- Lattice length: 10nm
- Wavelength: 1Å
- Au: $\delta=1.87e^{-5}$, $\beta=2.53e^{-6}$
- Si: $\delta=3.17e^{-6}$, $\beta=3.16e^{-8}$
- Detector: $\varphi$ in [-1, 1], $\alpha$ in [0, 2]
Exercise 2

- Polydisperse gold spheres on top of silicon substrate
- Hexagonal order
- Lattice length: 10nm
- Wavelength: 1Å
- Au: $\delta=1.87e-5$, $\beta=2.53e-6$
- Si: $\delta=3.17e-6$, $\beta=3.16e-8$
- Detector: $\varphi$ in [-1, 1], $\alpha$ in [0, 2]
- Radius distribution: lognormal with mean 5nm and scale parameter 0.15