BornAgain is a free and open source software package to simulate and fit small angle scattering at grazing incidence. It supports analysis of both X-ray and neutron data. Its name, BornAgain, indicates the central role of the distorted wave Born approximation in the physical description of the scattering process. The software provides a generic framework for modeling multilayer samples with smooth or rough interfaces and with various types of embedded nanoparticles.

Main features

Open source, multi-platform software
Inspired by established IsoGISAXS program [1]
Extended with
- support for multilayers
- Interface: roughness correlation
- Multiple types of nanoparticles in layers
- Particles with inner structure
- Polarized neutrons and magnetic scattering
Physical model based on Distorted Wave Born Approximation
- Multiple fitting engines (from ROOT and GSL)

Professional approach to software development
- Short release cycle
- Issue and bug tracking
- Version control
- Functional and unit tests
- Nightly builds

Scientific highlight

GISAXS experiment from mesocrystalline system of self-assembled iron oxide spherical nanoparticles [2]
- Nanoparticles have cylindrical shape and size about 1000 nm
- Nanoparticles are spherical with mean radius 5 nm and assemble into an FCC lattice

Quick start

http://apps.jcns.fz-juelich.de/BornAgain

on Unix platforms
1. Install third party software: Boost, GSL, fmri, numpy-devel
2. Download source code
3. Compile: cmake; make; make install
4. Run example: python CylindersAndPrisms.py

on Windows platforms
1. Install necessary Python modules
2. Run BornAgain installer
3. Run example, double-click CylindersAndPrisms.py

References:

Software design

- task driven rather then command driven approach
- high level of flexibility in sample construction
- modularity, extensibility, code reuse
- does not contain proprietary modules
- depends on only a few well-established open source libraries
- supports Python, C++, and C
- object oriented code
- dependency on third party libraries

Status

- Current release number 0.9.1
- Works under Linux, MacOS X and Windows
- IsGISAXS functionality is mostly in place, BornAgain fully agrees with IsoGISAXS
- Implemented support for neutron polarization and magnetic scattering, now validating
- Graphical User Interface is in prototyping stage

User interacts with BornAgain
- by running Python script
- through a graphical user interface (forthcoming)

Everyone is welcome to try it out