BornAgain - simulating and fitting X-ray and neutron scattering at grazing incidence.

User Guide version 0.1

Scientific Computing Group at FRM-II $\label{eq:July 17, 2013} \text{July 17, 2013}$

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Contents 0.1. Introduction

0.1 Introduction

BornAgain is a software to simulate and fit neutron and X-ray scattering at grazing incidence. It is a multi-platform open—source project that aims at supporting scientists in the analysis and fitting of their GISAS data, both for synchrotron (GISAXS) and neutron (GISANS) facilities. The name of the software, BornAgain indicates the central role of the distorted-wave Born approximation (DWBA) 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. In this way, it reproduces and enhances the functionality of the present reference software, IsGISAXS by R. Lazzari [?], and lays a solid base for future extensions in response to specific user needs.

To meet the growing demand for GISAS simulation of more complex structured materials, BornAgain has extended the IsGISAXS program's functionality by removing the restrictions on the number of layers and particles, by providing diffuse reflection from rough layer interfaces and by adding particles with inner structure.

The user guide starts with a brief description of steps necessary for compiling and running the simulation, Section 0.2. More detailed overview of software architecture and installation procedure is given in Section ??. General methodology of simulation with BornAgain and detailed usage examples are given in Section ??. Fitting tools provided by the frame work are presented in Section ??.

Contents 0.2. Quick start

0.2 Quick start

This section shortly describes how to build BornAgain from source and run first simulation. More details about software architecture and installation procedure are given in Section ?? and Section ??.

Step I: installing third party libraries

- boost library (≥ 1.48)
- GNU scientific library (≥ 1.15)
- fftw3 library ($\geq 3.3.1$)
- Eigen3 library ($\geq 3.1.0$), optional
- ROOT framework ($\geq 5.34.00$), optional

Step II: getting the source

```
git clone git://apps.jcns.fz-juelich.de/BornAgain.git
```

Step III: building the source

```
mkdir <build_dir>; cd <build_dir>;
cmake <source_dir> -DCMAKE_INSTALL_PREFFIX=<install_dir>
make
make check
make install
```

Step IV: running example

```
cd <install_dir>/Examples/python/ex001_CylindersAndPrisms
python CylindersAndPrisms.py
```

Bugs

License agreement

Directory layout

FAQ

Future development.