

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

User Guide
version 0.1

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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 0.4. 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 ???.

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 0.3 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_PREFIX=<install_dir>  
make  
make check  
make install
```

Step IV: running example

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

0.3 Software architecture

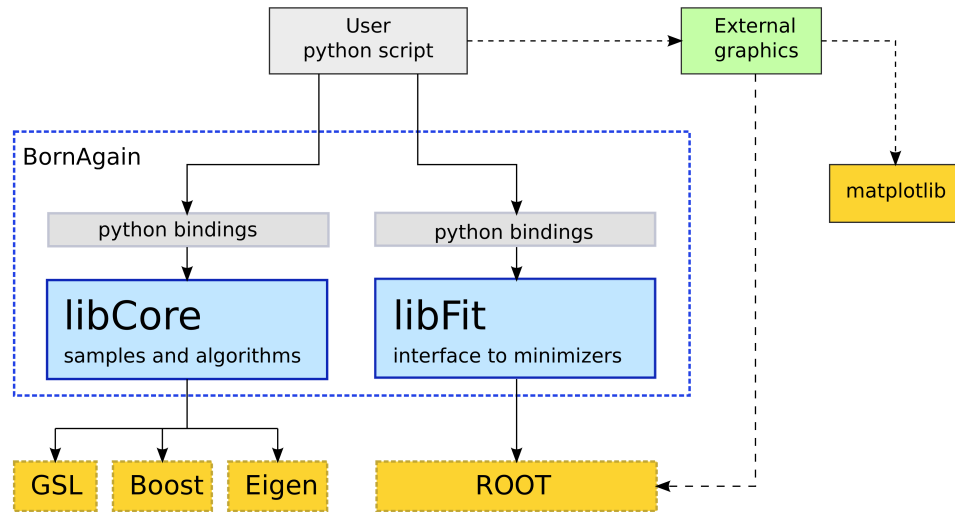


Figure 1: Left:

0.4 Installation

This section shortly describes how to build **BornAgain** from source and run first simulation.

0.4.1 Installation hints

In this section we give short installation instruction for several selected operation systems.

OpenSuse 12.3

Adding “scientific” repository

```
sudo zypper ar http://download.opensuse.org/repositories/science/
openSUSE_12.3 science
```

Installing obligatory packages

```
zypper install gsl-devel boost-devel fftw3-devel python-numpy-devel
```

Installing optional packages

```
sudo zypper install libroot-* root-plugin-* root-system-* root-ttf
libeigen3-devel
```