

# BornAgain

status report for ESS DMSC & reflectometry STAP, October 2020

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**Introduction**

Randolf Beerwerth

**Python API**

Gennady Pospelov

**new GUI**

Joachim Wuttke

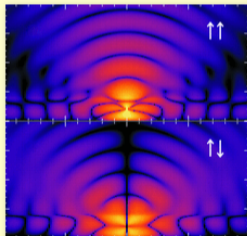
**Outlook**



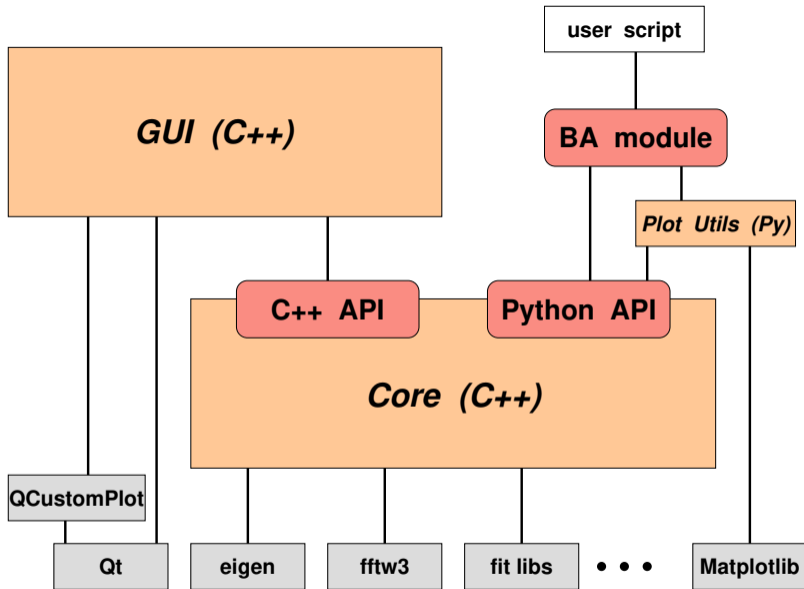
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## February 2020 issue



Cover illustration: An example application of the *BornAgain* software [Pospelov *et al.* (2020). *J. Appl. Cryst.* **53**, 262-276]. Polarized GISANS from vertically magnetized spherical nanoparticles on top of a substrate. The two simulations correspond to scattering (top) without and (bottom) with spin flip, assuming perfect vertical beam polarization and perfect polarization analysis.



## **Strong points** of current BornAgain GISAS GUI:

- tools to mask, project, fit 2D detector images
- graphical sample builder (LabView style)
- export to Python

## **Weak points:**

- no undo/redo
- no project back-compatibility
- strained architecture
- unusual workflow
- no way to build periodic multilayers

## Status

- new middleware Qt-MVVM is stable
- undo/redo works
- multilayer builder is complete

## Release 2.0 $\leq$ October 2021

- support full sample models
- support reflectometry fits

## Further milestones

- co-refinement
- polarized reflectometry
- off-specular and GISAS (terminate old GUI)

**Why BornAgain** though we have GenX, Motofit, Refnx, RasCAL, ...?

**How to win over users** from GenX, Motofit, Refnx, RasCAL, ...?

## **We have**

Windows, MacOS, Linux

Debian, Ubuntu, CentOS, ScientificLinux, Arch, ...

Fortran, C++, Python, Julia, ...

Word, LaTeX

McStas, Vitess, Geant4

IsGisaxs, BornAgain

## **And so we will have**

GenX, Motofit, Refnx, RasCAL, ..., and BornAgain



Overtake capitalism without catching up — Walter Ulbricht ca 1958

Implement union of functionality of extant software?

(we did it for IsGisaxs)

- **Too much:** some features never used
- **Too little:** won't win over seasoned users

The better path:

- Enable new data analyses
- Collaborate with domain experts (i. e. YOU)

## Limited resources

- 1–2 FTEs from JCNS
- ESS contribution to be specified
- other stakeholders?
- neutron money for x-ray software??

## Division of work

- JCNS computing group → engineering
- NN → implementation
- application experts (i.e. YOU) → theory & test data

## **Driven by internal logic**

Consolidate kernel, simplify API

Migrate to GUI2

Support co-refinement

Visualize SLD(z)

Work out polarized scattering by magnetic roughness

## **Respond to user requests**

We want YOUR data to challenge us

We need YOUR experience to build the right models