

BornAgain

software for reflectometry and GISAS, made by JCNS

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Non-functional requirements

- Fully open source
- Cross-platform (Windows, Linux, Mac)
- Long-term institutional commitment:
survived change of developer team
- Professional development practices:
version control, issue and bug tracking, code review, good test coverage, nightly builds, frequent releases
- C++ core for maximum speed
- Well documented:
2 papers; web site with API reference and huge example collection (covered by tests)

Functional requirements

- Reproduces and extends functionality of orphaned legacy code IsGisaxs
- Instruments: reflectometry, off-specular, GISAS, depthprobe
- Full support for polarized neutrons
- Sample: flexible user-controlled multilayer model, with rough interfaces and arbitrary assemblies of nanoparticles
- Numerically stable R&T computation
- Scattering simulation in DWBA
- Steered from GUI or Python script
- GUI highlights: detector masking, parameter sliding, real-space visualization, export to Python
- Various fit engines

Principal authors:

- Gennady Pospelov (2012-2021)
- Walter Van Herck (2012-2020)

Current maintainers:

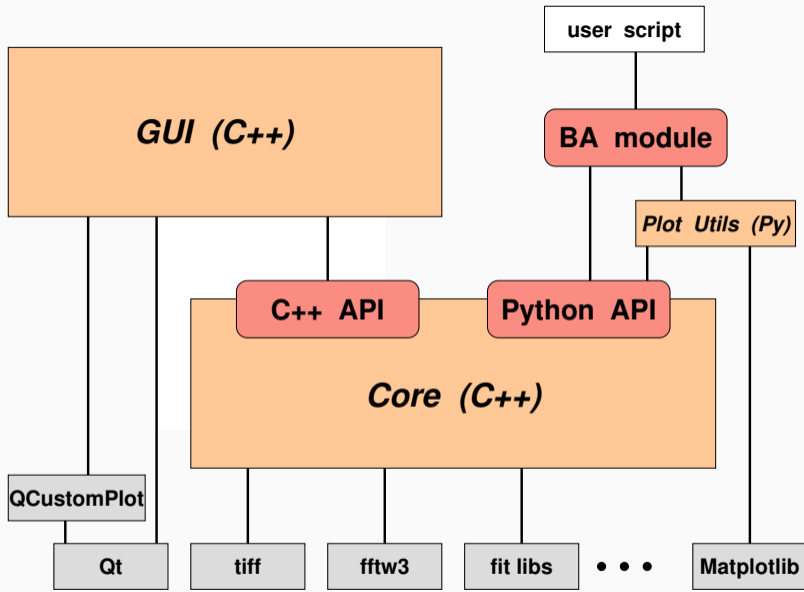
- Ammar Nejati (2021-)
- Mikhail Svechnikov (2022-)
- Joachim Wuttke (2012-)

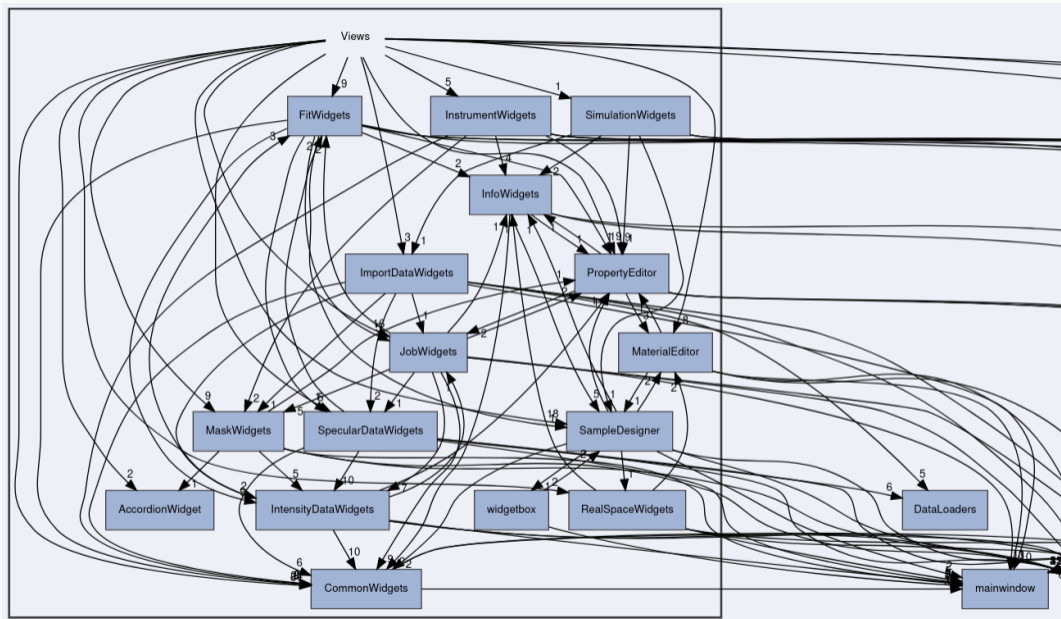
Former collaborators:

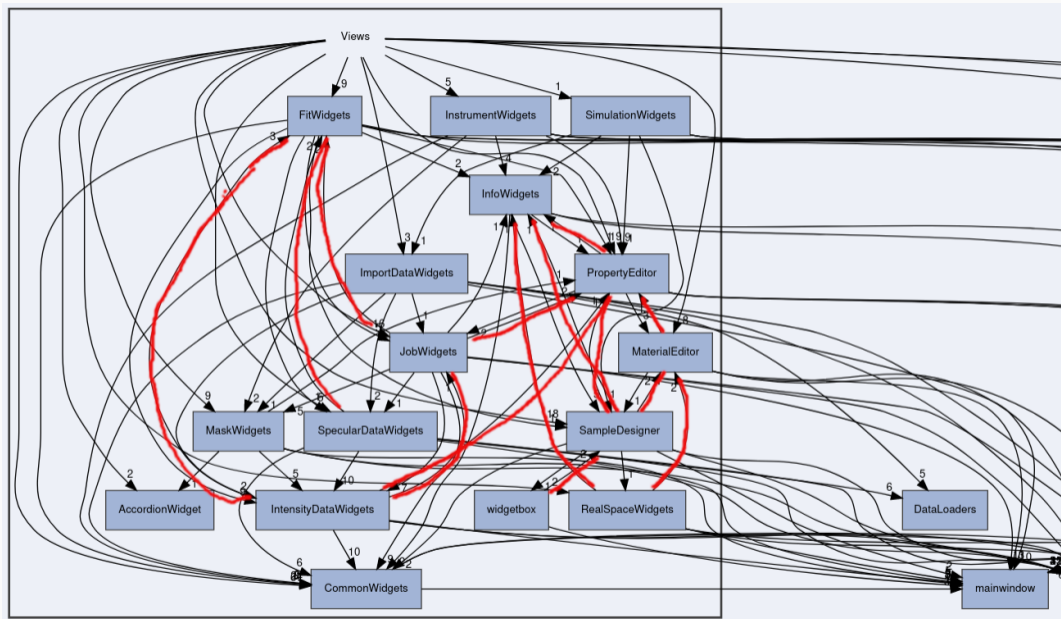
- Céline Durniak (2013-2015)
- Marina Ganeva (2013-2019)
- Jonathan Fisher (2016-2017)
- Jan Burle (2016-2017)
- Dmitry Yurov (2017-2019)
- Juan Carmona Loaiza (2018-2020)
- Alexander Schober (2020)
- Randolph Beerwerth (2020-2021)
- Matthias Puchner (2020-2022)
- Tobias Knopff (2021)

Timeline

2012		project started
2013	0.7.0	first preview
2015	1.0.0	first release
2017	1.8.0	fully reproduced IsGisaxs
2017–2021		ESS funding for extension to reflectometry
2019	1.16.0	paper → J Appl Cryst
2020	1.17.0	Van Herck departs
2021	1.19.0	Pospelov departs
2023	20.0 ... 21.1	deployment: binaries for Python 3.8–11 at PyPI paper → EPJ Web Conf
2024	21.2 ...	consolidation continues







BornAgain source code w/o tests, examples:

	v19.0 (mar21)	current (jul24)	
lines (w/o blank, comment)	107k	71k	−34%
files	1628	1145	−30%
classes	1166	700	−40%
“template”	387	152	−61%
“variant”	159	37	−77%
“dynamic_cast”	417	505	+21%

After v19.1, about 2k2 lines moved to libheinz, libformfactor.

- Continual user support
- Further simplification
- Support off-specular and ToF reflectometry
- Extend the sample model
- Improve usability

Not yet thought through

- Document actual computation in LaTeX / PDF
- Raise warnings if computation is questionable for given model and parameters
- Do better than Monte-Carlo for rapidly oscillation scattering function
- Do better than numeric integration for small / large q
- Improve support for parameter distributions
- How does scattering affect reflected and transmitted beam?