

# Plan of the school

## What's new in BornAgain

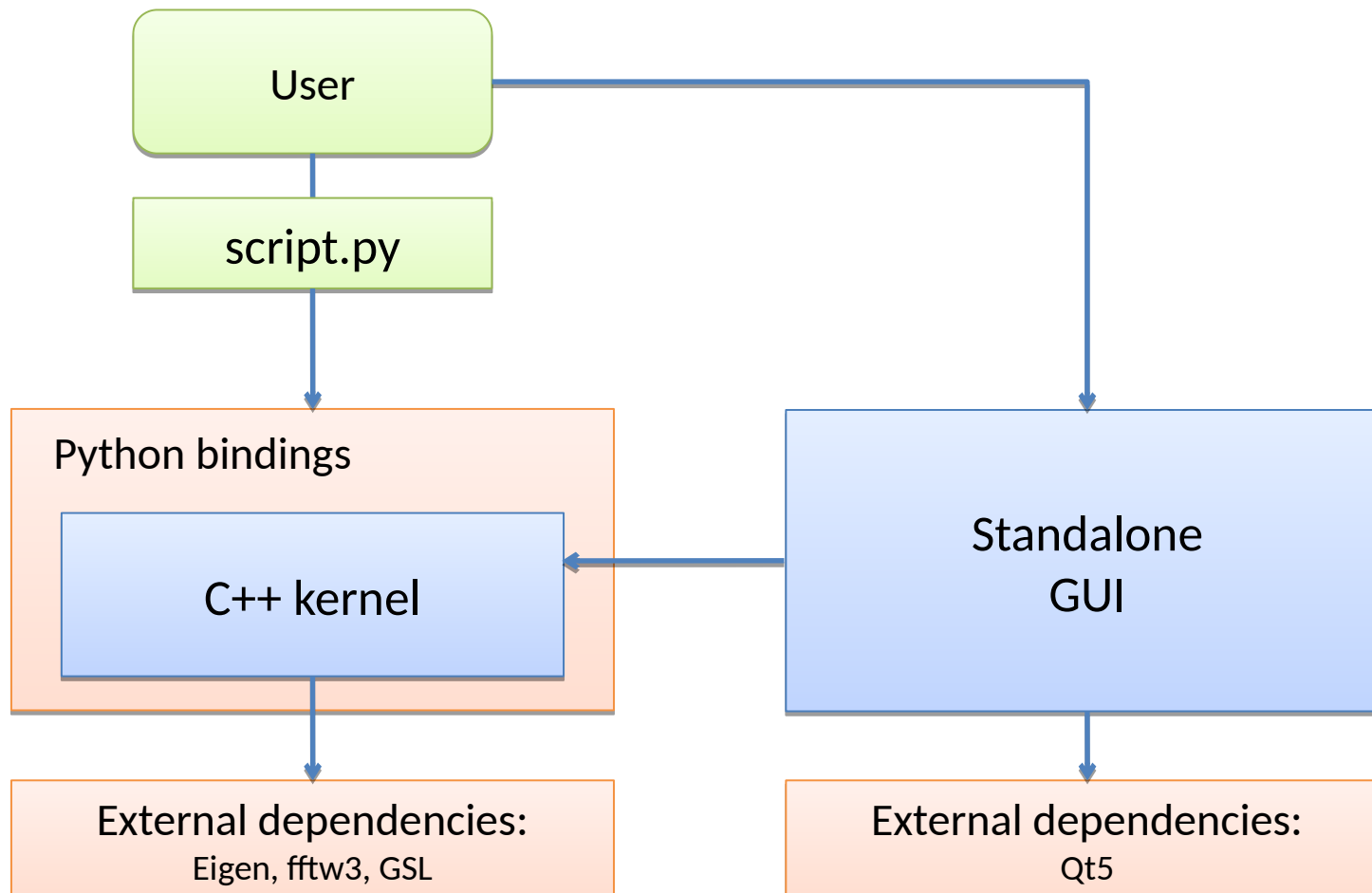
Gennady Pospelov  
Jülich Centre for Neutron Science at MLZ

BornAgain school and user meeting  
Garching, December 2018

day\_1

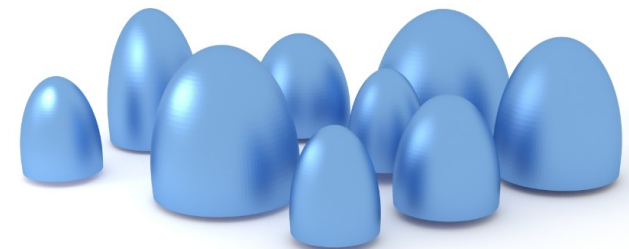
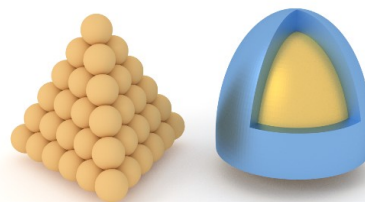
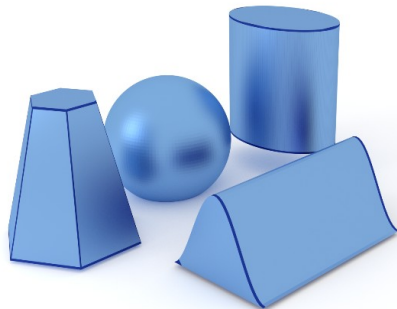
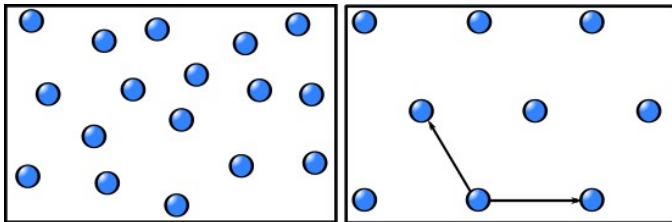
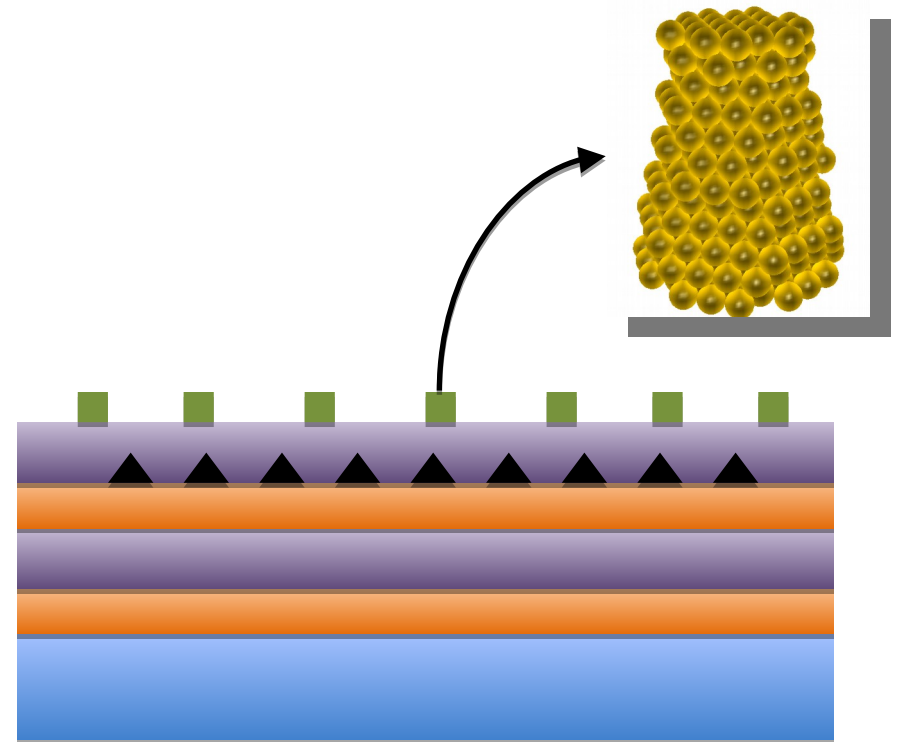
# Software architecture

- Open source, GPL3 license, 200k lines of code
- Multi platform: Windows, Mac OS, Linux
- C++ kernel for simulation/fitting, Python bindings, GUI

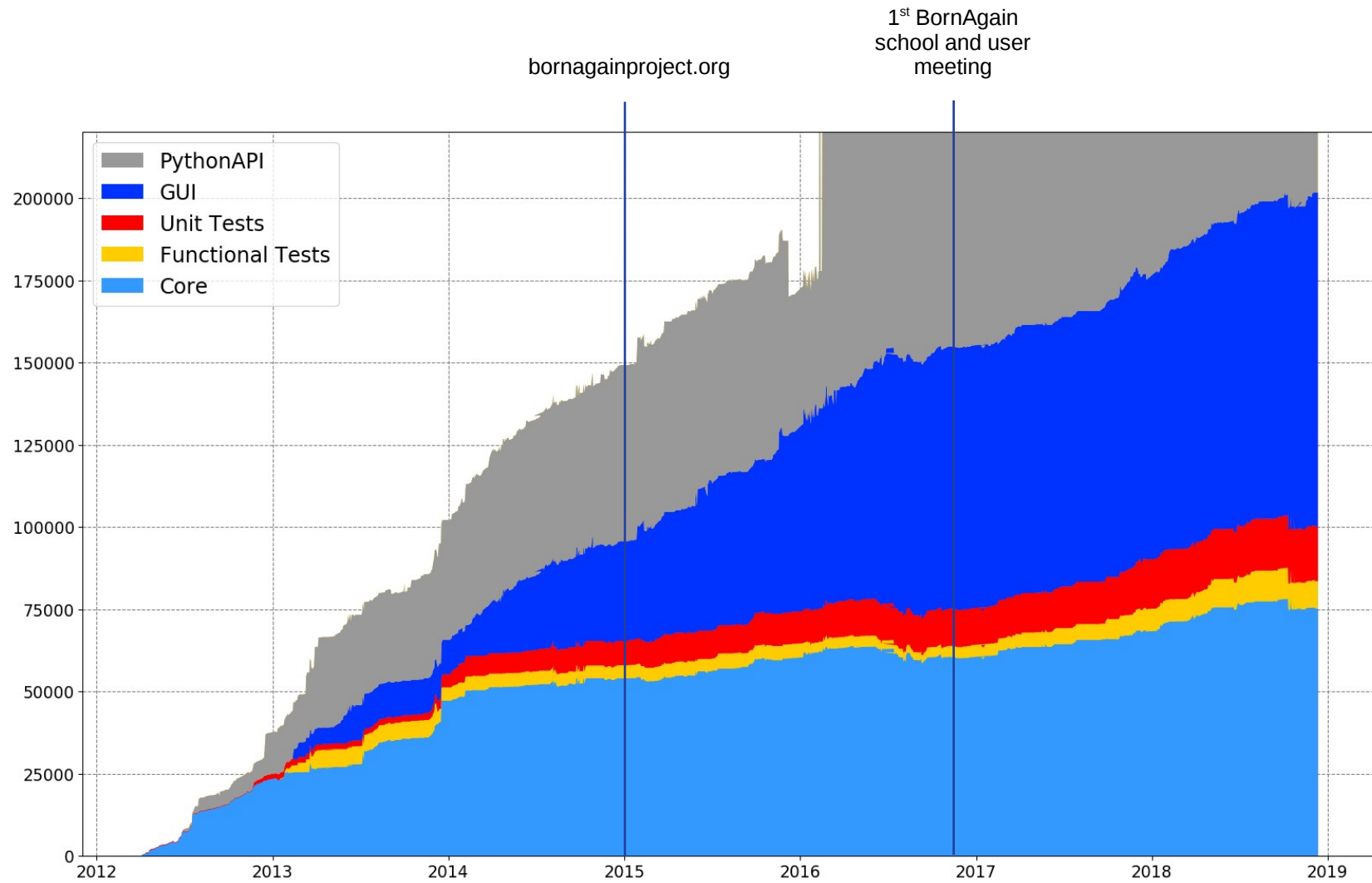


# Functionality overview

- X-rays, non-polarized and polarized neutrons
- Arbitrary number of layers
- Rough interfaces
- Simple and composite particles
- Correlated positions
- Nanoparticle assemblies
- Off-specular and specular setups
- Instrument effects



# Lines of code



# Release history

Version	Date	Features
1.0	Jan 2015	Graphical user interface, website <a href="http://bornagainproject.org">bornagainproject.org</a>
1.1	Apr 2015	New form factors, beam divergence in GUI, export GUI to Python
1.2	Jun 2015	Working on user manual, GUI real time
1.3	Jul 2015	New functional test machinery, new tutorials
1.4	Nov 2015	Rectangular detector, genetic fitting, fitting along slices, tutorials
1.5	Feb 2016	C++11 migration, GUI mask editor, new tutorials
1.6	Jun 2016	Python 3, GUI fitting beta, Windows 32 -> Windows 64
1.7	Nov 2016	BornAgain school and user meeting, specular peak, GitHub migration, new build server
1.8	Apr 2017	Graded interfaces, improved fitting support in GUI
1.9	Jul 2017	New magnetization formalism, GUI saving mechanism
1.10	Oct 2017	Mesocrystals in GUI, Plugin mechanism
1.11	Mar 2018	Off-specular simulation in GUI, specular in Core, SLD materials
1.12	May 2018	Specular simulation in GUI, depth probe simulation, new web site
1.13	Oct 2018	Fitting reflectometry in GUI, 3D View in GUI, external minimizers
1.14	Dec 2018	Material fitting, depth probe in GUI, import 1D data

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# School program

<https://indico.frm2.tum.de/event/150/>

<

Wed 19/12

Thu 20/12

Fri 21/12

All days

>

Print

PDF

Full screen

Detailed view

Filter

Session legend

Break

GISAS

GUI Basics

Introduction

see more...

09:00	<div><div><b>Python tutorial: Install BornAgain 1.14.0 and Python</b></div><div><i>Dr Alexander Schober</i></div><div>Conference room A (ground floor), gate Garching Technologie- und Gründerzentrum</div><div>09:00 - 10:00</div></div>
10:00	<div><div><b>Python tutorial: Part I</b></div><div><i>Dr Alexander Schober</i></div><div>Conference room A (ground floor), gate Garching Technologie- und Gründerzentrum</div><div>10:00 - 10:40</div></div>
	<div><div><b>Break: Coffee break</b></div><div>Conference room A (ground floor), gate Garching Technologie- und Gründerzentrum</div><div>10:40 - 11:00</div></div>
11:00	<div><div><b>Python tutorial: Part II</b></div><div>Conference room A (ground floor), gate Garching Technologie- und Gründerzentrum</div><div>11:00 - 13:00</div></div>
12:00	

# Plan of the school

## Day\_1 (today)

- GUI overview
  - setup instrument, sample construction, 3D-view, simulations
- GISAS theory
- GUI basics I
  - Particle positioning, rotation, embedded particles, particle composition
  - Particles with size distribution
- GUI basics II
  - Interference functions, graded interfaces, roughness
- GUI basics III
  - Fitting in GUI
- User session



# Plan of the school

## Day\_2 (tomorrow)

- Python API
  - Simulation from Python, complex lamellar example, new fitting API
- GISAS for soft matter
  - Lecture of Prof. P. Müller-Buschbaum
- Introduction to reflectivity I
  - Materials, theory
- Introduction to reflectivity II
  - Simulate/fit reflectivity from GUI
  - Reflectivity via Python API
- Polarized neutrons
  - Polarized SANS/GISANS, magnetic materials
- User session
- Optional “fit your own data”

# Plan of the school

## Day\_3 (Friday)

- Introduction to git and GitHub
- Complex samples
  - Mesocrystals, large particles, supperlattice
  - Density gradients, diffuse scattering
- Advanced geometry
  - Evanescent wave, off-specular simulation
- Advanced simulations with BornAgain API
  - Data generation for machine learning
  - Making GISAS movies

# School materials

<https://github.com/scgmlz/BornAgain-tutorial>

scgmlz / **BornAgain-tutorial**

Unwatch

5

Star

0

Fork

3

<> Code

Issues 0

Pull requests 0

Projects 0

Wiki

Insights

Settings

BornAgain tutorial

Edit

Manage topics

163 commits

2 branches

0 releases

5 contributors

GPL-3.0

Branch: master


New pull request

Create new file

Upload files

Find file

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 mganeva

 particles tutorial

Latest commit 7ec49e4 3 hours ago

bornagain-python	pdf go the talk	2 years ago
gennady/python-api	First part of PythonAPI tutorial	4 days ago
marina	particles tutorial	3 hours ago
python	delete obsolete latex slides	2 years ago
quickstart	ignore .DS_Store	6 days ago
talks	Add cross-correlation to roughness notebook	12 hours ago
.gitignore	Add notebook and helper functions for interference functions	4 days ago
LICENSE	Initial commit	2 years ago
Program.md	Program for 2018	6 days ago
README.md	Update README.md	2 years ago

README.md

# School materials

<https://github.com/scgmlz/BornAgain-tutorial>

scgmlz / **BornAgain-tutorial**

Unwatch ▾

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🔔 Issues 0

🔗 Pull requests 0

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BornAgain tutorial

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📄 163 commits

🌿 2 branches

📦 0 releases

👤 5 contributors

📄 GPL-3.0

Branch: master ▾


New pull request

Create new file

Upload files

Find file

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 mganeva particles tutorial Latest commit 7ec49e4 3 hours ago

📁 bornagain-python	pdf go the talk	2 years ago
📁 gennady/python-api	First part of PythonAPI tutorial	4 days ago
📁 marina	particles tutorial	3 hours ago
📁 python	delete obsolete latex slides	2 years ago
📁 quickstart	ignore .DS_Store	6 days ago
📁 talks	Add cross-correlation to roughness notebook	12 hours ago
📄 .gitignore	Add notebook and helper functions for interference functions	4 days ago
📄 LICENSE	Initial commit	2 years ago
📄 Program.md	Program for 2018	6 days ago
📄 README.md	Update README.md	2 years ago

📄 README.md

# School materials

Materials related to given topic are located in corresponding sub folder, for example

## School program

BornAgain-tutorials/talks/day\_1/plan\_of\_the\_school\_G  
school\_plan.pdf

## GISAS theory

BornAgain-tutorials/talks/day\_1/gisas\_theory\_W  
GISAS\_theory.ipynb

## GUI basics III

BornAgain-tutorials/talks/day\_1/gui\_basics\_3\_G  
gui\_basics\_3.pdf  
SpheresAtHexLattice

# BornAgain in a web browser

<https://bornagain.its.kfa-juelich.de>

20 virtual machines, Ubuntu 18.04, Python 3.6.7, BornAgain 1.14

Username: bornagain01 – bornagain40

Password: BornAgain.01 – BornAgain.40

