BornAgain: A software to simulate and fit GISAS

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Walter Van Herck, Joachim Wuttke

Garching, 21 nov 2016

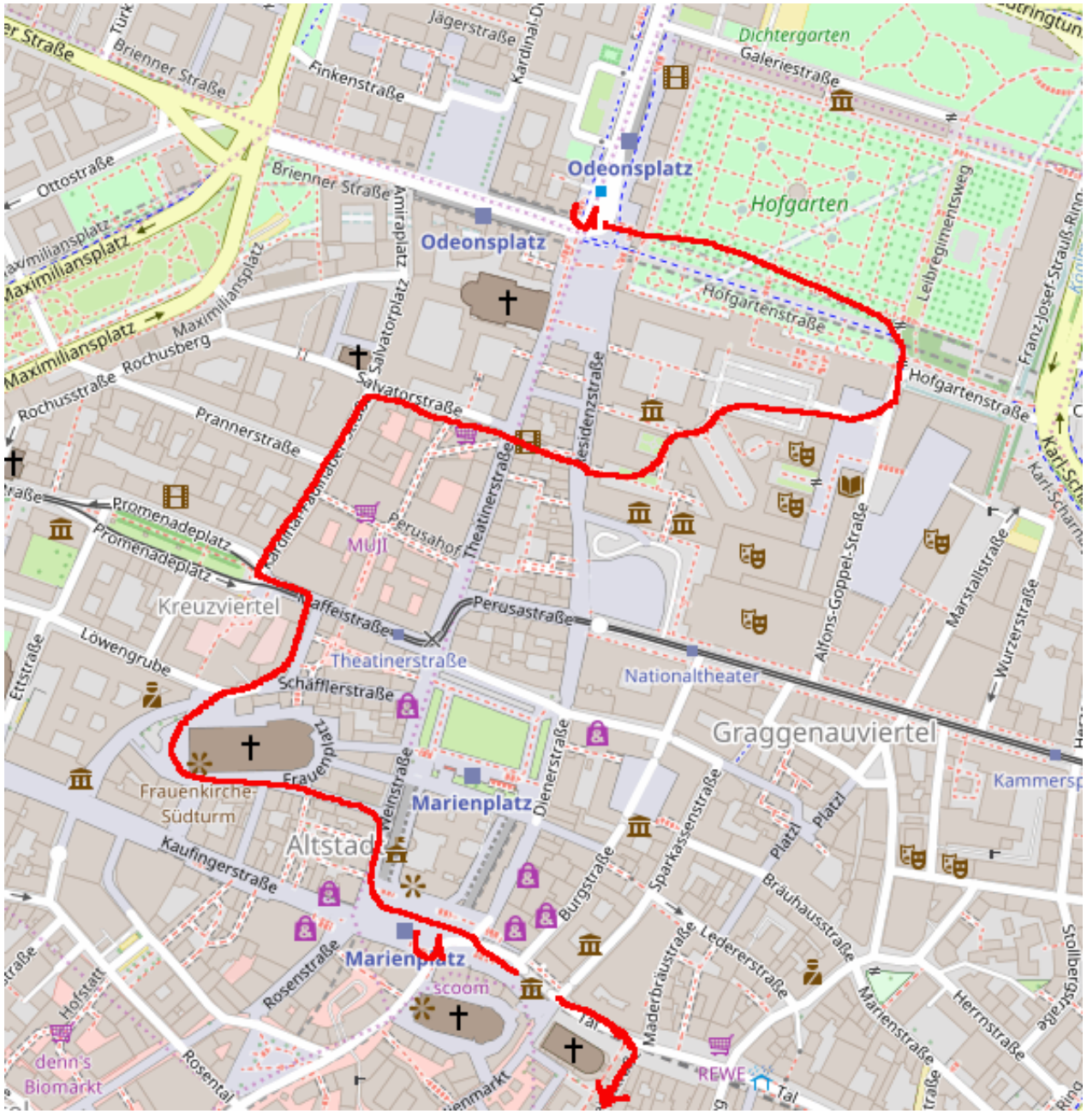
MLZ is a cooperation between

JÜLICH FORSCHUNGSZENTRUM

Helmholtz-Zentrum Geesthacht
Zentrum für Material- und Küstenforschung

Technische Universität München


WIRT


Odeonsplatz
Hofgarten
Dichtergarten
Galeriestraße
Brienner Straße
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Jägerstraße
Ottostraße
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Hofgartenstraße
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Franz-Josef-Strauß-Ring
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Rochusberg
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Prannerstraße
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Rosenstraße
Hofstatt
scoom
Mäderbräustraße
Marienstraße
Herrnstraße
Stollbergstraße
denn's Biomarkt
Rosental
Tal
REWE

Conference Dinner

Today 19h45, Marktwirt, Heiliggeiststraße 2

leave GATE	18h10	18h50
U6 Garching-Forschungszentrum	18h26	19h06
U6 Garching	18h29	19h09
U6 Garching-Hochbrück	18h31	19h11
U6 München-Odeonsplatz	18h50	
U6 München-Marienplatz		19h32
meet at Marktwirt	19h45	19h45

Conference Program

Mon	14-17	BornAgain introduction and tutorial
	17-18	Poster session
Tue	9-13	BornAgain tutorial ctd
	13-14	Lunch offered
	14-17	User talks, discussion

User Talks

Tuesday 14h

Hard matter

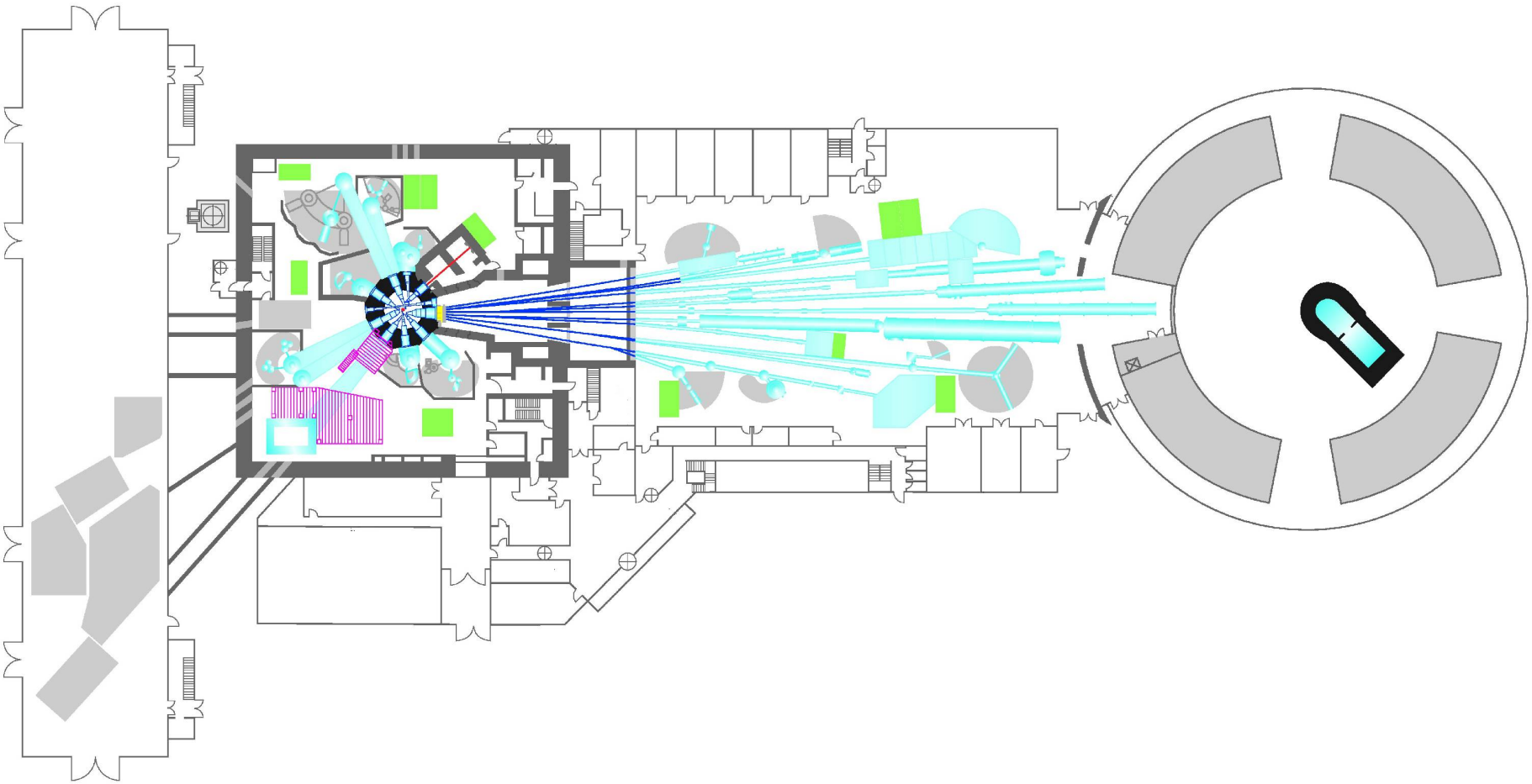
Emmanuel	Polarized GISANS from lateral spin correlations
Dieter	Dy/Y multilayers and off-specular magnetic scattering
Henrich	Resonator
Mika	Reconstruction of Structure Parameters

Soft matter

Deniza	Geometrical structure of ultrasmall Au9 nanoclusters
Jacqui	Dye aggregation in dye-sensitized solar cells
Olaf	Reverse hexagonal phase of self-assembled lipids

Final discussion

Artur	Real-world challenges in GISAS
Joachim	Outlook

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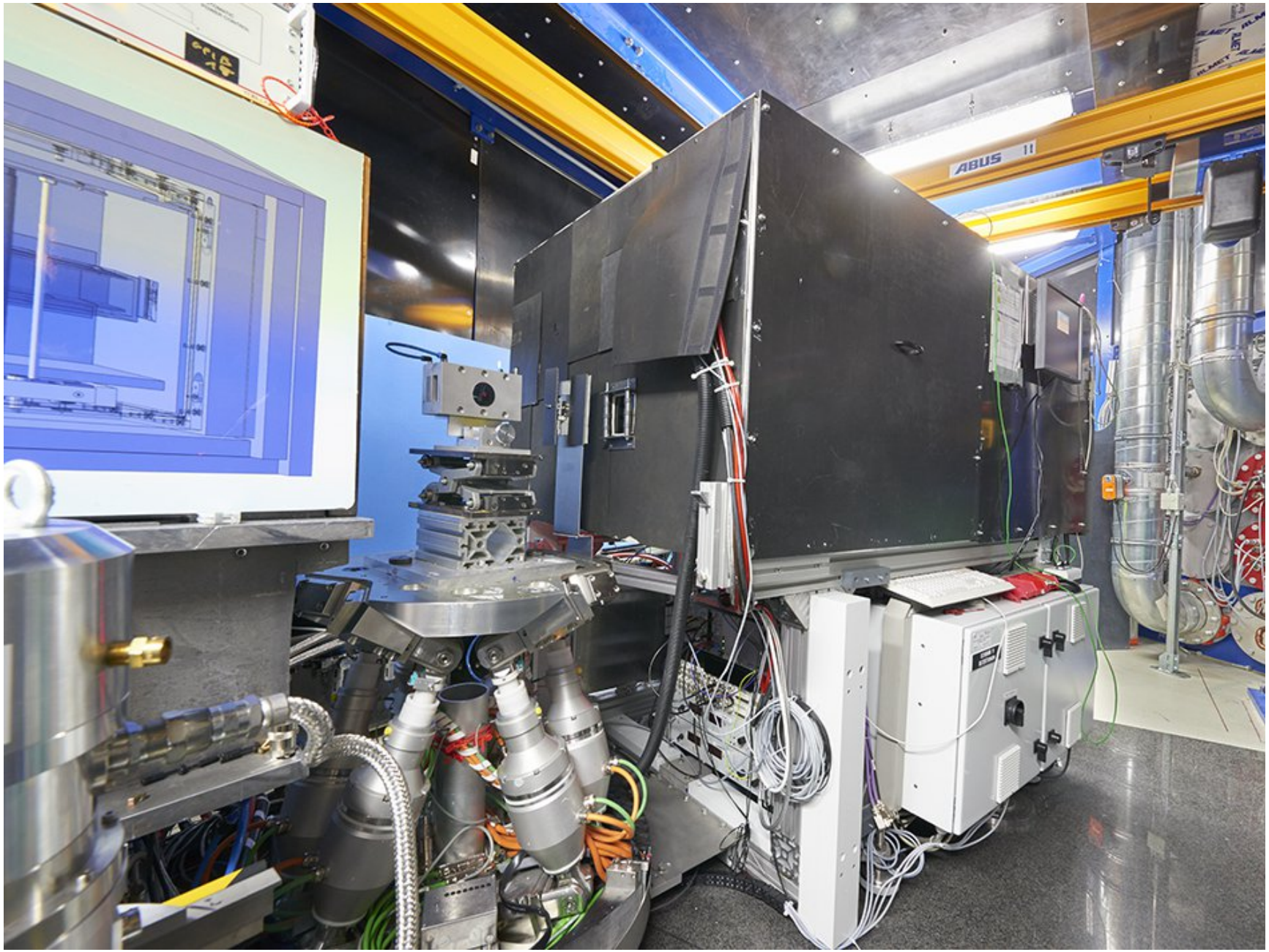
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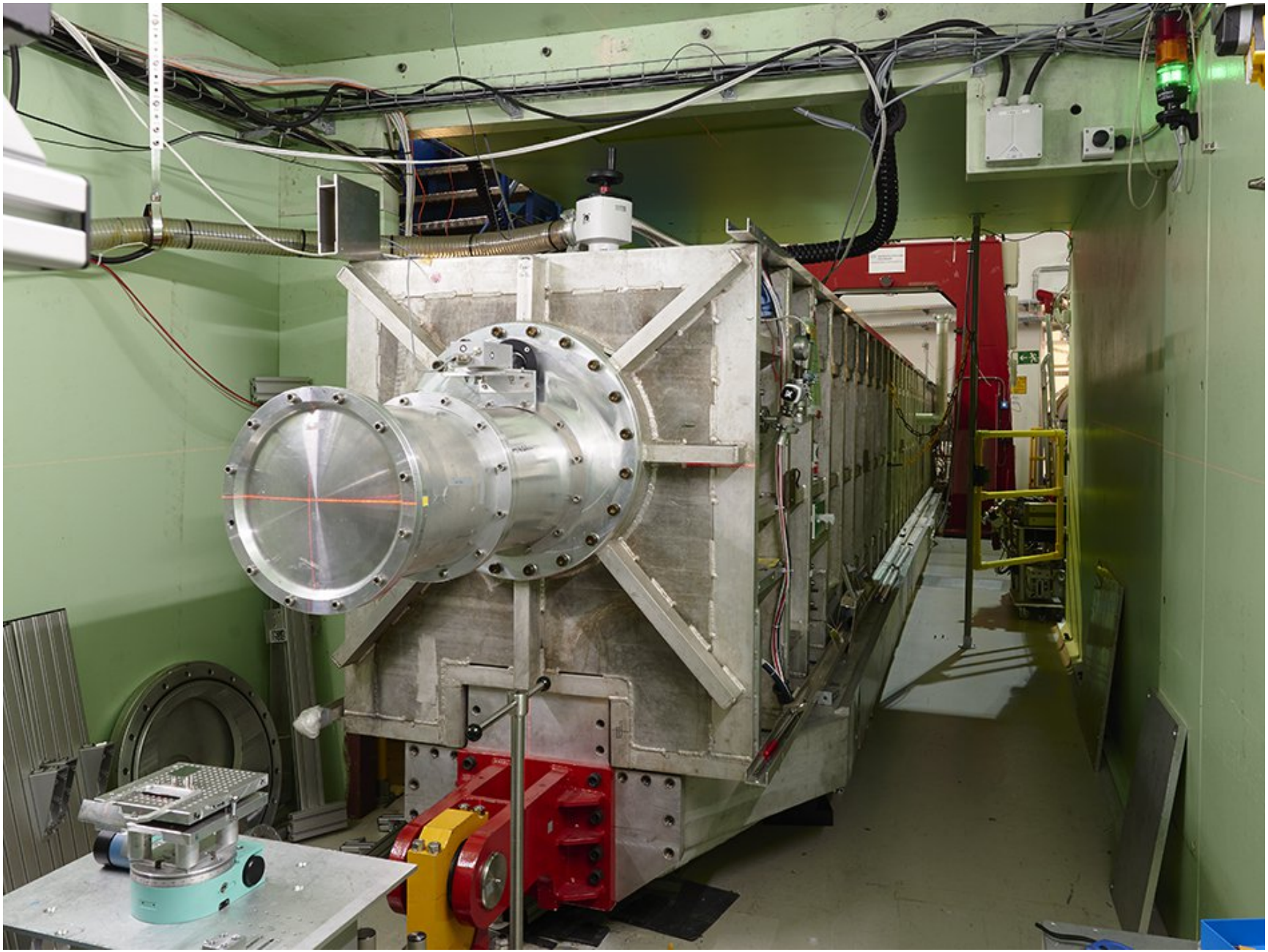

research reactor FRM II at Garching near Munich

scientific use through Heinz Maier-Leibnitz Zentrum (MLZ)

MLZ Heinz Maier-Leibnitz Zentrum

JÜLICH FORSCHUNGSZENTRUM

Helmholtz-Zentrum Geesthacht
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Scientific Computing Group at MLZ Garching

Mission:

- develop/adapt/maintain software
  for data reduction and analysis
  at neutron scattering instruments of MLZ

Staff:

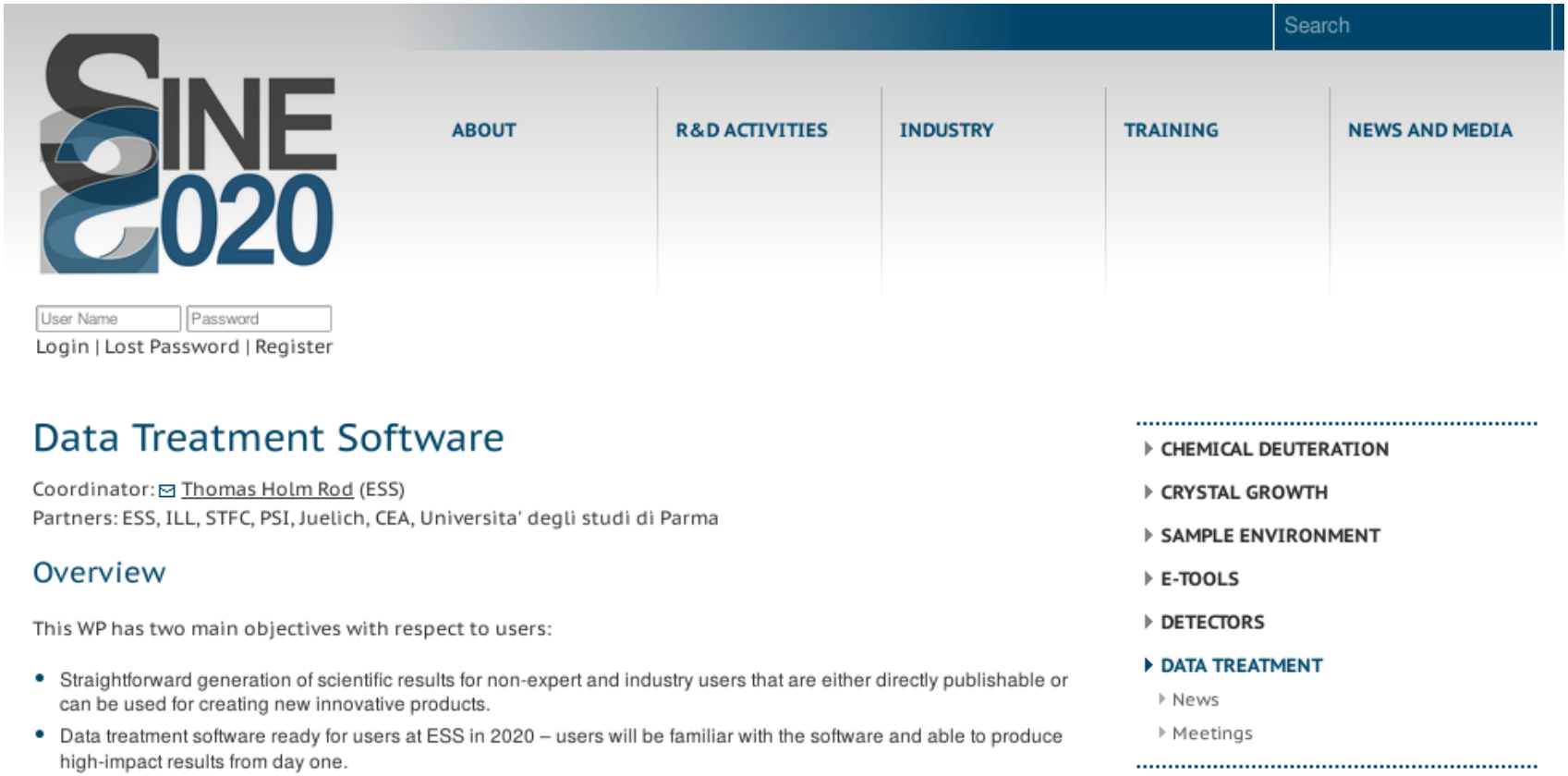
- five scientist-developers on core budget
- one position from EU SINE2020
- future collaborations with Univ Erlangen, ESS Lund

Initial projects:

- Data reduction for time-of-flight spectrometers
- Data reduction for materials diffractometer
- Simulation and fitting of GISAS

SINE2020

Science & Innovation with Neutrons in Europe in 2020



International division of tasks

SINE2020 workpackage 10: data treatment software

Technique	Facility	Software
Reflectometry	MLZ	BornAgain
QENS	ISIS	Mantid/Vates
Atomistic modelling	ILL	nMoldyn, DFT
SANS	ESS	SASView
Imaging	PSI	MuhRec/KipTool

Wishlist

Scientific software should be

- correct
- efficient
- easy to use
- documented (*and* have open code)
- adaptable, extensible (*also* by users)
- long-term available (*in extremis* by forking)

Scientific software development standards

Each software project should have

- clear licence status
- institutional support commitment
- no personal ownership, no dependence on single person
- well-chosen dependence on standard libraries and tools
- version control
- unit and functional test coverage
- automated builds and tests for all supported platforms
- web home page, mailing list, issue tracker
- short release cycles
- channels for user feedback

why GISAS simulation software?

- fit data
- support semi-quantitative or qualitative data analysis
- train experimentalists' intuition

why new GISAS simulation software?

to simulate

- multilayers
- polarized scattering
- magnetic domains

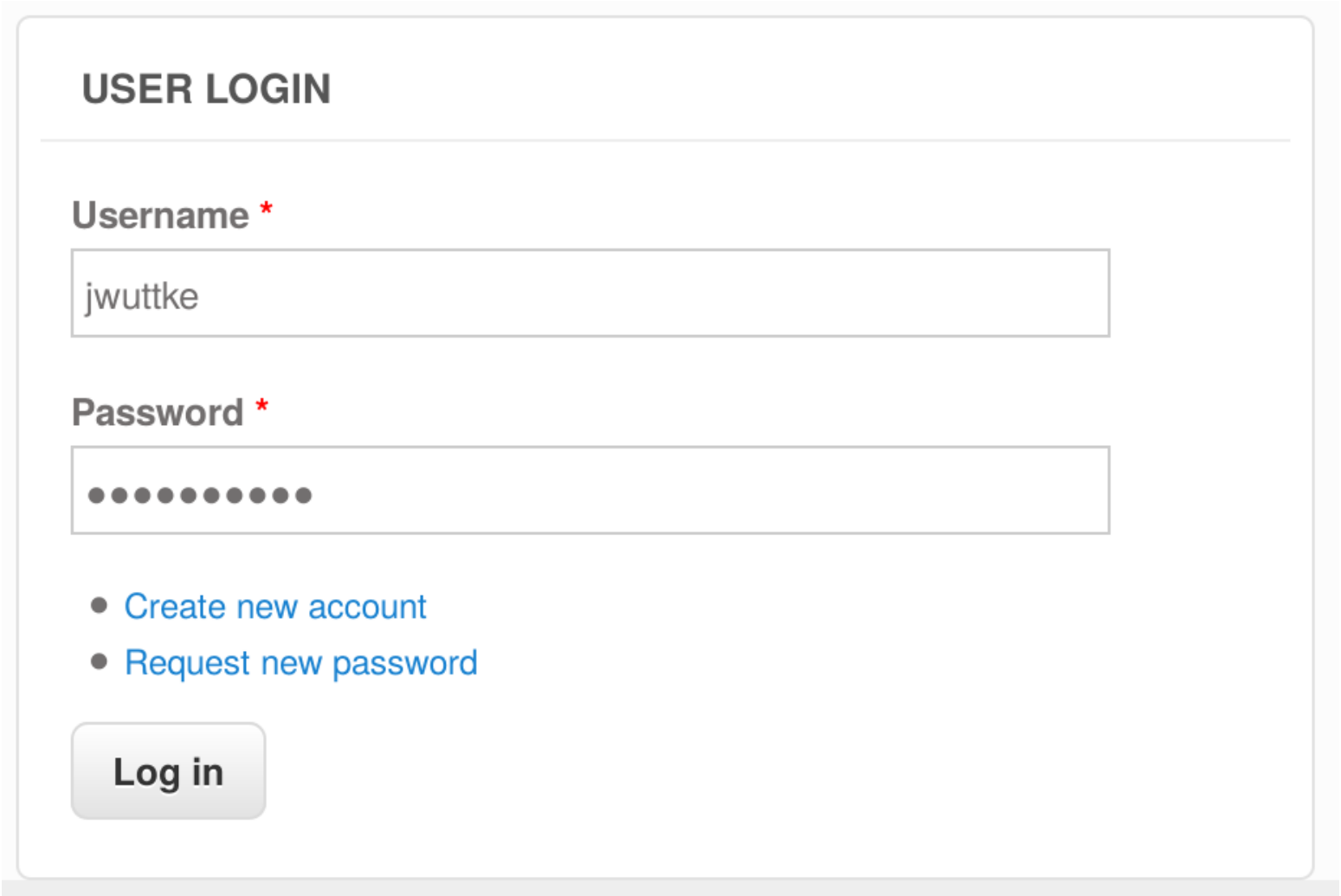
to support

- polarized neutron reflectometer MARIA
- X-ray reflectometer GALAXI
- in-house research
- user community at large


BornAgain
Simulate and fit grazing incidence small angle scattering
Home
Screenshots
Download
Documentation
Contact
Forums
About
Simulate your GISAS experiment
Welcome to BornAgain
BornAgain is a software package to simulate and fit small-angle scattering at grazing incidence. It supports analysis of both X-ray (GISAXS) and neutron (GISANS) data. Its name, BornAgain, indicates the central role of the distorted wave Born approximation 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.

Support

register to receive announcements or post to the forum



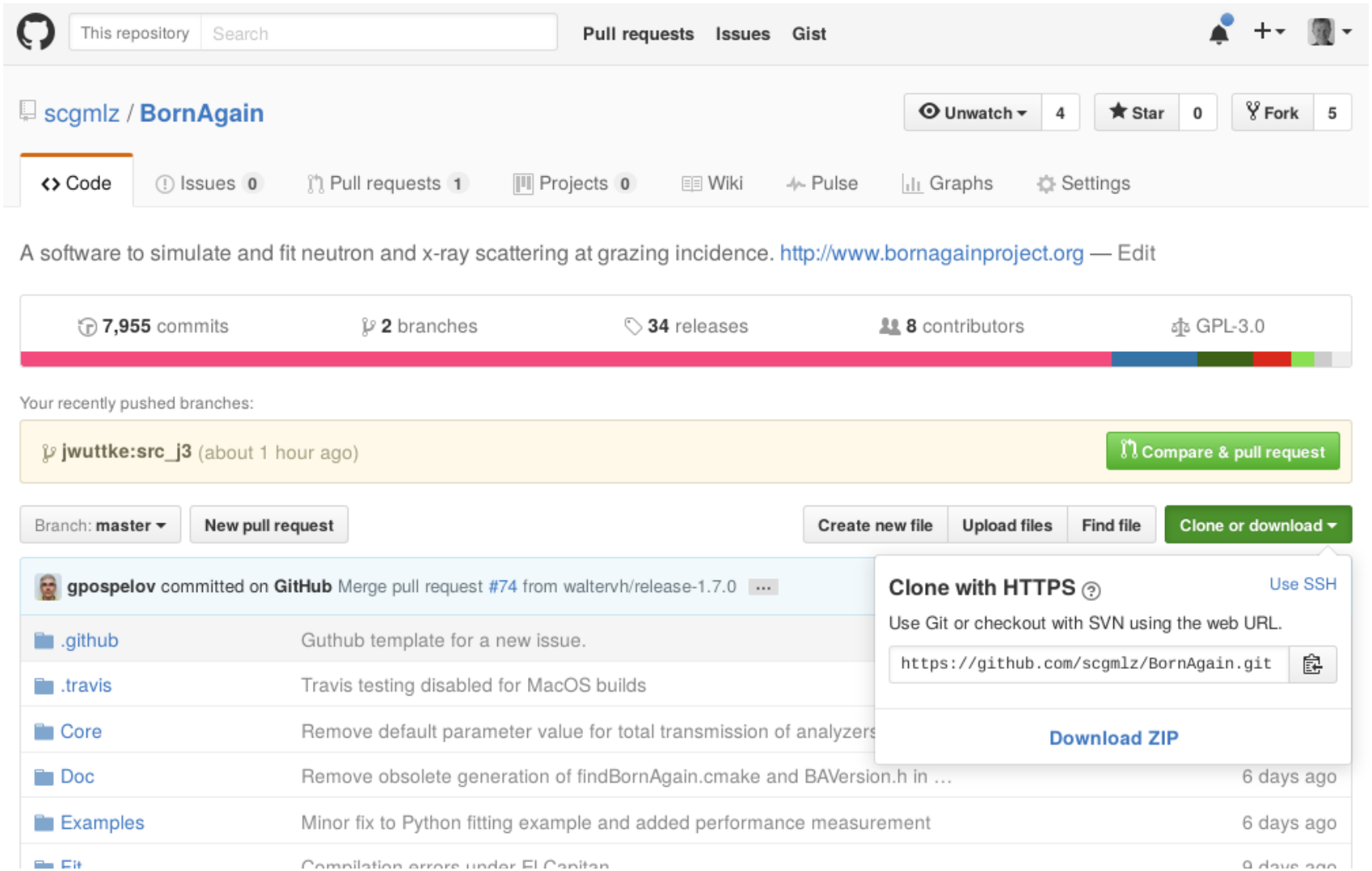
Download server

Download directory /src/BornAgain

Name	Last modified	Size
Parent Directory		-
experimental	15-Nov-2016 12:43	-
old	15-Nov-2016 12:42	-
BornAgain-1.7.0-macosx64-10.9+.dmg	14-Nov-2016 17:04	21M
BornAgain-1.7.0-win64.exe	14-Nov-2016 14:41	18M
BornAgain-1.7.0.tar.gz	14-Nov-2016 16:49	78M
BornAgainManual-1.7.0.html	15-Nov-2016 12:47	8.7M
BornAgainManual-1.7.0.pdf	15-Nov-2016 12:47	12M
CHANGELOG	15-Nov-2016 12:46	52K

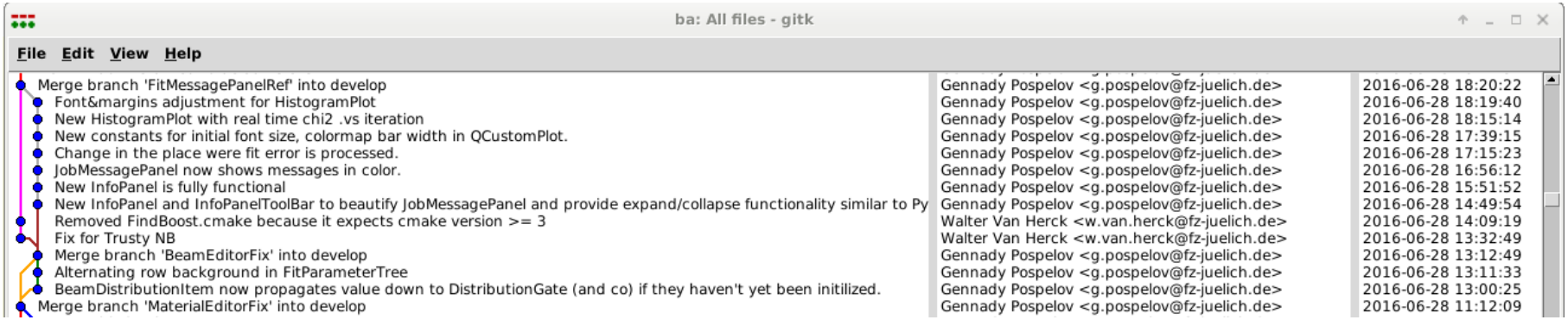
Source repository

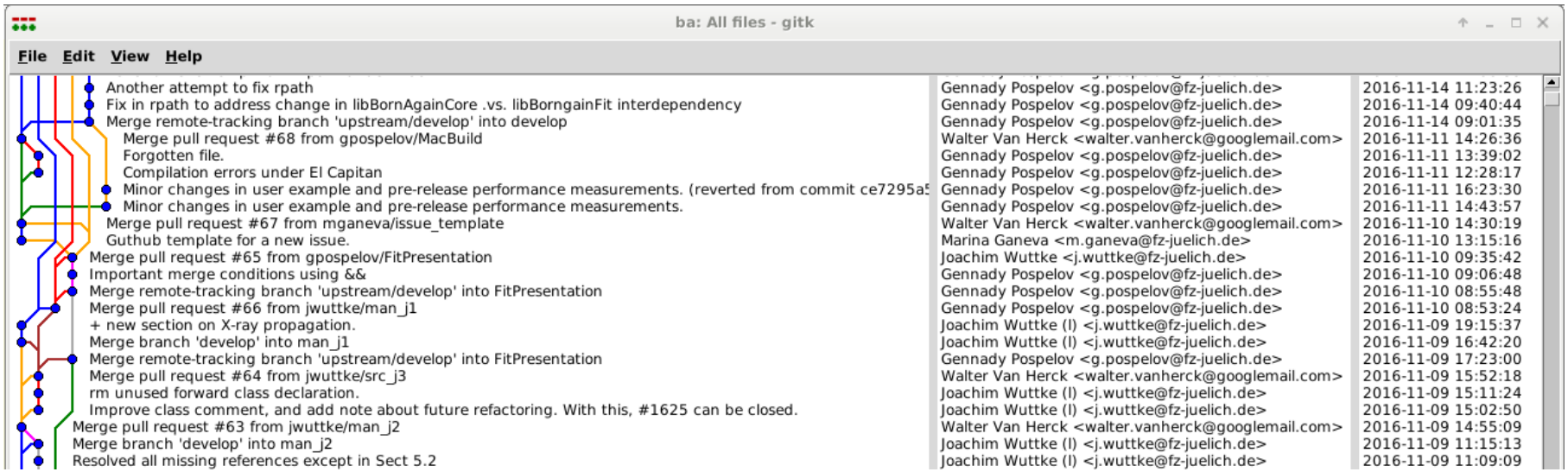
Get involved: report issues, propose patches



Source repository

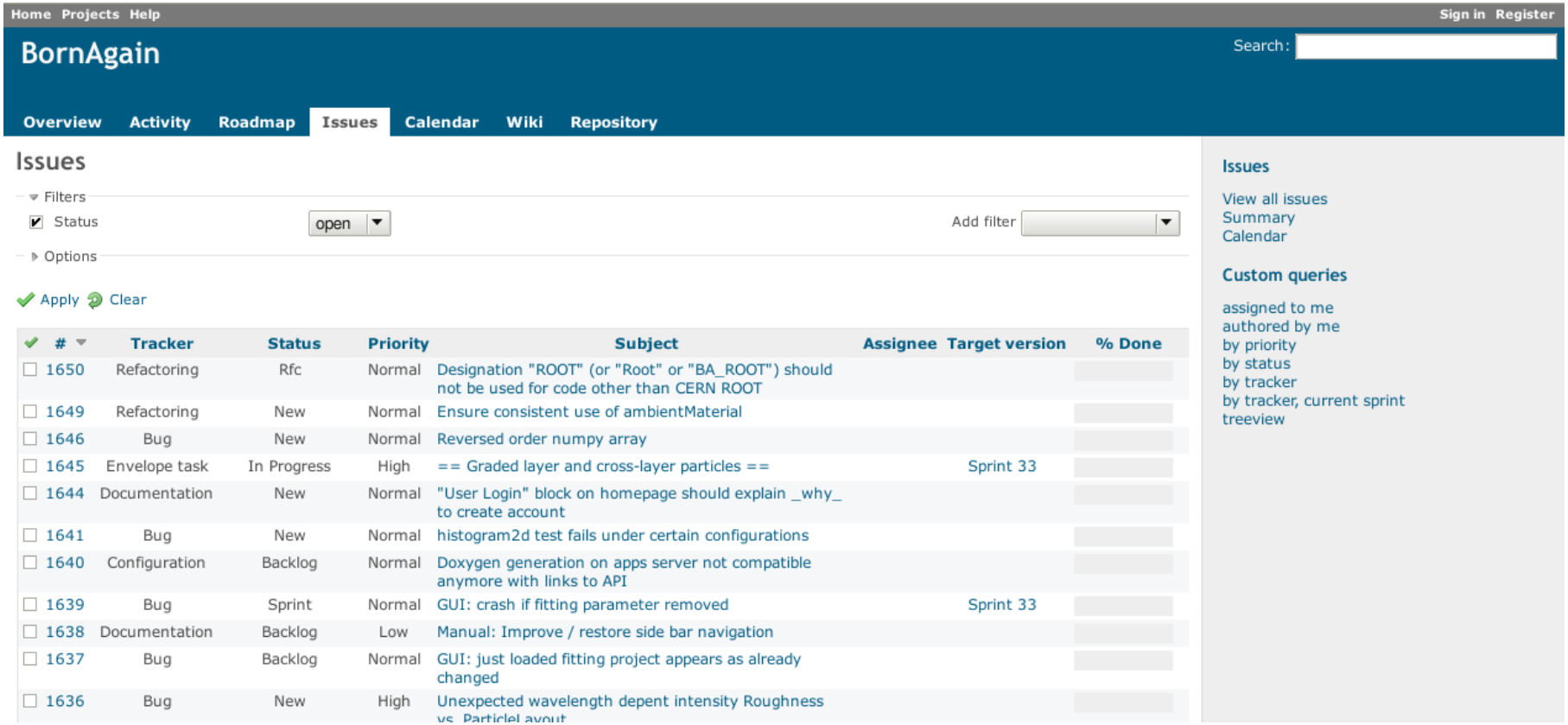
viewed with gitk





Internal issue tracker

public read access



The reference

IsGISAXS by Rémi Lazzari

IsGISAXS: a program for grazing-incidence small-angle X
of supported islands

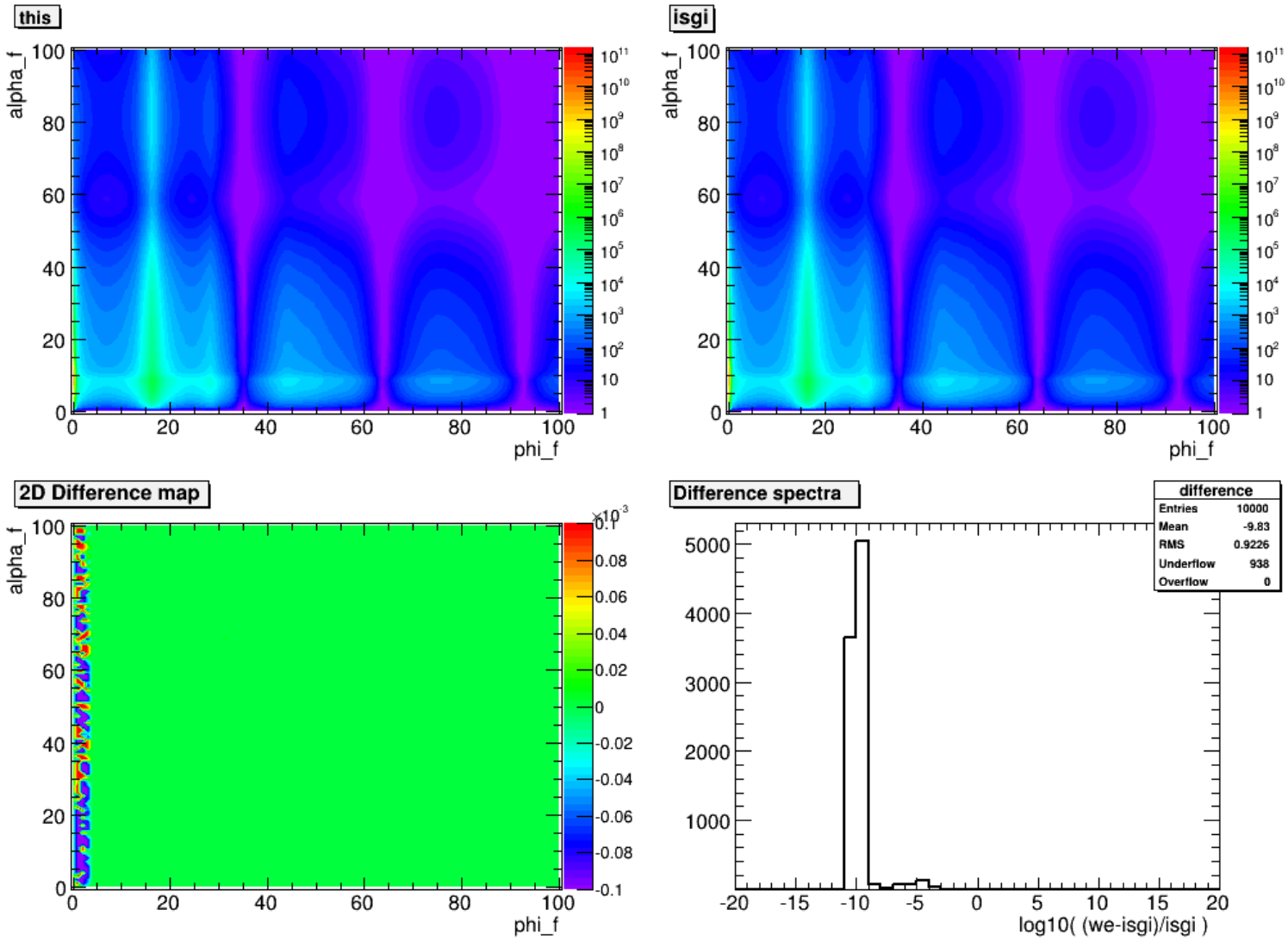
R **Lazzari** - Journal of Applied Crystallography, 2002 - scripts.iucr.org

This paper describes a Fortran program, IsGISAXS, for the simulation and
grazing-incidence small-angle X-ray scattering (GISAXS) of islands suppo
substrate. As is usual in small-angle scattering of particles, the scattering

Cited by 378 Related articles All 5 versions Import into BibTeX Save

Validation

BornAgain vs IsGISAXS



BornAgain functionality

Release 1.7 of Nov 15

Sample modelling:

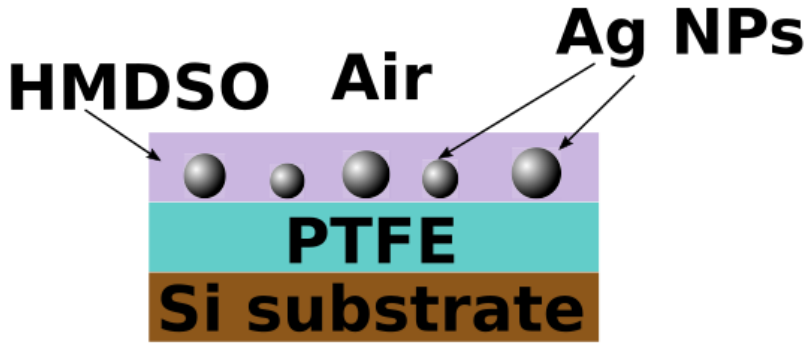
- IsGISAXS almost fully replicated
- arbitrary number of layers
- arbitrary particle layouts (shape $\otimes$ interference fct)
- compound particles
- mesocrystals
- polarized neutron propagation
- scattering by magnetic nanoparticles
- 2d fitting, masking
- off-specular scans

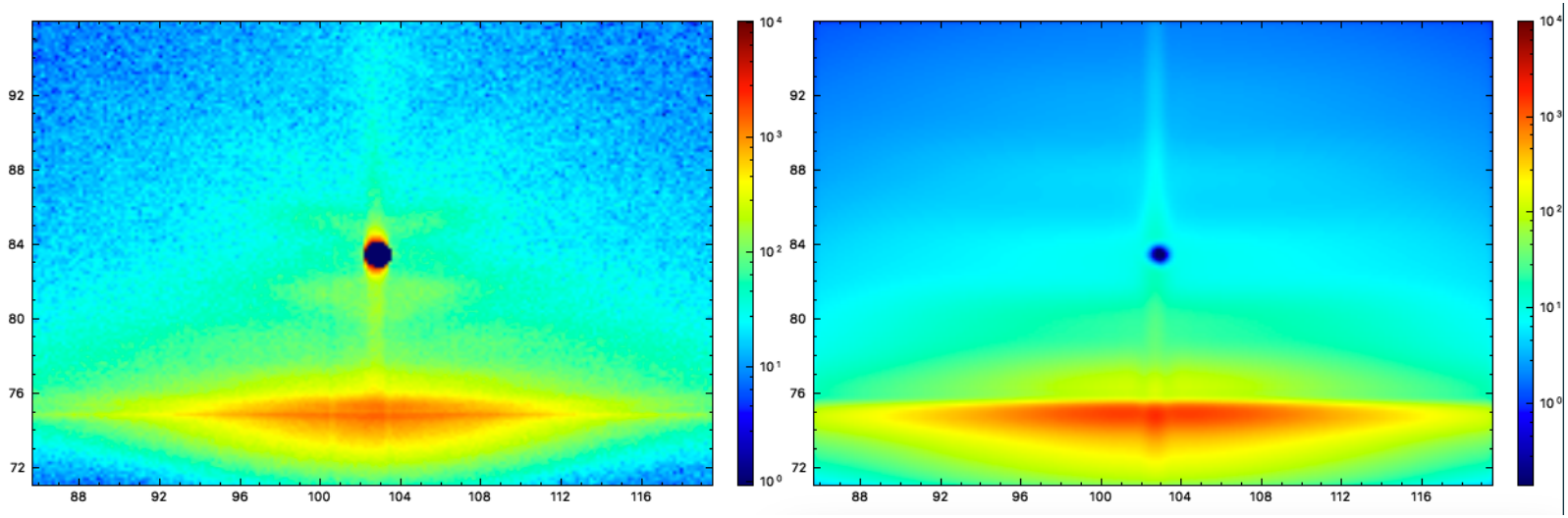
Usability:

- can be run from C++, Python, or GUI
- construct model in GUI, export to Python
- many examples, growing manual

HMDSO/Ag/PTFE nanocomposites

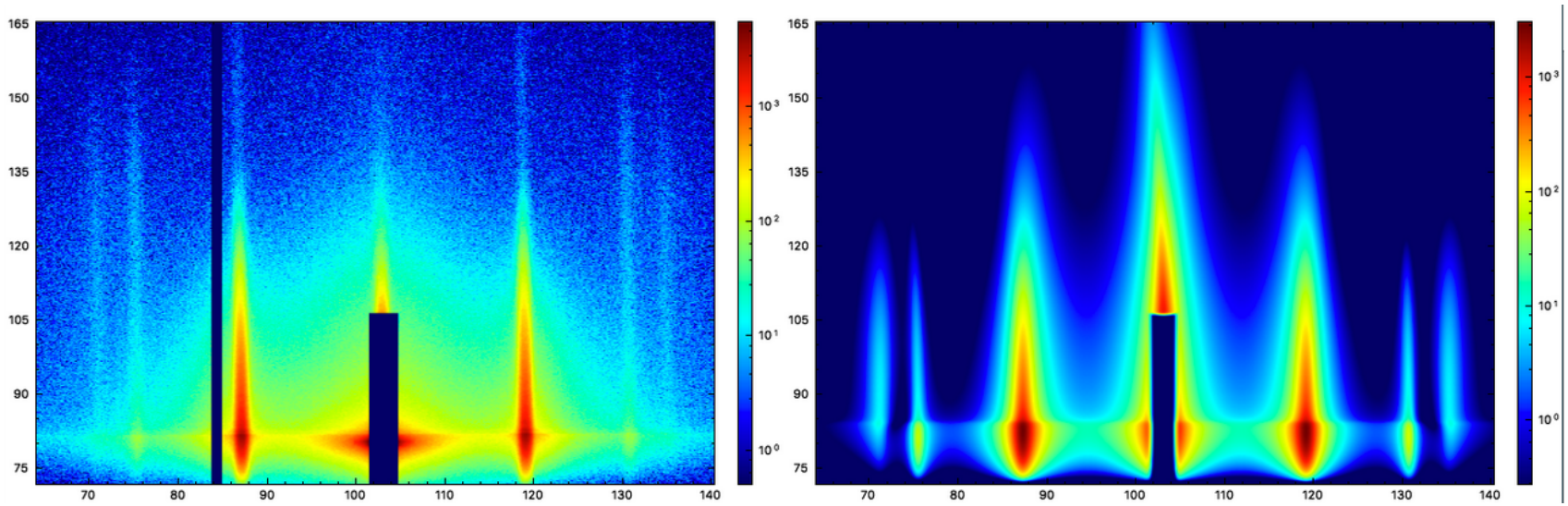
Layers have roughness. Nanoparticles have lognormal size distribution.





Ganeva et al, unpublished. Samples from Biederman group, Prague. Measured at GALAXI.

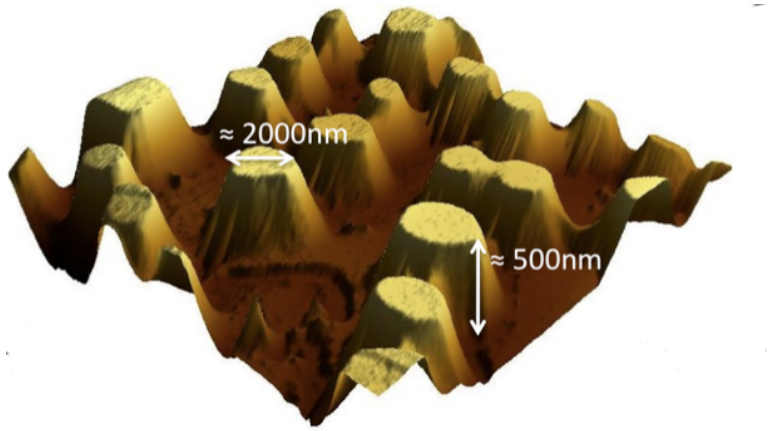
Co nanodots

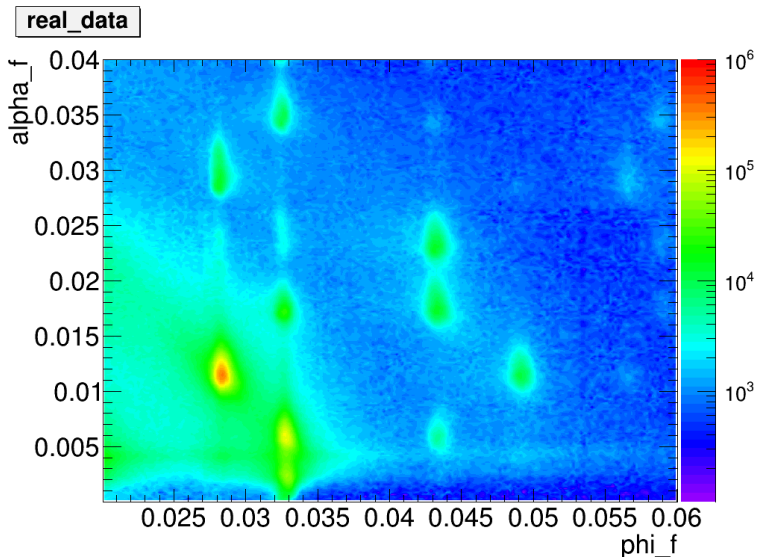


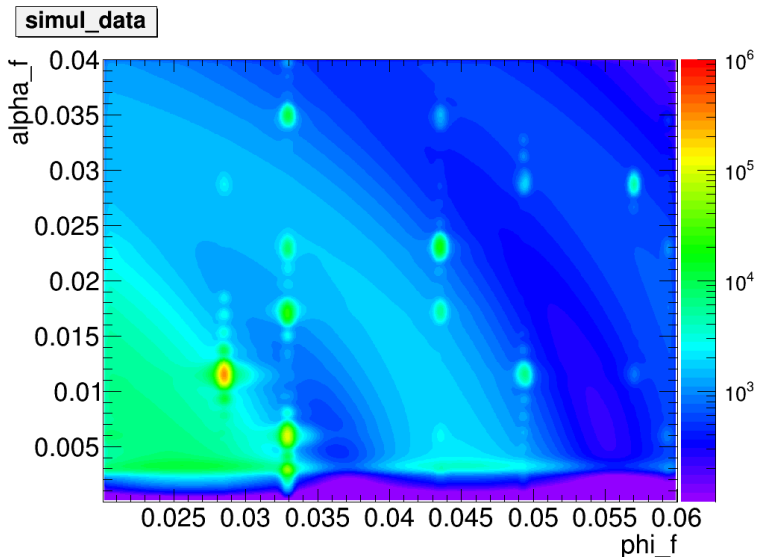
Alhroob, Ganeva, Kentzinger et al, unpublished. Measured at GALAXI.

Mesocrystal assembly

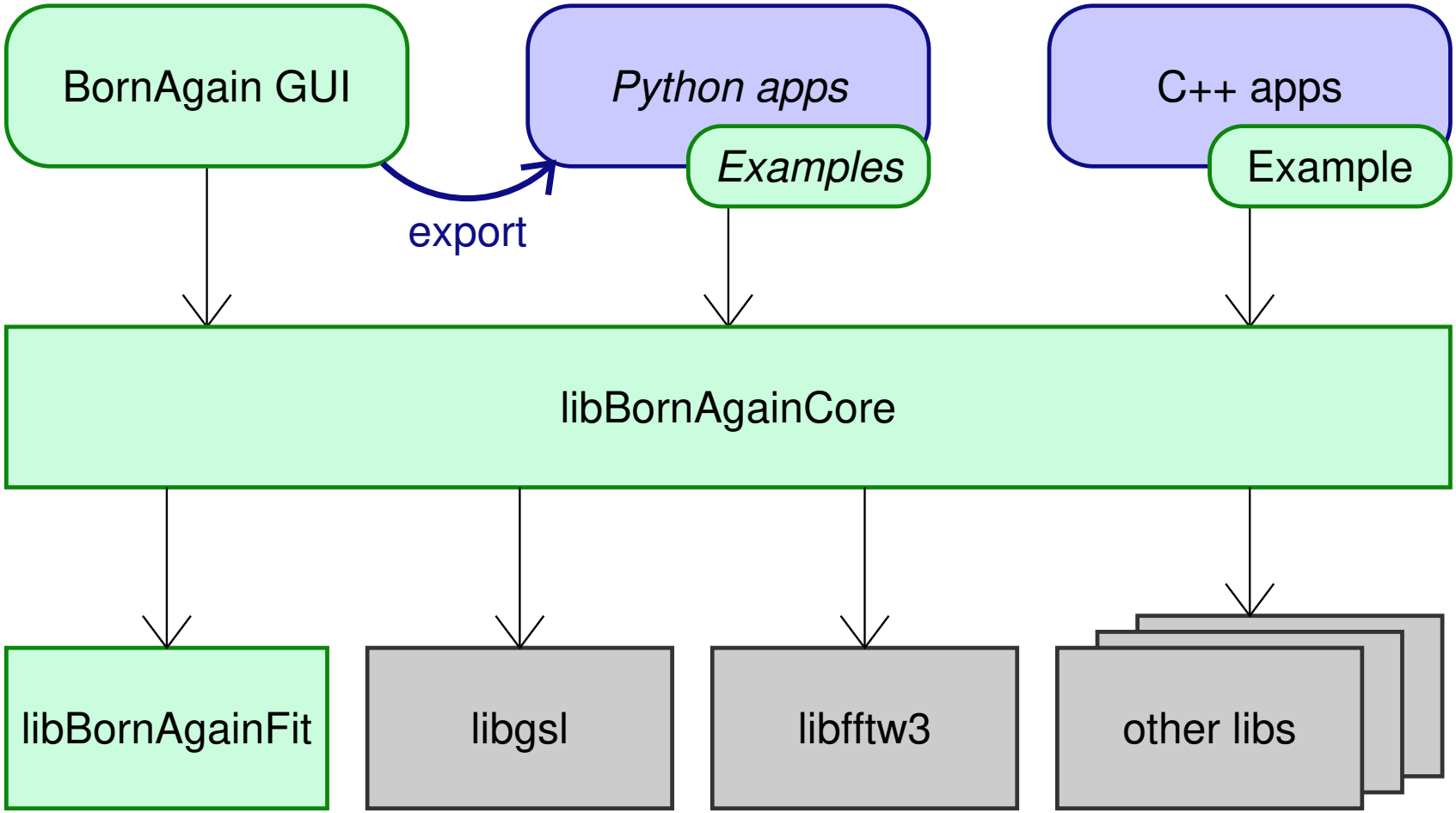
2D random assembly
of fcc mesocrystals of size $\sim$ 1 μm
of spherical particles of size 5 nm





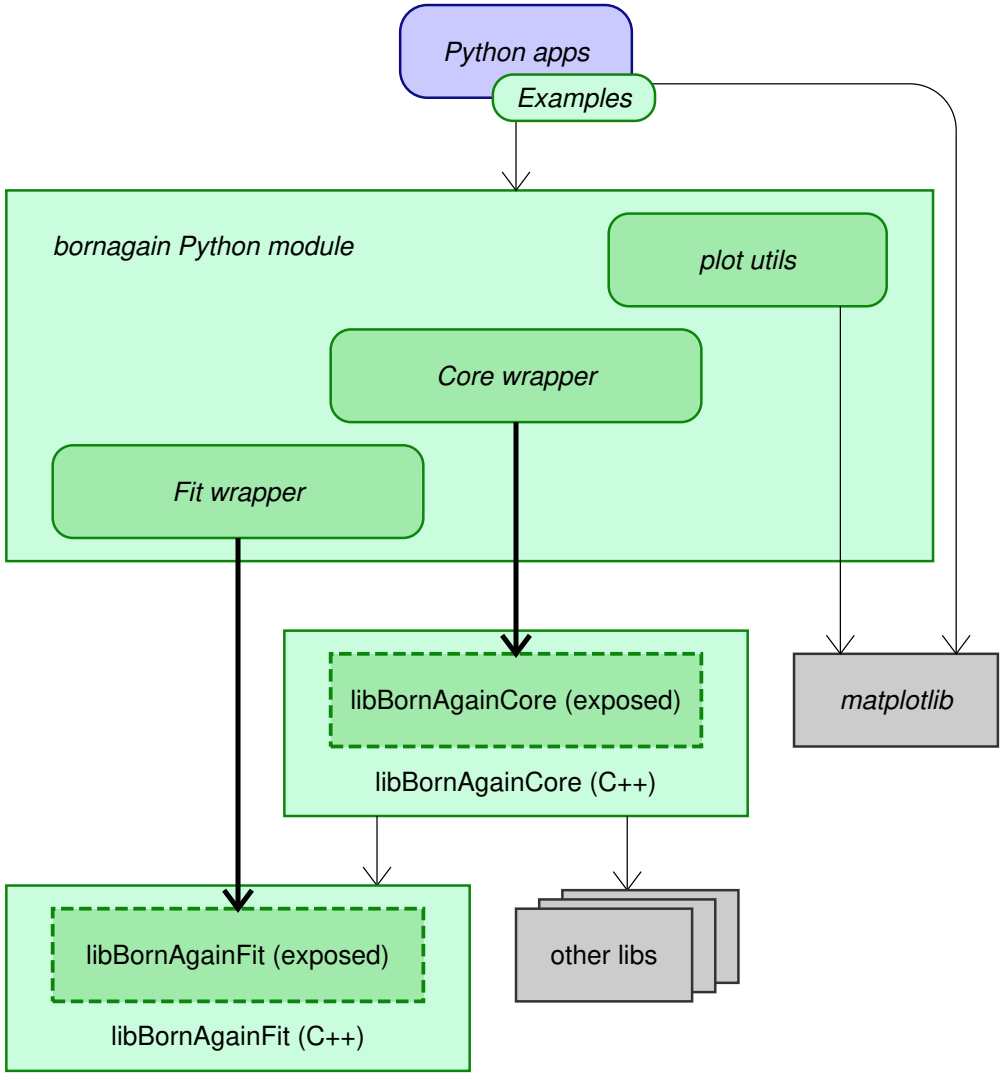


Architecture



Python module BornAgain

import bornagain as ba



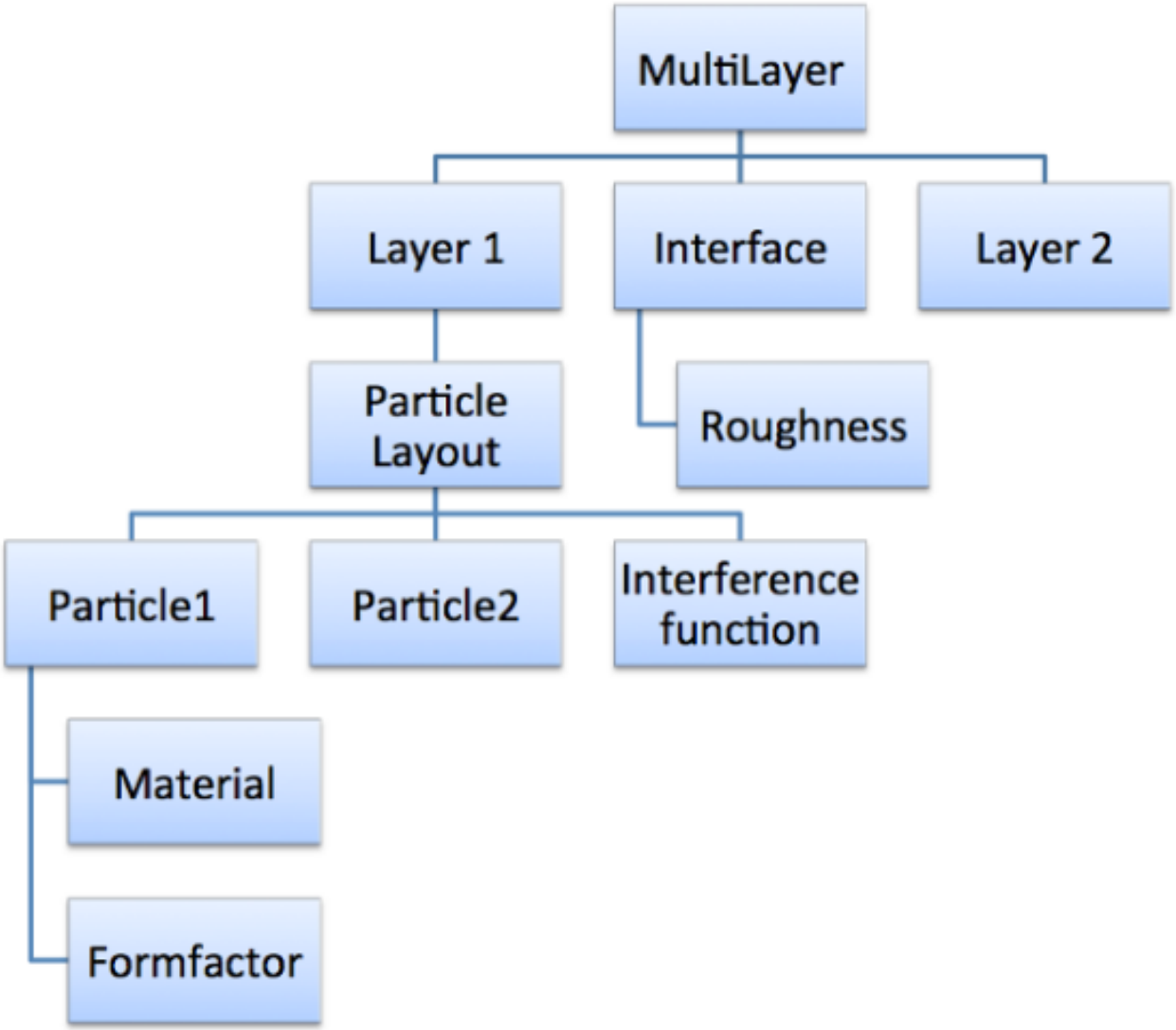
Basic simulation under Python

```
import bornagain as ba

sample = ba.MultiLayer()
...

simulation = ba.GISASSimulation()
simulation.setBeamParameters(
    1.0*angstrom, 0.2*deg, 0.0*deg)
simulation.setDetectorParameters(
    100, -1*deg, 1*deg, 100, -1*deg, 1*deg)
simulation.setSample(sample)

result = simulation.runSimulation()

ba.plot_intensity_data(result)
```

Hierarchical data structure

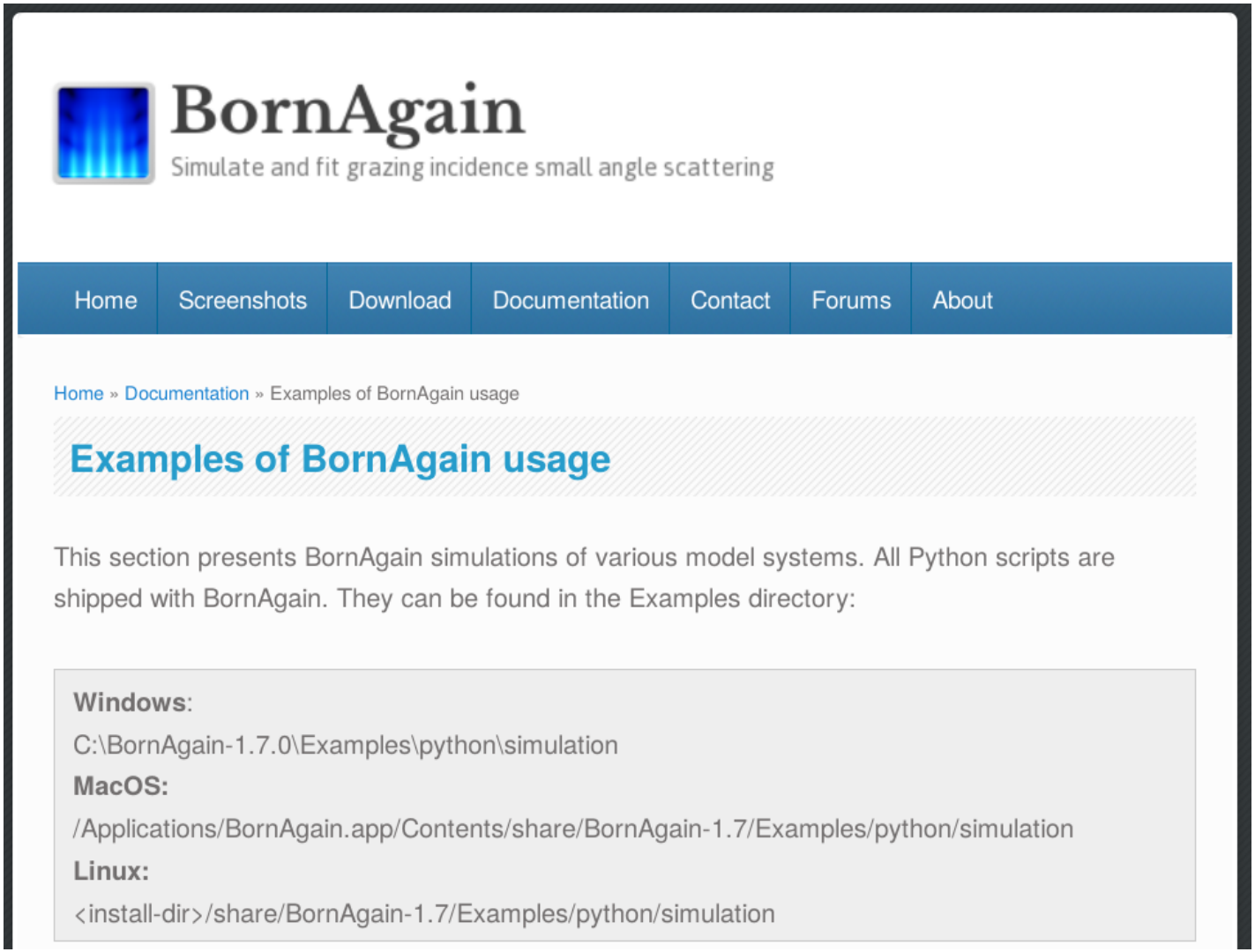
```
GISASSimulation
- Beam
- Detector
- Sample
   - Interface(s)
      - Roughness
   - Layer(s)
      - ParticleLayout
         - Particle(s)
            - Material
            - FormFactor
```

Hierarchical sample model



Application programming interface (API)

documented through usage examples



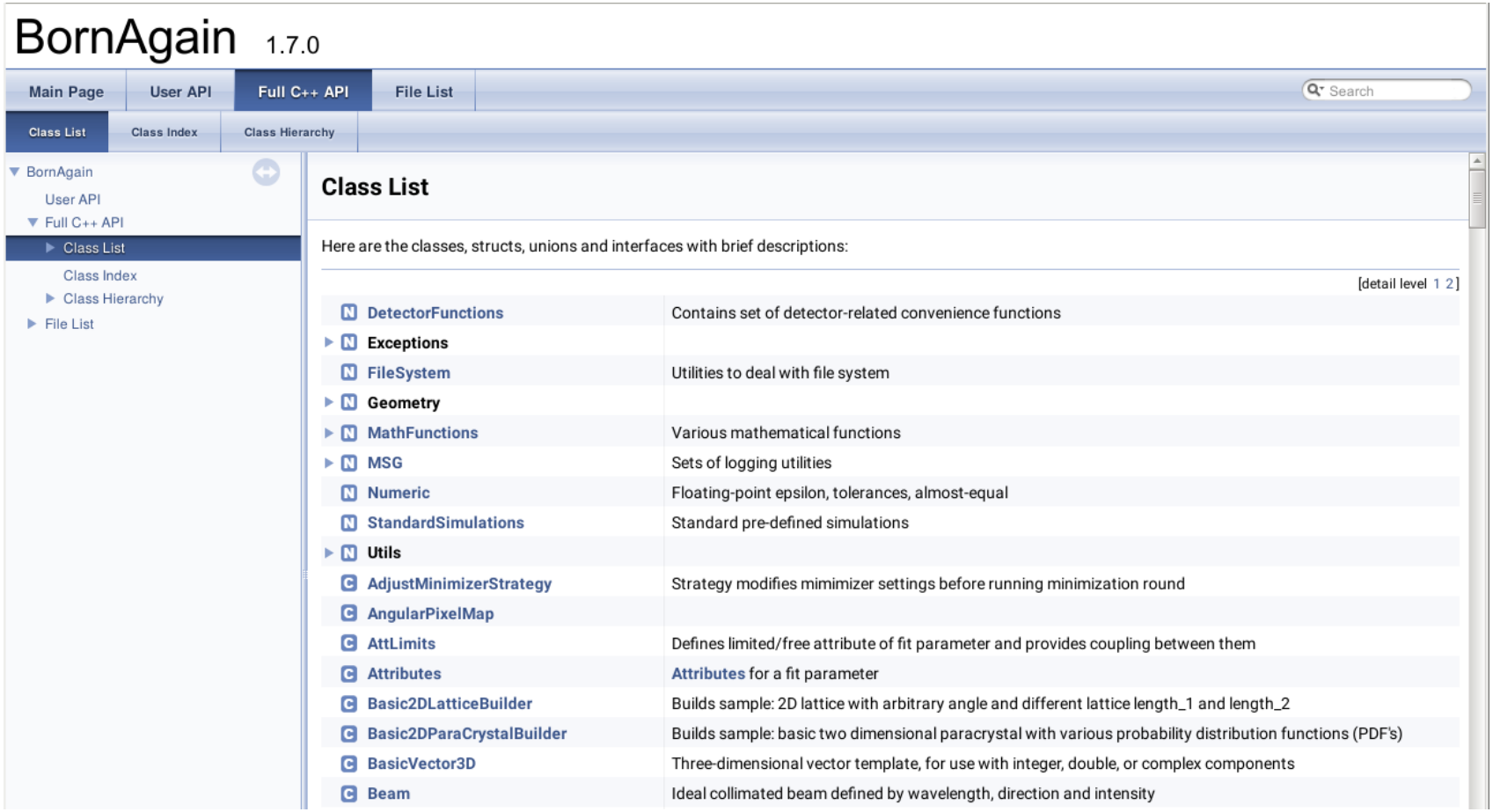
Application programming interface (API)

selective reference in User Manual, Part II

```
class Layer {
    Layer();
    Layer(const IMaterial& material, double
        thickness=0);
    void setThickness(double thickness);
    void setMaterial(const IMaterial& material);
    void addLayout(const ParticleLayout&
        decoration);
};
```

Application programming interface (API)

full reference automatically generated by Doxygen



Three parts of any simulation

```
# construct the model
simulation = ba.GISASSimulation()
simulation.setBeamParameters(
    1.0*angstrom, 0.2*deg, 0.0*deg)
simulation.setDetectorParameters(
    100, -1*deg, 1*deg, 100, -1*deg, 1*deg)
simulation.setSample(...)

# run the simulation
result = simulation.runSimulation()

# analyse the outcome
ba.plot_intensity_data(result)
```

Computing scattering intensities in DWBA

Precompute R & T coefficients

Loop over detector bins:

- Compute transmission to detector
- Compute scattering from rough interfaces
- Compute scattering from particle layout

Getting the hierarchical data to work

just a few out of many function calls

```
GISASSimulation.runSimulation()
-  MainComputation.run()
-  MainComputation.collectRTCoefficientsScalar()
   ...  -  SpecularMatrix.execute(sample, k, coeffs)
-  Multilayer.getLayer(i)
   -  Layer.getThickness()
   -  Layer.getRefractiveIndex()
   -  Layer.getLayout(j)
      -  ParticleLayout.getParticle(k)
      -  ParticleLayout.getAbundanceOfParticle(k)
         -  Particle(s).getFormFactor()
            -  Material.getRefractiveIndex()
            -  FormFactor.evaluate_for_q(q)
```

Distorted-Wave Born Approximation

leaves freedom in choice of distorted wave

Schrödinger equation, splitted for perturbation expansion:

$$\left\{\nabla^2 + \frac{2m\omega}{\hbar} - 4\pi\overline{V}(\boldsymbol{r})\right\}\psi(\boldsymbol{r}) = 4\pi\,\delta V(\boldsymbol{r})\,\psi(\boldsymbol{r})$$

$\overline{V} = \text{const}$:	plane-wave Born expansion
$\overline{V}(\boldsymbol{r})$ slowly varying:	distorted-wave Born expansion
$\overline{V}(z)$ slowly varying:	GISAS-DWBA
$\overline{V}(z)$ step function:	standard model in IsGISAXS, FitGISAXS, ..
$\overline{V}(z) = a + bz$:	BornAgain-1.8, hopefully
$\overline{V}(z)$ any slow function:	needed in BornAgain?

This talk online

https://github.com/scgmlz/BornAgain-tutorial → talks