BornAgain Python API

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Outline

Introduction to Python API	talking	pyapi01_introduction.pdf
Minimal simulation example	demo	pyapi02_minimal_example.py pyapi02_jupyter_example.ipynb
Simulating lamellar structure	demo	pyapi03_lamellar.py
Modifying lamellar example	task	pyapi04_lamellar_vertical_solution1.py pyapi04_lamellar_vertical_solution2.py

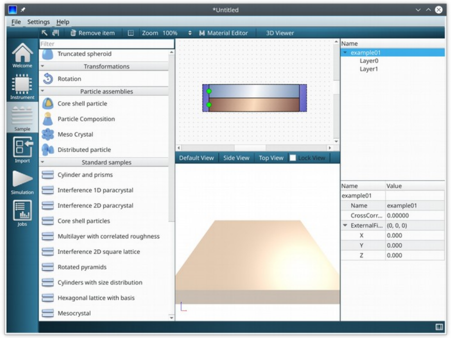
BornAgain Python API

Application Programming Interface (API) can be used to build and run simulations.

Advantages

- Complex sample construction
- Access to features non existing in GUI
- Possibility to reuse code in other projects
- Less back-compatibility problems
- Git based workflow

Minimal simulation example



GUI equivalent

```python
from bornagain import *

# --- sample ---

air = Layer(HomogeneousMaterial("Air", 0.0, 0.0))
substrate = Layer(HomogeneousMaterial("Substrate", 6e-6, 2e-8))

multi_layer = MultiLayer()
multi_layer.addLayer(air)
multi_layer.addLayer(substrate)

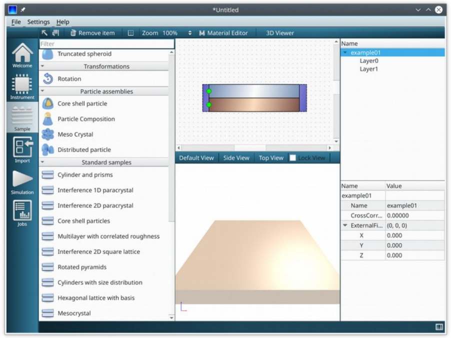
# --- simulation ---

simulation = GISASSimulation()
simulation.setDetectorParameters(100, -2.0*deg, 2.0*deg, 100, 0.0*deg, 2.0*deg)
simulation.setBeamParameters(1.0*angstrom, 0.2*deg, 0.0*deg)
simulation.setSample(multi_layer)

# --- run and plot ---

simulation.runSimulation()
plot_simulation_result(simulation.result())
```

Minimal simulation example



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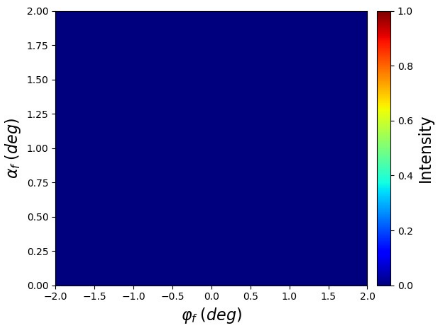
simulation.setSample(multi_layer)

# --- run and plot ---

simulation.runSimulation()
plot_simulation_result(simulation.result())
```

```
$ python pyapi02_minimal_example.py
```



Demo

Running trivial simulations

`pyapi02_minimal_example.py`

`pyapi02_jupyter_example.ipynb`

Structuring the code

```
import bornagain as ba

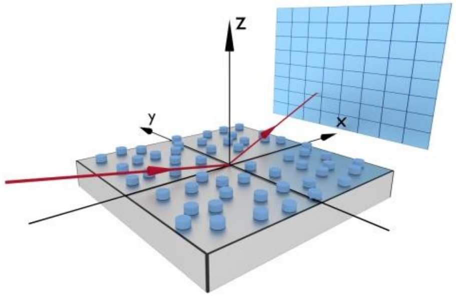

def get_sample():
    multi_layer = ba.MultiLayer()
    ...
    return multi_layer


def get_simulation():
    simulation = ba.GISASSimulation()
    ...
    sample = get_sample()
    simulation.setSample(sample)
    return simulation


def run_simulation():
    simulation = get_simulation()
    simulation.runSimulation()
    return simulation.result()


if __name__ == '__main__':
    result = run_simulation()
    ba.plot_simulation_result(result)
```

Example on sample construction



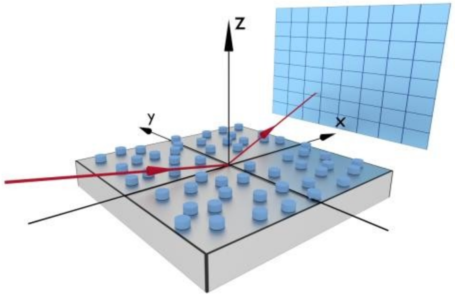

```python
import bornagain as ba


def get_sample():
    # defining materials
    air = ba.HomogeneousMaterial("Air", 0.0, 0.0)
    substrate = ba.HomogeneousMaterial("Substrate", 6e-6, 2e-8)
    gold = ba.HomogeneousMaterial("Gold", 6e-4, 2e-8)

    # creating particles
    cylinder_ff = ba.FormFactorCylinder(5*nm, 5*nm)
    cylinder = ba.Particle(gold, cylinder_ff)

    layout = ba.ParticleLayout()
    layout.addParticle(cylinder, 1.0)

    air_layer = ba.Layer(air)
    air_layer.addLayout(layout)
    substrate_layer = ba.Layer(substrate)

    multi_layer = ba.MultiLayer()
    multi_layer.addLayer(air_layer)
    multi_layer.addLayer(substrate_layer)
    return multi_layer
```

Material definition

Particle collection

MultiLayer construction

Example on sample construction




```
import bornagain as ba

def get_materials():
    # defining materials
    air = ba.HomogeneousMaterial("Air", 0.0, 0.0)
    substrate = ba.HomogeneousMaterial("Substrate", 6e-6, 2e-8)
    gold = ba.HomogeneousMaterial("Gold", 6e-4, 2e-8)
    return air, substrate, gold

def get_sample():
    air, substrate, gold = get_materials()

    # creating particles
    cylinder_ff = ba.FormFactorCylinder(5*nm, 5*nm)
    cylinder = ba.Particle(gold, cylinder_ff)

    layout = ba.ParticleLayout()
    layout.addParticle(cylinder, 1.0)

    air_layer = ba.Layer(air)
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    substrate_layer = ba.Layer(substrate)

    multi_layer = ba.MultiLayer()
    multi_layer.addLayer(air_layer)
    multi_layer.addLayer(substrate_layer)
    return multi_layer
```
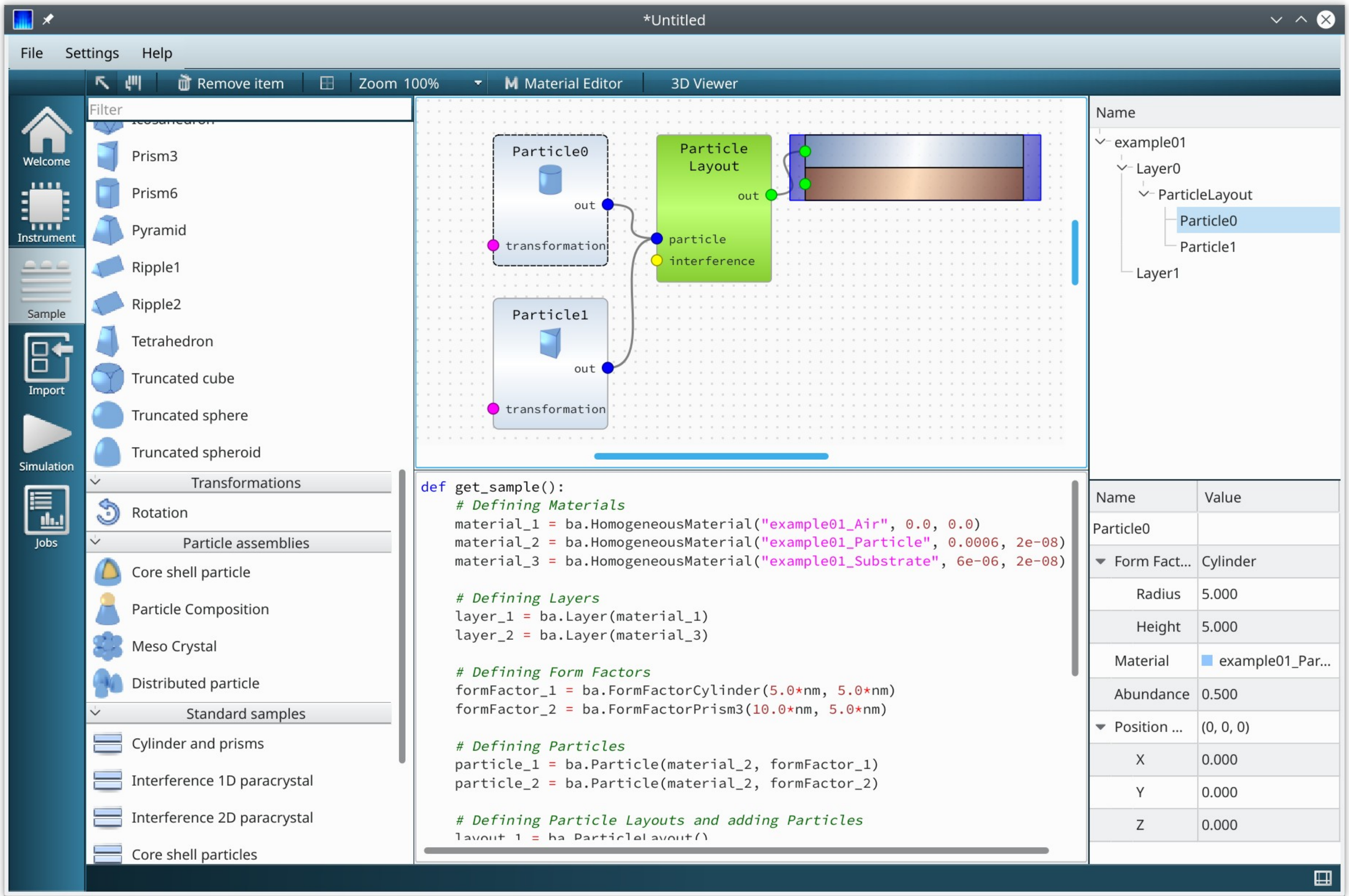

Material definition

Particle collection

MultiLayer construction

Where to start

Python viewer embedded in GUI



Where to start

Sample model reference on website

BornAgain

Home Gallery Download News Documentation Contact About

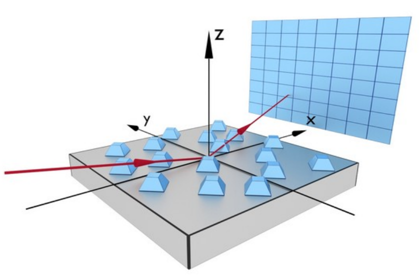
Home > Documentation > Sample model reference > Embedded particles > Rotated Pyramids

Rotated Pyramids

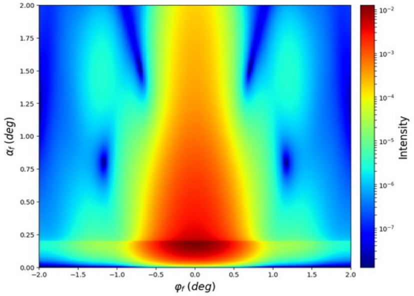
Scattering from a monodisperse distribution of rotated pyramids.

This example illustrates how the in-plane rotation of non-radially symmetric particles influences the scattering pattern.

- The sample is made of pyramids deposited on a substrate.
- Each pyramid is characterized by a squared-base side length of 10 nm, a height of 5 nm, and a base angle α equal to 54.73°.
- These particles are rotated in the (x, y) plane by 45°.
- There is no interference between the scattered waves.
- The wavelength is equal to 1 Å.
- The incident angles are $\alpha_i = 0.2^\circ$ and $\phi_i = 0^\circ$.



Real-space model

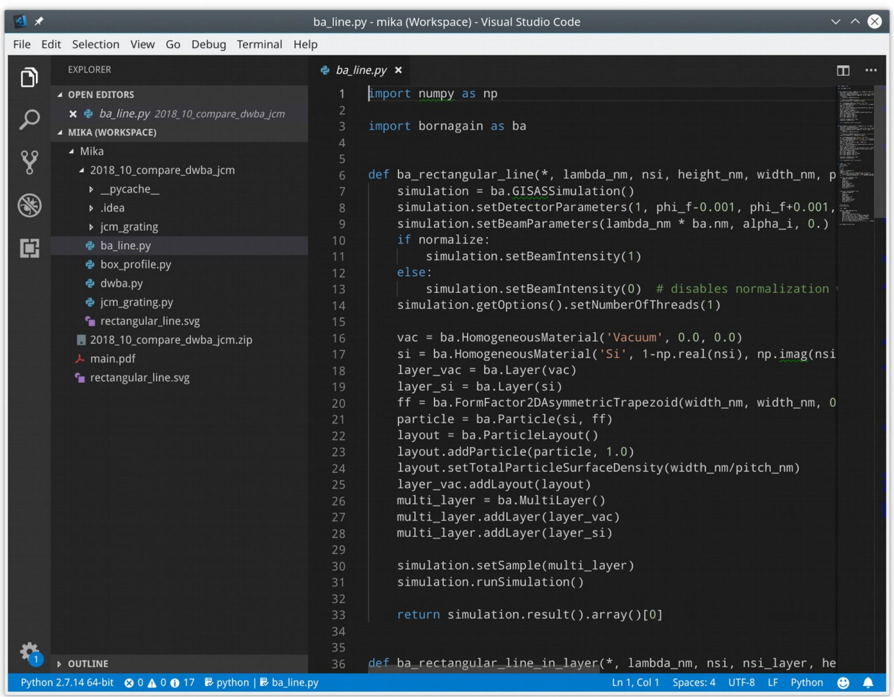


Intensity image

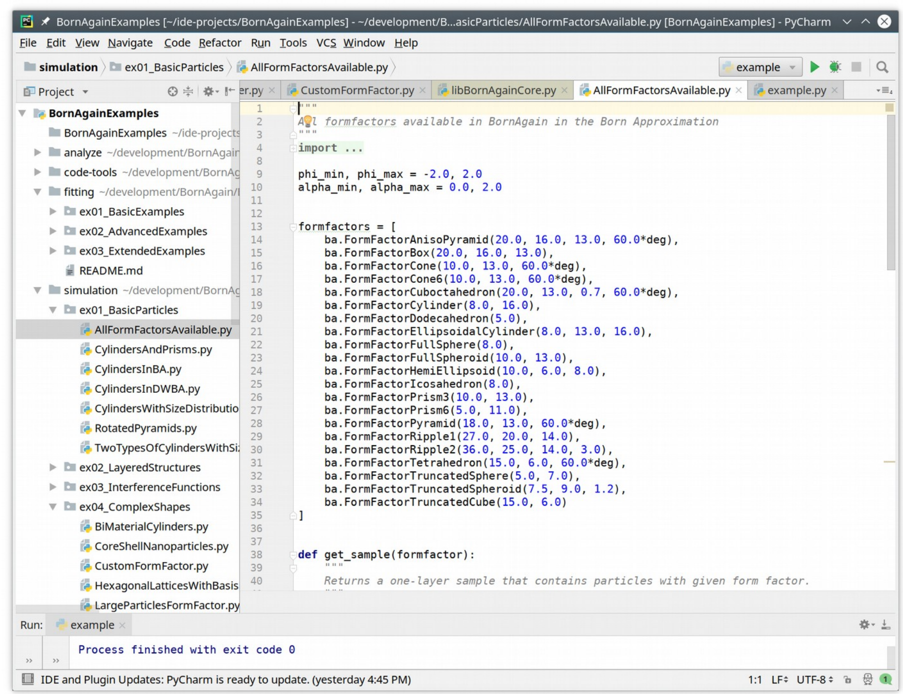
```python
"""
Rotated pyramids on top of substrate
"""
import bornagain as ba
from bornagain import deg, angstrom, nm


def get_sample():
```

Where to code

- Editor of your choice, Python interpreter
- Integrated development environment (IDE)
  - MS Visual Studio Code, PyCharm
  - Syntax and error highlighting, debug, code navigation
- Jupyter notebooks
  - Quick prototyping



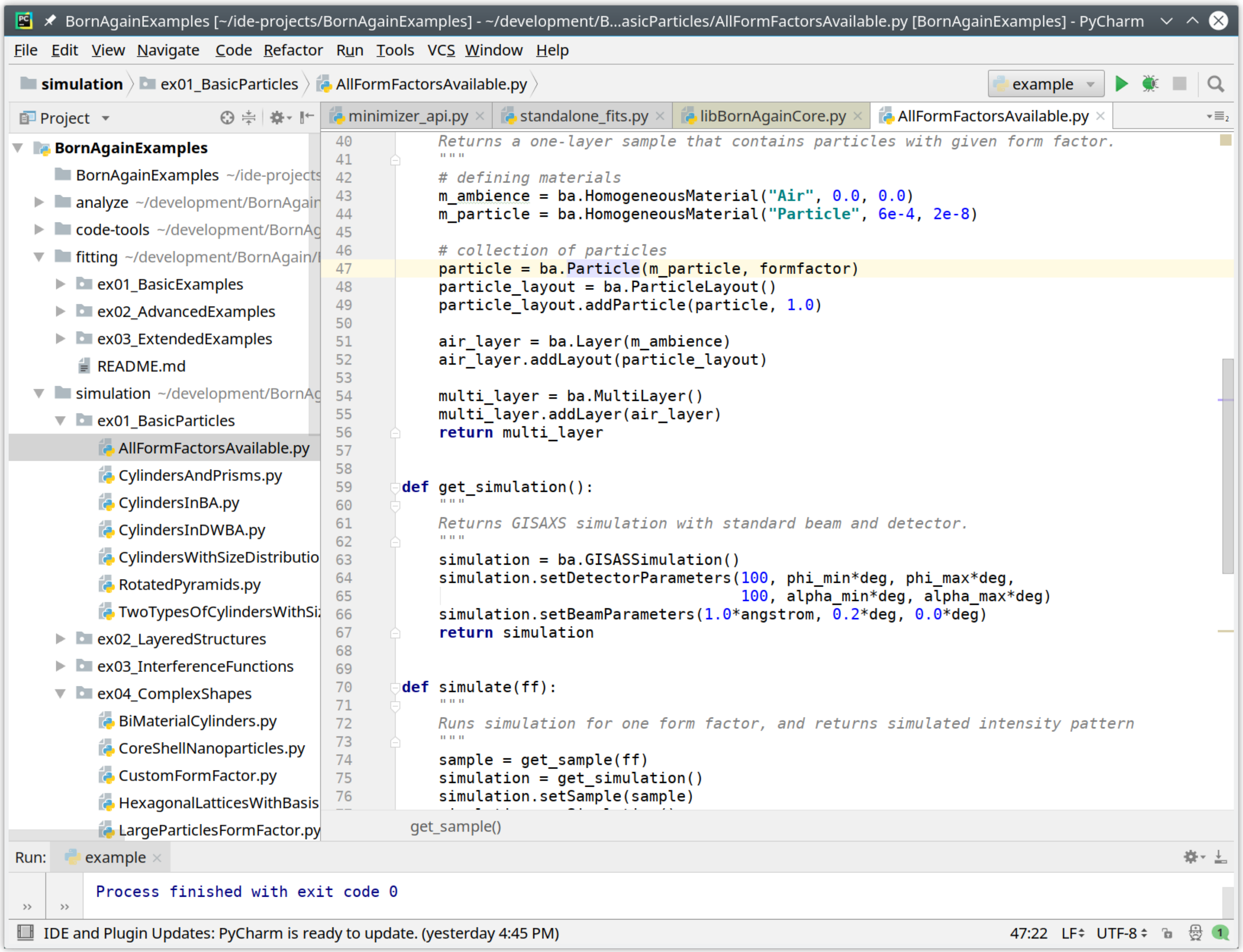
VS Code



PyCharm

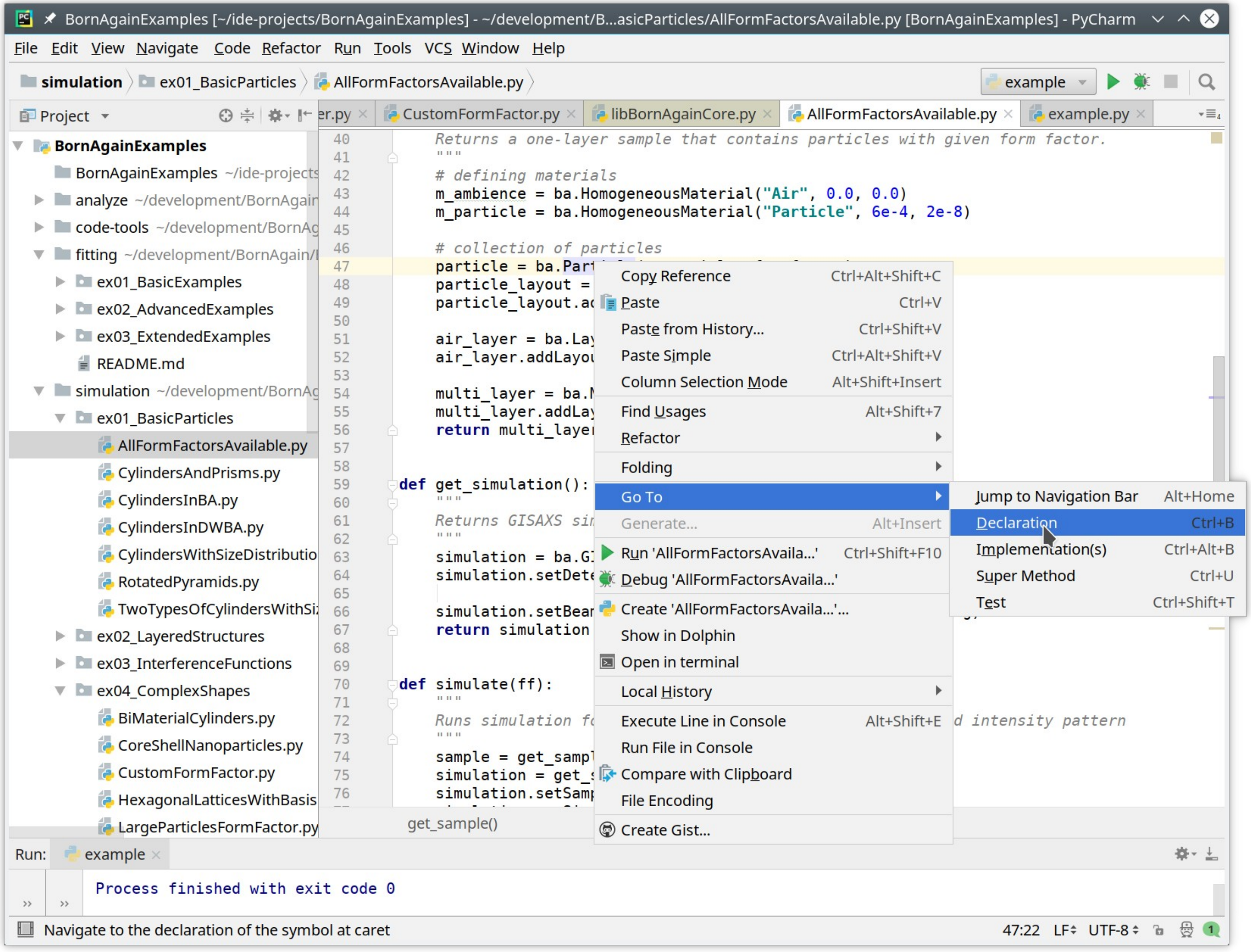
Python API technicalities

BornAgain Python API is automatically generated from C++ code



Python API technicalities

BornAgain Python API is automatically generated from C++ code



Python API technicalities

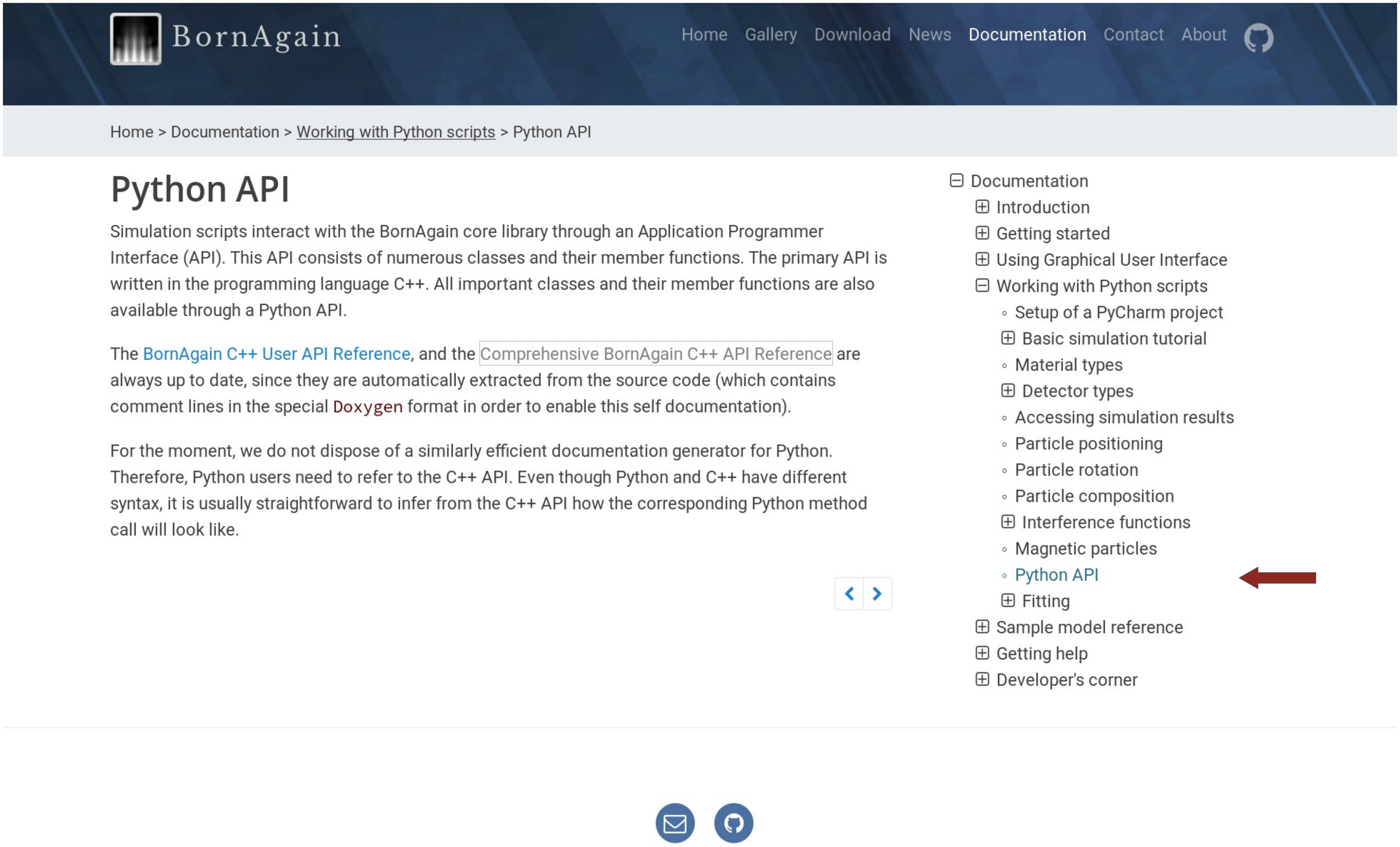
BornAgain Python API is automatically generated from C++ code

Python API internals looks unhuman

```python
class Particle(IParticle):
    """


    A particle with a form factor and refractive index.

    C++ includes: Particle.h

    """

    __swig_setmethods__ = {}
    for _s in [IParticle]:
        __swig_setmethods__.update(getattr(_s, '__swig_setmethods__', {}))
    __setattr__ = lambda self, name, value: _swig_setattr(self, Particle, name, value)
    __swig_getmethods__ = {}
    for _s in [IParticle]:
        __swig_getmethods__.update(getattr(_s, '__swig_getmethods__', {}))
    __getattr__ = lambda self, name: _swig_getattr(self, Particle, name)
    __repr__ = _swig_repr

    def __init__(self, *args):
        """
        __init__(Particle self) -> Particle
        __init__(Particle self, Material material) -> Particle
        __init__(Particle self, Material material, IFormFactor form_factor) -> Particle
        __init__(Particle self, Material material, IFormFactor form_factor, IRotation rota

        Particle::Particle(Material material, const IFormFactor &form_factor, const IRotat

        """
        this = _libBornAgainCore.new_Particle(*args)
        try:
            self.this.append(this)
        except __builtin__.Exception:
            self.this = this

```

Documentation on Python API

C++ API documentation sometimes might help …



Python API

Simulation scripts interact with the BornAgain core library through an Application Programmer Interface (API). This API consists of numerous classes and their member functions. The primary API is written in the programming language C++. All important classes and their member functions are also available through a Python API.

The BornAgain C++ User API Reference, and the Comprehensive BornAgain C++ API Reference are always up to date, since they are automatically extracted from the source code (which contains comment lines in the special `Doxygen` format in order to enable this self documentation).

For the moment, we do not dispose of a similarly efficient documentation generator for Python. Therefore, Python users need to refer to the C++ API. Even though Python and C++ have different syntax, it is usually straightforward to infer from the C++ API how the corresponding Python method call will look like.

BornAgain C++ API

Simulate and fit neutron and x-ray scattering at grazing incidence

Main Page | User API | Full C++ API | File List | Search

Class List | Class Index | Class Hierarchy

- BornAgain
  - User API
  - Full C++ API
    - Class List
    - Class Index
    - Class Hierarchy
  - File List

Class Index

A | B | C | D | E | F | G | H | I | K | L | M | N | O | P | R | S | T | U | V | W | Z

A

AnisoPyramid
AsymRippleBuilder
AttLimits
Attributes
AxesUnitsWrap
UnitConverterSimple::AxisData
AxisInfo

B

BaseMaterialImpl
Basic2DLatticeBuilder
Basic2DParaCrystalBuilder
BasicLattice
BasicVector3D
Beam
Bin1D
Bin1DCVector
Bin1DKVector
BiPyramid
Box
BoxCompositionBuilder
BoxCompositionRotateXBuilder
BoxCompositionRotateYBuilder
BoxCompositionRotateZandYBuilder
BoxCompositionRotateZBuilder
BoxesSquareLatticeBuilder
BoxStackCompositionBuilder

C

IntegratorReal::CallBackHolder
IntegratorMCMiser::CallBackHolder

FitStatus
FixedBinAxis
FootprintFactorGaussian
FootprintFactorSquare
FormatErrorException (Exceptions)
FormFactorAnisoPyramid
FormFactorBox
FormFactorCoherentPart
FormFactorCoherentSum
FormFactorComponents
FormFactorCone
FormFactorCone6
FormFactorCoreShell
FormFactorCrystal
FormFactorCuboctahedron
FormFactorCylinder
FormFactorDebyeBueche
FormFactorDecoratorDebyeWaller
FormFactorDecoratorMaterial
FormFactorDecoratorPositionFactor
FormFactorDecoratorRotation
FormFactorDodecahedron
FormFactorDot
FormFactorDWBA
FormFactorDWBAPol
FormFactorEllipsoidalCylinder
FormFactorFullSphere
FormFactorFullSpheroid
FormFactorGauss
FormFactorHemiEllipsoid
FormFactorIcosahedron
FormFactorLongBox
FormFactorLongBoxGauss

IClusteredParticles
IComputation
Icosahedron
IdentityRotation
IDetector
IDetector2D
IDetectorResolution
IDistribution1D
IDistribution1DSampler
IDistribution2DSampler
IFactory
IFootprintFactor
IFormFactor
IFormFactorBorn
IFormFactorDecorator
IFresnelMap
IFTDecayFunction1D
IFTDecayFunction2D
IFTDistribution1D
IFTDistribution2D
IFunctionAdapter (Fit)
IHistogram
IIntensityFunction
IIntensityNormalizer
IInterferenceFunction
IInterferenceFunctionStrategy
ILatticeOrientation
ILayerRTCoefficients
ILayout
IMinimizer
IMultiLayerBuilder
INamed
InfinitePlane

M

MagneticCylindersBuilder
MagneticMaterialImpl
MagneticParticleZeroFieldBuilder
MagneticRotationBuilder
MagneticSpheresBuilder
MagneticSubstrateZeroFieldBuilder
Material
MaterialBySLDImpl
PlainMultiLayerBySLDBuilder::MaterialData
MatrixFresnelMap
MatrixRTCoefficients
MesoCrystal
MesoCrystalBuilder
MillerIndex
MillerIndexOrientation
Minimizer (Fit)
MinimizerCatalogue
MinimizerFactory
MinimizerInfo
MinimizerOptions
MinimizerResult (Fit)
Minuit2Minimizer
MPISimulation
MultiLayer
MultilayerInfo
MultiLayerWithRoughnessBuilder
MultiOption
MultipleLayoutBuilder

N

NodeIterator

BornAgain C++ API

FormFactorBox Class Reference

Hard particles

Description

A rectangular prism (parallelepiped).

Definition at line 23 of file FormFactorBox.h.

Inheritance diagram for FormFactorBox:

Public Member Functions

	FormFactorBox (double length, double width, double height) Constructor of a rectangular cuboid. More...
FormFactorBox *	**clone** () const overridefinal Returns a clone of this **ISample** object.
void	**accept** (**INodeVisitor** *visitor) const overridefinal Calls the **INodeVisitor**'s visit method.
double	**getLength** () const
double	**getHeight** () const
double	**getWidth** () const
double	**radialExtension** () const overridefinal Returns the (approximate in some cases) radial size of the particle of this form factor's shape. More...
complex_t	**evaluate_for_q** (**cvector_t** q) const overridefinal Returns scattering amplitude for complex scattering wavevector q=k_i-k_f. More...

BornAgain C++ API

FormFactorBox.cpp

Go to the documentation of this file.

```
// ************************************************************************** //
//
//  BornAgain: simulate and fit scattering at grazing incidence
//
//! @file      Core/HardParticle/FormFactorBox.cpp
//! @brief     Implements class FormFactorBox.
//!
//! @homepage  http://www.bornagainproject.org
//! @license   GNU General Public License v3 or higher (see COPYING)
//! @copyright Forschungszentrum Jülich GmbH 2018
//! @authors   Scientific Computing Group at MLZ (see CITATION, AUTHORS)
//
// ************************************************************************** //

#include "FormFactorBox.h"
#include "BornAgainNamespace.h"
#include "Box.h"
#include "MathFunctions.h"
#include "RealParameter.h"

//! Constructor of a rectangular cuboid.
//! @param length: length of the base in nanometers
//! @param width: width of the base in nanometers
//! @param height: height of the box in nanometers
FormFactorBox::FormFactorBox(double length, double width, double height)
    : m_length(length), m_width(width), m_height(height)
{
    setName(BornAgain::FFBoxType);
    registerParameter(BornAgain::Length, &m_length).setUnit(BornAgain::UnitsNm).setNonnegative();
    registerParameter(BornAgain::Width,  &m_width).setUnit(BornAgain::UnitsNm).setNonnegative();
    registerParameter(BornAgain::Height, &m_height).setUnit(BornAgain::UnitsNm).setNonnegative();
    onChange();
}

complex_t FormFactorBox::evaluate_for_q(cvector_t q) const
{
    complex_t qzHdiv2 = m_height/2*q.z();
    return m_height*m_length*m_width *
        MathFunctions::sinc(m_length/2*q.x()) *  MathFunctions::sinc(m_width/2*q.y()) *
            MathFunctions::sinc(qzHdiv2) * exp_I(qzHdiv2);
}
```

Features available only in Python

Simulation

- Simulation with distributed parameters
- Some exotic interference functions

Fitting

- Fitting multiple data sets
- Fit along slices
- Third party minimizers
- Custom objective functions

Complex workflows

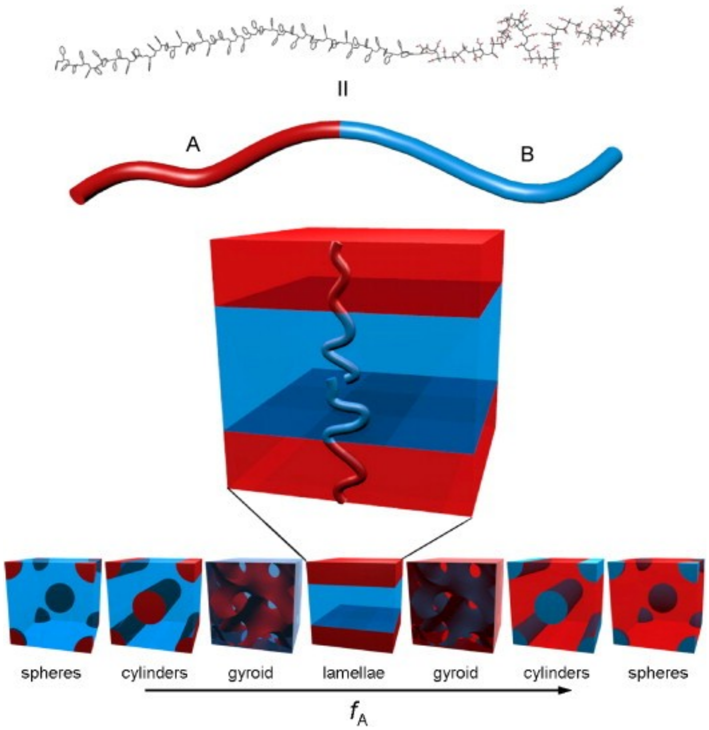
Demo

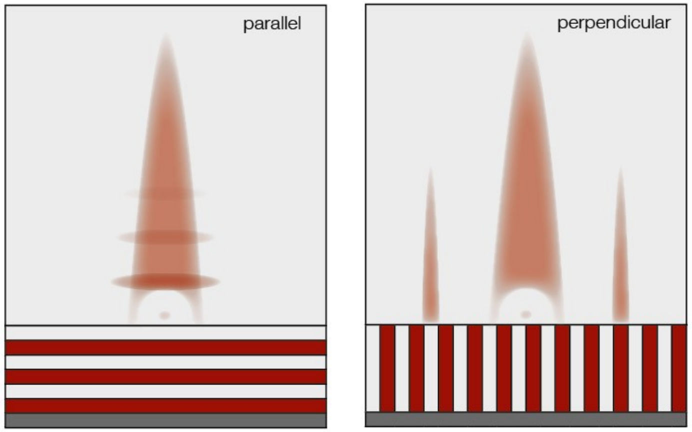
Simulating lamellar structure

`pyapi04_lamellar.py`

Simulating lamellar structures

- Represents one of ordered phase of block copolymers during self-assembly
- Alternating layers of different materials in the form of lamellae

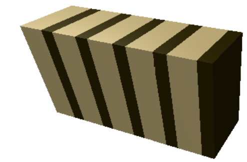




https://wiki.anton-paar.com/

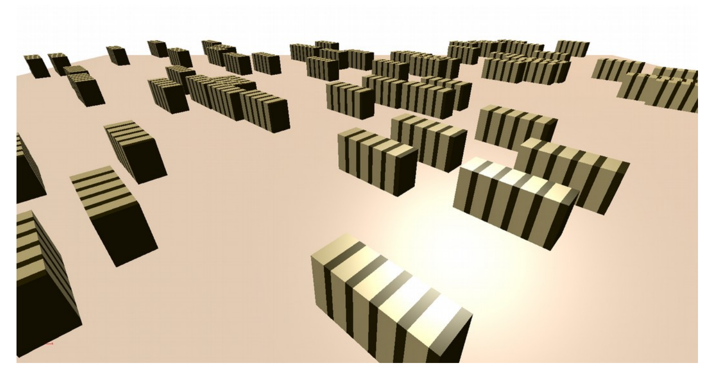
The resulting GISAS pattern depends on the size and arrangement of lamellar structure

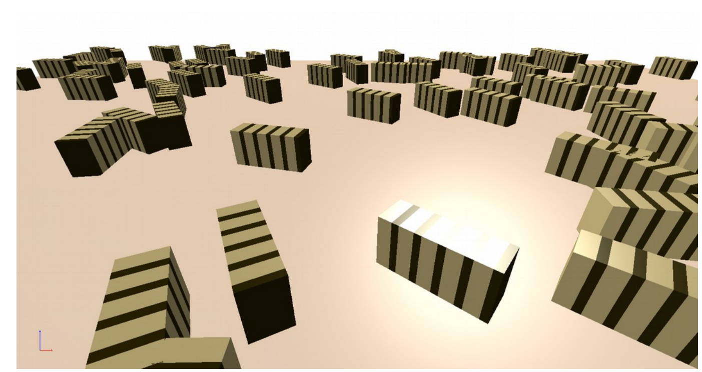
Simulating lamellar structures



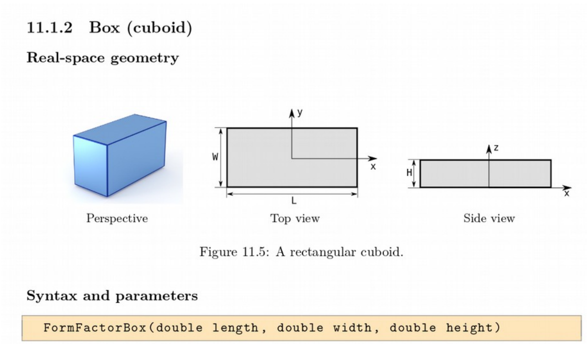
Steps to simulate vertically oriented lamellae in BornAgain using PythonAPI

- Define two materials
  - `HomogeneousMaterial`
- Define two boxes
  - `FormFactorBox`
- Define lamellar structure as stack of boxes
  - `ParticleComposition`
- Add rotation around Z
  - `RotationZ`
- Apply rotation angle distribution 0-180
  - `ParticleDistribution`





Simulating lamellar structures


11.1.2 Box (cuboid)

Real-space geometry

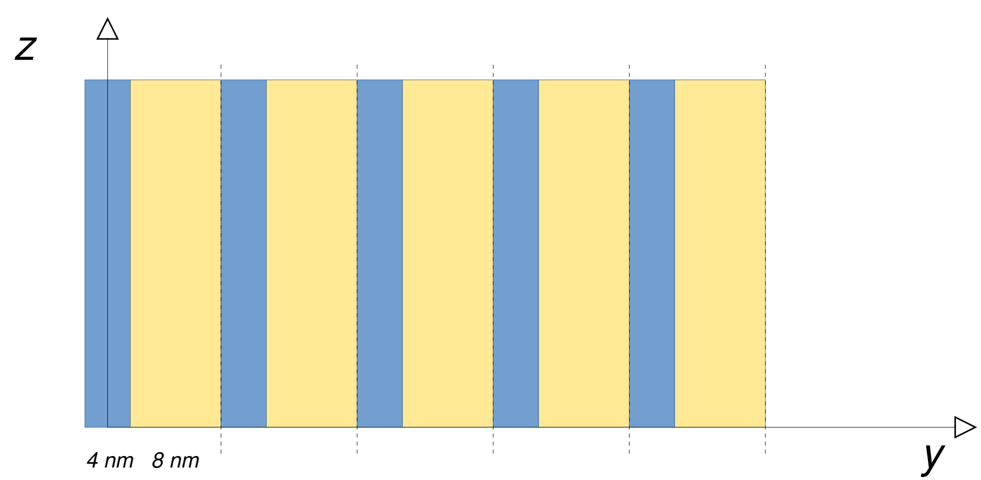
Perspective Top view Side view

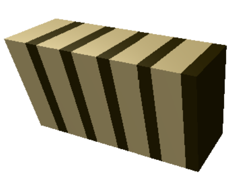
Figure 11.5: A rectangular cuboid.

Syntax and parameters

```
FormFactorBox(double length, double width, double height)
```

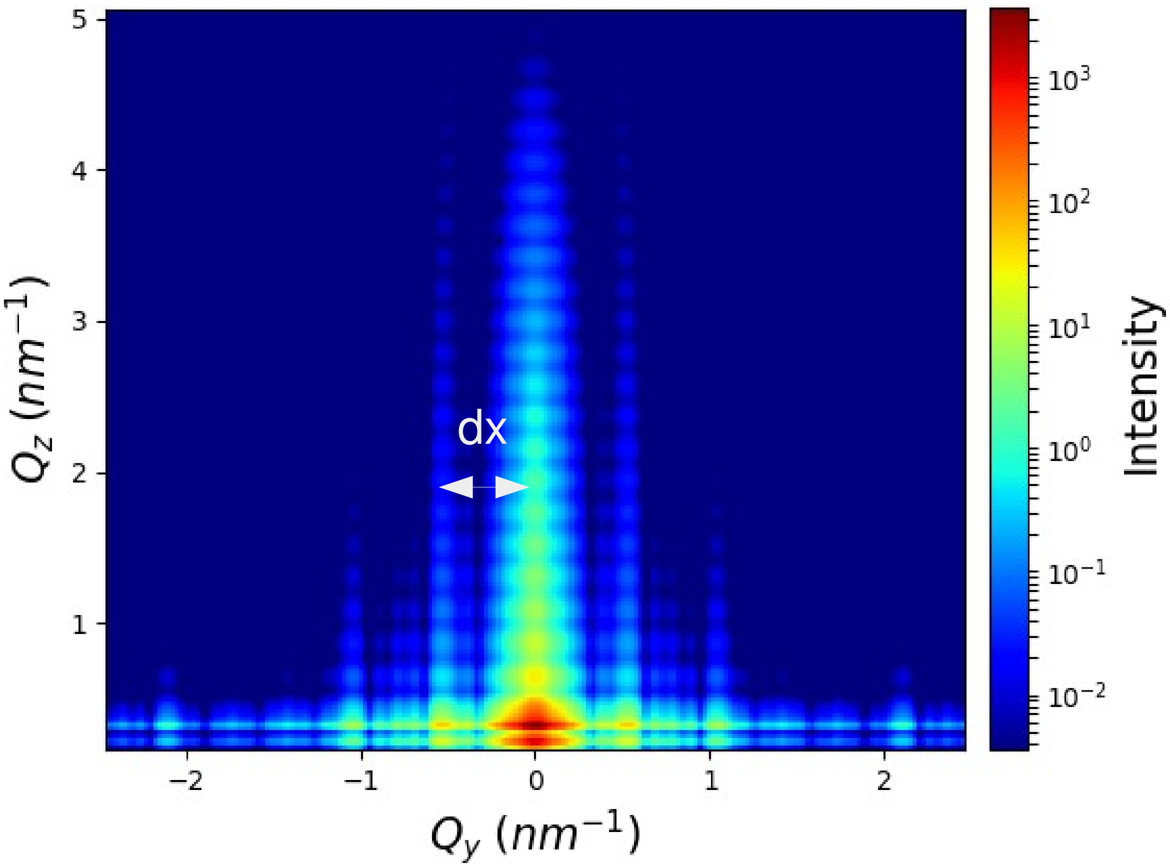
```
def get_horizontal_lamellar():
    mat_a = ba.HomogeneousMaterial("PTFE", 5.20508729E-6, 1.96944292E-8)
    mat_b = ba.HomogeneousMaterial("HMDSO", 2.0888308E-6, 1.32605651E-8)
    length = 30*nm
    width_a = 4*nm
    width_b = 8*nm
    height = 30*nm
    nstack = 5
    stack = ba.ParticleComposition()
    for i in range(0, nstack):
        box_a = ba.Particle(mat_a, ba.FormFactorBox(length, width_a, height))
        box_b = ba.Particle(mat_b, ba.FormFactorBox(length, width_b, height))
        stack.addParticle(box_a, ba.kvector_t(0.0, i*(width_a+width_b), 0.0))
        stack.addParticle(box_b, ba.kvector_t(0.0, (width_a + width_b)/2. + i*(width_a+width_b), 0.0))
```





Simulating lamellar structures

Results

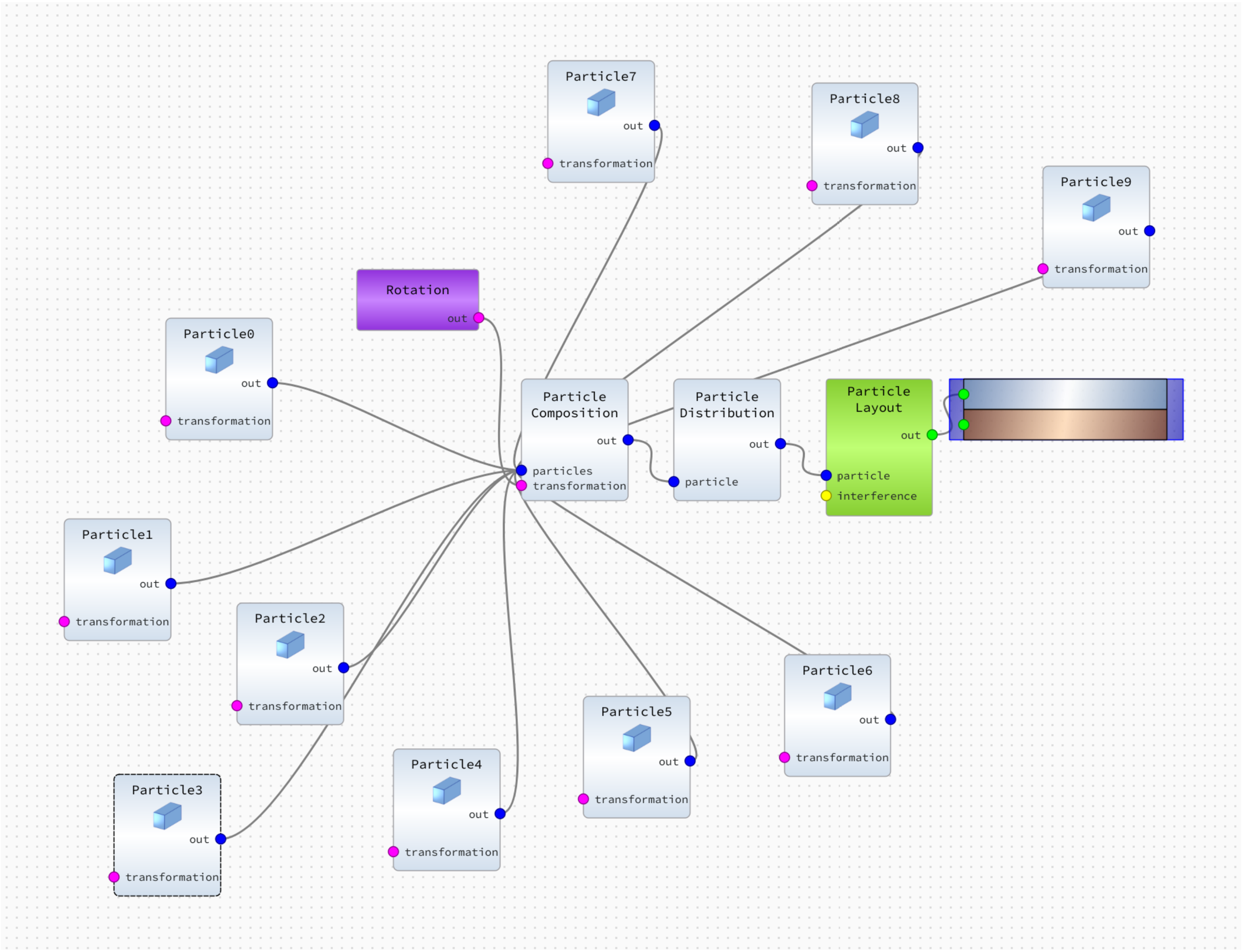


$2*\pi/dx = 12.0$ nm

the value coincide with lamellar period which was defined in simulation script

Simulating lamellar structures

If we would have to do it in GUI …



Task

Modifying lamellar example

`pyapi04_lamellar_vertical_solution1.py`

`pyapi04_lamellar_vertical_solution2.py`

Modifying lamellar example

Task: make lamellar parallel to surface