# BornAgain Python API

# Layout

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

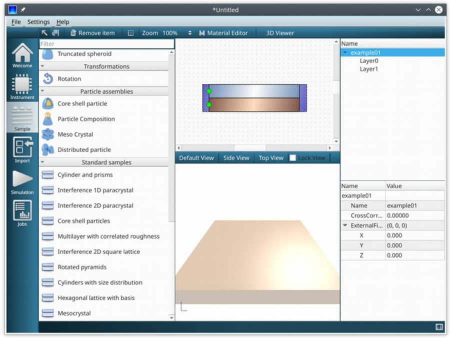
# BornAgain Python API

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

## Advantages

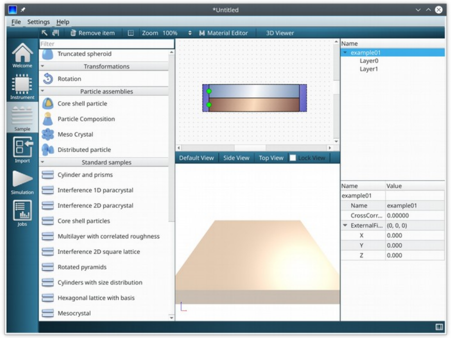
- Complex sample construction
- Access to features non existing in GUI
- Possibility to reuse code in other projects
- Less back-compatibility problems
- Git based workflow

# Minimal simulation example



```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())
```

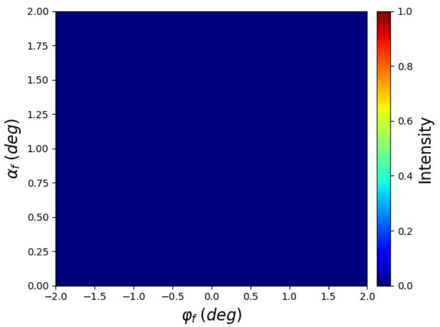
# Minimal simulation example



*GUI equivalent*

```
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())
```

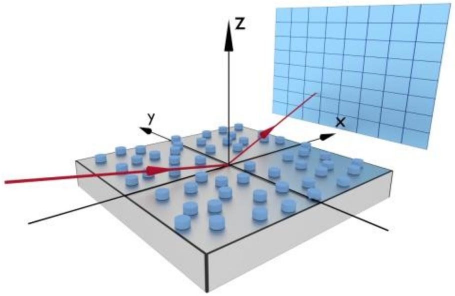
```
$ python pyapi02_minimal_example.py
```



# 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




```
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
```

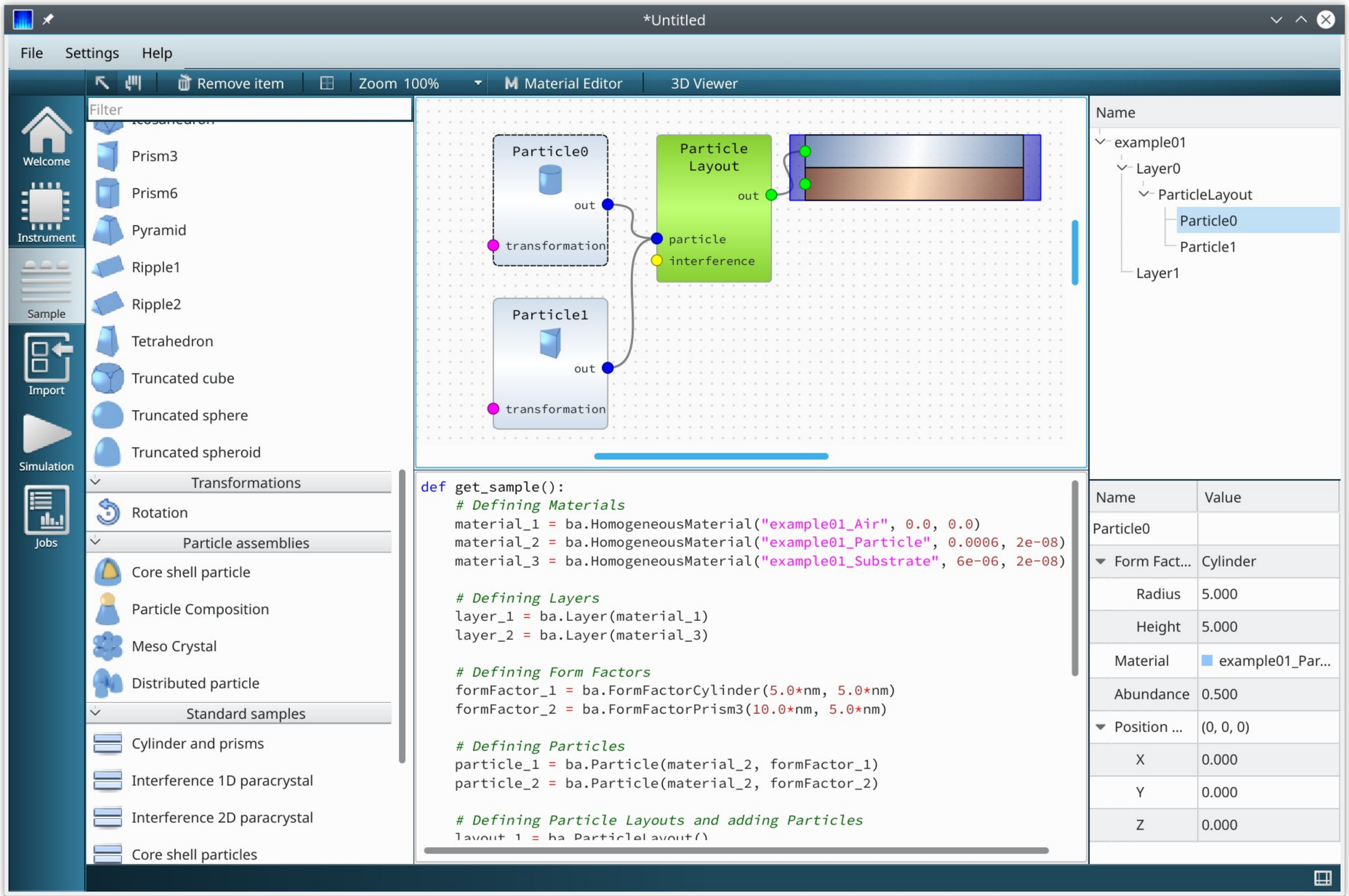
Material definition

Particle collection

MultiLayer construction

# Where to start

## Python viewer embedded in GUI



# Where to start

## Sample model reference on website

BornAgain  Home  Gallery  Download  News  **Documentation**  Contact  About

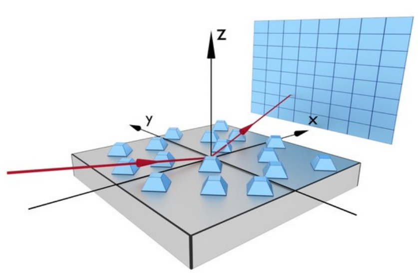
Home > Documentation > Sample model reference > Embedded particles > Rotated Pyramids

### Rotated Pyramids

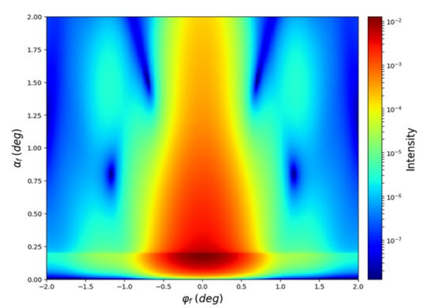
Scattering from a monodisperse distribution of rotated pyramids.

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 $\alpha$ equal to $54.73^\circ$.
- These particles are rotated in the $(x, y)$ plane by $45^\circ$.
- 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

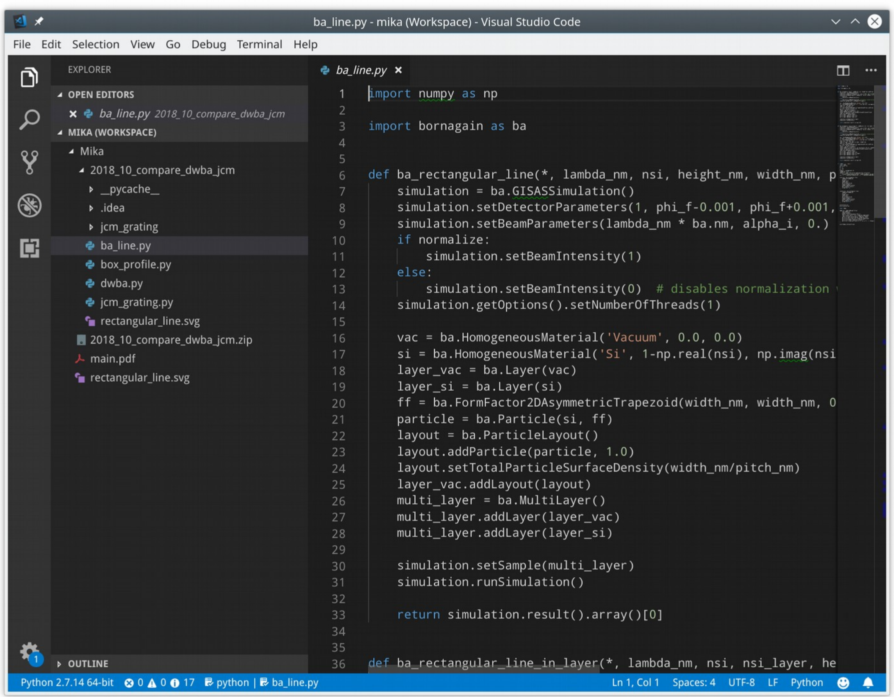



Intensity image

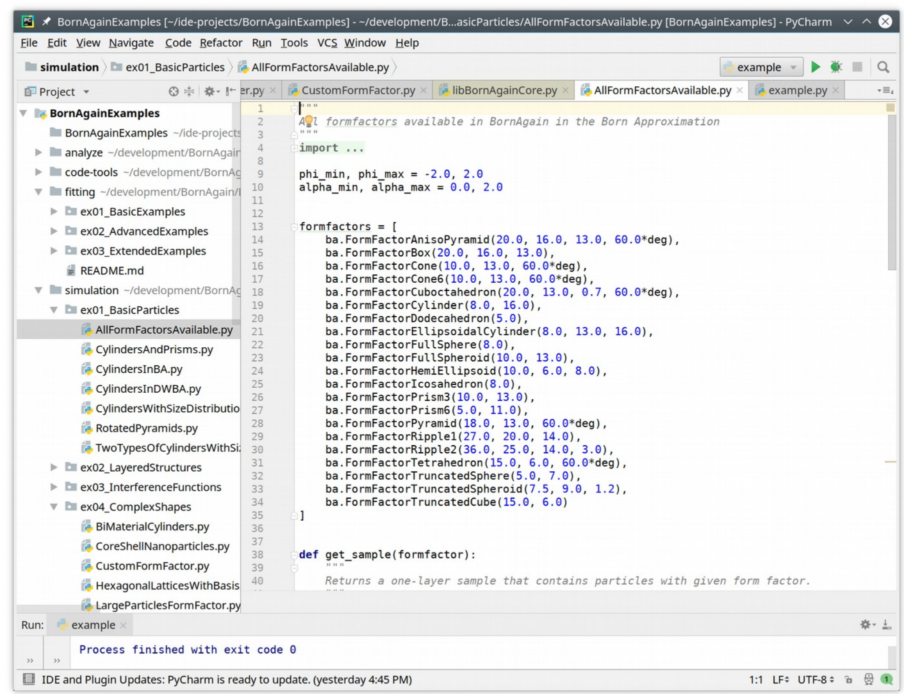
```python
"""
Rotated pyramids on top of substrate
"""
import bornagain as ba
from bornagain import deg, angstrom, nm


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



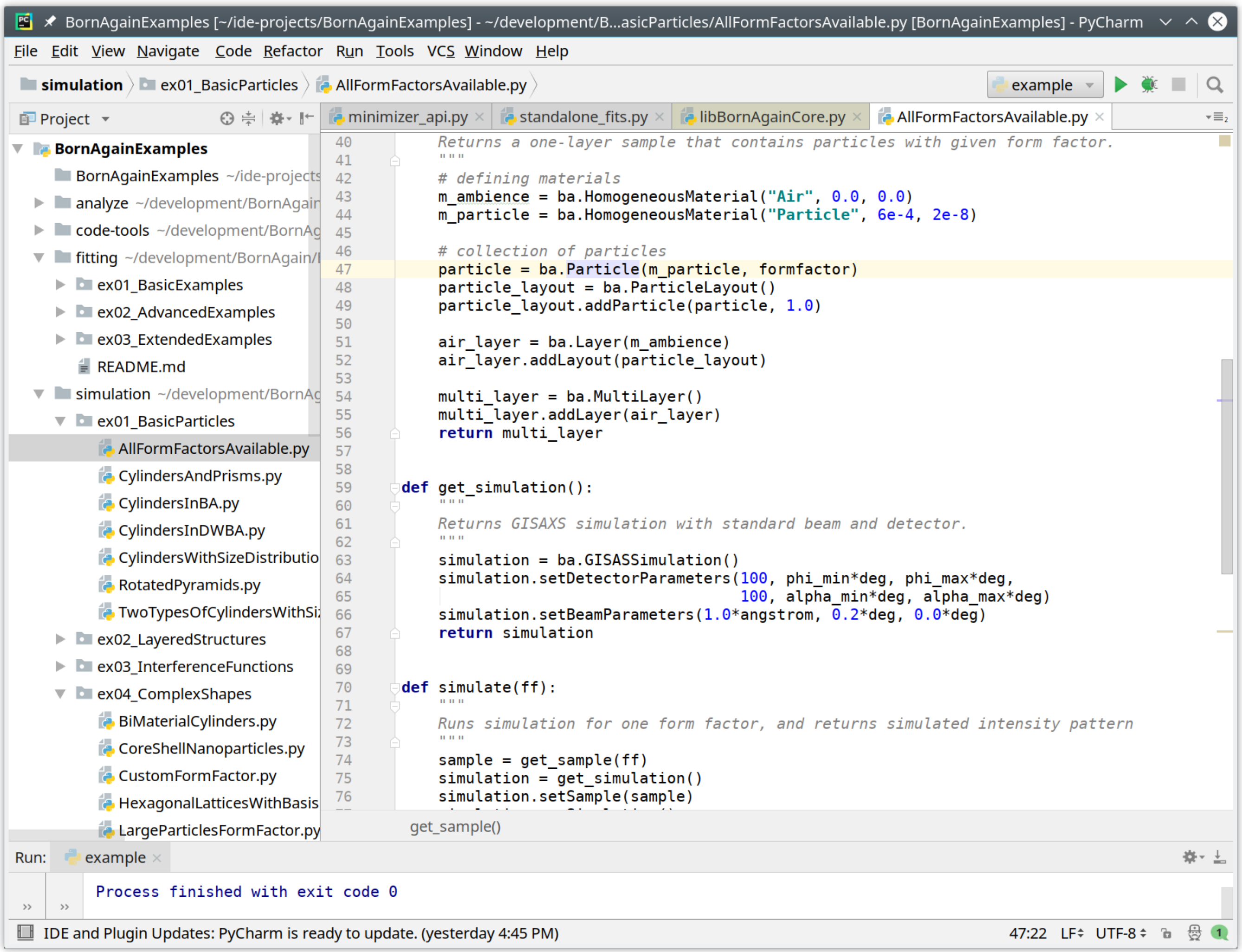

VS Code




PyCharm

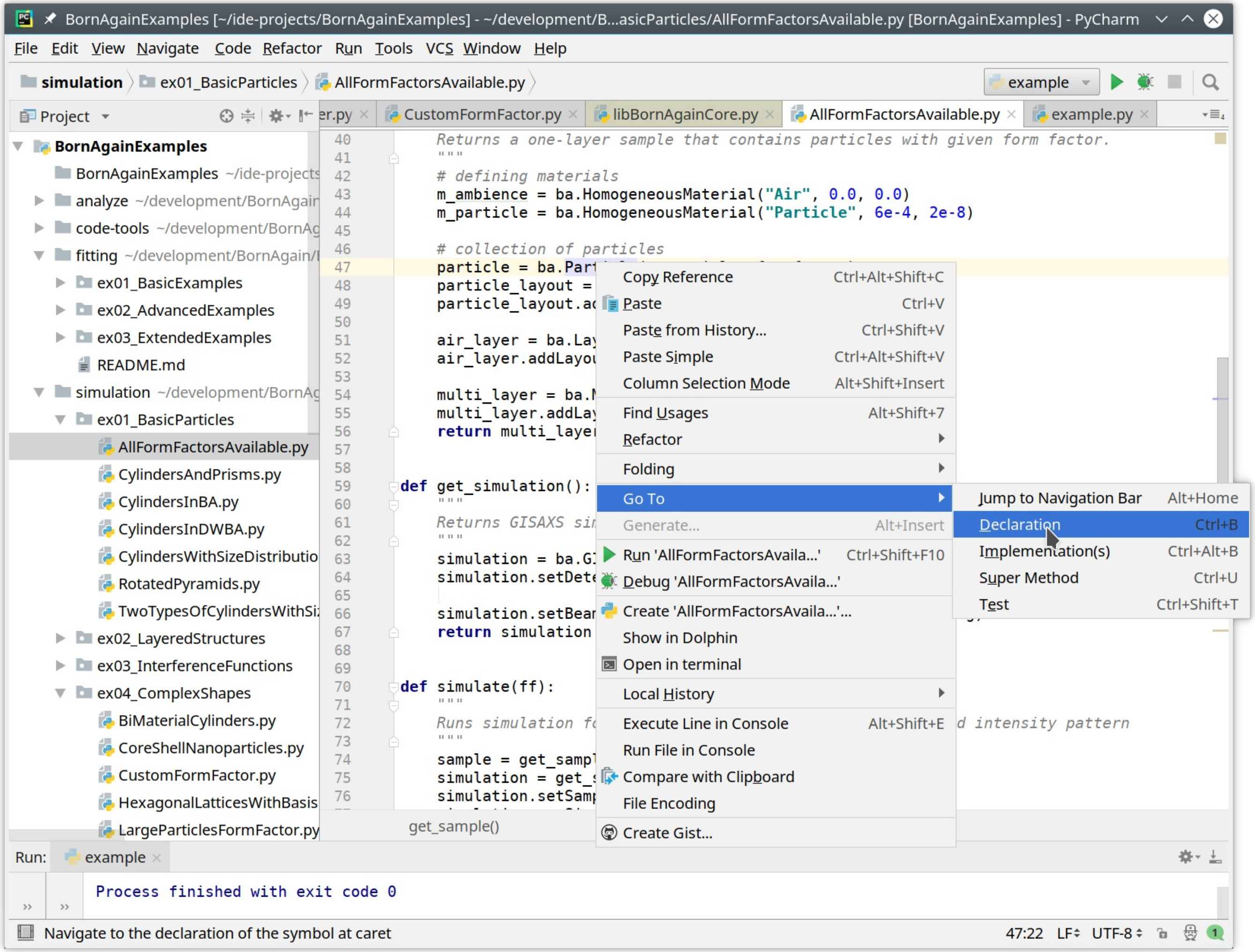
# Python API technicalities

BornAgain Python API is automatically generated from C++ code



# Python API technicalities

BornAgain Python API is automatically generated from C++ code



# Python API technicalities

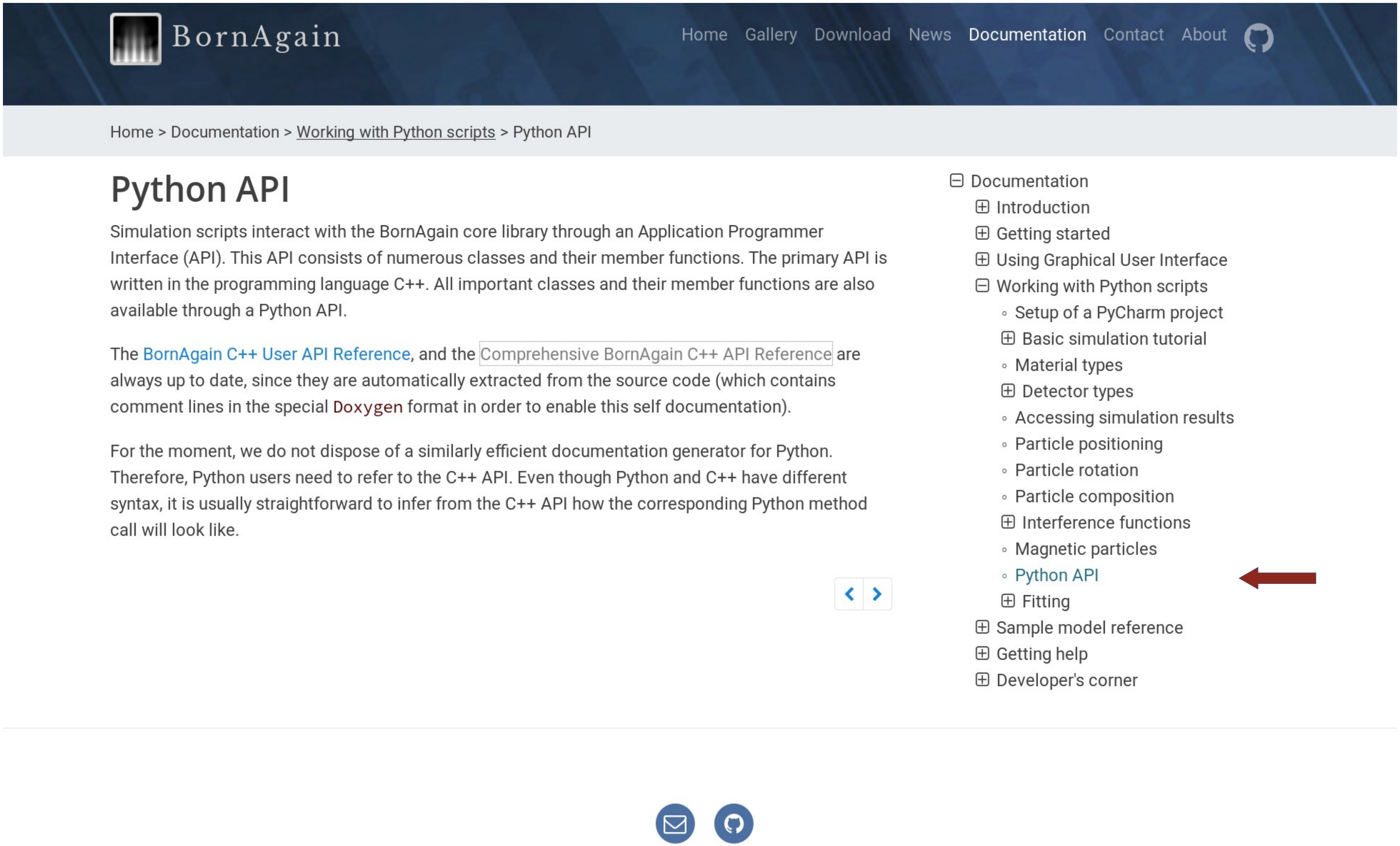
BornAgain Python API is automatically generated from C++ code

*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 …



BornAgain

Home Gallery Download News Documentation Contact About

Home > Documentation > Working with Python scripts > Python API

## 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.

- Documentation
  - Introduction
  - Getting started
  - Using Graphical User Interface
  - Working with Python scripts
    - Setup of a PyCharm project
    - Basic simulation tutorial
    - Material types
    - Detector types
    - Accessing simulation results
    - Particle positioning
    - Particle rotation
    - Particle composition
    - Interference functions
    - Magnetic particles
    - Python API
    - Fitting
  - Sample model reference
  - Getting help
  - Developer's corner

# BornAgain C++ API

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

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

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)<br>Constructor of a rectangular cuboid. More... |
| FormFactorBox * | clone () const overridefinal<br>Returns a clone of this ISample object. |
| void | accept (INodeVisitor *visitor) const overridefinal<br>Calls the INodeVisitor's visit method. |
| double | **getLength** () const |
| double | **getHeight** () const |
| double | **getWidth** () const |
| double | radialExtension () const overridefinal<br>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<br>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

Running trivial simulations

`pyapi02_minimal_example.py`

`pyapi02_jupyter_example.py`

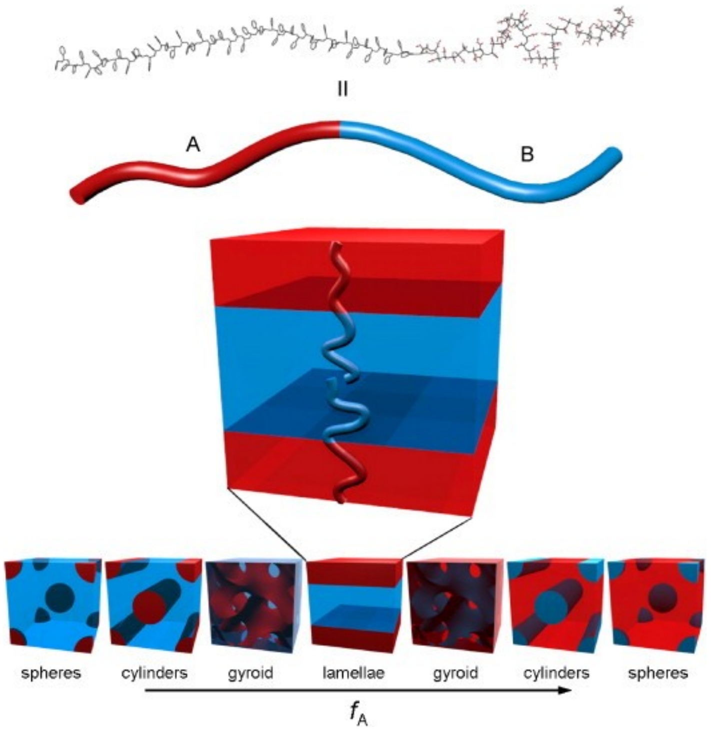
# Demo

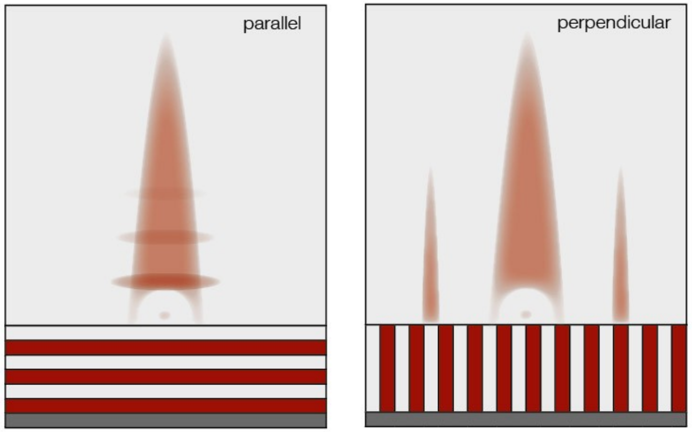
Simulating lamellar structure

`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

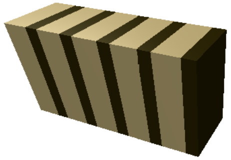



https://wiki.anton-paar.com/

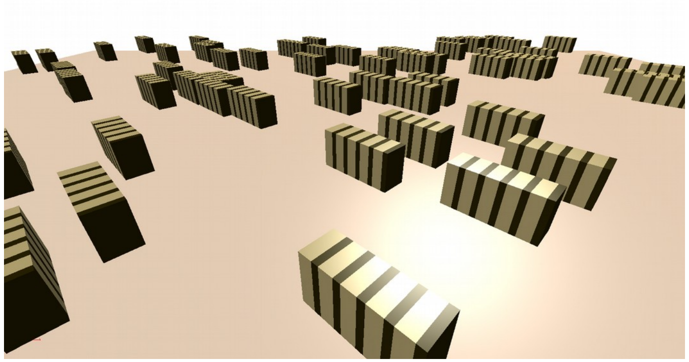
The resulting GISAS pattern depends on the size and arrangement of lamellar structure

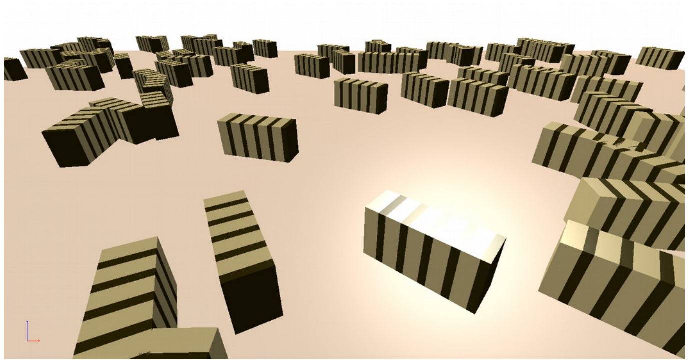
# Simulating lamellar structures



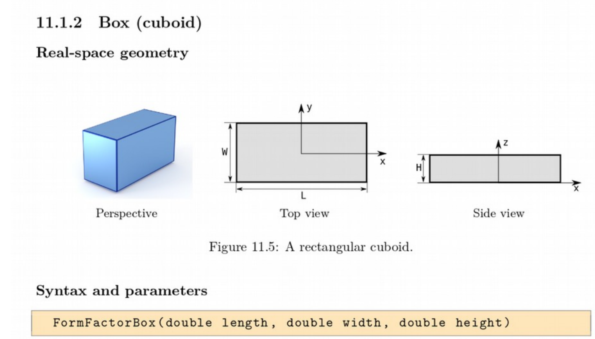
Steps to simulate vertically oriented lamellae in BornAgain using PythonAPI

- 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)

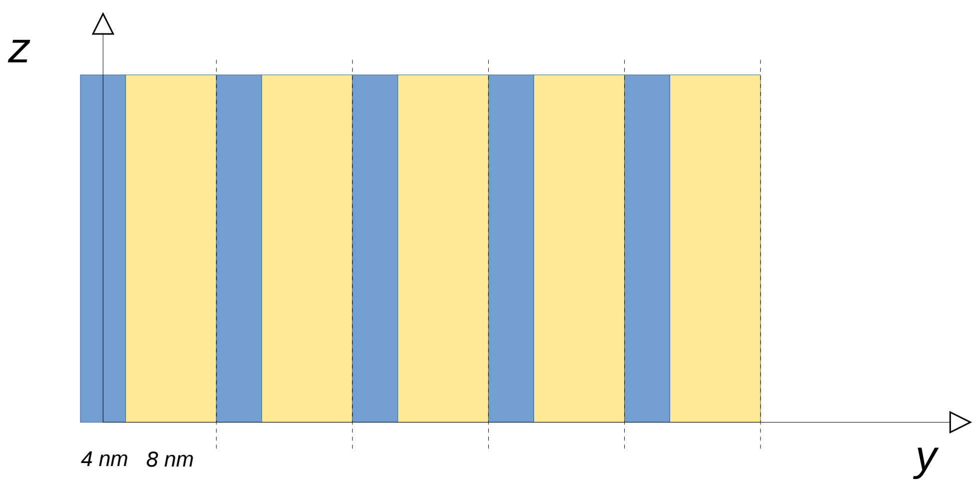
**Real-space geometry**

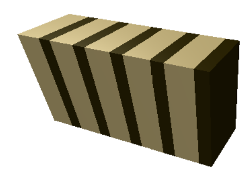

Figure 11.5: A rectangular cuboid.

**Syntax and parameters**

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

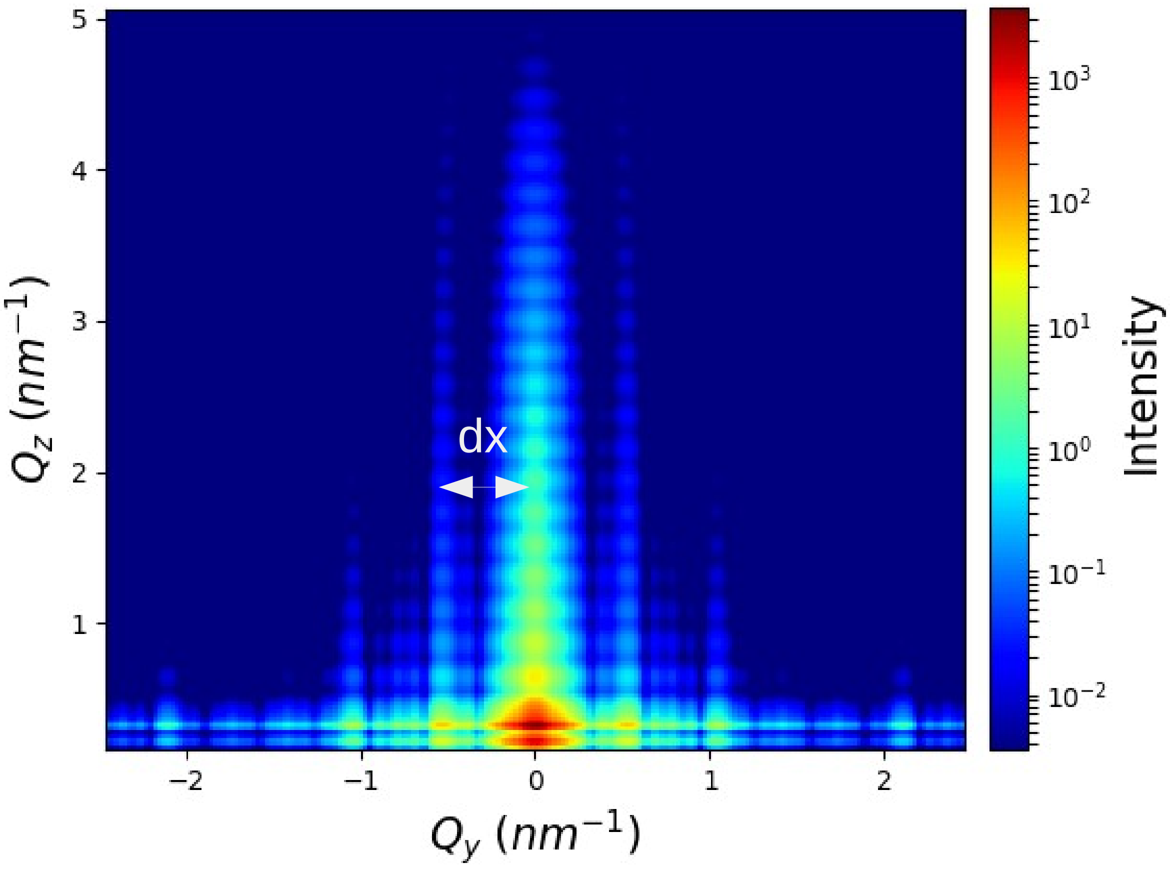
```
def get_horizontal_lamellar():
    mat_a = ba.HomogeneousMaterial("PTFE", 5.20508729E-6, 1.96944292E-8)
    mat_b = ba.HomogeneousMaterial("HMDSO", 2.0888308E-6, 1.32605651E-8)
    length = 30*nm
    width_a = 4*nm
    width_b = 8*nm
    height = 30*nm
    nstack = 5
    stack = ba.ParticleComposition()
    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

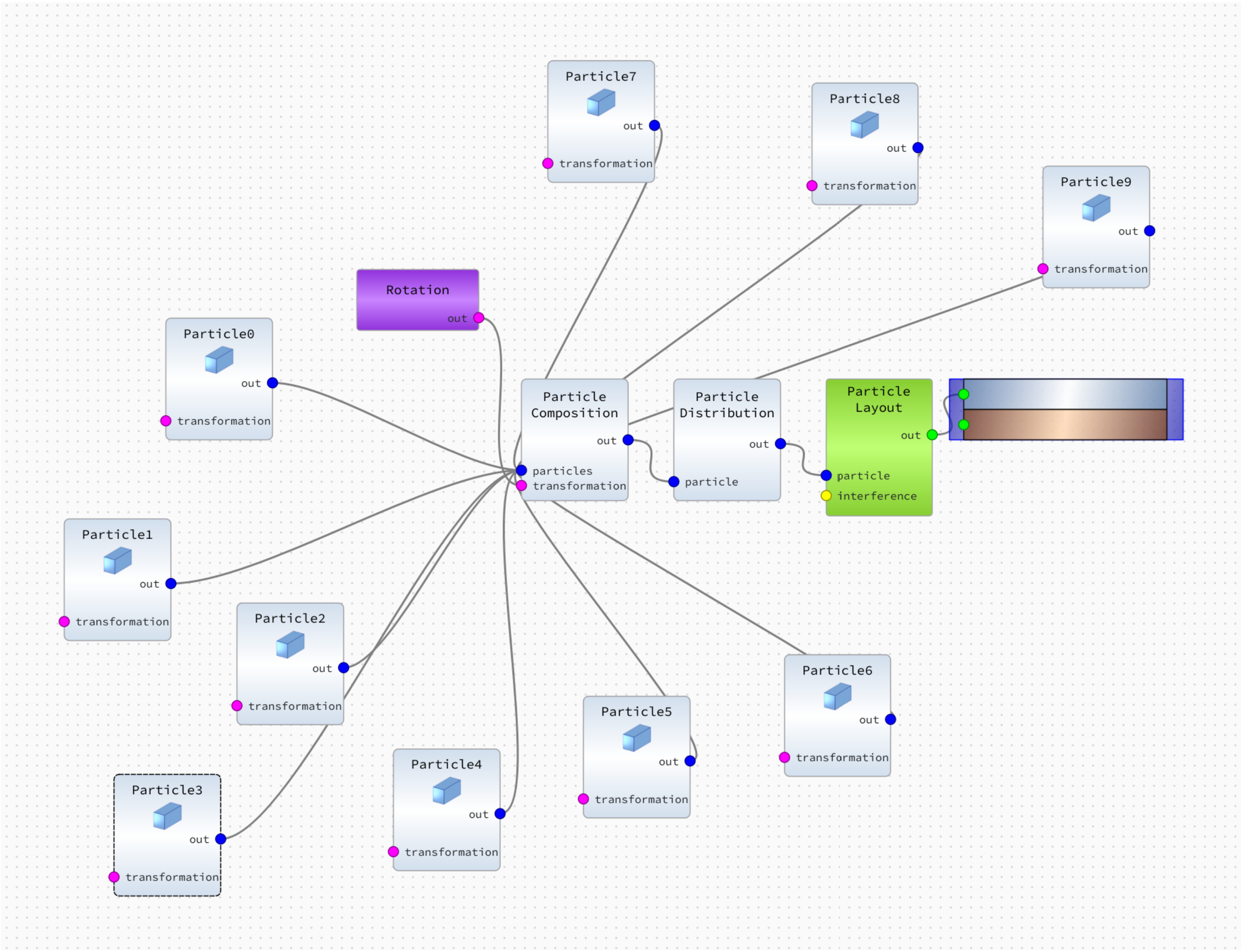



$2*\pi/dx = 12.0$ nm

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