

BornAgain Python API

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day_2

Outline

~/BornAgain-tutorial/talks/day_2/python_api_G

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
Introduction to fitting	talking	pyapi05_fitting.pdf
Fitting from Python outside BornAgain context	demo	pyapi06_rosenbrock_minimum.ipynb pyapi06_lmfit_decaying_wave.ipynb
Exact Python equivalent of GUI fit from day_1	demo	pyapi07_hexspheres_fit.py

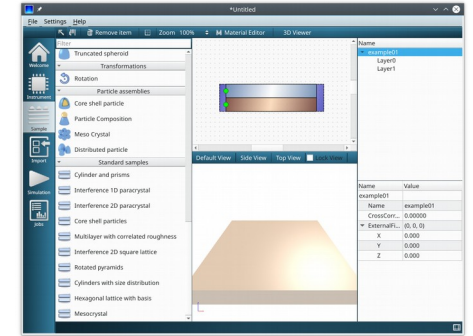
BornAgain Python API

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

```
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)

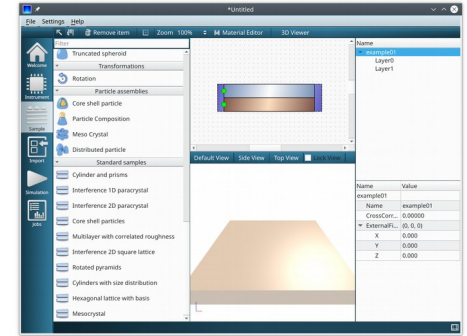
# --- simulation ---

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)

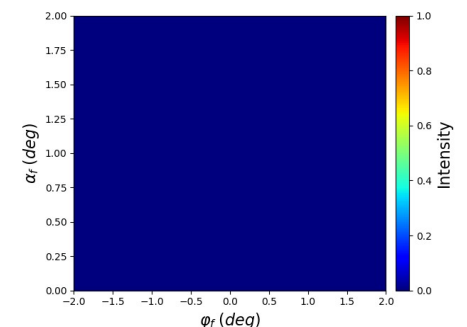
# --- simulation ---

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
```



Demo

Running trivial simulations

`pyapi02_minimal_example.py`

`pyapi02_jupyter_example.py`

Structuring the code

```
import bornagain as ba

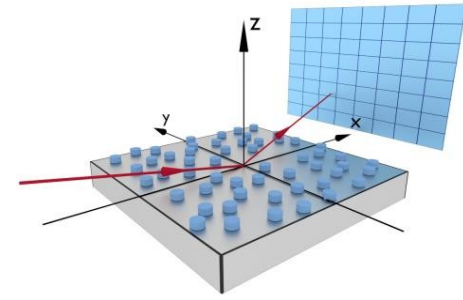
def get_sample():
    multi_layer = ba.MultiLayer()
    ...
    return multi_layer

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)
```

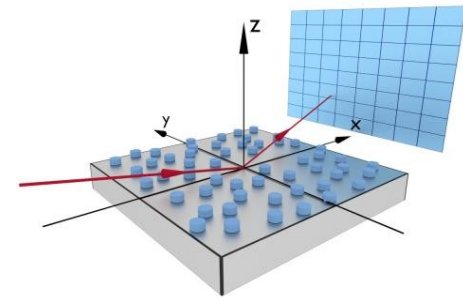
```
    return multi_layer
```

Material definition

Particle collection

MultiLayer construction

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
```

Material definition

```
def get_sample():  
    air, substrate, gold = get_materials()  
  
    # creating particles  
    cylinder_ff = ba.FormFactorCylinder(5*nm, 5*nm)  
    cylinder = ba.Particle(gold, cylinder_ff)
```

Particle collection

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

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

MultiLayer construction

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

Where to start

Python viewer embedded in GUI

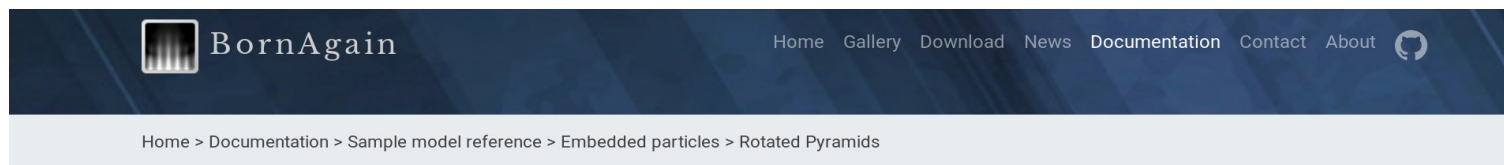
The screenshot shows a GUI application titled '*Untitled' with a menu bar (File, Settings, Help) and a toolbar (Remove item, Zoom 100%, Material Editor, 3D Viewer). The left sidebar contains a 'Filter' and a list of geometric shapes (Prism3, Prism6, Pyramid, Ripple1, Ripple2, Tetrahedron, Truncated cube, Truncated sphere, Truncated spheroid) and transformation options (Rotation, Particle assemblies, Standard samples). The main workspace displays a 3D visualization of a particle assembly with 'Particle0' and 'Particle1' connected to a 'Particle Layout' block. The bottom panel shows a Python code editor with a function 'def get_sample():' defining materials, layers, form factors, particles, and layouts. The right sidebar shows a hierarchical tree view of the assembly and a table of parameters for 'Particle0'.

```
def get_sample():  
    # Defining Materials  
    material_1 = ba.HomogeneousMaterial("example01_Air", 0.0, 0.0)  
    material_2 = ba.HomogeneousMaterial("example01_Particle", 0.0006, 2e-08)  
    material_3 = ba.HomogeneousMaterial("example01_Substrate", 6e-06, 2e-08)  
  
    # Defining Layers  
    layer_1 = ba.Layer(material_1)  
    layer_2 = ba.Layer(material_3)  
  
    # Defining Form Factors  
    formFactor_1 = ba.FormFactorCylinder(5.0*nm, 5.0*nm)  
    formFactor_2 = ba.FormFactorPrism3(10.0*nm, 5.0*nm)  
  
    # Defining Particles  
    particle_1 = ba.Particle(material_2, formFactor_1)  
    particle_2 = ba.Particle(material_2, formFactor_2)  
  
    # Defining Particle Layouts and adding Particles  
    layout_1 = ba.ParticleLayout()
```

Name	Value
Particle0	
Form Fact...	Cylinder
Radius	5.000
Height	5.000
Material	example01_Par...
Abundance	0.500
Position ...	(0, 0, 0)
X	0.000
Y	0.000
Z	0.000

Where to start

Sample model reference on website

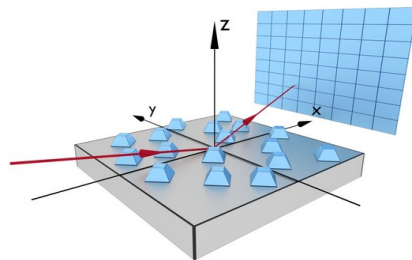


Rotated Pyramids

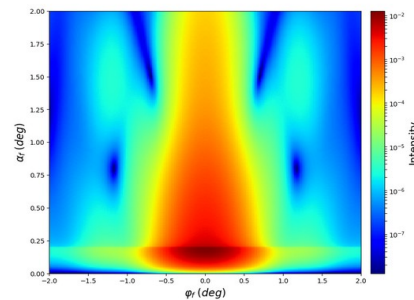
Scattering from a monodisperse distribution of rotated pyramids.

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



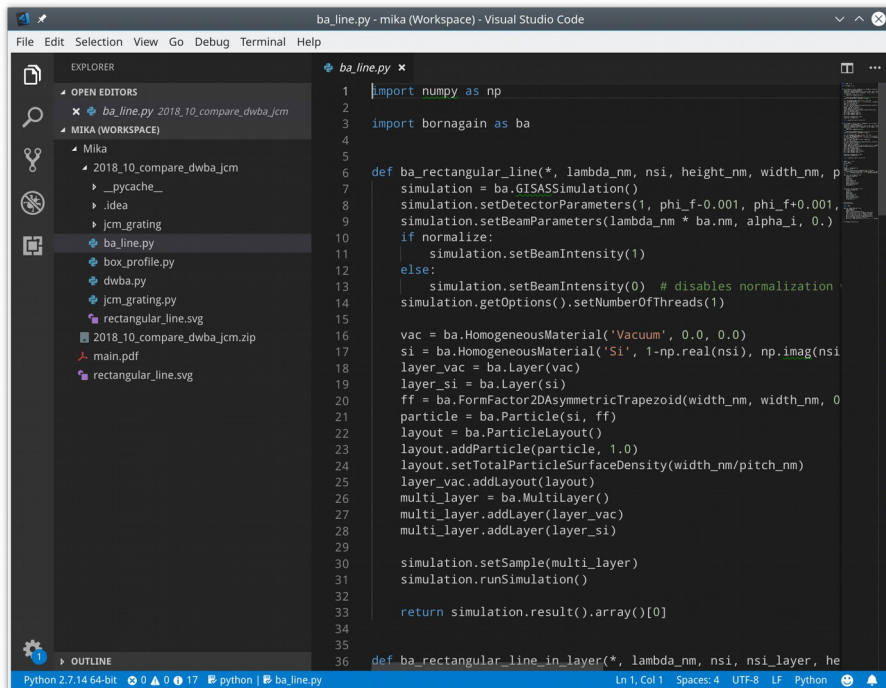
Intensity image

```
1  """
2  Rotated pyramids on top of substrate
3  """
4  import bornagain as ba
5  from bornagain import deg, angstrom, nm
6
7
8  def get_sample():
    ....
```

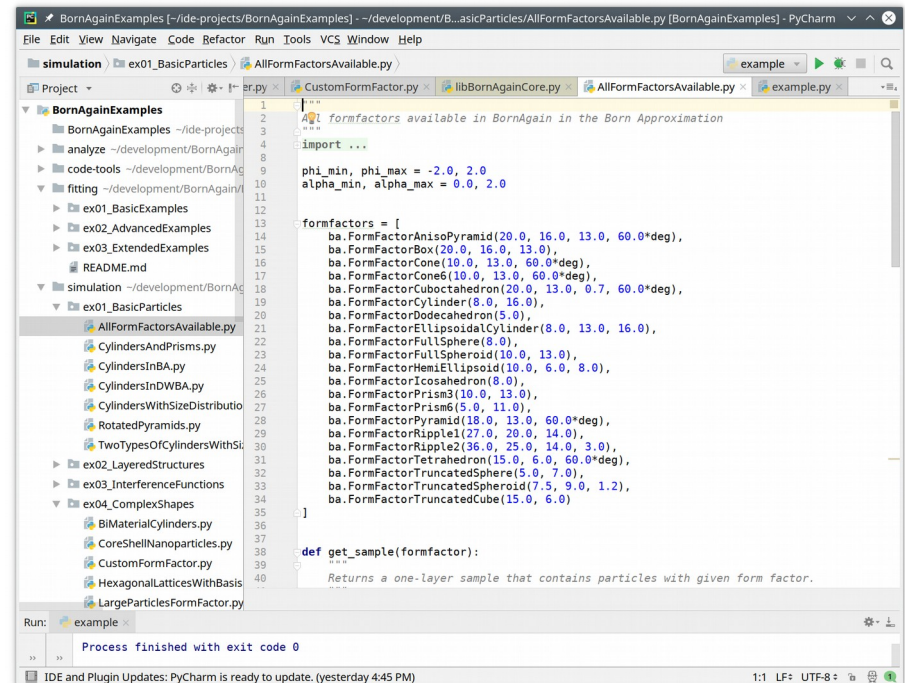
- [-] Documentation
 - [+] Introduction
 - [+] Getting started
 - [+] Using Graphical User Interface
 - [+] Working with Python scripts
 - [-] Sample model reference
 - [-] Embedded particles
 - Cylinders in Born Approximation
 - Cylinders in Distorted Wave Born Approximation
 - Cylinders with size distribution
 - Two types of cylinders with size distribution
 - Rotated Pyramids
 - Cylinders and Prisms
 - All available form factors
 - [+] Layered structures
 - [+] Interference functions
 - [+] Complex shapes
 - [+] Beam and detector
 - [+] Reflectometry
 - [+] Fitting
 - [+] Miscellaneous
 - [+] Getting help
 - [+] Developer's corner

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

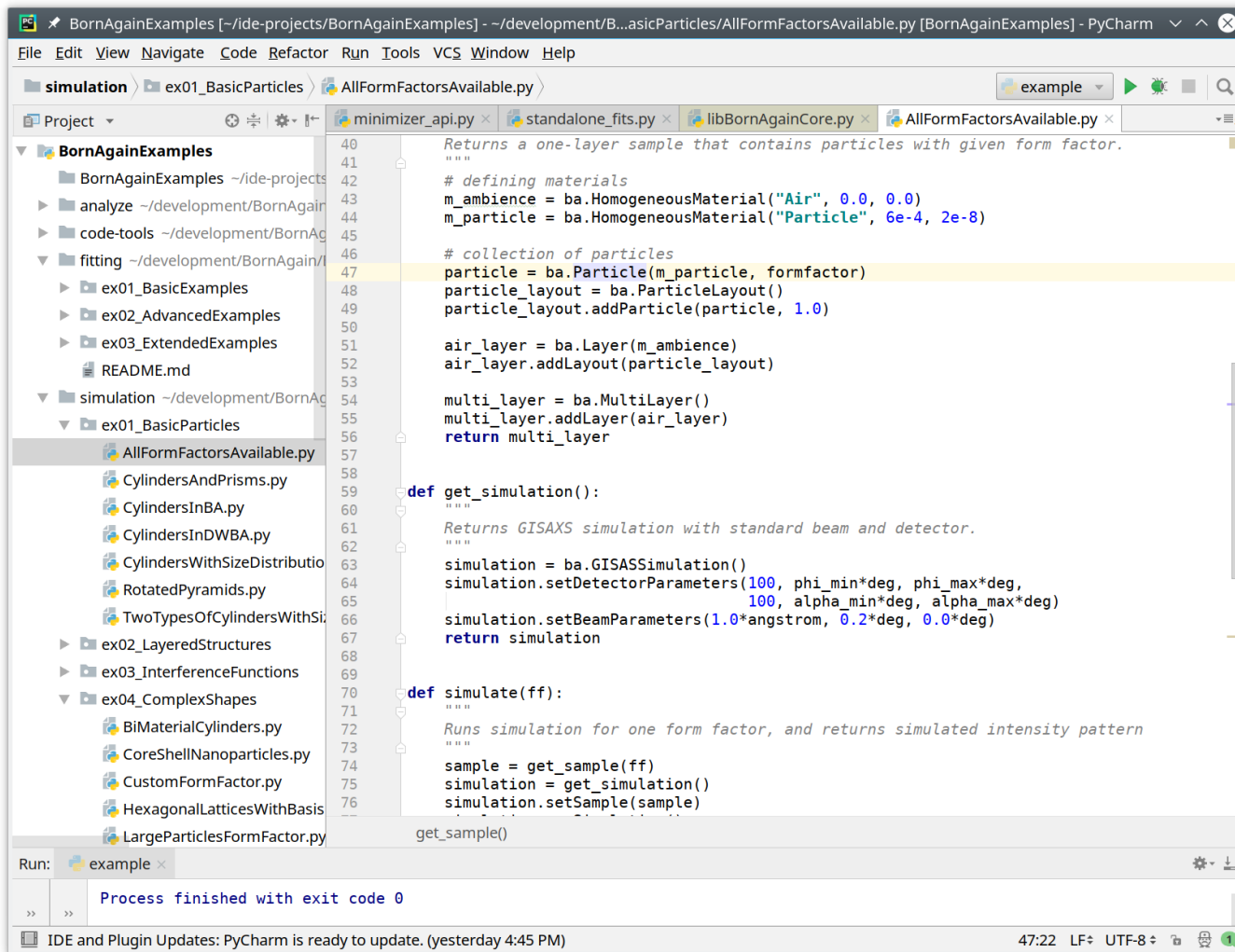


VS Code



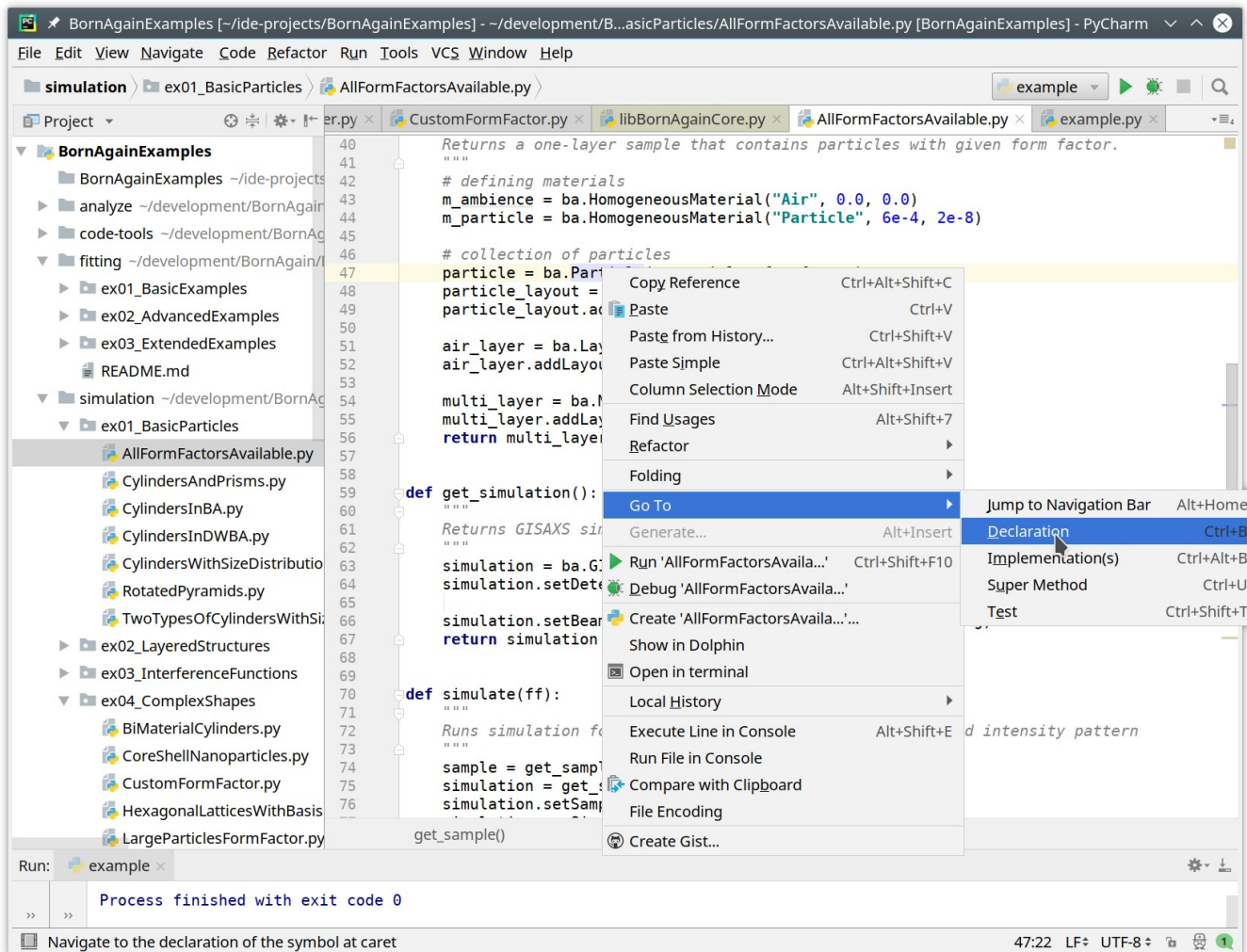
Python API technicalities

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*

```
26223 class Particle(IParticle):
26224     """
26225
26226     A particle with a form factor and refractive index.
26227
26228     C++ includes: Particle.h
26229
26230     """
26231
26232     __swig_setmethods__ = {}
26233     for _s in [IParticle]:
26234         __swig_setmethods__.update(getattr(_s, '__swig_setmethods__', {}))
26235     __setattr__ = lambda self, name, value: __swig_setattr(self, Particle, name, value)
26236     __swig_getmethods__ = {}
26237     for _s in [IParticle]:
26238         __swig_getmethods__.update(getattr(_s, '__swig_getmethods__', {}))
26239     __getattr__ = lambda self, name: __swig_getattr(self, Particle, name)
26240     __repr__ = __swig_repr
26241
26242
26243 def __init__(self, *args):
26244     """
26245     __init__(Particle self) -> Particle
26246     __init__(Particle self, Material material) -> Particle
26247     __init__(Particle self, Material material, IFormFactor form_factor) -> Particle
26248     __init__(Particle self, Material material, IFormFactor form_factor, IRotation rota
26249
26250     Particle::Particle(Material material, const IFormFactor &form_factor, const IRotat
26251
26252     """
26253     this = _libBornAgainCore.new_Particle(*args)
26254     try:
26255         self.this.append(this)
26256     except __builtin__.Exception:
26257         self.this = this
26258
```

Documentation on Python API

C++ API documentation sometimes might help ...

 BornAgain

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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.

[<](#) [>](#)

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- ⊕ Using Graphical User Interface
- ⊖ Working with Python scripts
 - Setup of a PyCharm project
 - ⊕ Basic simulation tutorial
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 - ⊕ 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

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FormFactorCrystal

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FormFactorCylinder

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FormFactorDecoratorMaterial

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FormFactorDodecahedron

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FormFactorEllipsoidalCylinder

FormFactorFullSphere

FormFactorFullSpheroid

FormFactorGauss

FormFactorHemiEllipsoid

FormFactorIcosahedron

FormFactorLongBox

FormFactorLongBoxGauss

IClusteredParticles

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Icosahedron

IdentityRotation

IDetector

IDetector2D

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IDistribution1D

IDistribution1DSampler

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IFactory

IFootprintFactor

IFormFactor

IFormFactorBorn

IFormFactorDecorator

IFresnelMap

IFTDecayFunction1D

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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.](#)

```
1  // ***** //  
2  //  
3  // BornAgain: simulate and fit scattering at grazing incidence  
4  //  
5  ///! @file      Core/HardParticle/FormFactorBox.cpp  
6  ///! @brief     Implements class FormFactorBox.  
7  ///!  
8  ///! @homepage  http://www.bornagainproject.org  
9  ///! @license   GNU General Public License v3 or higher (see COPYING)  
10 ///! @copyright  Forschungszentrum Jülich GmbH 2018  
11 ///! @authors   Scientific Computing Group at MLZ (see CITATION, AUTHORS)  
12 //  
13 // ***** //  
14 //  
15 #include "FormFactorBox.h"  
16 #include "BornAgainNamespace.h"  
17 #include "Box.h"  
18 #include "MathFunctions.h"  
19 #include "RealParameter.h"  
20 //  
21 ///! Constructor of a rectangular cuboid.  
22 ///! @param length: length of the base in nanometers  
23 ///! @param width: width of the base in nanometers  
24 ///! @param height: height of the box in nanometers  
25 FormFactorBox::FormFactorBox(double length, double width, double height)  
26     : m_length(length), m_width(width), m_height(height)  
27 {  
28     setName(BornAgain::FFBoxType);  
29     registerParameter(BornAgain::Length, &m_length).setUnit(BornAgain::UnitsNm).setNonnegative();  
30     registerParameter(BornAgain::Width, &m_width).setUnit(BornAgain::UnitsNm).setNonnegative();  
31     registerParameter(BornAgain::Height, &m_height).setUnit(BornAgain::UnitsNm).setNonnegative();  
32     onChange();  
33 }  
34 //  
35 complex_t FormFactorBox::evaluate_for_q(cvector_t q) const  
36 {  
37     complex_t qzHdiv2 = m_height/2*q.z();  
38     return m_height*m_length*m_width *  
39         MathFunctions::sinc(m_length/2*q.x()) * MathFunctions::sinc(m_width/2*q.y()) *  
40         MathFunctions::sinc(qzHdiv2) * exp_I(qzHdiv2);  
41 }  
42
```

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

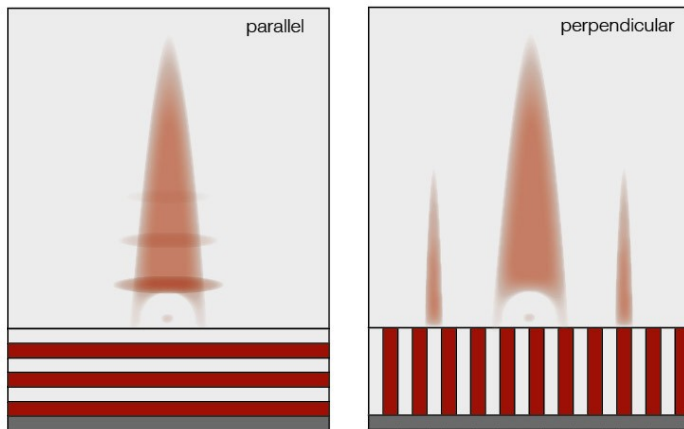
Demo

Simulating lamellar structure

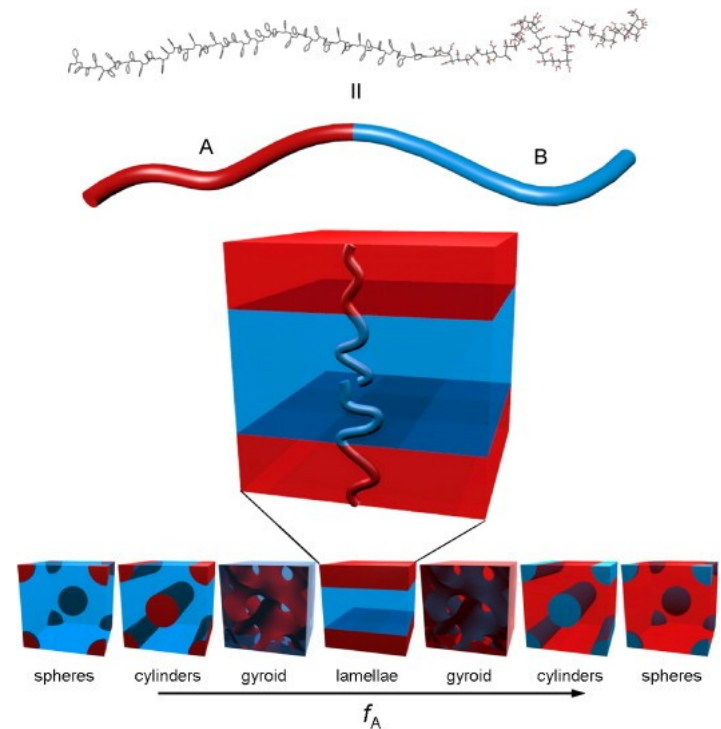
`pyapi04_lamellar.py`

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/>

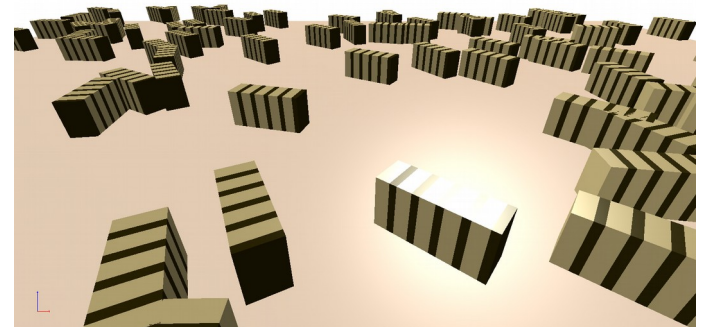
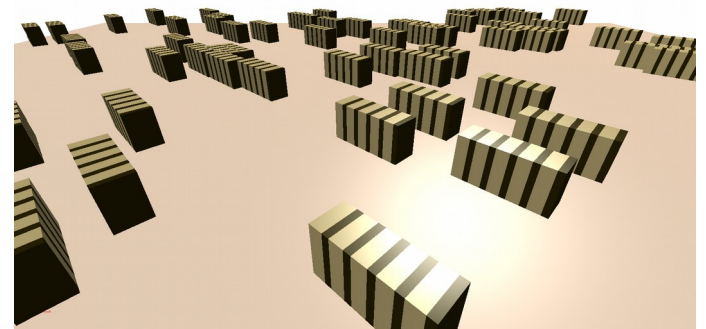
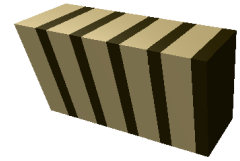


The resulting GISAS pattern depends on the size and arrangement of lamellar structure

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

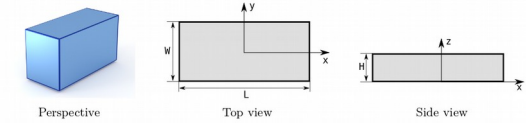
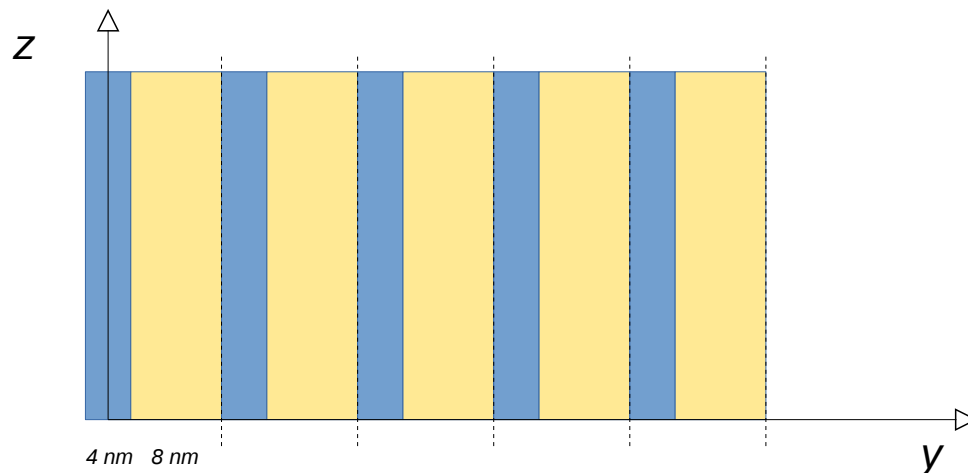


Figure 11.5: A rectangular cuboid.

Syntax and parameters

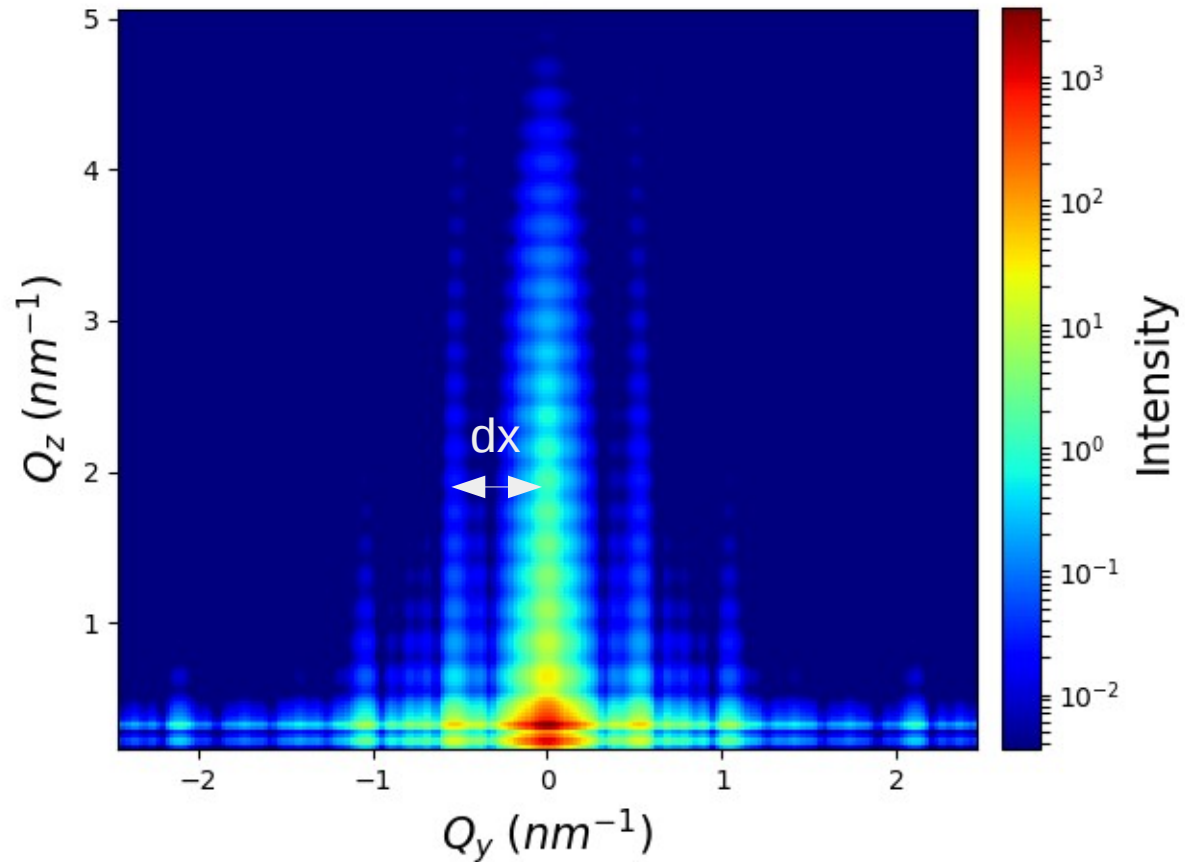
```
FormFactorBox(double length, double width, double height)
```

```
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

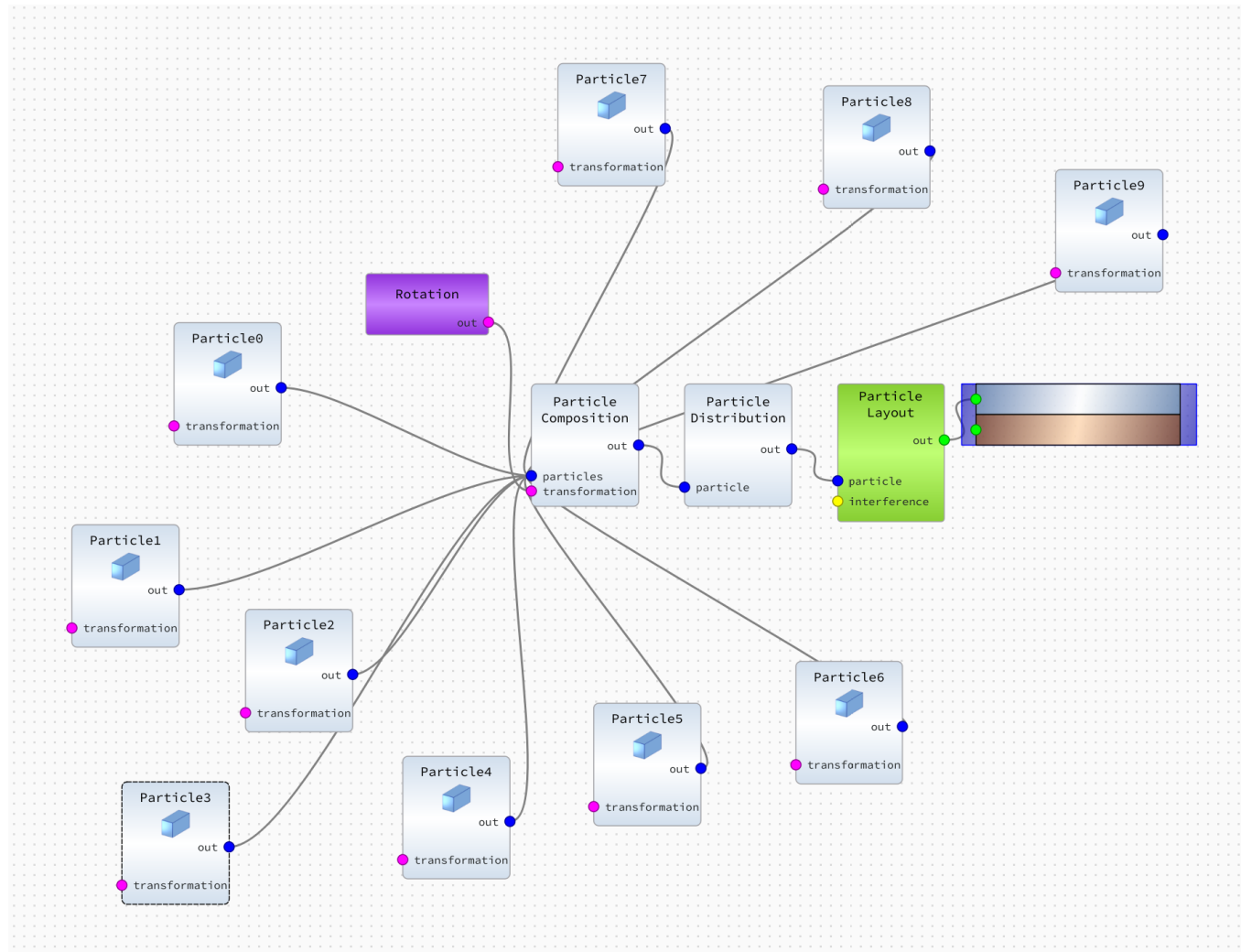


$$2 \cdot \pi / dx = 12.0 \text{ nm}^{-1}$$

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

