

Status of a new reflectometry GUI

for ESS DMSC & reflectometry STAP

October 21, 2020

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Reflectometry in BornAgain

The screenshot shows the BornAgain software interface. The main workspace contains a diagram with the following components:

- Particle** block: A blue box with an 'out' port connected to the 'particle' port of the Particle Layout block.
- Particle Layout** block: A green box with an 'out' port connected to the 'Interference' port of the Interference 2DLattice block. It is also connected to a material stack.
- Interference 2DLattice** block: A yellow box with an 'out' port.
- Material Stack**: A stack of three layers: 'example06_Air' (blue), 'Default' (green), and 'example06_Substrate' (brown).

The Python code at the bottom of the workspace defines the simulation setup:

```
def get_sample():  
    # Defining Materials  
    material_1 = ba.HomogeneousMaterial("example06_Air", 0.0, 0.0)  
    material_2 = ba.HomogeneousMaterial("example06_Particle", 0.0006, 2e-08)  
    material_3 = ba.HomogeneousMaterial("Default", 0.001, 1e-05)  
    material_4 = ba.HomogeneousMaterial("example06_Substrate", 6e-06, 2e-08)  
  
    # Defining Layers  
    layer_1 = ba.Layer(material_1)  
    layer_2 = ba.Layer(material_3)
```

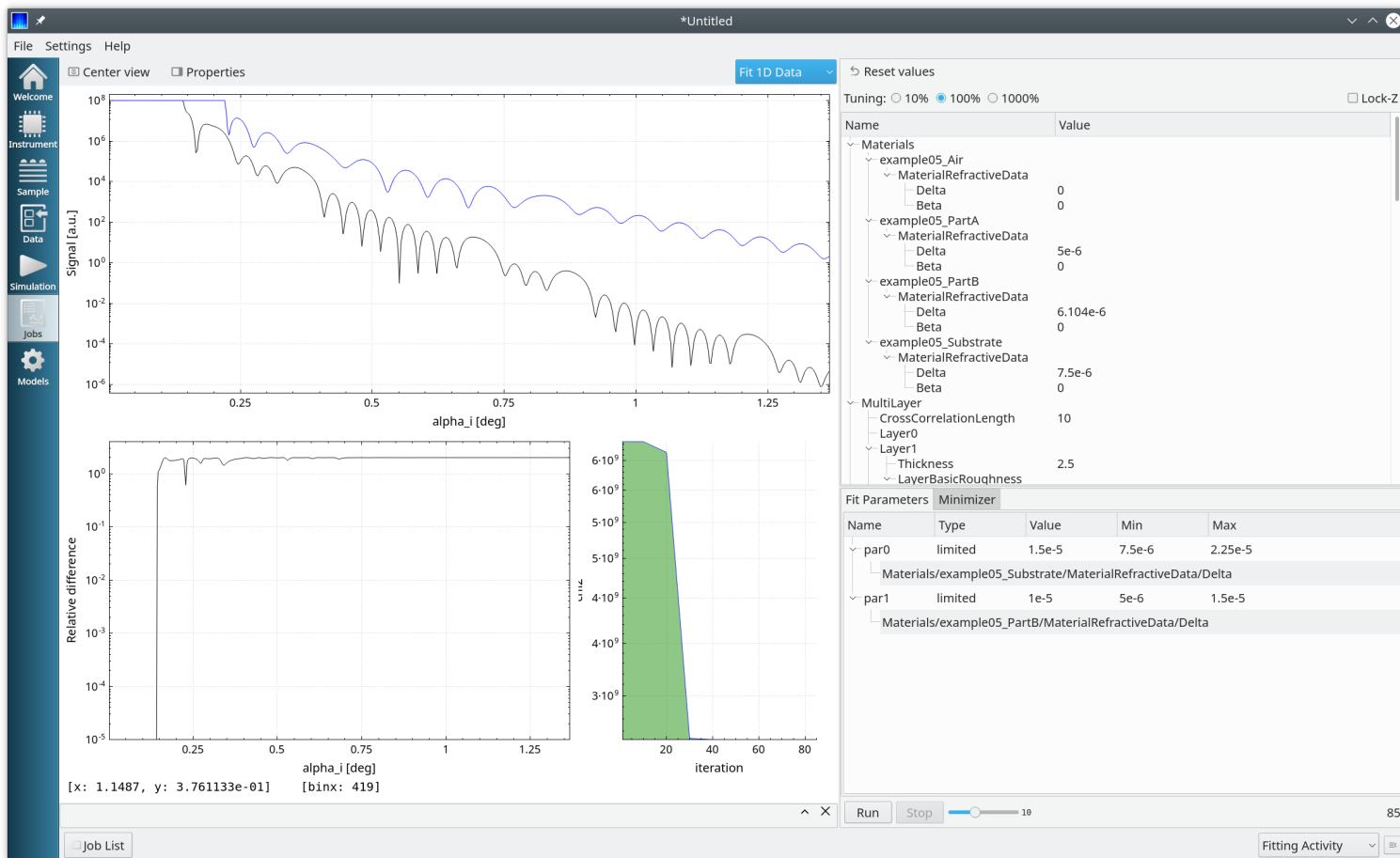
The right sidebar shows a tree view of the simulation structure:

- example06
 - Layer0
 - ParticleLayout
 - Particle
 - Interference2DLattice
 - Layer1
 - Layer2

Below the tree view is a table of parameters:

Name	Value
Interference...	
PositionV...	0.000
LatticeType	Square
Lattice...	10.000
Xi	0.000
Decay Fun...	Cauchy 2D
Decay...	47.746
Decay...	15.915
Gamma	0.000
Integratio...	<input type="checkbox"/> False

Reflectometry in BornAgain



Reflectometry in BornAgain

The screenshot displays the BornAgain software interface. The central 3D viewer shows a layered sample model with the following components:

- example05_Air
- example05_PartA
- example05_PartB
- example05_PartA
- example05_PartB
- example05_PartA
- example05_PartB
- example05_PartA
- example05_PartB
- example05_PartA
- example05_PartB
- example05_Substrate

The left sidebar contains a 'Filter' section and several categories of options:

- Instrument:** Prism3, Prism6, Pyramid, Tetrahedron, Truncated cube, Truncated sphere, Truncated spheroid, Ripples
- Sample:** Box, BarGauss, BarLorentz, Ripple1Box, Ripple1Gauss, Ripple1Lorentz, Ripple2Box, Ripple2Gauss, Ripple2Lorentz
- Simulation:** Rotation, Particle assemblies (Core shell particle, Particle Composition, Meso Crystal, Distributed particle), Standard samples (Cylinder and prisms, Interference 1D paracrystal, Interference 2D paracrystal, Core shell particles, Multilayer with...lated roughness, Interference 2D square lattice, Rotated pyramids, Cylinders with size distribution, Hexagonal lattice with basis, Mesocrystal)

The right sidebar shows a tree view for 'example05' with layers Layer0 through Layer11. Below it is a table of parameters:

Name	Value
example05	
Name	example05
CrossCorr...	10.00000
ExternalFlu...	(0, 0, 0)
X	0.000
Y	0.000
Z	0.000

At the bottom, a code editor shows the following Python code:

```
def get_sample():  
    # Defining Materials  
    material_1 = ba.HomogeneousMaterial("example05 Air", 0.0, 0.0)  
    material_2 = ba.HomogeneousMaterial("example05 PartA", 5e-06, 0.0)  
    material_3 = ba.HomogeneousMaterial("example05 PartB", 1e-05, 0.0)  
    material_4 = ba.HomogeneousMaterial("example05 Substrate", 1.5e-05, 0.0)  
  
    # Defining Layers  
    layer_1 = ba.Layer(material_1)  
    layer_2 = ba.Layer(material_2, 2.5)  
    layer_3 = ba.Layer(material_3, 5)
```

The demo

Prototype of reflectometry GUI

Currently implemented

- Save/load projects
- Import data from multi-column ASCII file
- Create materials, assemble multi-layers with repetitions
- Setup simple Q-scan
- Run simulations based either on simple Q-scan, or on imported data
 - With simulation kernel being a replica of BornAgain reflectometry kernel
- Tune SLD and roughness in real-time editor
- Show simulated specular curve together with imported curve

Planned

- First round of user reviews followed by necessary adjustments
- Fitting