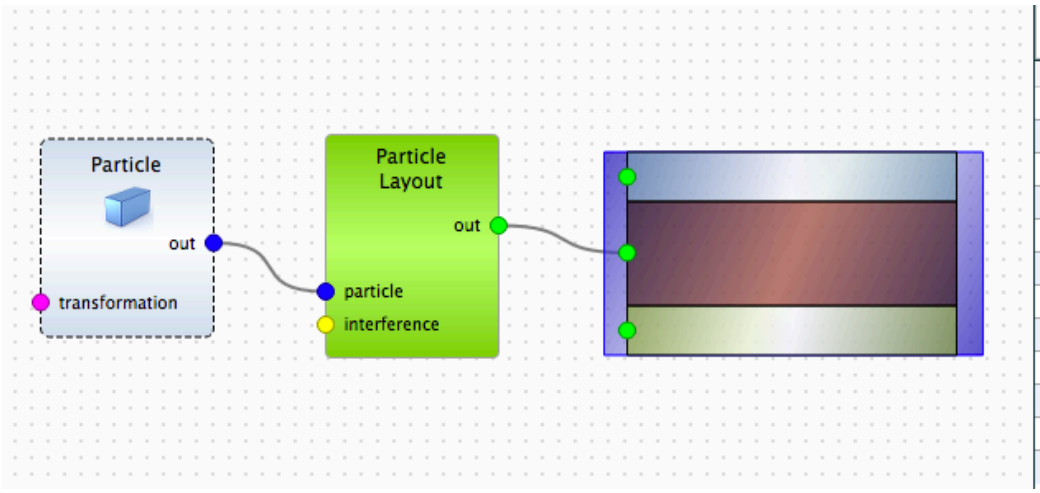
Exercise 3: particle rotation

Tasks

Use the sample from exercise2. Particles should be placed on the bottom of the polymer layer.



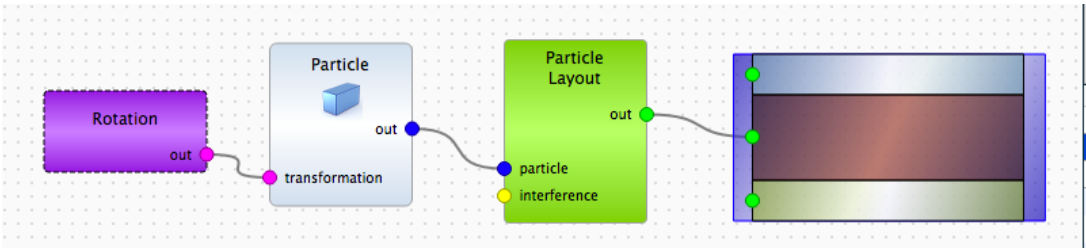
Property	Value
Particle	
Form Factor	Box
Length	20.000
Width	20.000
Height	10.000
Material	Si
Abundance	1.000
Position Offset	(0, 0, -50)
X	0.000
Y	0.000
Z	-50.000

1. Rotate particles around X axis by 45 degree. Does the particle position need to be adjusted? Set the correct value for the particle position.
2. Repeat the same for Y and Z axes.
3. **Advanced:** Create Euler rotation which turns the particle upside down and rotates it by 30 degree around Z axis. How to represent the same transformation with the set of consequent simple rotations? Adjust the particle position if needed.

Particle rotation documentation

Solution

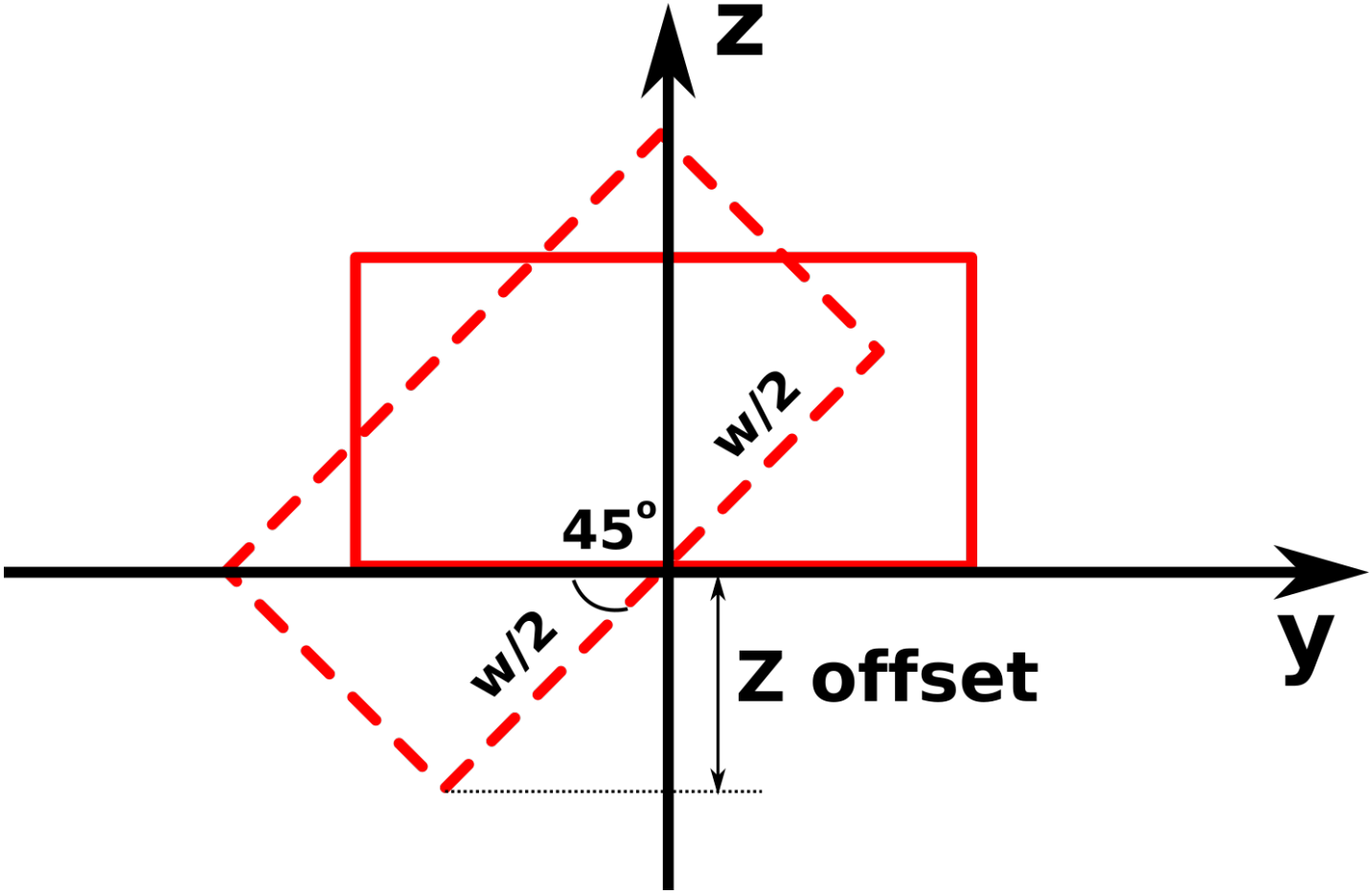
Rotate particles around X axis by 45 degree



Property	Value
Rotation	
Rotation type	X axis Rotation
Angle	45.000

Initial particle position was on the bottom of the polymer layer (-50 nm). Rotation around the X axis has

shifted the particle bottom by 0.5 * width * sin(45) = 7.1 nm down. The position need to be adjusted to $Z = -50 + 7.1 = -42.9$ nm to keep particles on the bottom of the layer.



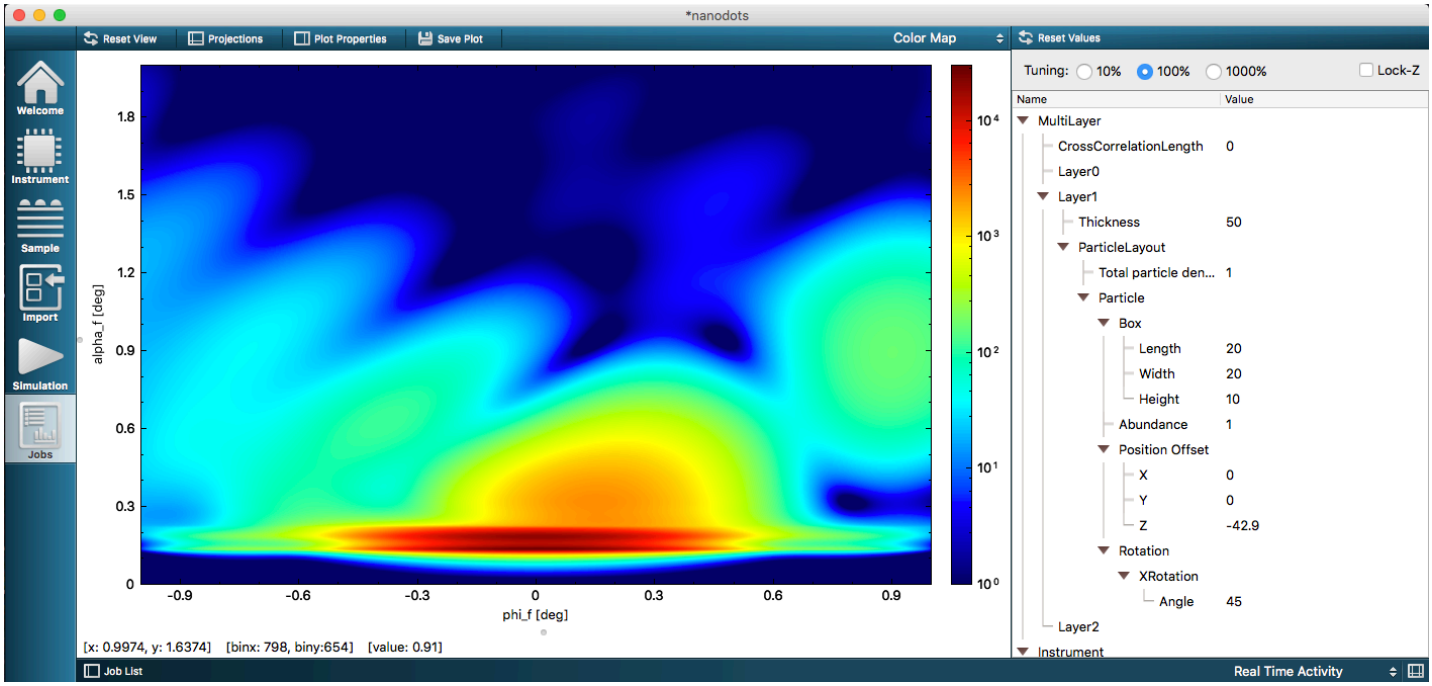
To define a particle rotation in Python, use `RotationX`, `RotationY` or `RotationZ` statement as:

```
particle_1_rotation = ba.RotationX(45.0*deg)
particle_1.setRotation(particle_1_rotation)
```

The full `getSample()` function will look like:

```
def getSample():
    # Defining Materials
    material_1 = ba.HomogeneousMaterial("Air", 0.0, 0.0)
    material_3 = ba.HomogeneousMaterial("Si", 7.6e-06, 1.7e-07)
    material_2 = ba.HomogeneousMaterial("Polymer", 2.0e-06, 1.3e-08)

    # Defining Layers
    layer_1 = ba.Layer(material_1)
    layer_2 = ba.Layer(material_2, 50)
    layer_3 = ba.Layer(material_3)

    # Defining Form Factors
    formFactor_1 = ba.FormFactorBox(20.0*nm, 20.0*nm, 10.0*nm)

    # Defining Particles
    particle_1 = ba.Particle(material_3, formFactor_1)
    particle_1_rotation = ba.RotationX(45.0*deg)
    particle_1.setRotation(particle_1_rotation)
    particle_1_position = kvector_t(0.0*nm, 0.0*nm, -42.9*nm)
    particle_1.setPosition(particle_1_position)

    # Defining Particle Layouts and adding Particles
    layout_1 = ba.ParticleLayout()
    layout_1.addParticle(particle_1, 1.0)
    layout_1.setTotalParticleSurfaceDensity(1)

    # Adding layouts to layers
    layer_2.addLayout(layout_1)

    # Defining Multilayers
    multiLayer_1 = ba.MultiLayer()
    multiLayer_1.addLayer(layer_1)
    multiLayer_1.addLayer(layer_2)
    multiLayer_1.addLayer(layer_3)
    return multiLayer_1
```

The result of the simulation:

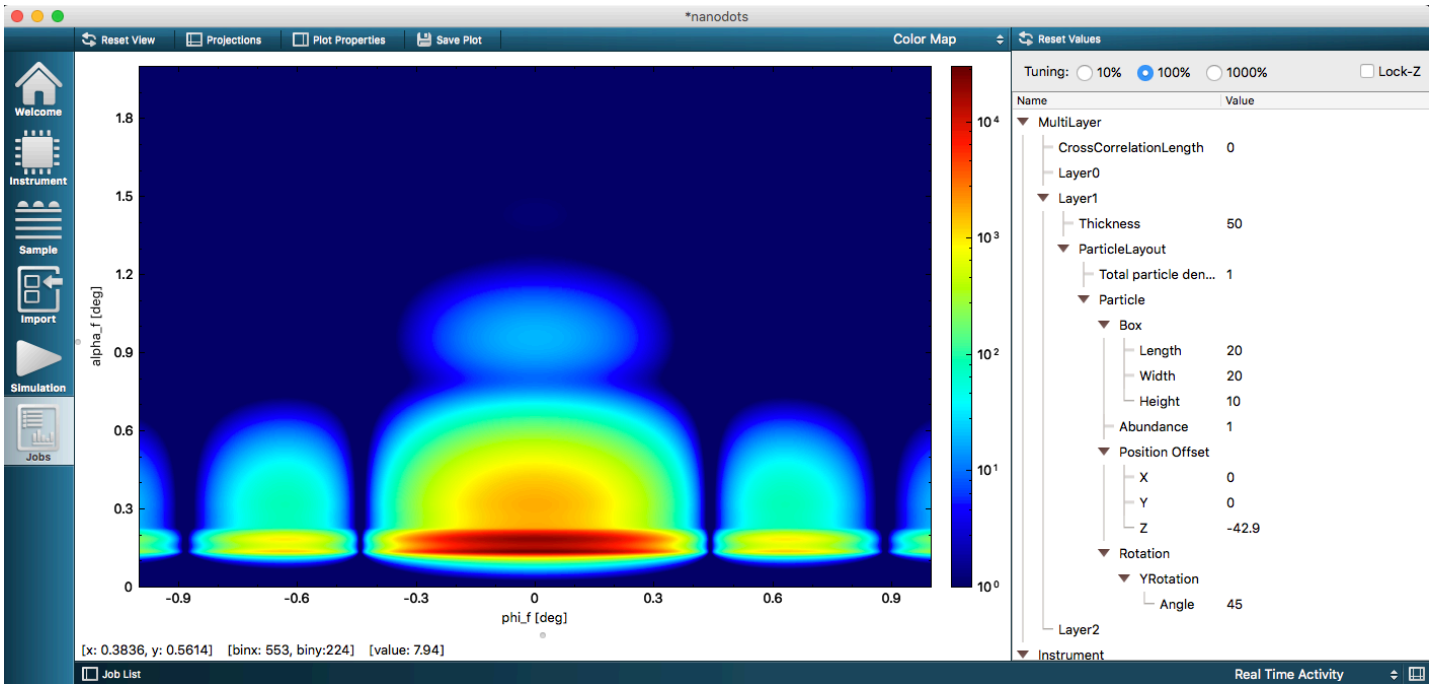


Rotate particles around Y axis by 45 degree

Replace X rotation by Y rotation in graphical user interface or in the Python script.

```
particle_1_rotation = ba.RotationY(45.0*deg)
particle_1.setRotation(particle_1_rotation)
```

Rotation around the Y axis has shifted the particle bottom by 0.5 * length * sin(45) = 7.1 nm down. The position need to be adjusted to $Z = -50 + 7.1 = -42.9$ nm to keep particles on the bottom of the layer.

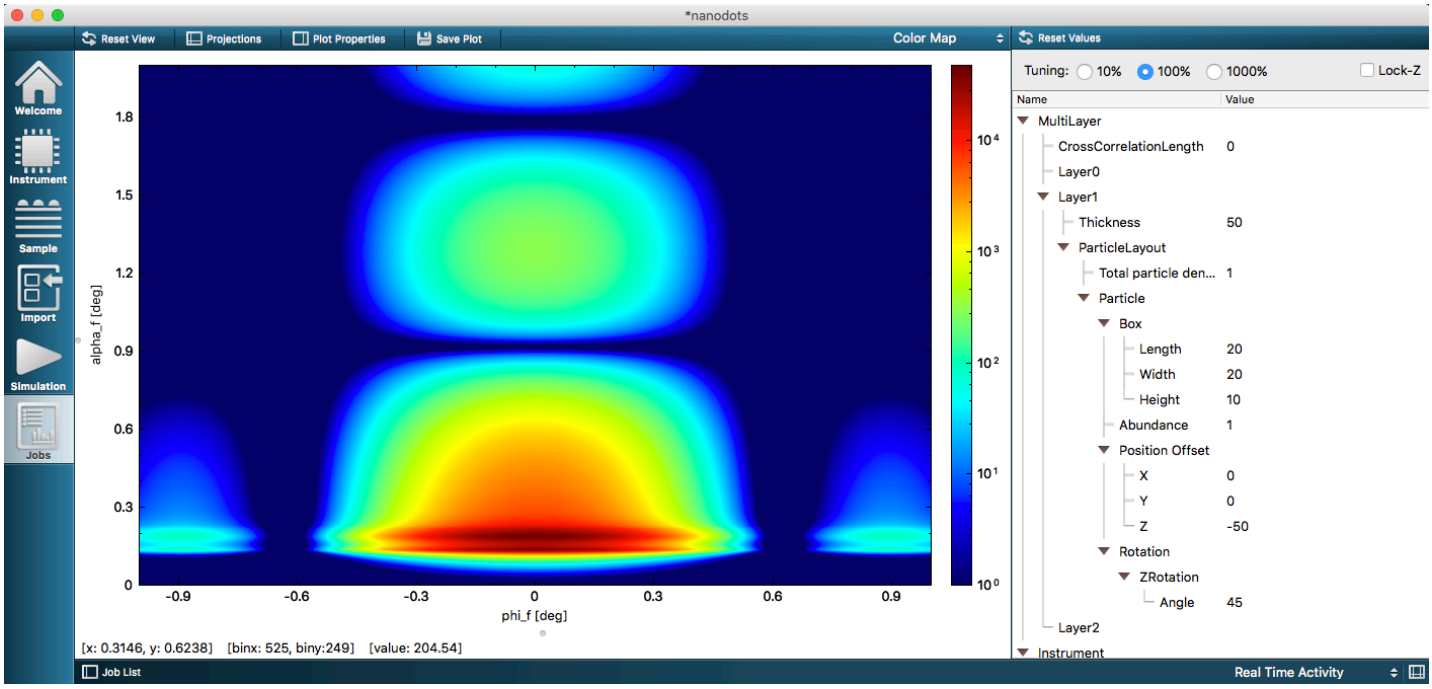


Rotate particles around Z axis by 45 degree

Replace X rotation by Y rotation in graphical user interface or in the Python script.

```
particle_1_rotation = ba.RotationZ(45.0*deg)
particle_1.setRotation(particle_1_rotation)
```

Rotation around the Z axis dies not shift the particle. No position adjustment is needed.

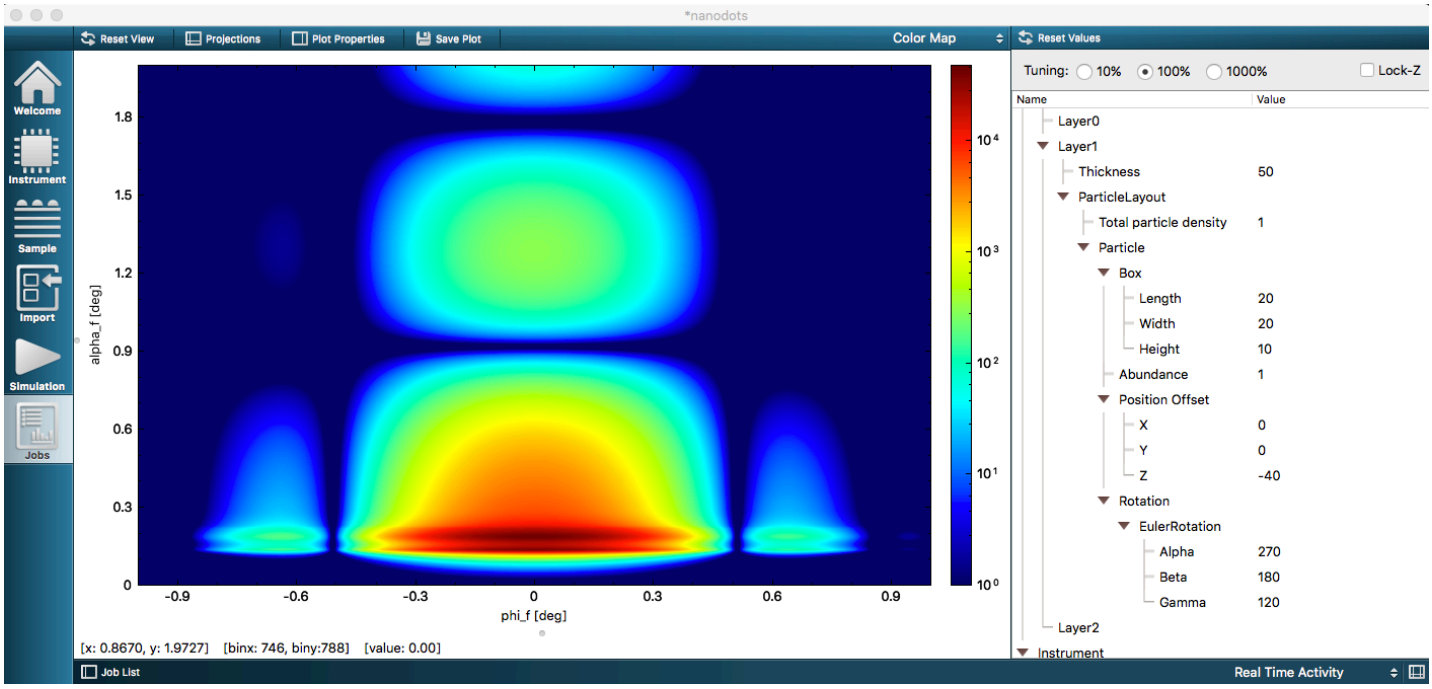


Euler rotation

To turn the particle upside down and rotate it by 30 degree, Euler rotation with the following angles can be applied:

- $\alpha = -90^\circ = 270^\circ$
- $\beta = 180^\circ$
- $\gamma = 120^\circ$

Particle position must be adjusted by the height of the particle: $Z = -50 + 10 = -40$ nm.



In Python:

```
particle_1_rotation = ba.RotationEuler(-90.0*deg, 180.0*deg, 120.0*deg)
particle_1.setRotation(particle_1_rotation)
particle_1_position = kvector_t(0.0 * nm, 0.0 * nm, -40.0 * nm)
particle_1.setPosition(particle_1_position)
```

The same result can be achieved by combining of the rotation around Y by 180 degree and rotation around Z by 30 degree. For the moment, it is possible only in Python:

```
particle_1_rotationY = ba.RotationY(180.0 * deg)
particle_1.setRotation(particle_1_rotationY)
particle_1_rotationZ = ba.RotationZ(30.0 * deg)
particle_1.applyRotation(particle_1_rotationZ)
particle_1_position = kvector_t(0.0 * nm, 0.0 * nm, -40.0 * nm)
particle_1.setPosition(particle_1_position)
```