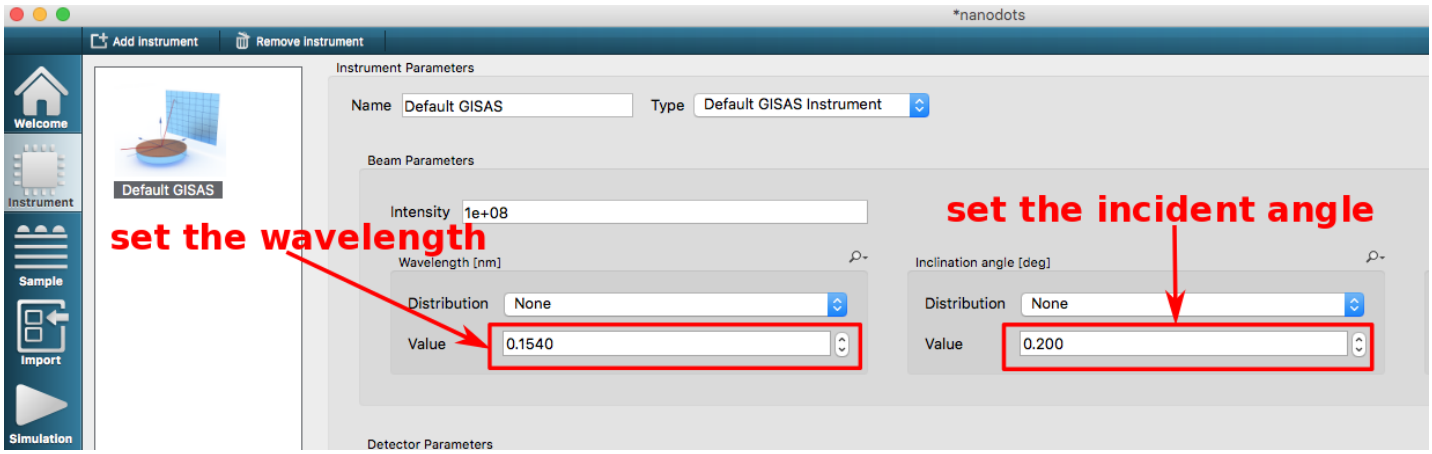
Exercise 1: Simulate Si nano dots on Si substrate

Sample simulation parameters

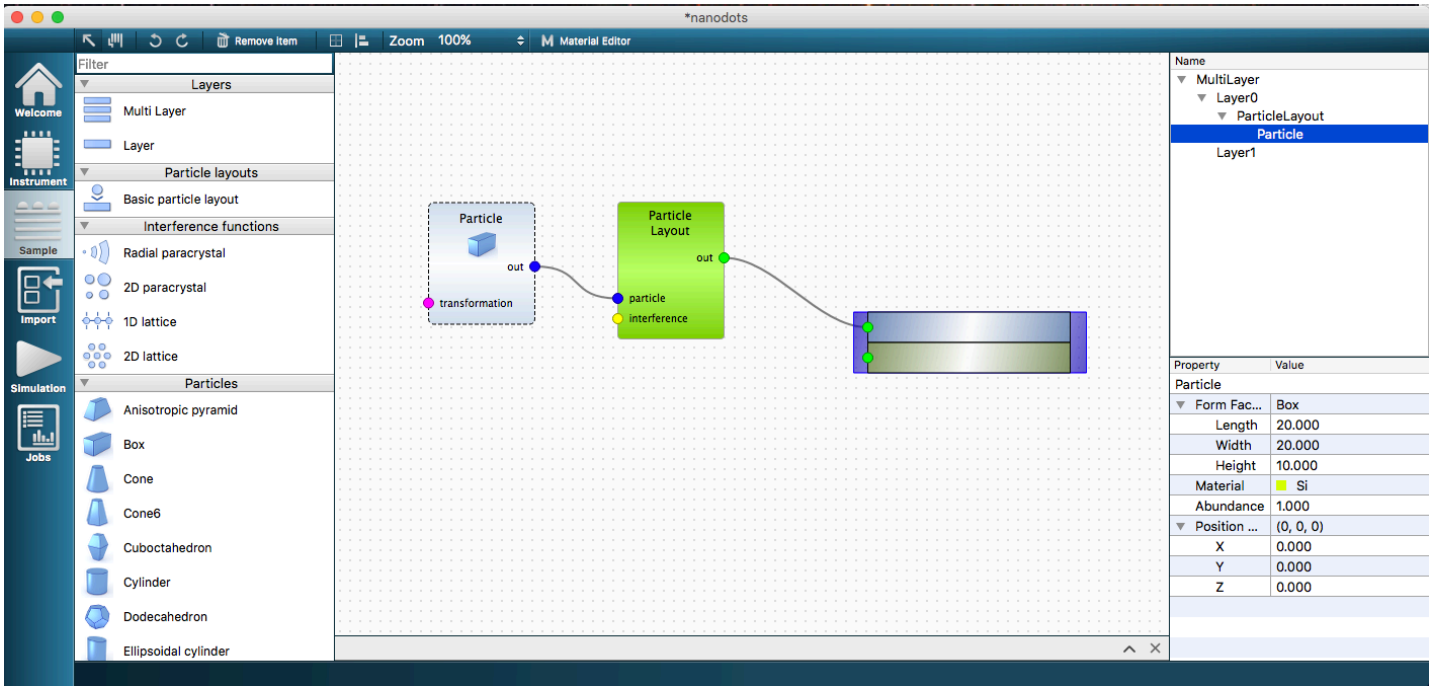
- Beam wavelength $\lambda = 1.54\mathring{\mathrm{A}}$
- Incident angle $\alpha_i = 0.2^{\circ}$
- Index of refraction for Si: $\delta = 7.6 \times 10^{-6}$, $\beta = 1.7 \times 10^{-7}$
- Particle shape: box with length = 20 nm, width = 20 nm and height = 10 nm
- No interference between particles

Solution

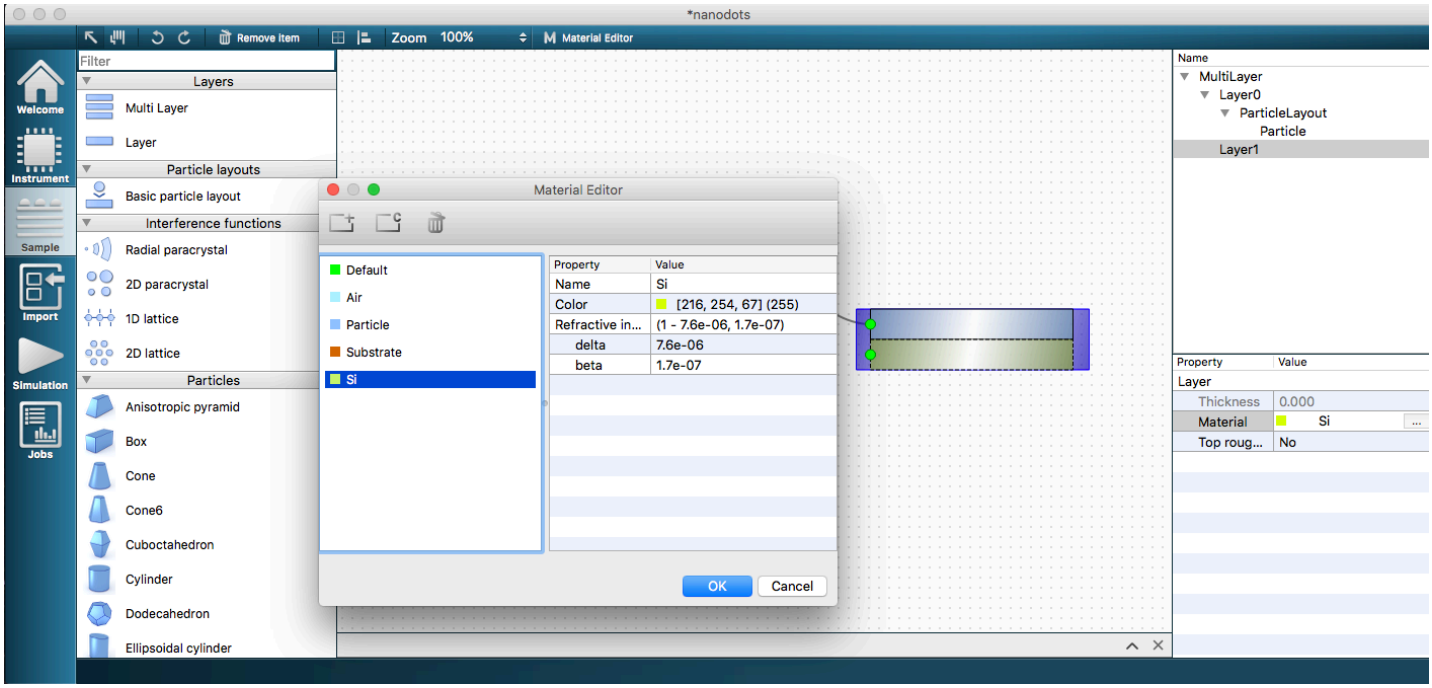
Set the beam parameters



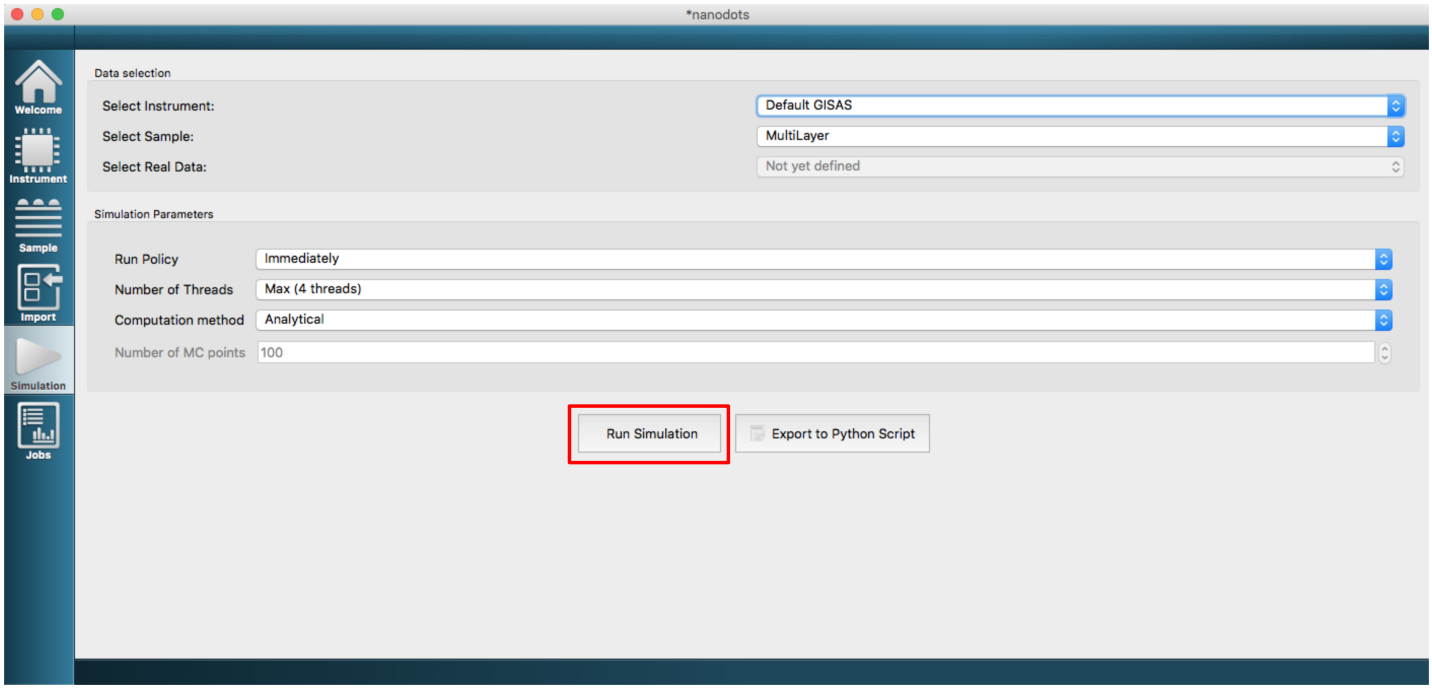
Define sample



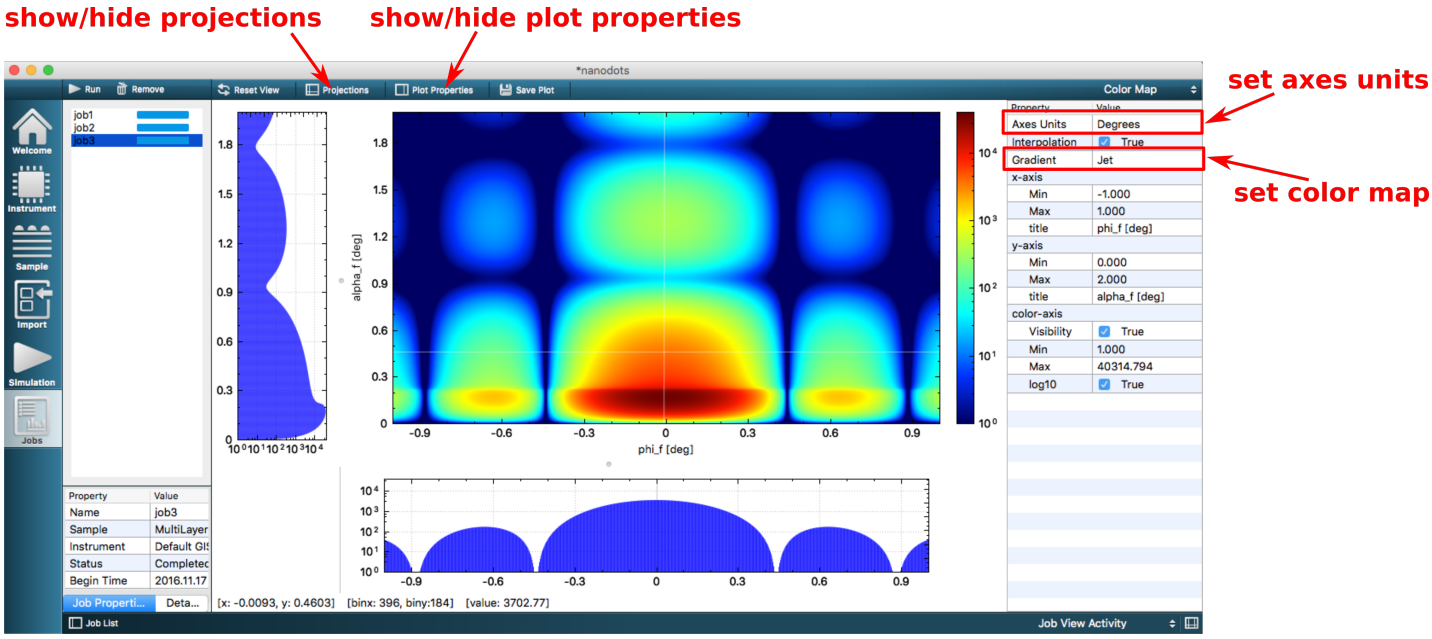
Create Material Si and assign it to particles and to substrate



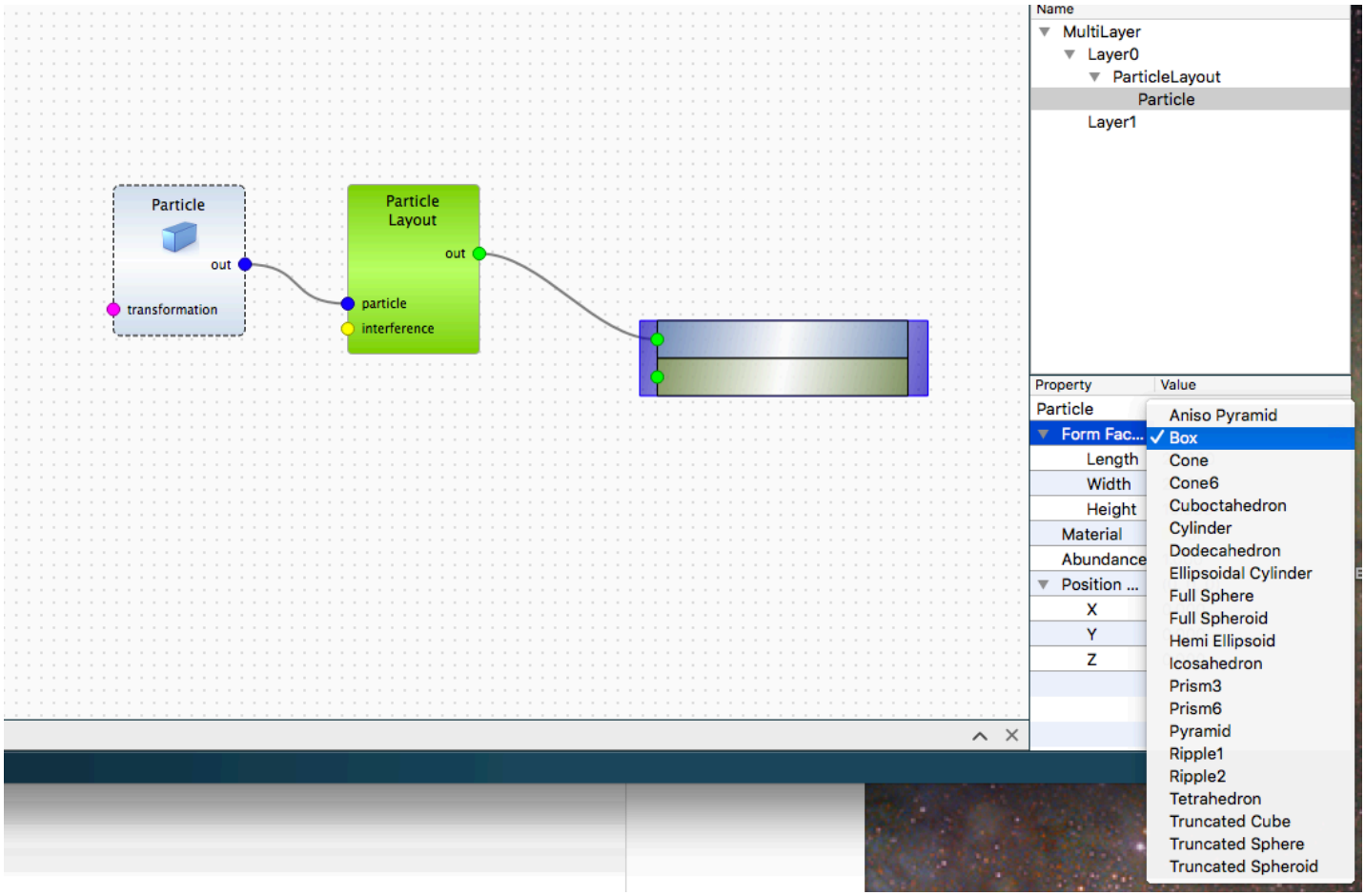
Run simulation



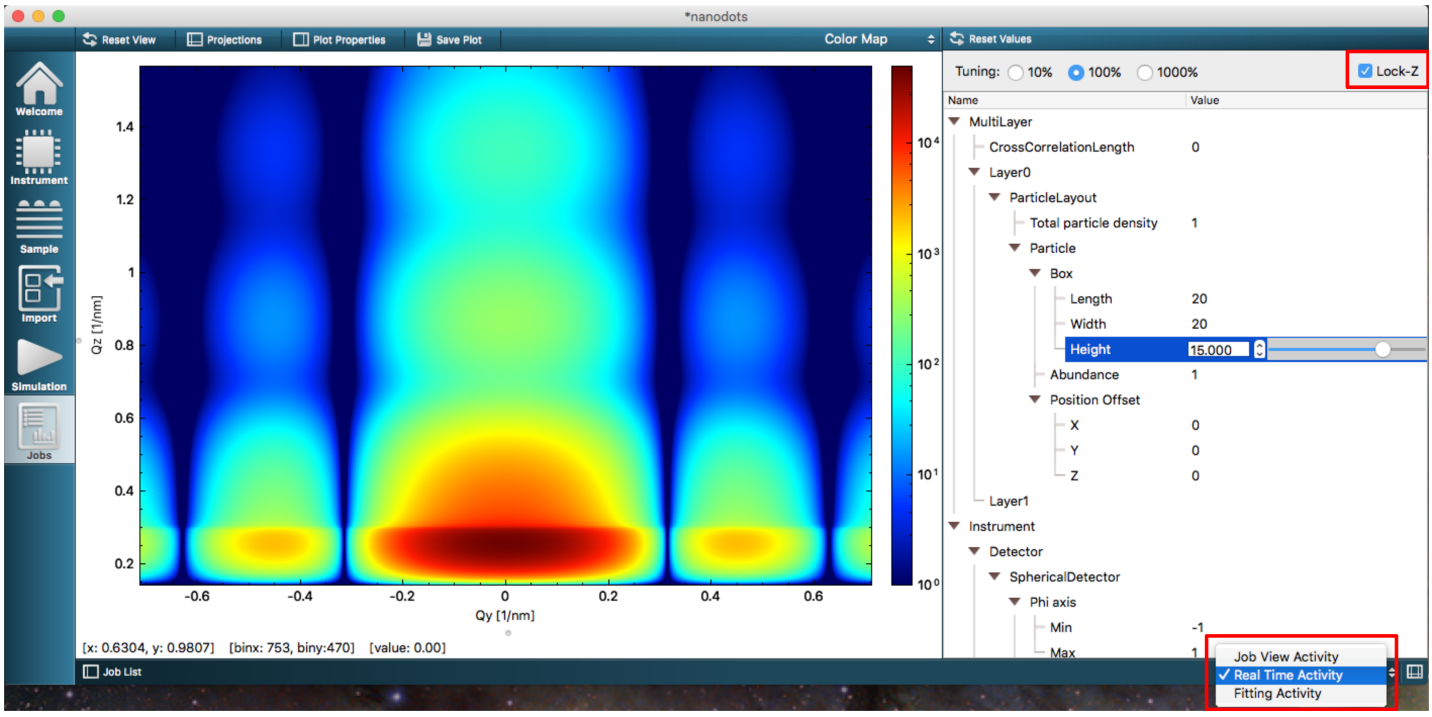
Change the plot axes to Q_y, Q_z, change the color map. Save plot to the file. Review the saved plot.



Change the particle form factor, run simulation and compare the simulation result to the previous one. Repeat for different form factors.

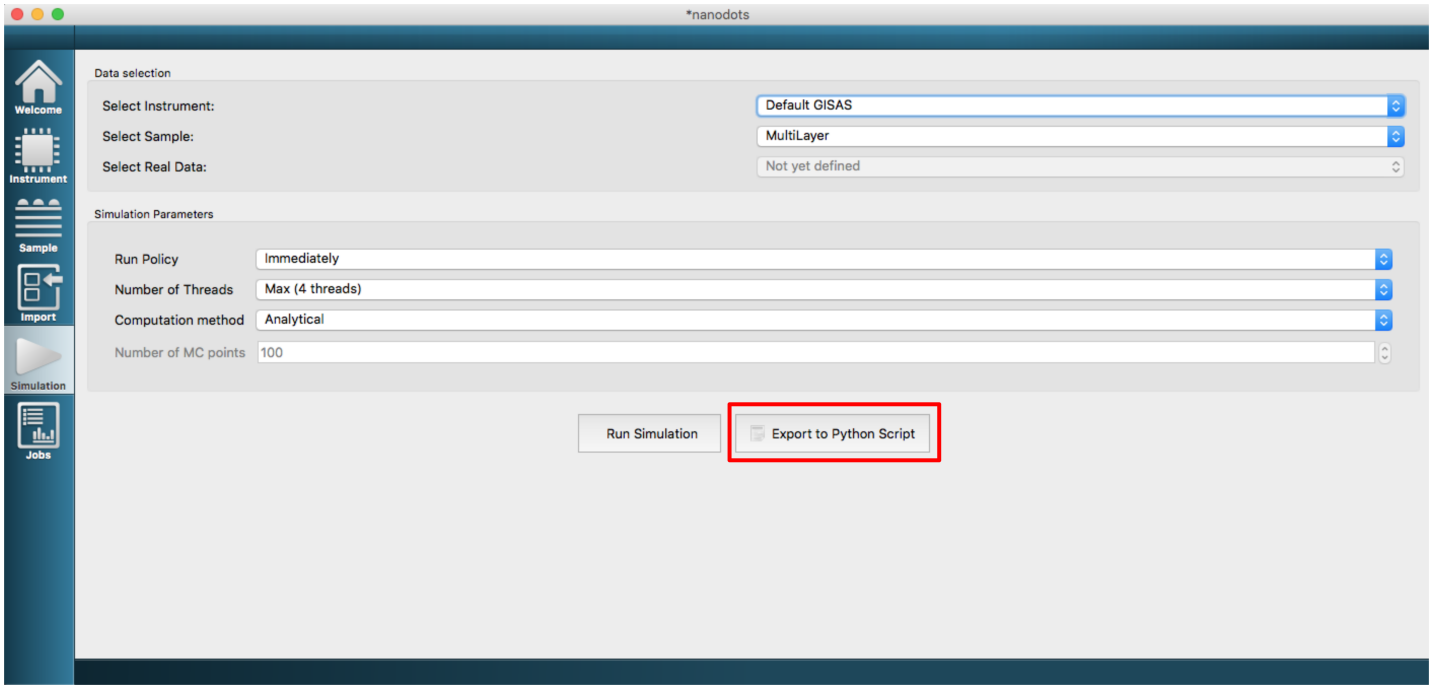


Switch to the real time activity. Set and lock Z axis range. Change particle size. See the changes of simulated pattern.

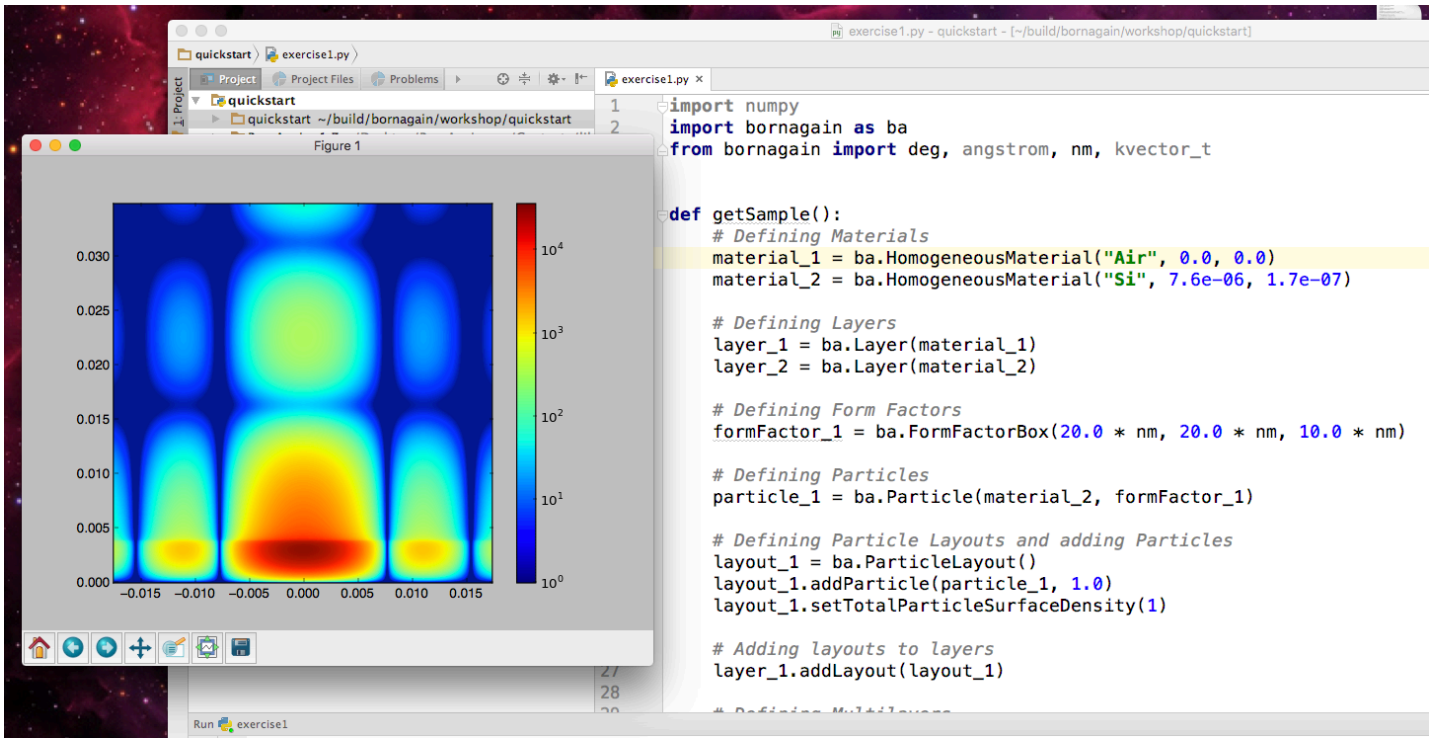


Switch to the "Simulation" tab. Click `Export to Python Script` and save

the script to the directory with your PyCharm project.



Open the saved Python script in PyCharm. Run simulation.



The code of your Python script should look approximately like this:

```
import numpy
import bornagain as ba
from bornagain import deg, angstrom, nm, kvector_t
```

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

    # Defining Layers
    layer_1 = ba.Layer(material_1)
    layer_2 = ba.Layer(material_2)

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

    # Defining Particles
    particle_1 = ba.Particle(material_2, formFactor_1)

    # 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_1.addLayout(layout_1)

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

def getSimulation():
    simulation = ba.GISASSimulation()
    simulation.setDetectorParameters(200, -1.0*deg, 1.0*deg, 200, 0.0*deg, 2.0*deg
)

    simulation.setBeamParameters(0.154*nm, 0.2*deg, 0.0*deg)
    simulation.setBeamIntensity(1.0e+08)
    return simulation


def plot(intensities):
    import matplotlib.colors
    from matplotlib import pyplot as plt
    im = plt.imshow(intensities.getArray(), norm=matplotlib.colors.LogNorm(1, inte
nsities.getMaximum()), extent=[-1.0*deg, 1.0*deg, 0.0*deg, 2.0*deg])
    plt.colorbar(im)
    plt.show()
```

```
def simulate():
    # Run Simulation
    sample = getSample()
    simulation = getSimulation()
    simulation.setSample(sample)
    simulation.runSimulation()
    return simulation.getIntensityData()


if __name__ == '__main__':
    ba.simulateThenPlotOrSave(simulate, plot)
```

Change the particle form factors and sizes of particles. Compare simulation results.

The form factors can be changed in the line 16.

`formFactor_1 = ba.FormFactorBox(20.0 * nm, 20.0 * nm, 10.0 * nm)`