Carleton University

ELEC 4700 - Assignment #2

Finite Difference Models for Electrostatic Potentials

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supervised by

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February 26, 2018

1 Question #1

Please refer to Question1.m for the code for this section.

1.1 Part 1

Using finite difference, Laplace's equation $\nabla^2 V = 0$ was solved. The boundary conditions were set so that $V = 1$ for when $x = 0$ and $V = 0$ for $x = L$ where L in this case was chosen to be 50. The following figure describes the distribution of a potential field along the x dimension:

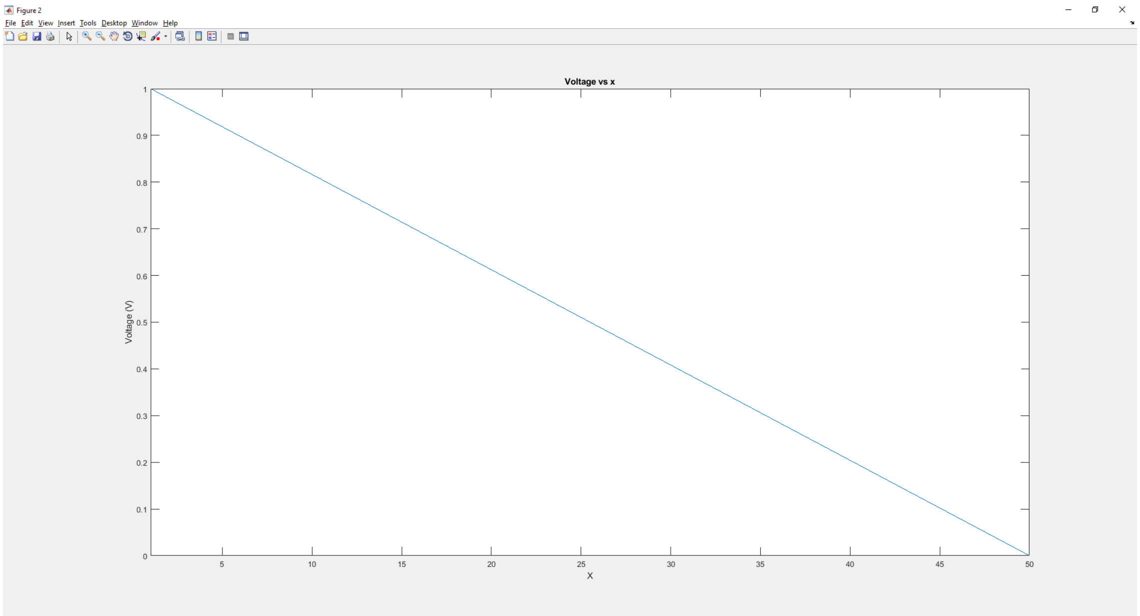

Figure 1: Finite Difference Solution to Laplace's Equation in One Dimension

1.2 Part 2

The previous problem was expanded into two dimensions to investigate the accuracy of finite difference analytical solutions. The boundary conditions were set so that $V = 1$ for when $x = 0$, $V = 0$ for $x = L$ and $V = 0$ for both $y = 0$ and $y = W$. The dimensions were set such that $L = 3/2 \times W$ so in this case $L = 50$ and $W = 75$. The following diagram is the solution to Laplace's equation with the given boundary conditions:

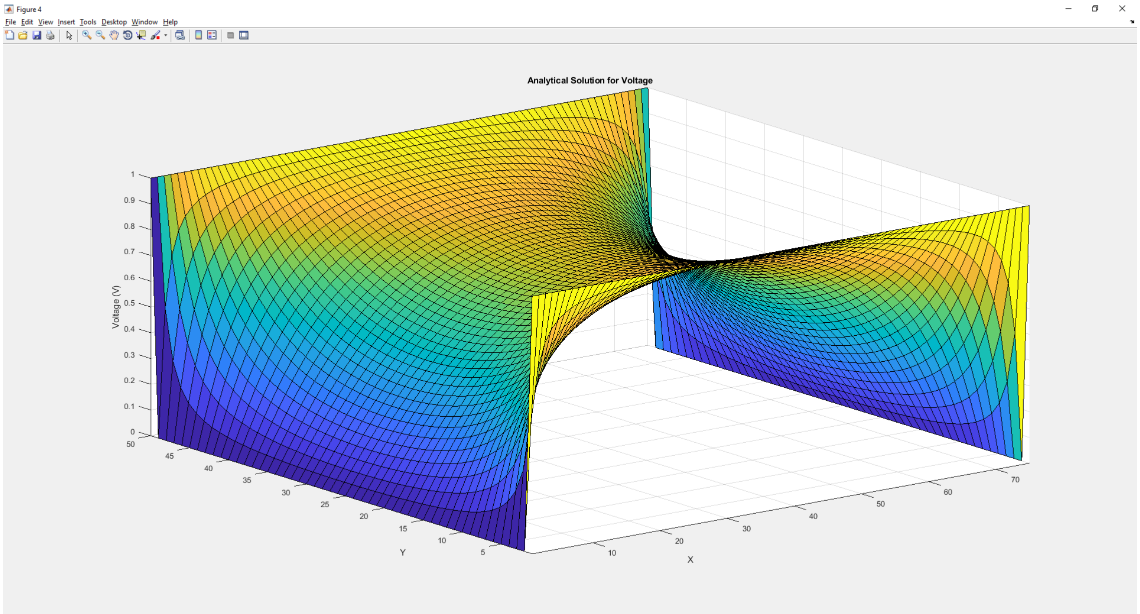

Figure 2: Analytical Solution to Laplace's Equation in Two Dimension

To compare the accuracy of the analytical solution, the following numerical solution was evaluated:

$$V(x,y) = \frac{4V_0}{\pi} \sum_{n=1,3,5,\ldots}^{\infty} \frac{1}{n} \frac{cosh(\frac{n\pi x}{a})}{cosh(\frac{n\pi b}{a})} sin\left(\frac{n\pi y}{a}\right) \tag{1}$$

When the numerical solution was evaluated to $n = 100$, the following curve was generated:

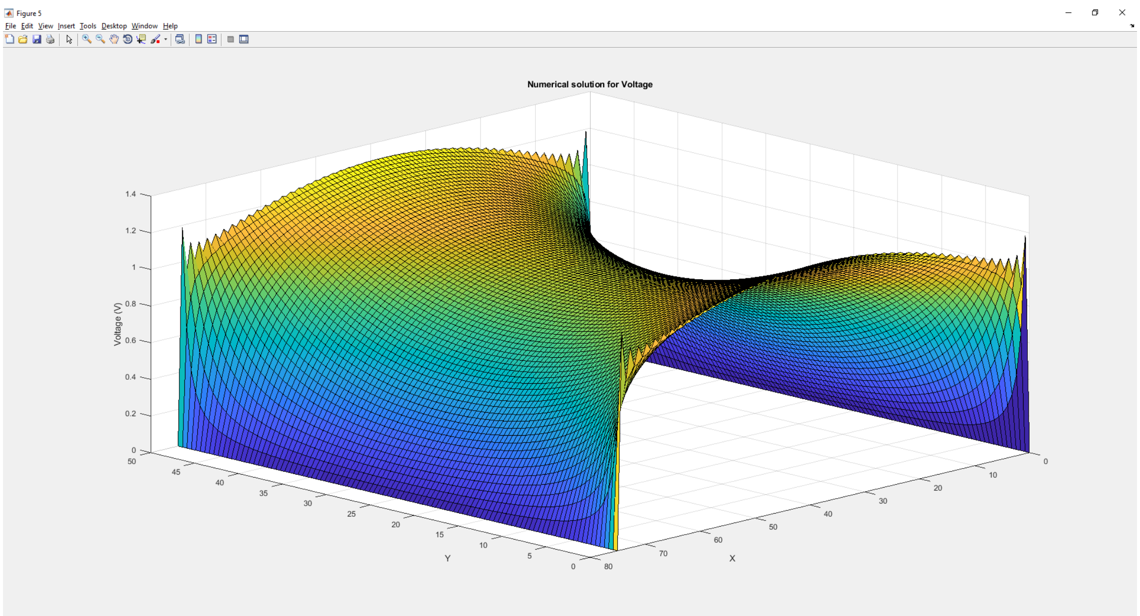

Figure 3: Numerical Solution to Laplace's Equation in Two Dimension

It is important to note that both analytical and numerical solutions are approximations for the true solutions of Laplace's equation with the given geometry. In the case of the analytic solution, the mesh size and shape plays an important role in solution's accuracy. As the density of the mesh grid increases, the solution will tend closer to the actual solution to Laplace's equation. The shape of the mesh also determines the how well the analytical solution is represented. In this case, a square mesh was used while it can be proposed that a triangular mesh would be more ideal to express the solutions around regions where the potential changes rapidly.

The numerical solution is distinct from the analytical solution in that there are many peaks around the $y = 0$ and $y = W$ boundaries. This is a consequence of the periodic functions used in equation (1) being summed together to form a square wave. A truly square function requires an infinite sum or a piecewise function to express mathematically. This formula is also limited in that the $cosh(\frac{n\pi b}{a})$ term begins to diverge around $n = 500$. When terms beyond $n = 500$ are added to the solution, parts of the solution disappear and the solution collapses.

2 Question #2

Please refer to Question2.m for the code for this section. Unless otherwise stated in this section, the boundary conditions were set so that $V = 1$ for when $x = 0$, $V = 0$ for $x = L$ while the y boundary were no flow regions. Unless otherwise stated, the dimensions were set such that $L = 3/2 \times W$ and in this case $L = 50\mu m$ and $W = 75\mu m$.

2.1 Part 1

Current flow through a choke-point was evaluated by adding low conductivity regions in the center of the plane of interest. In this case, two boxes were placed in the center with a conductivity of $\sigma_{x,y} = 0.01$ while the rest of the region has a conductivity of $\sigma_{x,y} = 1$. The following plot demonstrates where the conductivity regions are located.

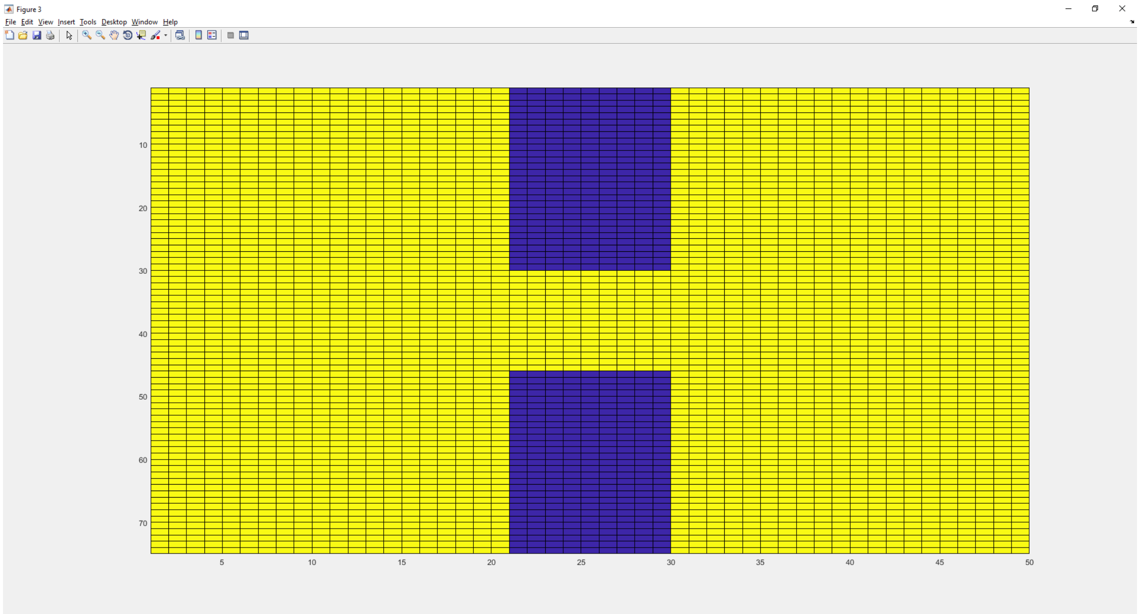

Figure 4: Conductivity of the Region of Interest

The region in purple represents the low conductivity region while the yellow regions is the high conductivity region.

By solving the modified version of Laplace's equation $\nabla(\sigma_{x,y}\nabla V) = 0$, the potential of the region of interest can be evaluated while taking into account the conductivity of the different regions. The following plot is the analytical solution of the given geometry using the modified version of Laplace's equation:

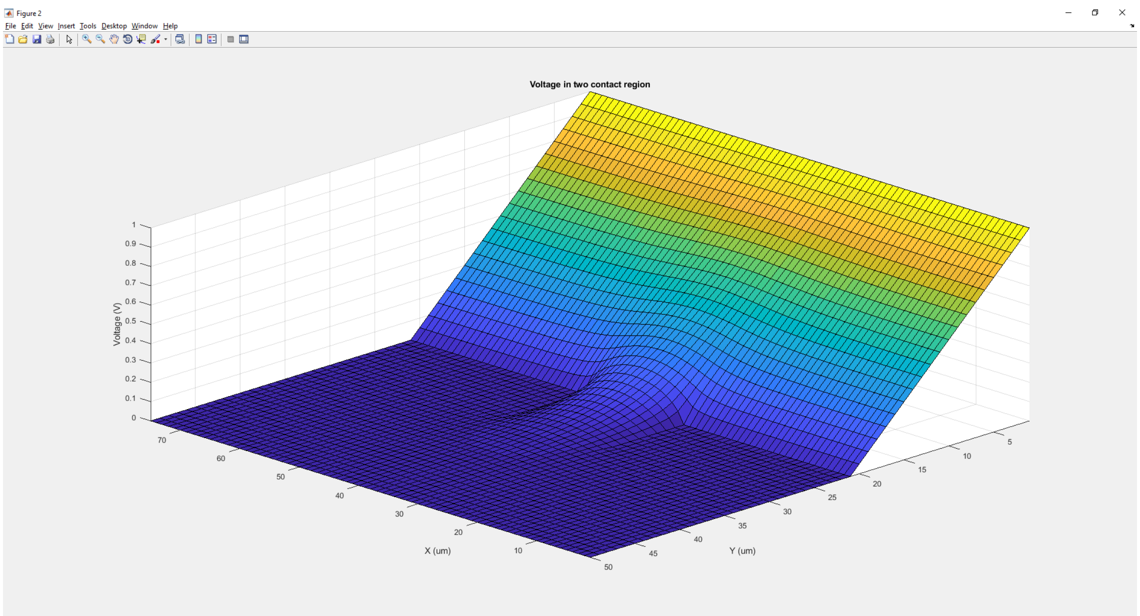

Figure 5: Electric Potential Within a Region with Low Conductivity Contacts

Notice that the electric potential in the region between the two low conductivity boxes creates a "bottleneck" effect.

The electric field of the given geometry can be calculated with a time invariant electrodynamics equation $E = -\nabla V$. The two dimensions are taken into account by splitting up the equation into its x and y components and using vector addition to evaluate the total electric field.

$$E_x = -\frac{\partial V_x}{\partial x} \tag{2}$$

$$E_y = -\frac{\partial V_y}{\partial y} \tag{3}$$

$$E_{x,y} = -\sqrt{E_x^2 + E_y^2} \tag{4}$$

The resulting equations produce the following electric field distribution:

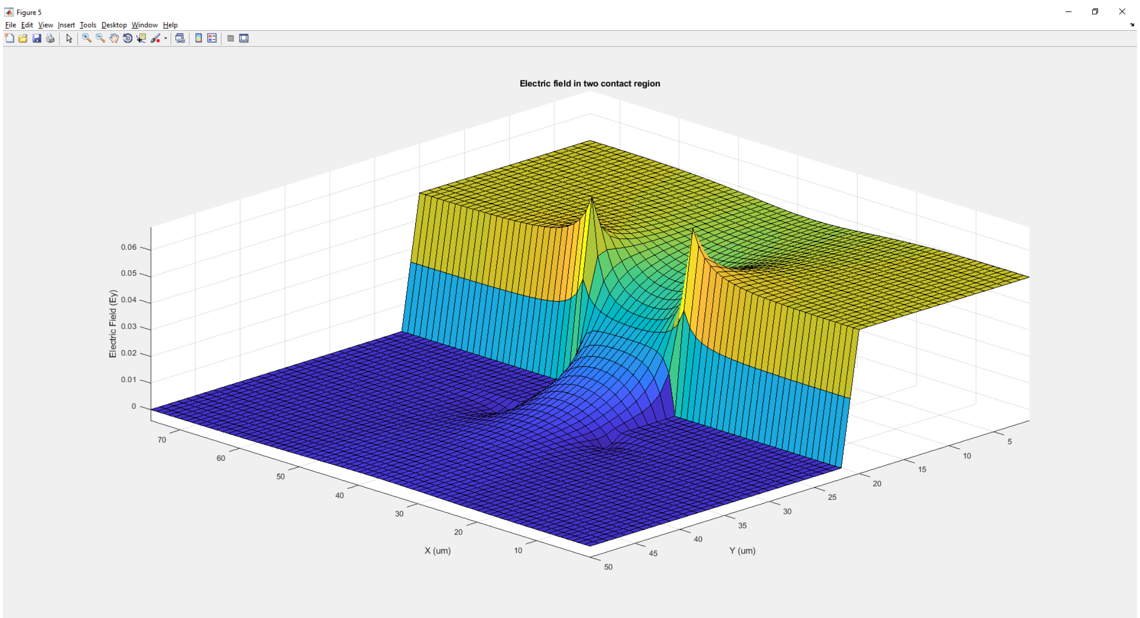

Figure 6: 2-D particle trajectory plot of 10 particles over 5 ps with scattering

Notice the large peaks that are found are the ends of the choke-point. This is a result of the abrupt change in conductivity that is present in the system. This is not a physically accurate model of what it would be in reality and a gradual shift in conductivity would be worth investigating in a future version of the code.

The current density equation $J_{x,y} = \sigma_{x,y} E_{x,y}$ can be used to evaluate the current inside the choke-point. The following plot depicts the current density of the system:

The total current that is present in the bottleneck region can be evaluated by summing the current density within the choke-point. By multiplying the current density by the area of the choke-point, the current was calculated.

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The current between the contacts is 5.061259e-10 A
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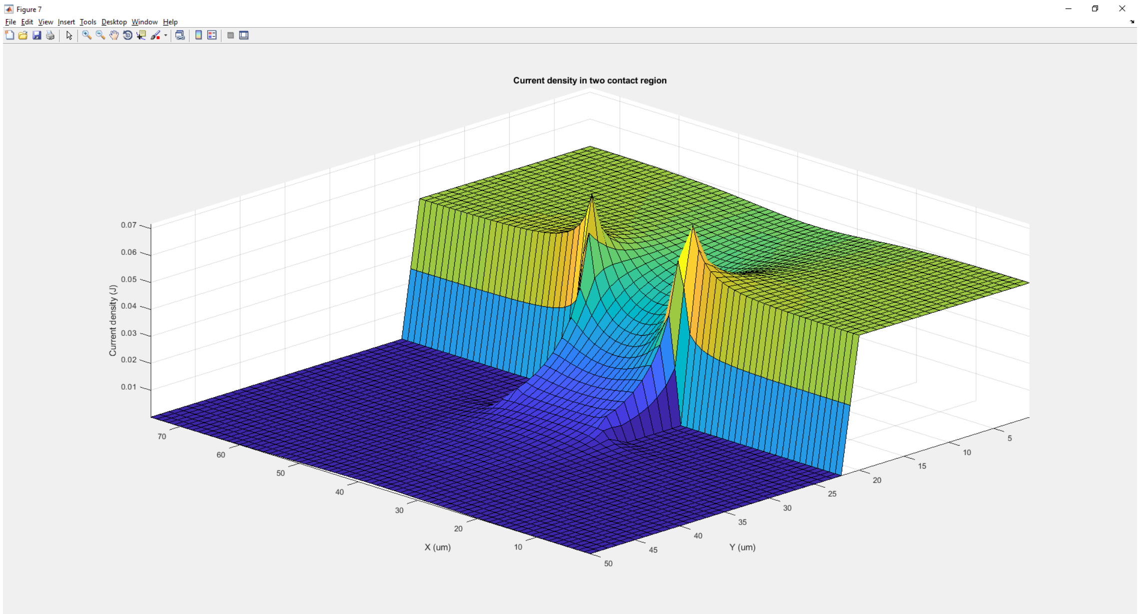

Figure 7: 2-D particle trajectory plot of 10 particles over 5 ps with scattering

2.2 Part 2

An investigation into the mesh size was conducted to determine its effect on the current in the choke-point. The geometry of the system was changed so that the x length L was set to $10\mu m$ and increase by $10\mu m$ until it reached $100\mu m$. The width was kept to the same proportion of $L = 3/2 \times W$. The current in the bottleneck region was evaluated with each mesh geometry.

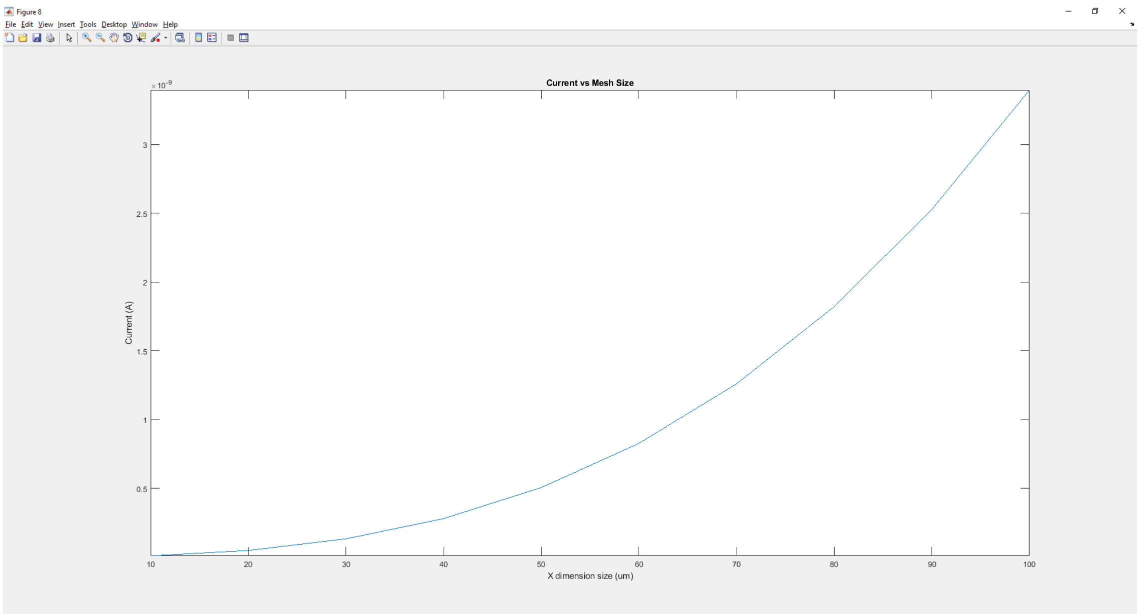

Figure 8: Mesh density versus current in choke-point

It should be expected that if the mesh were to increase toward infinity that it should converge to a single value. There are limitations in the simulation as the mesh size computation time is an N^2 process which results in slower simulations for larger mesh sizes. Further investigation can be done for this geometry using more computation power.

2.3 Part 3

The low conductivity regions have remained to be 0.2L wide and 0.4W long for each simulation. For this investigation the length of the contacts was modified while the width of the contacts remained the same. The length was changed such that the choke-point gap varied from $73\mu m$ to $1\mu m$.

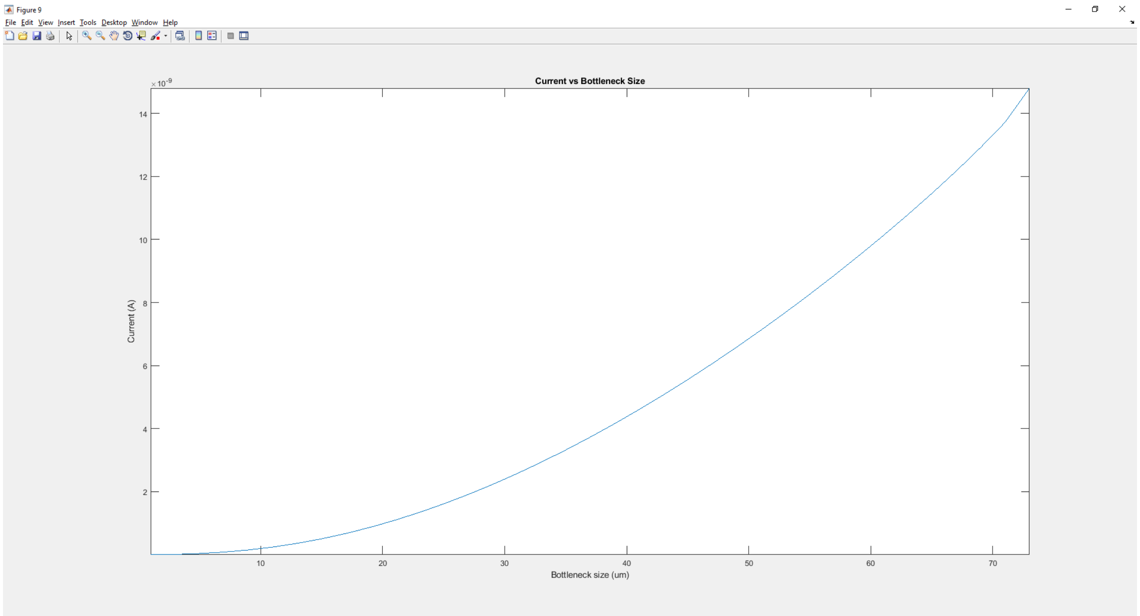

Figure 9: Bottleneck distance versus Current in choke-point

In a physical sense, the results of this investigation are sound. As the bottleneck becomes more narrow, more current will be squeezed into a smaller area resulting in a higher current.

2.4 Part 4

The conductivity of the contacts was varied to investigate the impact on bottleneck current. The contacts conductivity was changed from 0.1 to 1.

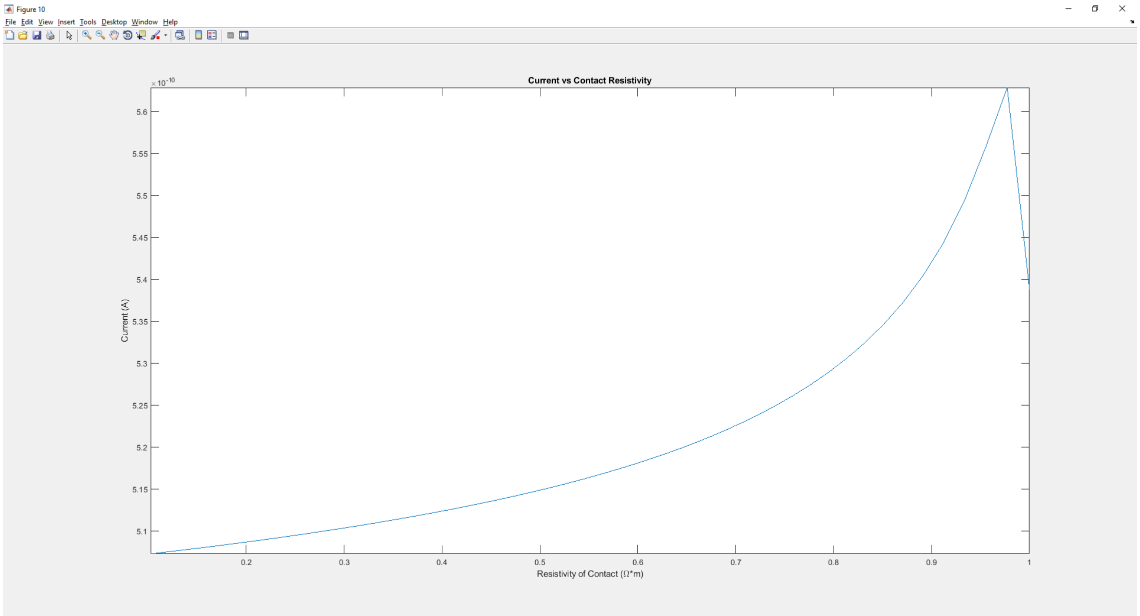

Figure 10: Contact Conductivity versus Current in choke-point

One can notice that there is a spike of current that is present when the conductivity is around 0.95. This should not be the case. The expected result is that the current in the bottleneck should be small for a contact conductivity similar to the region conductivity. This would be due to the electrons having the capability to jump to cross the lower conductivity contacts rather than crossing the bottleneck. The current should increase as the conductivity in the contacts decreases until it converges to a maximum current. The opposite result has been found in Figure 10. As the conductivity decreases, the current in the bottleneck decreases. One result that is consistent with electron transport theory is that the once the contact conductivity equals the system conductivity, there is a sharp decline in current in the bottleneck. Please consult the Assignment2.m file to determine the cause of the problem.