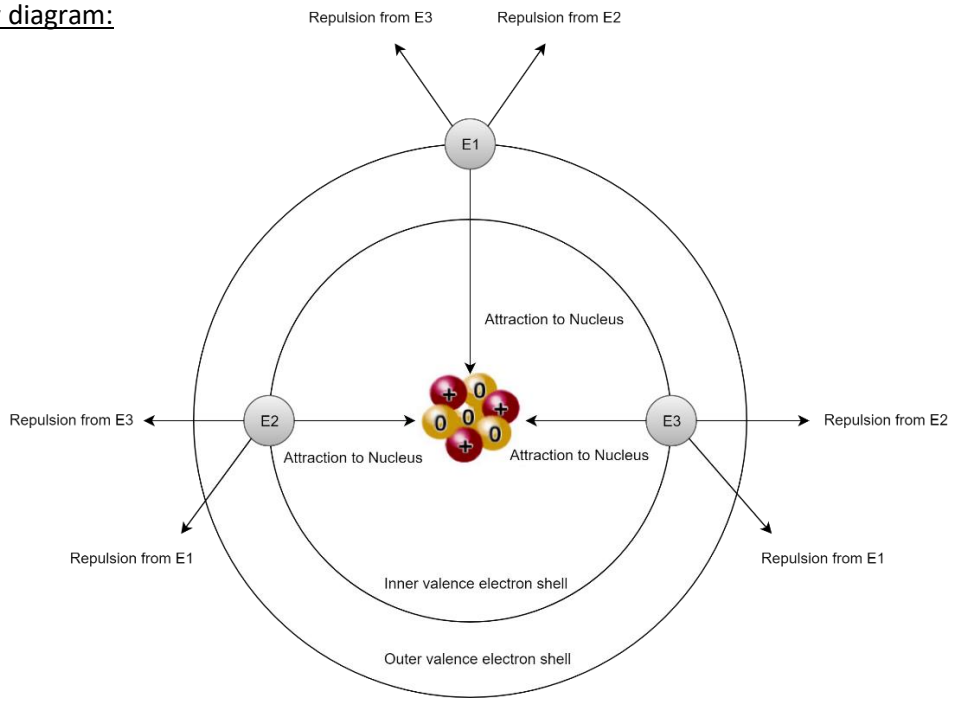
Introduction

Simulating the movement of electrons within an atom involves many complex interactions between every charged particle in the atom. Modeling such a system is achieved by using a simplified model of an atom, Bohr's model, to create movement similar to planetary orbit. When only one electron is present, the forces at work are almost identical to planetary motion, with the positive charge of the nucleus attracting the negative charge of the electron. When more than one electron is involved, an additional force is added, as the electrons' negative charges repel each other.

Free body diagram:



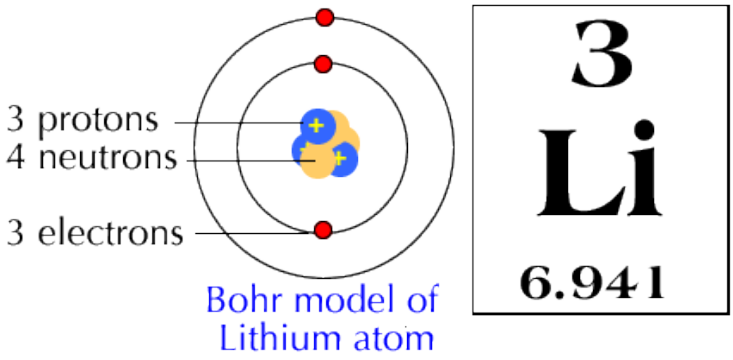
The attraction or repulsion from the electrons and the nucleus can be modeled using Coulomb's law:

$$|F_1| = |F_2| = K_e \frac{|q_1 \, x \, q_2|}{d^2}$$

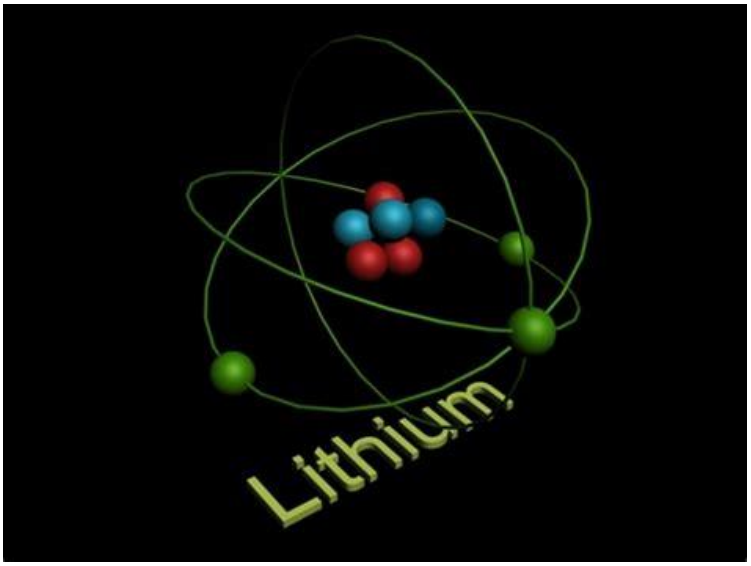
The distance (d) in Coulomb's law can be found by using the distance formula in-between both charges:

$$d = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$$

Once the system is implemented, it can be compared to the accepted Bohr's model for the lithium atom.



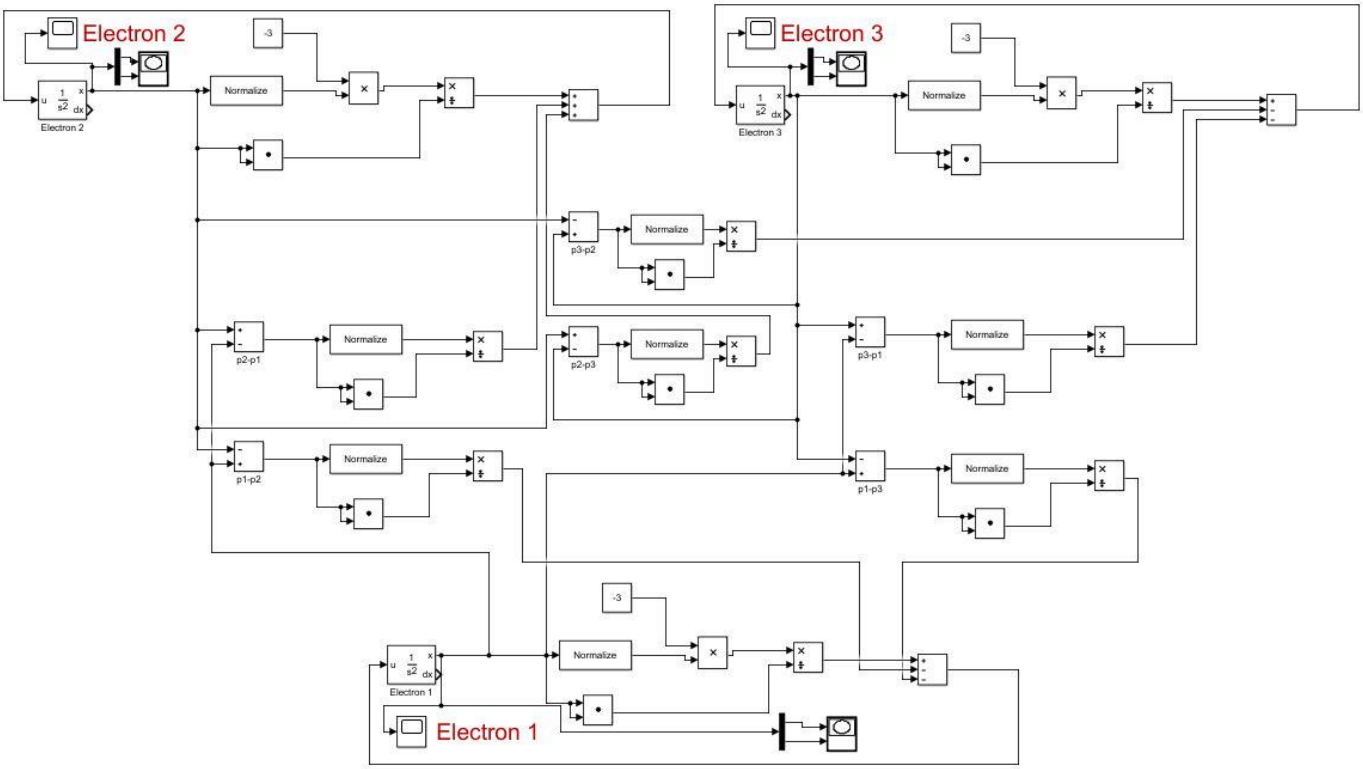
The last issue that arises from the model is one of translating a three-dimensional model to two dimensions. The only stable orbit for the Lithium atom when taking the real physics equations into account relies heavily on movement within the z axis. The three-dimensional model for comparison takes this into account.



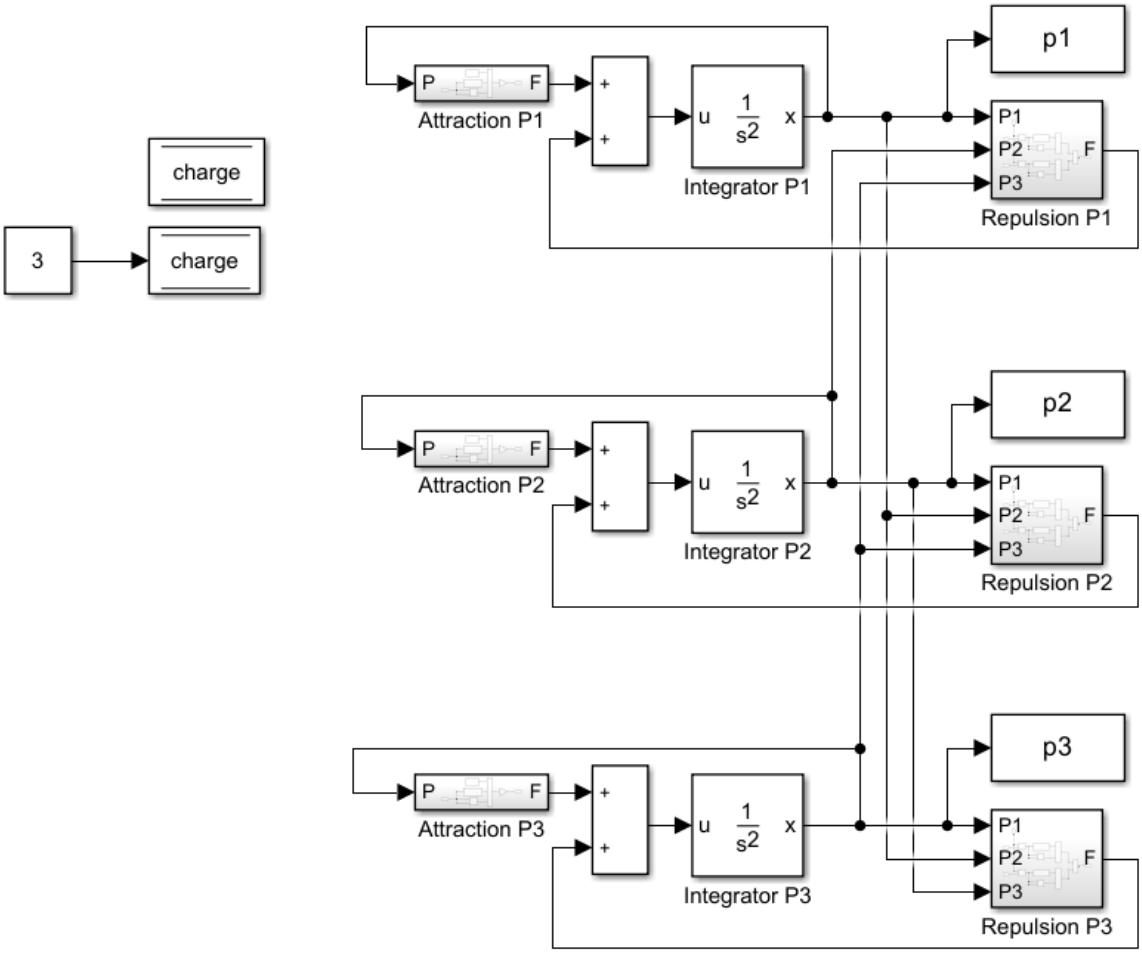
Procedure

State Space Model: $$f''[P_i] = -\widehat{P_i} * \frac{3}{\|P_i\|^2} + \sum_j^{j \neq i} (\widehat{P_i - P_j}) * \frac{1}{[\![P_i - P_j]\!]^2}$$

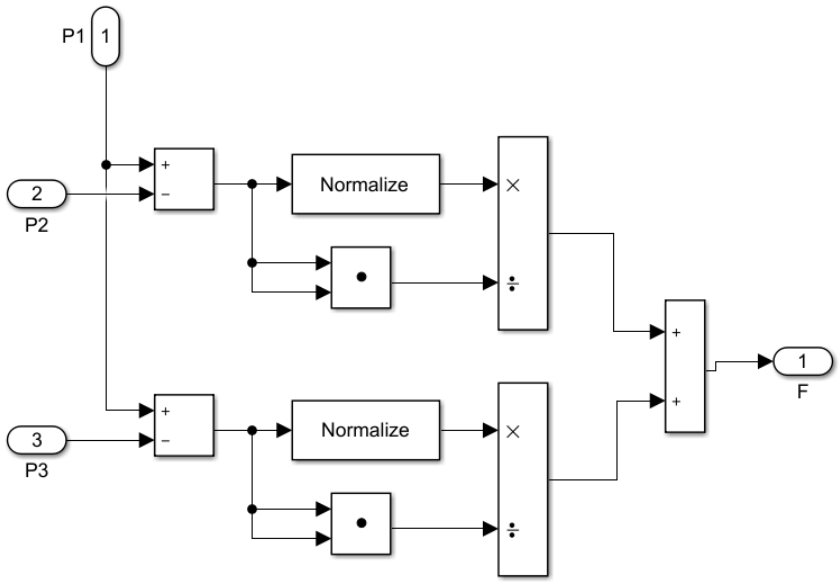
Simulink Diagram (2d Model):



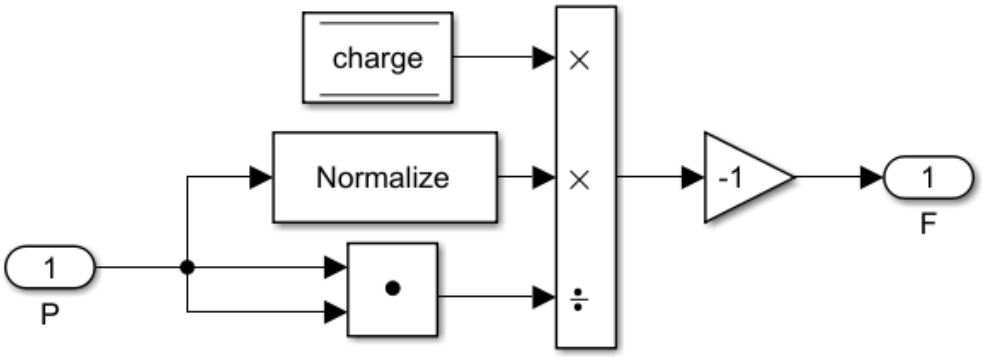
Simulink Diagram (3d Model):



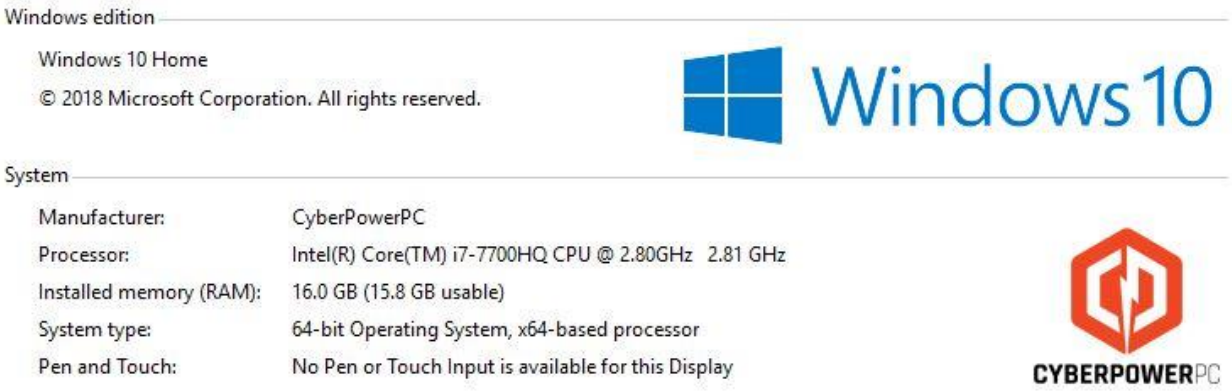
Inside of repulsion block within 3d Model:



Inside of attraction block within 3d Model:



Hardware used for testing:



Two different models were prepared within MATLAB's Simulink program, one to represent the two-dimensional model of this system, and the other to represent the three-dimensional model. The two-dimensional model was slightly modified for verification and validation purposes, to match the accepted Simulink model for the Helium atom. The modified blocks in the two-dimensional model were as follows: deleting every block associated with electron 3, changing the -3-constant block to a value of -2, changing the final sum block from three inputs to two, and modifying the initial conditions to the ones given for the Helium model.

Given initial values for the Helium model (2d model verification/validation)		
	Electron 1	Electron 2
Position: (X, Y) coordinate	(3, 0)	(1, 0)
Velocity: (X, Y) value	(0, 0.4)	(0, -1)

The desired accuracy of this simulation should be within 1 nanometer of the accepted solution. Modifying the tolerance of the simulation drastically changes its output, so the ideal tolerance will be the highest possible value that still gives an error of less than 1 nanometer. Numerous trials were also conducted using various methods to determine the ideal parameters of this model using the generated and accepted solutions for the Helium atom. The chosen methods used in order to simulate this model were Runge-Kutta 4, Runge-Kutta 4/5, and the trapezoidal method. The Runge-Kutta 4 method is an explicit, fixed step, 4th order method with the following equations:

$$k_1 = f(x_i, y_i)$$
$$k_2 = f(x_i + 0.5h,\ y_i + 0.5k_1 h)$$
$$k_3 = f(x_i + 0.5h,\ y_i + 0.5k_2 h)$$
$$k_4 = f(x_i + h,\ y_i + k_3 h)$$
$$y_{i+1} = y_i + \tfrac{1}{6}h(k_1 + 2k_2 + 2k_3 + k_4)$$

The Runge-Kutta 4/5 method is an explicit, variable step, 5th order method with the following equations:

$$\vec{k_1} = \vec{u}(t_n, \vec{x_n})$$
$$\vec{k_2} = \vec{u}(t_n + \frac{h}{4}, \vec{x_n} + \frac{\vec{k_1}}{4})$$
$$\vec{k_3} = \vec{u}(t_n + \frac{3h}{8}, \vec{x_n} + \frac{3k_1}{32} + \frac{9k_2}{32})$$
$$\vec{k_4} = \vec{u}(t_n + \frac{12h}{13}, \vec{x_n} + \frac{1932}{2197}\vec{k_1} - \frac{7200}{2197}\vec{k_2} + \frac{7296}{2197}\vec{k_3})$$
$$\vec{k_5} = \vec{u}(t_n + h, \vec{x_n} + \frac{439}{216}\vec{k_1} - 8\vec{k_2} + \frac{3680}{513}\vec{k_3} - \frac{845}{4104}\vec{k_4})$$
$$\vec{k_6} = \vec{u}(t_n + \frac{h}{2}, \vec{x_n} - \frac{8}{27}\vec{k_1} + 2\vec{k_2} - \frac{3544}{2565}\vec{k_3} + \frac{1859}{4104}\vec{k_4} - \frac{11}{40}\vec{k_5})$$
$$\vec{x}_{n+1}^{[4]} = \vec{x_n} + \left(\frac{25}{216}\vec{k_1} + \frac{1408}{2565}\vec{k_3} + \frac{2197}{4104}\vec{k_4} - \frac{1}{5}\vec{k_5}\right)$$
$$\vec{x}_{n+1}^{[5]} = \vec{x_n} + \left(\frac{16}{135}\vec{k_1} + \frac{6656}{12825}\vec{k_3} + \frac{28561}{56430}\vec{k_4} - \frac{9}{50}\vec{k_5} + \frac{2}{55}\vec{k_6}\right)$$

The Trapezoidal method is an implicit, variable step, 2nd order method with the following equation:

$$y_{n+1} = y_n + \frac{1}{2}h\Big(f(t_n, y_n) + f(t_{n+1}, y_{n+1})\Big)$$

The trial with the smallest error compared to the accepted solution would be the parameters chosen for the simulation of the lithium atom.

Test parameter values (2d helium model)				
Trial	Stop time (sec)	Solver method	Fixed/Variable step	Step size/ Rel Error
1	161	Runge-Kutta 4	Fixed step	0.01
2	161	Trapezoidal	Variable step	1E-7
3	161	Runge-Kutta 4/5	Variable step	1E-7

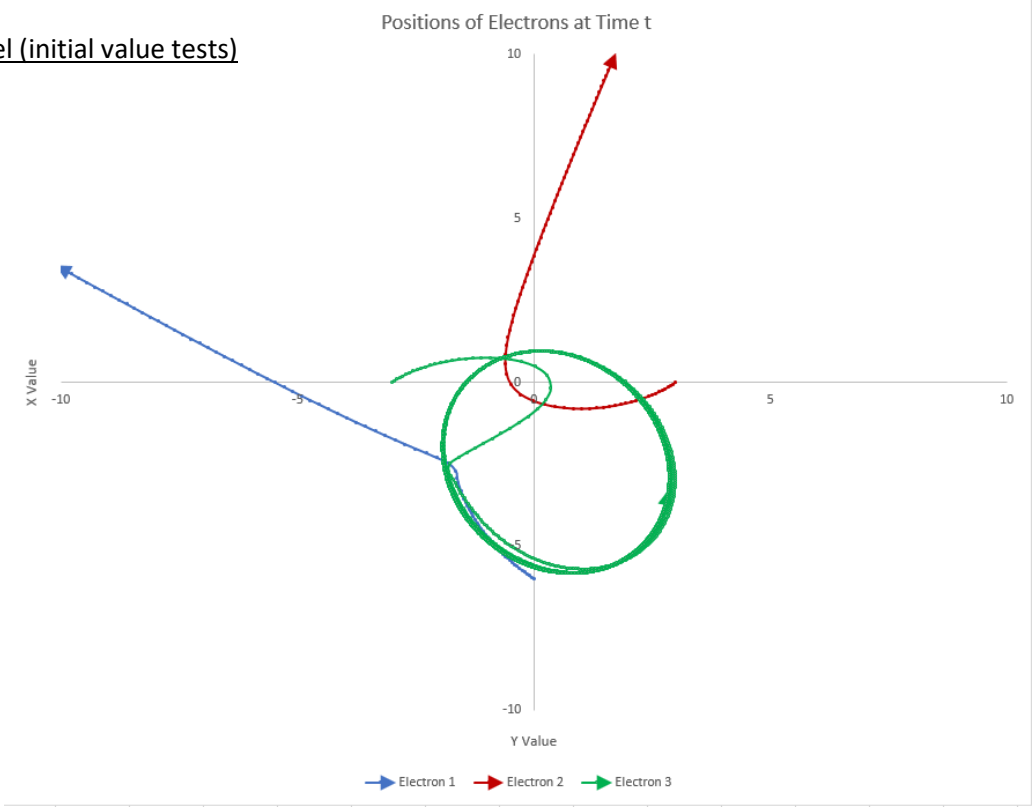
In order to determine the initial conditions, the parameters determined by the helium atom model would be used while modifying the electrons so that they fall into a stable orbit. The time needed for these trials was increased to 500 seconds for the observation of these orbital patterns. Three trials were then conducted to find the initial conditions, using slight modifications to the initial conditions used for the helium model. The most accurate values were those that remained the most stable. The initial values of the three-dimensional model were obtained in the same manner.

Initial values (2d model)			
Trial 1	Electron 1	Electron 2	Electron 3
Position: (X, Y) coordinate	(0, -6)	(-3, 0)	(-3, 0)
Velocity: (X, Y) value	(-0.5, 0.5)	(-0.5, -0.5)	(0.5, 0.5)
Trial 2	Electron 1	Electron 2	Electron 3
Position: (X, Y) coordinate	(0, -6)	(3, 0)	(-3, 0)
Velocity: (X, Y) value	(-0.5, 0.5)	(-0.5, -1.5)	(0.5, 0.5)
Trial 3	Electron 1	Electron 2	Electron 3
Position: (X, Y) coordinate	(1, 0)	(0, 3)	(-1, 7)
Velocity: (X, Y) value	(0, -1)	(0.6, -0.2)	(-0.3, -0.1)
Initial values (3d model)			
	Electron 1	Electron 2	Electron 3
Position: (X, Y, Z) coordinate	(1, 0, 0)	(0, 3, 0)	(0, 0, 20)
Velocity: (X, Y, Z) value	(0, 1, 0)	(0, 0, 1)	(-0.3, 0, 0)

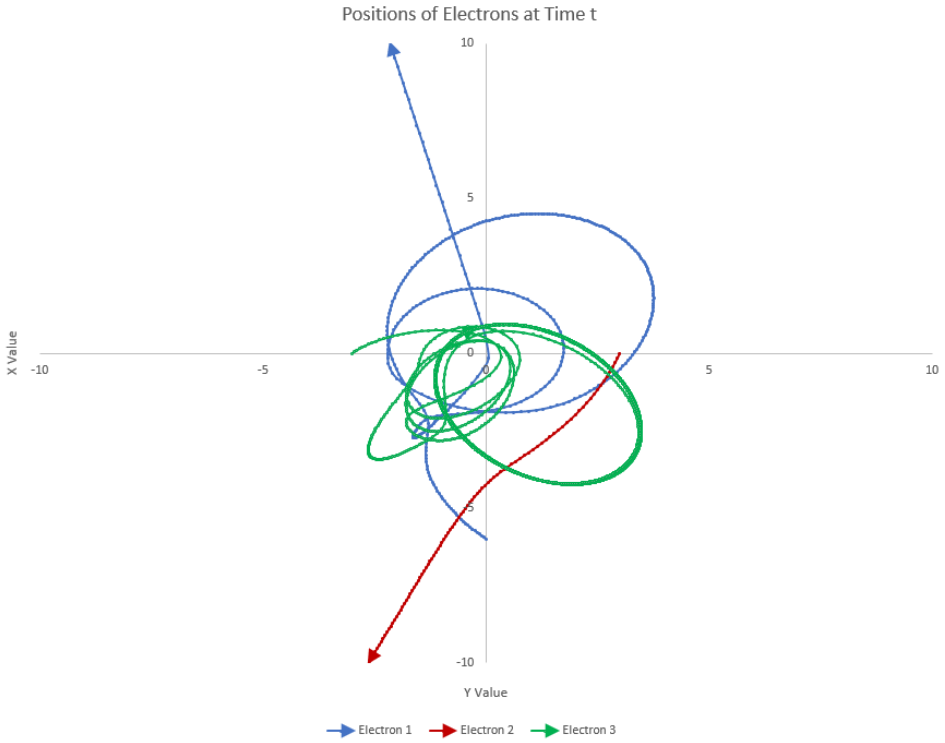
Results

2d model (initial value tests)

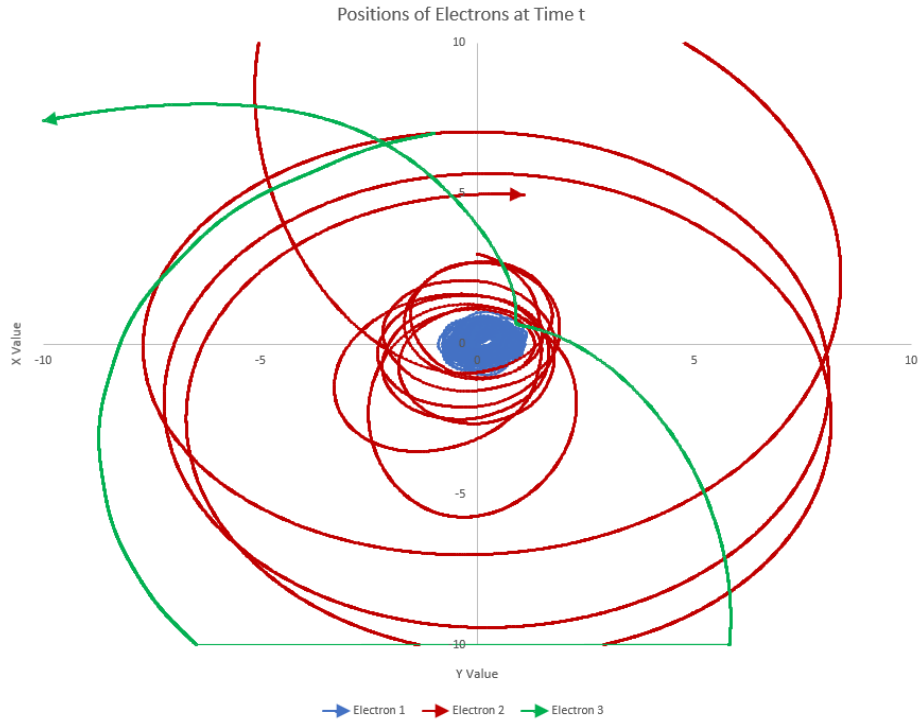
Trial 1:



Trial 2:

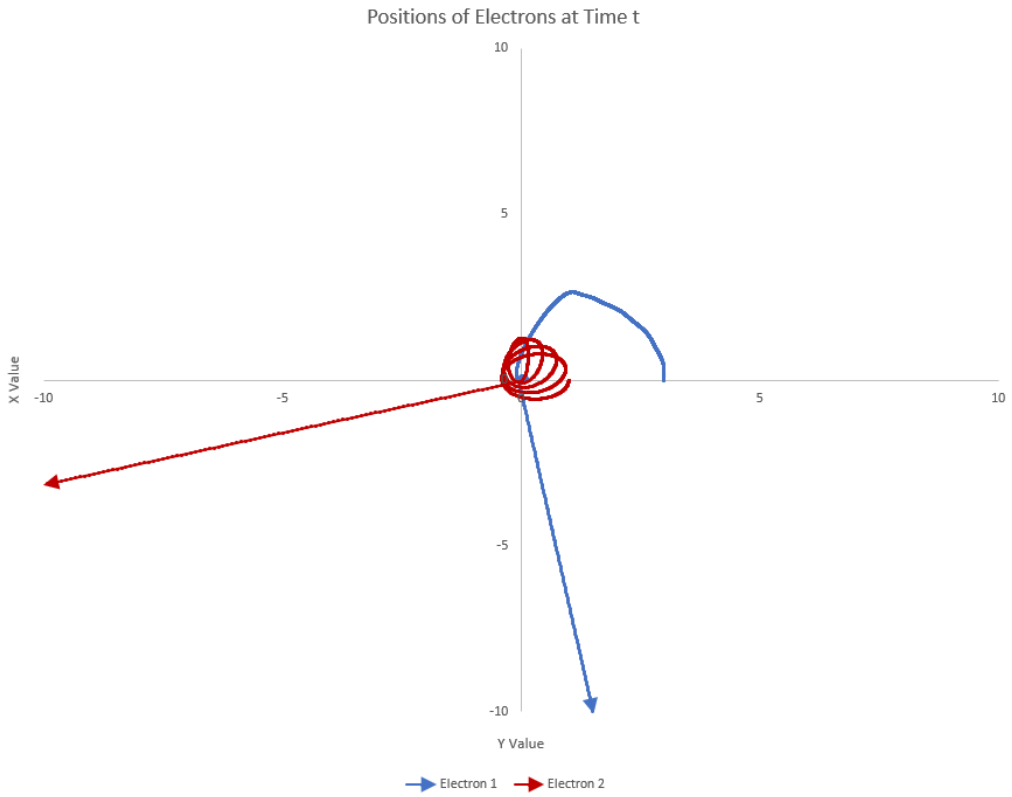


Trial 3:

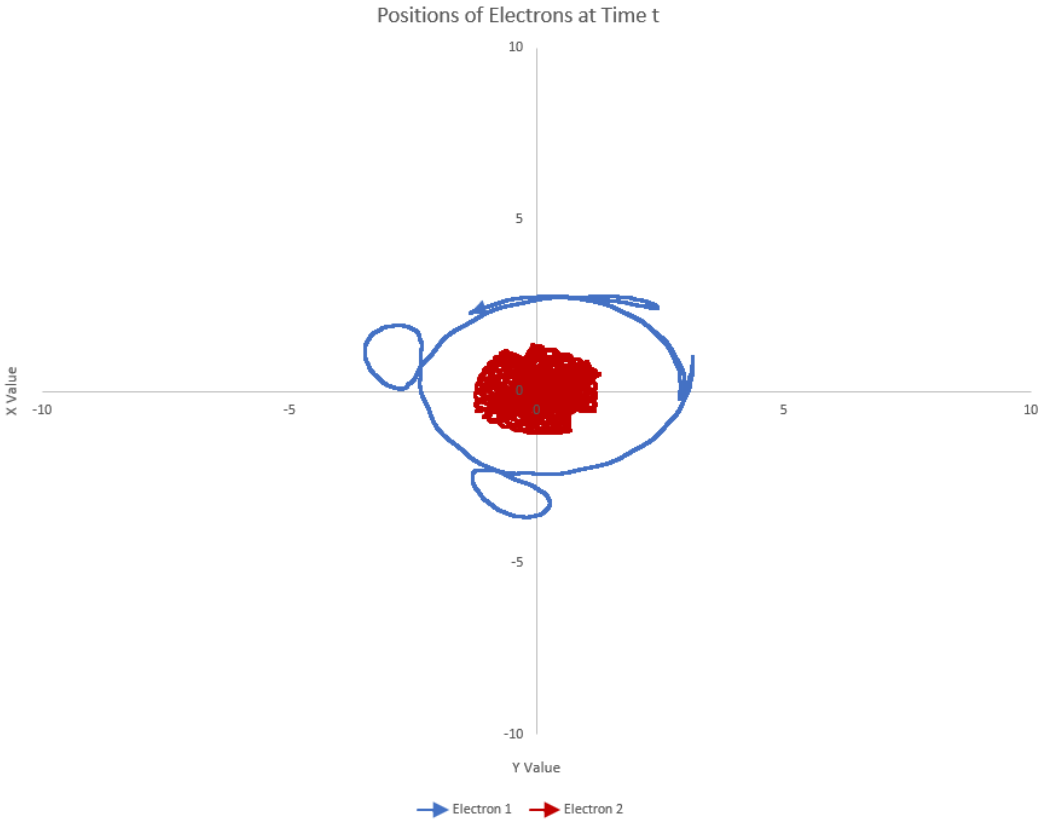


2d model (parameter tests on Helium atom)

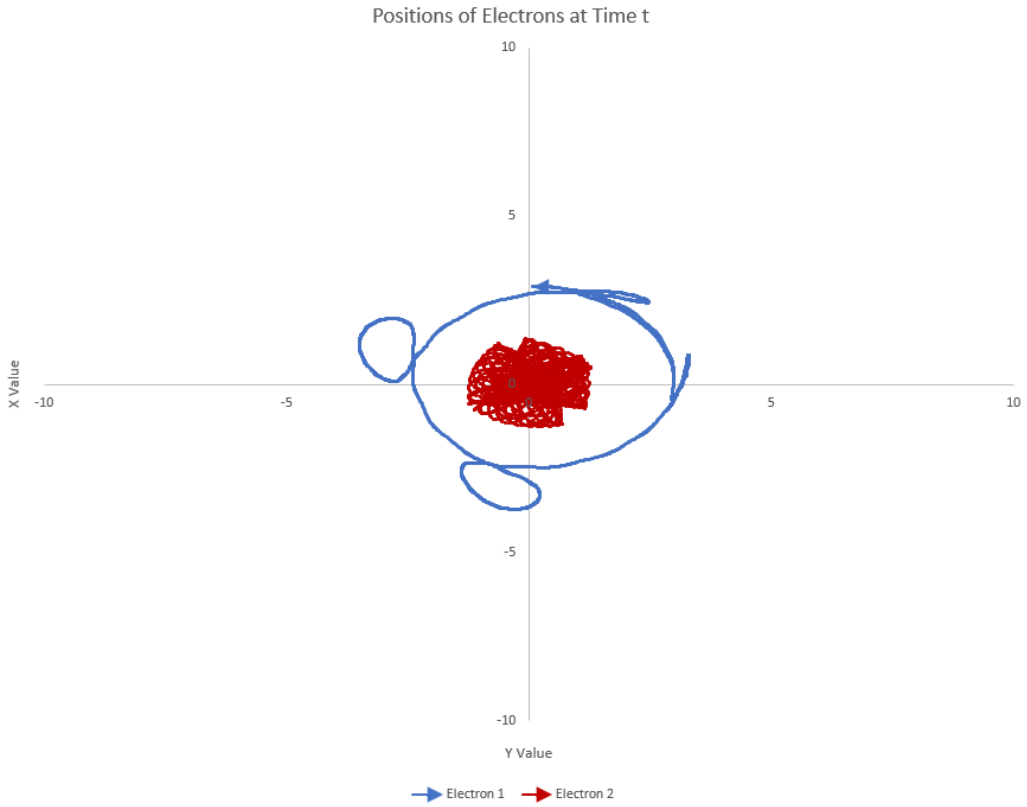
Trial 1:



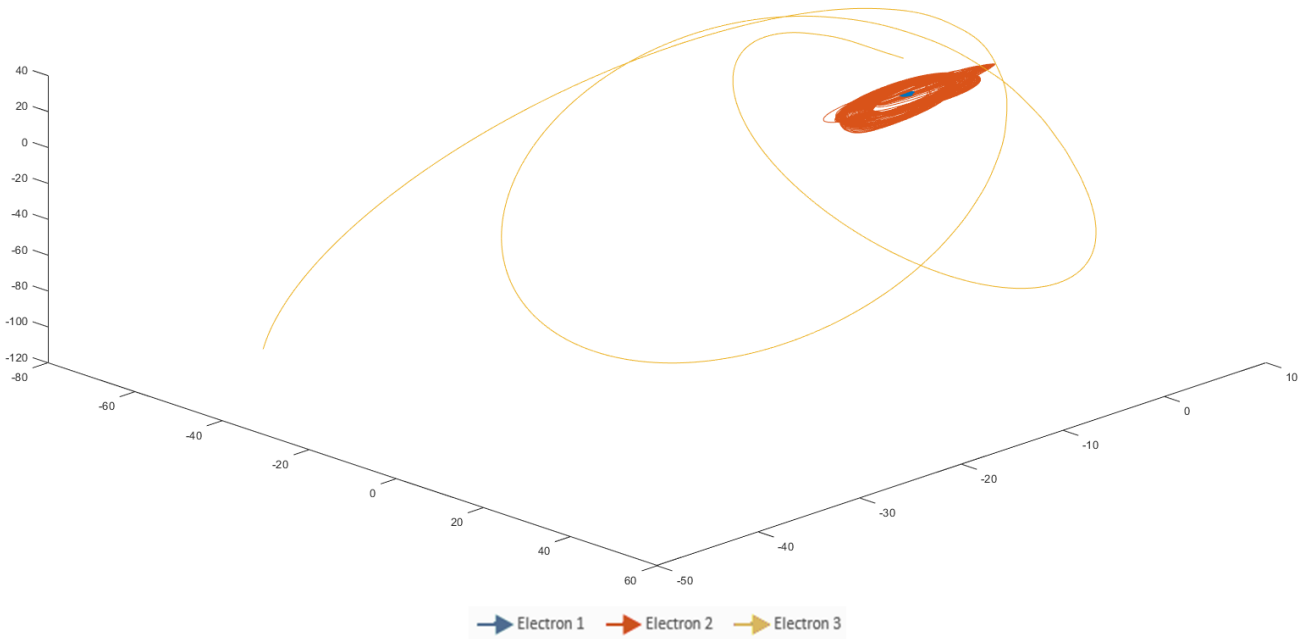
Trial 2:



Trial 3:



3d model

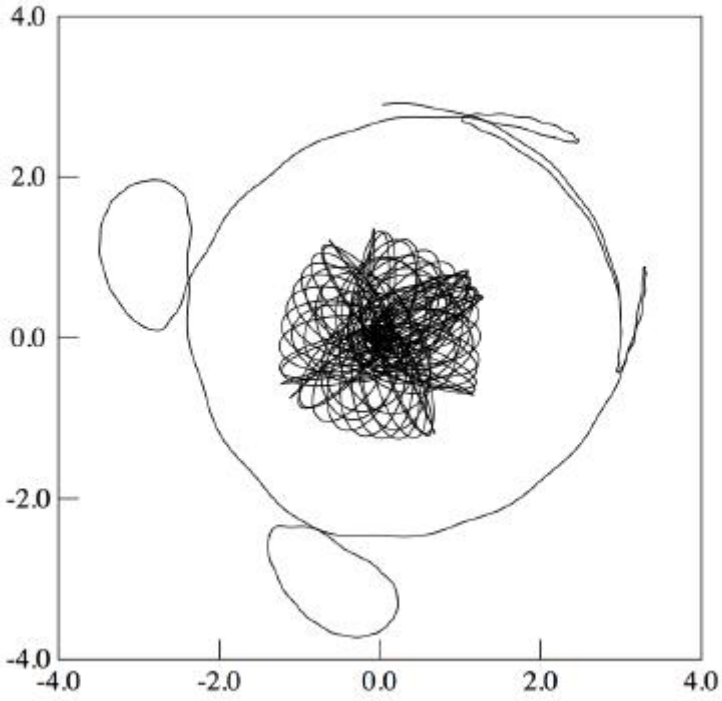


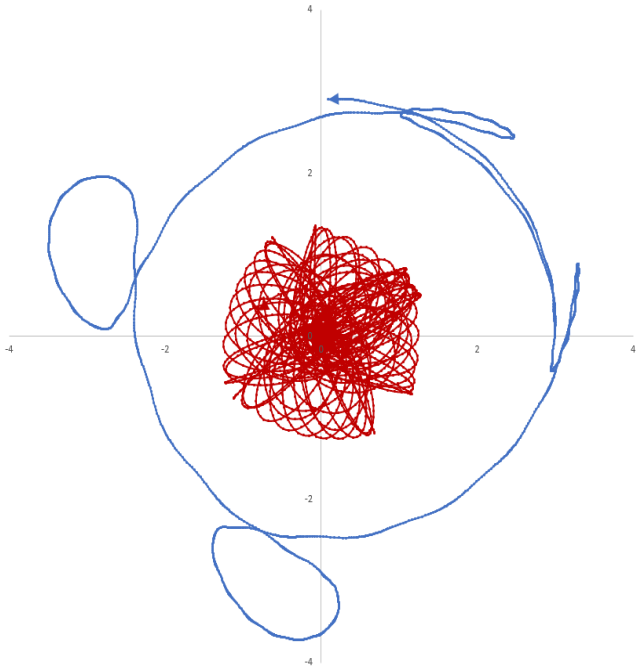
Analysis/Conclusions

Trial:	Point	Time (sec)	Electron 1 Error	Electron 2 Error
1 (parameter test)	1	0	0	0
	2	16	2.074939	0
Runge-Kutta 4	3	32	26.02657	70.5318
	4	48	684.9468	238.6409
	5	64	93.17771	334.7539
	6	80	126.0785	3301.417
	7	96	152.0055	844.1735
	8	112	199.459	2437.843
	9	128	377.8003	1499.844
	10	144	6758.26	876.0609
	11	160	257.4616	907.1902
	12	161	257.0115	2674.084
Average Electron 1 Error:	744.5252291		Average Electron 2 Error:	1273.859011
Global Relative Error:			624.75953895	
2 (parameter test)	1	0	0	0
	2	16	0.006006	0.016894
Trapezoidal	3	32	0.005586	0.196709
	4	48	0.133239	0.777624
	5	64	0.011341	1.011361
	6	80	0.198131	1.106972
	7	96	0.105877	2.619298
	8	112	2.496727	4.619597
	9	128	0.116417	0.241572
	10	144	0.440296	14.63853
	11	160	1.569231	1.367724
	12	161	8.137176	0.451669
Average Electron 1 Error:	1.101669015		Average Electron 2 Error:	2.253996375
Global Relative Error:			0.549836916	
3 (parameter test)	1	0	0	0
	2	16	0	0
Runge-Kutta 4/5	3	32	0	0
	4	48	0	0
	5	64	0	0
	6	80	0	0
	7	96	0	0
	8	112	0	0
	9	128	0	0
	10	144	0	0
	11	160	0	0
	12	161	0	0
Average Electron 1 Error:	0		Average Electron 2 Error:	0
Global Relative Error:			0.0	

To validate this model, the accepted model for the helium atom was compared with the generated model for the helium atom to verify consistency with given physics laws. The same parameters were then used by adding one more electron to the atom and increasing the charge of the nucleus to three.

Helium atom: Given model vs. generated model:





After running the two separate trials, the Runge-Kutta 4/5 method worked the best, with an error size of 1E-7, and the initial conditions found in the third trial. The system was not stiff, as any modifications to the values made the system react erratically and unpredictably. The two-dimensional system was not stable, as the only way this atom reaches stability in the real system is by the inclusion of the z-axis. In other words, this atom can not be stable unless it is three-dimensional. This is later reflected in the generated three-dimensional system, in which all of the electrons reach stability.

The most cost-effective method was also the Runge-Kutta 4/5, as the trapezoidal method took far longer than both other methods combined to run, in addition to its higher error over RK4/5. This

expensive run time was likely due to the 119,121 steps it took for completion for a total of 238,242 function calls. In comparison, the RK4/5 method only took 5,604 steps and 33,624 function calls, while the RK4 took 16,101 steps and 64,404 function calls.

The two-dimensional model was the main model of focus due to the verification and validation that could be applied, even though the solution is ultimately unstable compared to the three-dimensional model. This was the biggest trade-off undertaken in using the accepted solution directly in implementation of the system.

The initial conditions can be corrected further for the three-dimensional model and the two-dimensional model, and this is a source of still existing errors in the simulation. Additional errors may be caused by the non-inclusion of the k-constant in Coulomb's law, as this constant was assumed to simply speed up the simulation. An additional assumption was that electrons could be placed anywhere around the atom, and would eventually fall into place in a nice, steady orbit. The most important lesson to be learned from the lithium atom is that initial conditions can make all the difference from a steady and stable orbit, to an erratic and -likely radioactive- outcome.