Phys 410 Project1

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1 Introduction

The Thomson Problem is a Electrostatic problem proposed by physicist, J.J. Thomson in 1904[1]. The goal of the problem was to determine the configuration of electrons on a charged unit sphere to minimize the electrostatic potential energy of the system. The primary motivating factor behind this problem was to study the geometry of minimal energy charge configurations, and how the configurations would look like for large number of charges.

Due to the nontrivial solution to the differential equations that describe the motion of the charges (which will covered in the section below), computational methods using Finite Difference Approximation were developed to solve the Thomson problem. The derivation and implementation of this computational solution to the Thomson problem will be covered in this paper as well as an analysis of the results and comparative accuracy to previous computational solutions to the Thomson Problem

2 Notation and Normalization

Before we proceed with the derivation and implementation of the solution to the Thomson problem it is worthwhile to define notation to express the position and velocities of specific charges at given times.

Consider a charge q_i where i denotes it is charge i out of N charges. At any given time step – n out of nt – the charge has position $\mathbf{r_i^n}$ and velocity v_i^n where $\mathbf{r_i^n} = [x_i^n, y_i^n, z_i^n]$.

Also, because the charges exist on the surface of a unit sphere, at any given time, n: $r_i^n \equiv \mathbf{r_i^n} = \sqrt{(x_i^n)^2 + (y_i^n)^2 + (z_i^n)^2} = 1$

3 Mathematical Background

First we should define the equation of motion for a charge described by $\mathbf{r_i}$ where it is charge number i in a system of N charges denoted, such that:

$\mathbf{r_i} \equiv r_i[x(t), y(t), z(t)], \quad i = 1, 2, ..., N$

From here we can construct the equation of acceleration over time for r_i:

$$\frac{d^2\mathbf{r}_i^n}{dt^2} = -\sum_{j=1,j\neq i}^{N} \frac{\mathbf{r}_{if}^n}{(r_{ij}^n)^3} - \gamma\frac{dr_i^n}{dt}; \quad i = 1, 2, ...N; \quad 0 \leq N \leq t_{max} \quad (1)$$

where γ is an is an adjustable parameter that controls the magnitude of the velocity-dependent dissipative force.

Now we can utilize Finite Difference Approximation equations:

$$\frac{dr_i^n}{dt} \mid_{t=t^n} \rightarrow \frac{r_i^{n+1} - r_i^{n-1}}{2\Delta t} \quad (2)$$

$$\frac{d^2r_i^n}{dt^2} \mid_{t=t^n} \rightarrow \frac{r_i^{n+1} - 2r_i^n + r_i^{n-1}}{\Delta t^2} \quad (3)$$

We can set eq (1) = eq(2) and substitute in (3) to produce a single expression for r_i^{n+1} (with some rearranging):

$$r_i^{n+1} = \frac{2\Delta t}{2+\gamma} * (-\sum_{j=1,j\neq i}^{N} \frac{\mathbf{r}_{ij}^n}{+}\gamma * \frac{(r_i^{n-1})}{2\Delta t} + 2(r_{ij}^n) - \frac{(r_i^{n-1})}{\Delta t} \quad (4)$$

Now we have expressions for $r(t)$ described be eq (4) and $v(t)$ described by eq (2) which we can implement

Also, We can use Electric Potential as a 'diagnostic' quantity to verify our simulation is accurate:

$$V(t^n) = \sum_{i=2}^{N}\sum_{j=1}^{i-1} \frac{1}{r_{ij}^n} \quad (5)$$

where $lim_{t\rightarrow \inf} V(t)$ is a minimum

Finally, there is one last mathematical concept useful in this project: equivalence classes. Two charges belong to an equivalence class if the difference in the sorted distances to charges vectors are less that the defined tolerance ϵ_{ec}. The implementation of checking equivalence classes will be discussed in the following computational methods section.

4 Computational Methods

The main function 'charges' takes in 5 positional arguements: (r0, tmax, level, gamma, epsec). r0 is the initial position, tmax is the max time, level describes how many time steps to iterate over, gamma is the previously discussed adjustable parameter that controls the dissapative force, and epsec is the tolerance for checking if two charges belong in an equivalence class. This function is divded into four main parts:

Initializing arrays and Initial Conditions:
The first array that is initialized in the charges function is the time array. The number of time steps in the array is defined to be $nt = 2^{level} + 1$, and from here a time array can be initialized as a meshgrid from 0 to tmax with nt steps. After time the first two position and first velocity steps are initializes with:

$$r_i^1 = r_0; \quad r_i^2 = r_0; \quad v_i^1 = 0$$

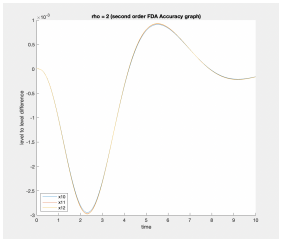
The logic is that the initial charges do not have an initial velocity so it is a fair assumption to set the first two position increments to r0.
Updating r(t) and v(t):
The next thing done in the charges function is to iterate through nt and update the charges position and velocity. This is done using the derived equattions (4) and (2) for position and velocity respectively.
Updating V(t): The third thing that's happening is updating the Potential V(t). This is done using the eq(5). This is being done inside the same time for loop that is updating the position and velocity.
Checking Equivalence Relations: As described earlier, two charges are in an equivalence class in the magnitude difference in the vectors of their sorted distance vector to other charges is less than ϵ_{ec}. The implementation of this includes two sets of double for loops: the first double for loop initializes an nc by nc matrix of sorted distances from charges to other charges. Then the second double for loop iterates through the rows of this sorted nc by nc matrix and checks if two charges belong in an equivalence class by the method described in the first sentence. If so then both charges are removed from the matrix to avoid double counting.

5 Results And Analysis

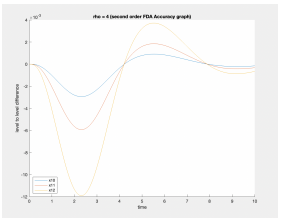
I will go through and explain the requested 'calculations to perform' and their results.
4-level convergence test:
To reproduce run 'convtest.m':
Using the requested initial conditions and 4 sets of levels described in the project assignment[3] with the results:

$$\delta x_{10}, \quad \rho\delta x_{11}, \quad \rho^2\delta x_{12}$$

We can graph these results and see convergence for $\rho = 2$ if our FDA is first-order accurate, and $\rho = 4$ if our FDA is second-order accurate. Running this file we get the graphs:



(a) $\rho = 2$, First Order Accuracy



(b) $\rho = 4$, Second Order Accuracy

Figure 1: Comparing First and Second Order Accuracy

Comparing The results of the 4-level Convergence, it is clear that our computational solution to the Thomson problem is of **First Order Accuracy**, due to the convergence in the different levels.

Time Evolution of potential for 12-charge calculation:
To reproduce run 'plotv.m':
To help us get a visual understanding of the convergence of the Potential we can make an example of N=12 charges and graph the potential over time. We expect the graph to converge at a horiznotal line:

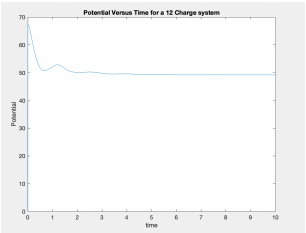


Figure 2: Potential versus Time for N=12

This graph shows the convergence of the potential value for N=12 as time goes on. This represents the charges reaching an equilibrium on the surface of the sphere which turns out to roughly 49.1652530576 for N=12. Comparing with the Wikipedia page for Thomson Potentials [2] we can see we are very close, and that our computational solution is ready to survey multiple configurations of charges.

Survey of V (tmax; N) and vec(N) for various values of N:
To reproduce run 'survey.m':
Using the scaffolding given in the project description[3] in addition to the charges function, the only critical decision for this script is to decide on an appropriate tmax and levels. In order oprimize the chances that the charges will converge,

tmax was made to 500, and level to be 12. As a result running the file Survey.m took about 25 minutes on my computer but resulted a relatively accurate table of $V(t_max : N)$ and v_{ec}, where $V(t_max : N)$ is the potential of the system for N charges, and v_{ec} is the vector of ordered equivalence classes.

Table of $V(t_max : N)$ and v_{ec} combined:

N Charges	Potential at tmax	Eq Class Vector
2	0.5000000000	[2]
3	1.7320508076	[3]
4	3.6742346142	[4]
5	6.4746914947	[3 1 1]
6	9.9852813742	[6]
7	14.4529774813	[1 1 1 1 1 1 1]
8	19.6752878612	[8]
9	25.7599865313	[3 2 4]
10	32.7169494601	[8 2]
11	40.5964505082	[1 2 4 2 1 1]
12	49.1652530576	[12]
13	58.8532306117	[2 2 3 1 2 1 1 1]
14	69.3063632966	[12 2]
15	80.6702441143	[6 4 1 1 3]
16	92.9116553025	[12 4]
17	106.0504048286	[5 8 2 1 1]
18	120.0844674475	[8 6 2 1 1]
19	135.0894683273	[1 2 2 2 1 2 1 1 2 1 1 2 1]
20	150.8815683338	[6 6 3 1 2 1 1]
21	167.6416224009	[2 2 1 1 2 1 1 2 1 1 2 1 1 1 1 1]
22	185.2875361493	[12 3 3 2 1 1]
23	203.9301906629	[6 5 3 2 4 1 1 1]
24	223.3470740518	[24]
25	243.8127650759	[1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1]
26	265.1333263174	[1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1]
27	287.3026150330	[10 2 5 4 2 1 1 1 1]
28	310.4915423582	[12 7 1 6 1 1]
29	334.6344399209	[2 2 2 2 2 2 1 1 1 2 1 1 1 1 2 1 1 1 1 2]
30	359.6039459038	[2 2 2 2 2 1 2 1 1 1 2 1 2 1 1 1 1 1 1 1 1 1]
31	385.5308380633	[3 3 6 1 1 5 3 1 1 2 2 1 1 1]
32	412.2612746505	[20 4 6 1 1]
33	440.2040578594	[1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1]
34	468.9048532813	[4 3 3 3 3 3 4 1 1 3 1 3 1 1]
35	498.5698724908	[2 2 2 2 2 2 1 1 1 2 2 2 1 1 1 1 2 1 1 2 1 1 1 1]
36	529.1224095902	[2 2 2 2 2 2 2 1 1 2 1 2 1 1 1 1 1 2 1 1 2 1 1 1 1]
37	560.6188877310	[10 8 6 4 2 2 2 1 2]
38	593.0385035665	[12 8 6 5 3 2 1 1]
39	626.4409584107	[2 2 1 2 1 2 2 2 1 2 1 2 1 2 2 1 1 1 1 2 1 1 1 1 2 1 1]

N Charges	Potential at tmax	Eq Class Vector
40	660.7253044014	[2 2 2 2 2 2 2 2 2 1 1 1 1 1 2 2 2 1 2 1 1 1 1 2 1 1]
41	695.9167443419	[6 5 4 3 3 6 2 4 1 1 2 1 1 1 1]
42	732.0781075437	[10 9 6 4 5 2 2 1 1 1 1]
43	769.1908469096	[2 2 2 2 1 1 2 1 1 2 2 2 2 1 1 1 1 2 1 2 1 1 1 1 1 1 1 1 1 1 1 1]
44	807.1742630846	[12 3 7 6 1 3 6 1 1 3 1]
45	846.1884017453	[2 2 2 2 2 2 2 1 2 2 1 1 2 2 1 2 1 1 1 1 2 1 2 1 1 1 1 1 1 1 1]
46	886.1714324245	[2 2 1 2 2 2 2 2 2 2 1 2 2 2 2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1]
47	927.0622696713	[1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1]
48	968.7134553438	[24 10 10 3 1]
49	1011.5571826536	[3 3 2 3 2 2 3 2 3 3 2 2 3 2 2 1 1 1 1 2 1 1 1 2 1]
50	1055.1823147263	[12 10 8 5 1 6 3 3 1 1]
51	1099.8192903189	[3 6 6 6 3 1 2 4 4 3 1 2 2 1 1 1 2 2 1]
52	1145.4189643193	[3 3 3 3 2 2 2 1 3 1 1 2 1 1 2 3 1 3 2 2 1 1 1 1 3 1 1 1 1]
53	1191.9222905021	[2 2 2 2 2 1 2 2 1 2 2 2 2 2 1 1 2 1 1 2 2 1 1 2 1 1 1 1 1 1 1 1 1 1 1 1 1]
54	1239.3711922688	[1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1]
55	1287.7772608069	[4 2 3 4 3 2 3 2 3 2 1 2 2 1 2 2 1 1 1 1 1 2 1 1 1 2 1 1 1 1 1]
56	1337.0953482671	[2 2 2 2 2 1 2 1 2 2 2 2 2 1 1 2 2 2 2 1 1 1 2 1 2 2 1 1 1 1 1 1 1 1 1 1 1]
57	1387.3832292528	[6 6 6 6 5 2 3 3 2 2 3 1 3 1 1 2 1 1 2 1]
58	1438.6381050033	[1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1]
59	1490.7907730924	[2 2 2 2 2 2 2 2 1 2 2 1 2 2 2 1 2 2 1 1 1 1 1 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1]
60	1543.8350995985	[2 2 2 2 1 2 1 2 1 2 1 2 2 2 2 2 2 2 2 1 2 1 1 1 1 1 2 1 1 2 1 1 1 1 1 1 1 1 1 2 1]

Analysis of the Table: In analyzing the previous table we see that the Potential(tmax) of the charges holds with reasonable accuracy (≥ 5 decimal points) until we reach N=39 at which my values start to diverge with Wikipedia's values[2]. It is also at this point that the equivalence classes start to be become non-absolute. Or in other words if I run survey again I might get different values for the equivalence classes for around N=39 onwards. I theorize it is around this point that the needed iterations to achieve true equilibrium and equivalence convergence is so exhaustive that I would need an improved operating device. Regardless, this table demonstrates that our computation holds reasonably well for the first 39 charge configurations. We can also scan the table for meaningful results. For example, in analyzing the rate that the potential increases we can see it rouhgly proportional to just under the change in of the charges in the system. For example the difference in the potential difference between N=60 and N=59 is roughly 53 which 36 N=20 and N=21 which is 17. This is an interesting observation: as we increase the number of charges N by n we will increase the potential at tmax by a amount roughly smaller than n. Another interesting result that occurs as we increase N is the equivalence relation vector holding less charges in each equivalence class. For example, there are multiple Ns for $N > 50$ with the maximum charges in an equivalence class being either 1 or 2. This is interesting because I would have hypothesized that as we increase N there would more charges in the same equivalence class since there are more charges on the same sphere. However, this shows that even despite high number of charges, the charges will still try to space out as much as possible which results in isolated charges and thus a long Equivalence Class Vector.

Video of sample evolution:
To reproduce ruin 'main.m':

For the requested charges video I decided to use the initial conditions: nc = 45, tmax =15, gamma=1, epsec = 0.00001, level = 8. I coded this in 'main.m', and the animation video is saved to the default file name, 'charges.avi'. I chose 45 because it was large enough that you could actually see the configuration of charges start to resemble a sphere as they moved away from each other. If I wanted true convergence I would choose levels to be on the order of 15-20 and tmax to be 500, but for the purpose of an informative animation the current parameters work fine.

6 Conclusion

Through the combination of the equations of the acceleration of charges in the presence of other charges with the methods of Finite Difference Approximation, I was able to computationally solve the Thomson Problem with reasonable accuracy for the first 39 charge configurations. In 'convtest.m', we demonstrated that our results converged to a first order FDA accuracy. In 'plotv.m', we

demonstrated visually how the potential of a charge distribution converges to V(tmax). In 'survey.m', we constructed a table for the first 60 charge configurations calculating V(tmax) and the equivalence relations vector for each configurations. We found that our results were reasonably accurate for the first 39 charges and started decreasing in accuracy beyond that point which could be explained by a more exhaustive time array is needed to reach convergence. And finally in 'main.m' and 'charges.avi' we animated the (rough) equilibrium of a N=45 charge system to get a visual sense of the charges occupying a configuration of minimum electrostatic potential energy. Future efforts could be made towards optimizing the computations for higher order charge configurations, and standardization of equilibrium classes.

7 References

(1) Thomson, J. J.(1904) 'XXIV. On the structure of the atom: an investigation of the stability and periods of oscillation of a number of corpuscles arranged at equal intervals around the circumference of a circle; with application of the results to the theory of atomic structure', Philosophical Magazine Series 6, 7: 39, 237 — 265

(2) Wikimedia Foundation. (2022, October 17). Thomson problem. Wikipedia. Retrieved October 19, 2022, from https://en.wikipedia.org/wiki/Thomson$_problem$

(3) Phys 410 Project 1 Description http://laplace.physics.ubc.ca/410/homework/pr1.pdf