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PHYS 410 - Computational Physics - Project 1

Introduction

In this project I consider collections of N identical charges which are confined to the surface of a sphere, but which can move over that surface under the influence of their mutual electrostatic interactions. By modeling such a system using finite difference approximations of the equations of motion with a velocity dependent retarding force, I find properties and characterizations of equilibrium configurations an arbitrary *N*. I catalogue these properties, which include the electrostatic potential and equivalence classes. Finally, the model and approximations used will be examined to understand their accuracy and convergence.

Review of Theory

Setup

Given N charges, index each identical point charges by the variable

$$i = 1,2, \dots, N \tag{1}$$

Without loss of generality, I non-dimensionalize by setting the mass and charge of each particle, as well as Coulomb's constant, to be 1. Define the position vector of each particle to be

$$\boldsymbol{r}_i(t) \equiv [x_i(t), y_i(t), z_i(t)]. \tag{2}$$

We confine the charges to the unit sphere, and thus the norm of the position vectors is 1. Associated with the position vectors are the unit separation vectors, given by

$$\boldsymbol{r}_{ij} = \boldsymbol{r}_j - \boldsymbol{r}_i \tag{3}$$

Equations of Motion

We begin by establishing the exact second order ordinary differential equation that governs the motion of the charges. We have

$$m_i \boldsymbol{a_i} = -k_e \sum_{j=1, j\neq i}^{N} \frac{q_i q_j}{r_{ij}^3} \boldsymbol{r}_{ij} - \gamma \boldsymbol{v}_i, \qquad 0 \le t \le t_{max} \tag{4}$$

where $\boldsymbol{a}_i = \frac{d^2 \boldsymbol{r}_i}{dt^2}$ and $\boldsymbol{v}_i = \frac{d\boldsymbol{r}_i}{dt}$, k_e is the Coulomb constant, γ controls the magnitude of the velocity-dependent dissipative force, $\gamma \boldsymbol{v}_i$, and t_{max} is the final time of the evolution. Rewriting in terms of r_i and simplifying,

$$\frac{d^2 \boldsymbol{r}_i}{dt^2} = -\sum_{j=1, j\neq i}^{N} \frac{\boldsymbol{r}_{ij}}{r_{ij}^3} - \gamma \frac{d\boldsymbol{r}_i}{dt}, \qquad 0 \le t \le t_{max}. \tag{5}$$

Finite Differencing

To numerically model charge systems, we solve **Eq. 5** via finite difference approximations. We replace the continuum values of *t* with a temporal mesh of integer level parameter *l*. We define

$$n_t = 2^l + 1, \tag{6}$$

$$\Delta t = \frac{t_{max}}{n_t - 1} = 2^{-l} t_{max}, \tag{7}$$

$$t^n = (n-1)\Delta t, \qquad n = 1,2, \dots, n_t, \tag{8}$$

and introduce the finite difference notation for a grid function,

$$\boldsymbol{r}_i^n \equiv \boldsymbol{r}_i(t_n). \tag{9}$$

Recalling the $O(\Delta t^2)$ accurate FDAs for the first and second time derivatives of position,

$$\boldsymbol{r}_i'(t^n) \approx \frac{\boldsymbol{r}_i^{n+1} - \boldsymbol{r}_i^{n-1}}{2\Delta t}, \tag{10}$$

$$\boldsymbol{r}_i''(t^n) \approx \frac{\boldsymbol{r}_i^{n+1} - 2\boldsymbol{r}_i^n + \boldsymbol{r}_i^{n-1}}{\Delta t^2}, \tag{11}$$

we can fully discretize **Eq. 4**:

$$\frac{\boldsymbol{r}_i^{n+1} - 2\boldsymbol{r}_i^n + \boldsymbol{r}_i^{n-1}}{\Delta t^2} = -\sum_{j=1, j\neq i}^{N} \frac{\boldsymbol{r}_{ij}}{r_{ij}^3} - \gamma \frac{\boldsymbol{r}_i^{n+1} - \boldsymbol{r}_i^{n-1}}{2\Delta t}. \tag{12}$$

Isolating for $\boldsymbol{r}_i^{n+1}$, we get

$$\boldsymbol{r}_i^{n+1} = \frac{-\Delta t^2 \sum_{j=1, j\neq i}^{N} \frac{\boldsymbol{r}_j^n - \boldsymbol{r}_i^n}{\left|\boldsymbol{r}_j^n - \boldsymbol{r}_i^n\right|^3} + 2\boldsymbol{r}_i^{n-1} - \boldsymbol{r}_i^{n-2} + \frac{\gamma \Delta t}{2}\boldsymbol{r}_i^{n-2}}{1 + \frac{\gamma \Delta t}{2}}. \tag{13}$$

Finally, we enforce that the charges must stay on the unit sphere by normalizing the vector

$$\hat{\boldsymbol{r}}_i^{n+1} = \frac{\boldsymbol{r}_i^{n+1}}{\left|\boldsymbol{r}_i^{n+1}\right|} \tag{14}$$

Properties of Charge System

The total potential energy of the system, $V(t)$, after non-dimensionalization is given by

$$V(t) = \sum_{i=2}^{N} \sum_{j=1}^{N} \frac{1}{r_{ij}} \tag{15}$$

For a stable equilibrium solution, $\lim_{n\to\infty} V(t)$ is a local minimum. It may be the global minimum, depending on the number of charges and initial conditions.

We can further characterize the symmetry of the equilibrium distribution by examining the pairwise distances between the charges. For each charge, express the distances to every other charge as a distance list with elements sorted in ascending order. We say that two charges are in the same equivalence class if the elementwise absolute difference between their distance lists is less than or equal to some tolerance ϵ_{ec}. This in turn implies that the two charges are indistinguishable in the equilibrium configuration.

Numerical Approach and Implementation

Charge Modeling

In *charges.m*, I implemented **Eqs. 13, 14** numerically to model the position of an arbitrary number of charges. The particle positions in the first two time steps were assigned the initial particle positions, assuming the initial velocity of the particles is zero. The initial positions are generated via a uniform distribution over the volume $-1 \leq x, y, z \leq 1$ and then normalized to be on the unit sphere (*generate_r0.*m). Then, the charges positions are found by iterating over the charges on a specific time step, and then time step is then incremented. While it may seem intuitive to compute the summation in the numerator of **Eq. 13** via iteration, doing so would

result in three nested loops. Instead, vector and matrix operations, which are far more efficient in MATLAB, were used to compute the sum. See the code snippet below:

```
rij = r(:, :, n-1) - r(i, :, n-1);
norms = sqrt(sum(rij.^2, 2));
norms(i) = inf;
r(i, :, n) = r(i, :, n) + sum(rij ./ norms.^3, 1);
```

In addition, the function calculates and records the electrostatic potential of the system over time. This is done by calling the function in *potential.m*, which simply computes the potential via iteration using **Eq. 15**. Simple calculations in two nested loops is less computationally intensive compared to modeling particle positions.

Finally, the function computes the equivalence classes in the system by calling the function in *equivalence.m*. It represents the result in a descending vector, the equivalence class count, where each element is the number of charges in a particular equivalence class. The distance list of each charge is examined in order, and it is compared with previously examined unique distance lists. We check if an equivalent distance list has been encountered before. If so, the element corresponding to the equivalence class is incremented. Otherwise, a new equivalence class is added with a count of 1.

Simulations and calculations

So far, I've discussed how the model is implemented, but how can the accuracy be verified? For some values of t_{max}, l, and γ, the model may not converge in time or have unsatisfactory oscillations. In particular, the survey of $V(t_{max}; N)$ displays potential values to 10 decimal places, which is a reasonable goal to set for the absolute error in the final step. This absolute error can be computed over some number of iterations for a charge model (*v_error.m*). Since for the same values of t_{max}, l, and γ, a smaller N generally converges faster, an satisfactory absolute error for the model with largest N should ensure the accuracy of the results for the required simulations and calculations.

Results

To reproduce the results, change the working directory to *Simulations and Results*. Relevant function calls will be included.

The convergence of the FDA seems to be linear in Δt. This is because for $\rho = 2$ the curves get closer for higher level differences (**Fig. 1**). The tight convergence further implies that the FDA is reliable. Recall that the per time step accuracy of our derivative discretization in **Eqs. 10,11** is $O(\Delta t^2)$ accurate. Since we take a total of n_t steps, where $(n_t - 1) \propto \frac{1}{\Delta t}$, the FDA is $O(\Delta t)$ accurate over the interval $0 \leq t \leq t_{max}$. The convergence of the voltage can also be observed. Take a model with 12 charges, t_{max} = 10, l = 12, γ = 1. The potential converges to 49.165, reaching an equilibrium configuration.

Computed equilibrium potential values match with the theoretically calculated ones (**Table 1**.). I chose t_{max} = 500, l = 12, γ = 1, and epsec = 1.0e-5. I confirmed the parameters by running *v_error(60, 500, 12, 1, 1.0e-5, 10)*, which yielded an absolute less than 1.0e-10. Notice I chose to run this function for N = 60, as it is the model I expect to converge slowest. The equivalence class value show that for N = 2, 3, 4, 6, 8, 12, all particles are in the same equivalent class. In addition, for some values of N there are many equivalence classes with very few particles in each class. Many equivalence classes have the same number of particles belonging to that class for a specific N. In general, the number of equivalence classes increases.

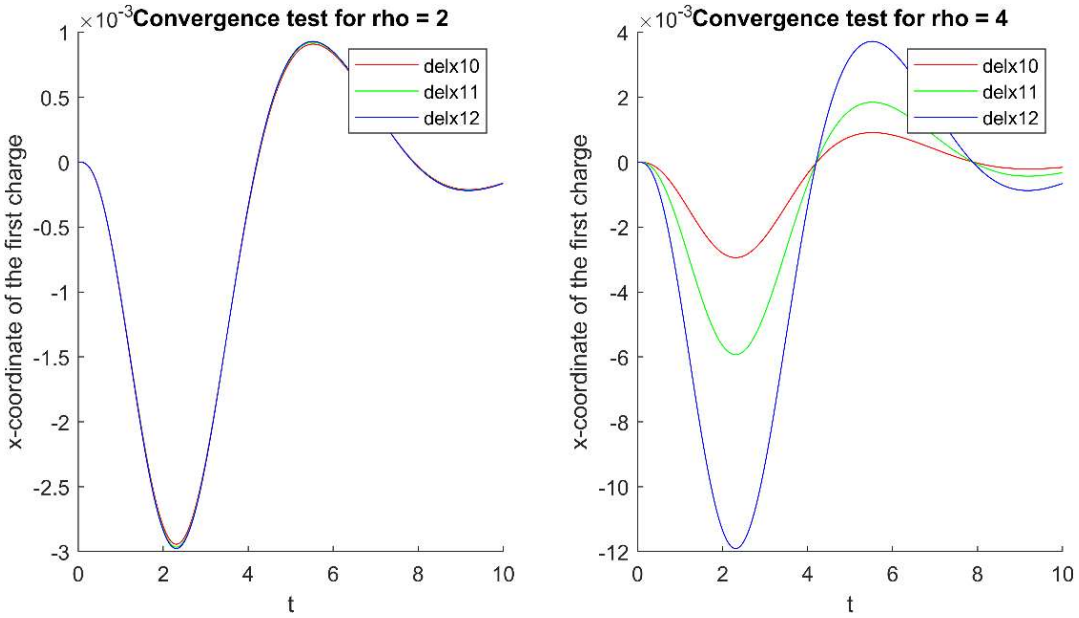

Figure 1. Convergence Test: X-Coordinate of the First Particle Over Time. The lines represent the differences between approximations at adjacent levels of 10, 11, 12, and 13. Produced by calling *convtest()*.

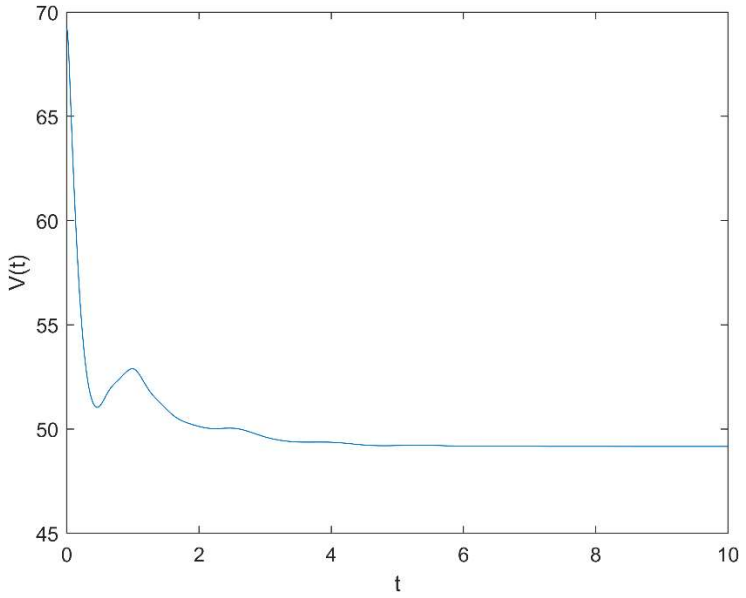

Figure 2. Voltage of 12 Charge System Over Time. The voltage asymptotically approaches a value. Produced by calling *plotv()*.

Table 1. Equilibrium Voltage of N-Particle System for N = 2 to 60.

N	**Actual**	**Computed**	***N***	**Actual**	**Computed**	***N***	**Actual**	**Computed**
2	0.5	0.5	22	185.2875361	185.2875361	42	732.0781075	732.0781075
3	1.732050808	1.732050808	23	203.9301907	203.9301907	43	769.1908465	769.1908465
4	3.674234614	3.674234614	24	223.3470741	223.3470741	44	807.1742631	807.1742631
5	6.474691495	6.474691495	25	243.8127603	243.8127609	45	846.1884011	846.1884147
6	9.985281374	9.985281374	26	265.1333263	265.1333263	46	886.1671136	886.170216
7	14.45297741	14.45297751	27	287.302615	287.302615	47	927.0592707	927.0592707

8	19.67528786	19.67528786	28	310.4915424	310.4915424	48	968.7134553	968.7134553
9	25.75998653	25.75998653	29	334.6344399	334.6344399	49	1011.557183	1011.557183
10	32.71694946	32.71694946	30	359.6039459	359.6039459	50	1055.182315	1055.182315
11	40.59645051	40.59645051	31	385.5308381	385.5308381	51	1099.81929	1099.81929
12	49.16525306	49.16525306	32	412.2612747	412.2612747	52	1145.418964	1145.437597
13	58.85323061	58.85323061	33	440.2040574	440.2040578	53	1191.92229	1191.92229
14	69.3063633	69.3063633	34	468.9048533	468.9048533	54	1239.361475	1239.361475
15	80.67024411	80.67024411	35	498.5698725	498.5698725	55	1287.772721	1287.777261
16	92.9116553	92.9116553	36	529.1224084	529.1224103	56	1337.094945	1337.095348
17	106.0504048	106.0504048	37	560.6188877	560.6279731	57	1387.383229	1387.383229
18	120.0844674	120.0844674	38	593.0385036	593.0385036	58	1438.618251	1438.633708
19	135.0894676	135.0894679	39	626.389009	626.389009	59	1490.773335	1490.774386
20	150.8815683	150.8815683	40	660.6752788	660.6752788	60	1543.830401	1543.8351
21	167.6416224	167.6416224	41	695.9167443	695.9167443			

Table 2. Equivalence Class Count for N = 2 to 60.

N	**Equivalence Class Count**
2	2
3	3
4	4
5	3 2
6	6
7	1 1 1 1 1 1 1
8	8
9	6 3
10	8 2
11	4 2 2 2 1
12	12
13	4 2 2 2 2 1
14	12 2
15	6 6 3
16	12 4
17	10 5 2
18	8 8 2
19	2 2 2 2 2 2 2 2 2 1
20	6 6 6 2
21	2 2 2 2 2 2 2 1 1 1 1 1 1 1
22	12 6 4
23	6 6 6 3 2
24	24
25	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	2 2 2 2 2 2 2 2 2 2 2 2 2
27	10 10 5 2

28	12 12 4
29	6 6 6 6 3 2
30	2 2 2 2 2 2 2 2 2 2 2 2 2 2 1 1
31	6 6 3 3 3 3 3 3 1
32	20 12
33	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	4 4 4 4 4 4 4 4 2
35	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 1
36	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
37	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
38	12 12 12 2
39	12 6 6 6 6 3
40	12 12 12 4
41	12 6 6 6 6 3 2
42	10 10 10 10 2
43	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1 1 1 1 1 1
44	16 16 12 8
45	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 1
46	4 4 4 4 4 4 4 4 2 2 2 2 2 2 1 1
47	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1 1 1 1
48	24 24
49	3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 1
50	12 12 12 12 2
51	6 6 6 6 6 6 6 6 3
52	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
53	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 1
54	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
55	4 4 4 4 4 4 4 4 4 4 2 2 2 2 2 2 2 1
56	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
57	6 6 6 6 6 6 6 6 6 3
58	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
59	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 1
60	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2

Discussion/Conclusions

In this project, I modeled and examined the properties of N identical charged particles on a unit sphere by applying finite difference approximations. The model has accuracy $O(\Delta t)$ over a specified time period and converges well both in particle positions and electrostatic potential. I compared the computed values of equilibrium potentials with known values and found general trends in the equivalence class counts.

I had no particular problems with the assignment and no generative AI was used.