Designing and Simulating Paul Traps: An Introductory Guide to Computational Electromagnetism

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In this paper, we design and simulate a Paul trap to confine charged particles in a region in space with an electric field varying periodically. We model the charge distribution on the electrodes to calculate the potential and electric field they create, and use them to describe the trajectories of the particles. We also determine the range of frequencies for the variation of the electric field under which the trap works for different trap parameters

I. INTRODUCTION

A static electric field cannot be used to trap charged particles, since it would require the potential to have a maxima or minima, depending on the sign of the charge of the ion. A 3D potential, however, cannot have neither maxima nor minima. Instead, the potential will have a saddle point, which isn't a stable equilibrium point of the electric field.

A Paul trap is a quadrupole ion trap with an AC potential. It uses two hyperbolic capacitors to traps ions in an area around a saddle point, which is inverted every time the electric field (periodically) changes sign.

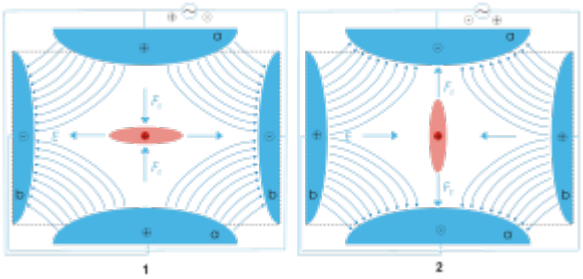

FIG. 1. Idea behind the Paul trap

II. MODELLING THE PROBLEM

A. Integral equation for the potential

In this section, we will cover the steps to model the charge distribution on a capacitor, which we will use to calculate the potential at any given point in space. We start from Poisson's equation for the potential:

$$\nabla^2\phi(\vec{r}) = -\frac{q(\vec{r})}{\varepsilon} \tag{1}$$

The Green's function G for the ∇^2 operator is known, and as such, we can solve it as follows.

$$\phi(\vec{r}) = q(\vec{r}) * G = \int_S q(\vec{r}\,')\frac{1}{4\pi\varepsilon|\vec{r}-\vec{r}\,'|}d\vec{r}\,'$$

Where S is the surface of the electrodes. Finally, applying the boundary condition $\phi(\vec{r})|_S = V_0$, we obtain the integral equation.

$$\int_S q(\vec{r}\,')\frac{1}{4\pi\varepsilon|\vec{r}-\vec{r}\,'|}d\vec{r}\,'\Big|_S = V_0 \tag{2}$$

Applying the same process to the 2D problem, we obtain another integral equation.

$$\frac{-1}{2\pi\varepsilon}\int_C q(\vec{\rho}\,')ln(\vec{\rho}-\vec{\rho}\,'|)d\vec{\rho}\,'\Big|_C = V_0 \tag{3}$$

B. Method of Moments

In order to solve the integral equation, we will use a discretization method called the method of moments (MoM) [1], which will discretize equation (2) ((3) for the 2D cases) into a linear system

$$[Z][a] = [b] \tag{4}$$

We discretize the unknown function $q(\vec{r})$ as $\sum_{n=1}^{N} q_n x_n(\vec{r})$, where the coefficients q_n are the unknowns of the linear system, $[a]$. We will have $[b] = V_0$. And, since our integral equation is defined by a linear operator $\mathcal{L}$, $\mathcal{L}(q(\vec{r})) = \sum_{n=1}^{N} q_n \mathcal{L}(x_n(\vec{r}))$.

We define the residual error $R(\vec{r}) = V_0 - \sum_{n=1}^{N} q_n \mathcal{L}(x_n(\vec{r}))$. In order to minimize $R(\vec{r})$, we force its inner product with a set of weighting functions $w_m{}_{m=1}^{N}$ to be zero: $< w_m(\vec{r}), R(\vec{r}) >= 0$. We will be using $w_m(\vec{r}) = \delta(\vec{r}-\vec{r}_m)$. This is known as point matching, because it forces the residual error on the discretization points to be zero.

$$R(\vec{r}_m) = 0 \implies \sum_{n=1}^{N} q_n \mathcal{L}x_n(\vec{r}_m) = V_0(\vec{r}_m) \tag{5}$$

As such, the components of the matrix Z of the linear system take the form $Z_{mn} = \mathcal{L}x_n(\vec{r}_m)$. The functions x_n are called basis functions. We will use different basis

functions for the 2D and 3D problems. Let us find Z_{mn} for both cases.

For 2D, we go back to equation (3). When we discretize q, we take N points along the curve C, and consider $q = q_n$ on an interval of length h_n and center $\vec{\rho}_n$. We will consider $h = h_n \ \forall n$. Then our basis function will be $x_n(\vec{\rho}) = \Pi(\frac{\vec{\rho}}{h})ln(|\vec{\rho}|)$. Finally, for $m \neq n$,

$$\mathcal{L}x_n(\vec{\rho}_m) = \frac{-1}{2\pi\varepsilon}\int_C \Pi(\frac{\vec{\rho}' - \vec{\rho}_n}{h})ln(\vec{\rho}_m - \vec{\rho}'|)d\vec{\rho}'$$

$$Z_{mn} \approx \frac{-h}{2\pi\varepsilon}ln(|\vec{\rho}_m - \vec{\rho}_n|) \quad (6)$$

For $m = n$, we have to solve the integral analytically, resulting in the following expression.

$$Z_{mm} = \frac{-h}{2\pi\varepsilon}\left(ln\left(\frac{h}{2}\right) - 1\right) \quad (7)$$

Regarding the 3D case, we will model the geometry of the electrodes with N triangles T_n with centers $\vec{r}_n$, and consider $q = q_n$ constant in each triangle. Then, taking into account equation (2), we will use a set of basis functions such that,

$$\mathcal{L}x_n(\vec{r}_m) = \int_{T_n} \frac{1}{4\pi\varepsilon|\vec{r}_m - \vec{r}'|}d\vec{r}' \quad (8)$$

This integral can be computed analytically, as shown in [2]. Solving this integral gives us the expression for Z_{mn} for a 3D problem.

III. VALIDATION OF RESULTS FOR SIMPLE CASES

In this section we will validate that we can reproduce well-known results for simple cases, both in 2D and 3D, as well as a simple study of the convergence.

Firstly, we will use our model to calculate the capacitance of two identical infinite cylinders, which is given by $C = \frac{Q}{V_0} = \frac{1}{V_0}\sum_{n=1}^{N} hq_n$, which should coincide with the capacitance given by the exact expression $C = \frac{\pi\varepsilon}{arccosh(d/R)}$, with $2d$ the distance between the centers of the cylinders, and R their radius. Figure 2 shows that our model converges properly. Figure 3 shows how our precision doubles when we double the points of our discretization.

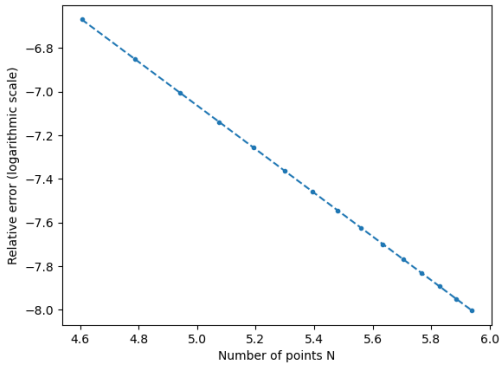

FIG. 2. Convergence for the capacitance of a two cylinder capacitor

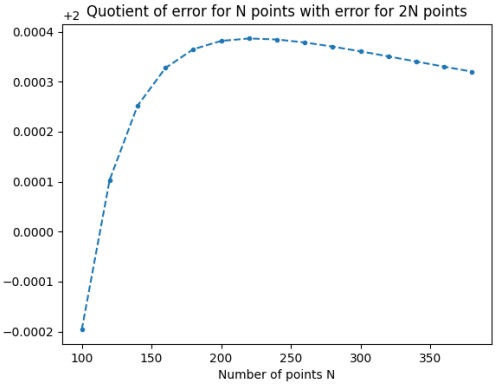

FIG. 3. Quotient between relative errors for N and 2N points for a two cylinder capacitor

The second test for our model will be the calculation of the capacitance for a 3D plane capacitor. Using a similar mesh size than what we will use for the hyperbolic capacitors, we had a relative error of 3.616%.

IV. GEOMETRY DESIGN

The Paul trap we designed consists of a two-sheets hyperboloid along the z-axis and a one-sheet hyperboloid around the z-axis. To construct the one-sheet hyperboloid we built separately the top and bottom part, in both cases we start by generating equally distributed points on circumferences of increasing radius on the XY plane and then projecting them on the Z coordinate according to the hyperbolic equation:

$$z = \pm\sqrt{0.5(x^2 + y^2) + 1} \quad (9)$$

Plus in the case of the top and minus in the bottom part. Once we have the points of the mesh, using the delaunay_2D function we obtain a complete triangular mesh

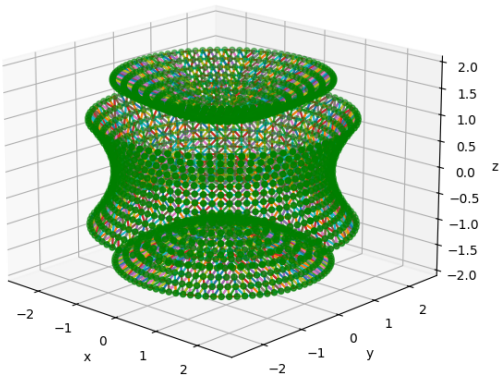

FIG. 4. Geometry of the electrodes with the barycenter of each triangle

of the surfaces with the mesh points already organized in triangles, and then we calculated the barycenters. In the case of the one sheet hyperboloid, we used the cylindrical symmetry. We produced a mesh of equally spaced cylindrical points, making the radial component follow the hyperboloid equation:

$$r = 2\sqrt{0.5 \cdot z^2 + 1} \tag{10}$$

We used again delaunay to obtaine the triangular mesh and then calculated the barycenters.

V. CHARGE DISTRIBUTION IN THE ELECTRODES: POTENTIAL AND FIELD

Next, we applied the method of moments to the triangular mesh to find the charge density in each triangle, solving equation (4). For that, one has to find the elements of the matrix Z, which are given by the expression (8). In order to calculate these integrals, we used the method described in [2].

Once we finally have a charge q_n associated to each triangle in the mesh, we can create a spatial grid and compute the potential V in each point using equation (2) and the charge distribution $q = \sum_{n=1}^{N} q_n x_n$:

$$V(\vec{r}) = \sum_{n=1}^{N} q_n \int_{T_n} \frac{1}{4\pi\varepsilon|\vec{r} - \vec{r}\,'|} d\vec{r}\,' \tag{11}$$

We can observe the results in the following images. In Figure 5, we can observe the potential in the planes $x = 0$, $y = 0$ and $z = 0$, and the cones represent the electric field, which is computed with the function *numpy.gradient*. In Figure 6, we also see the electric field and level surfaces of potential, that is to say, surfaces where the potential is constant. Specially, we can

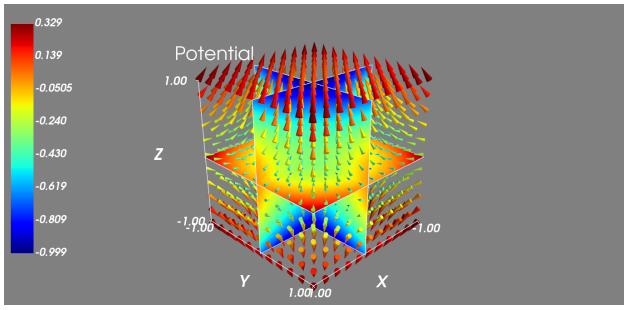

FIG. 5. Potential along the axe's in V and electric field, flowing from the positive charged plate to the negative one

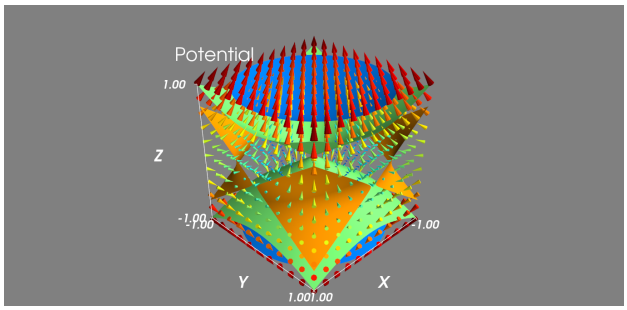

FIG. 6. Level surfaces with constant value of the potential created by the electrodes and the electric field represented with cones.

see that one of the level surfaces is a perfect cone, that is very characteristic of the hyperboloid geometry.

VI. IONS TRAJECTORIES

Once we already have calculated the potential in all space due to the electrodes, we can move on to study the behavior of ions in this potential and try to trap them, which is the main goal. We solved the equation of motion for the ions numerically.

We can determine the ions trajectories from the initial positions and velocities, and the force acting on them over time. The force on an ion is just $\vec{F} = \frac{q\vec{E}}{m} = -\frac{q\nabla V}{m}$, where q is the ion charge and m the ion mass.

To trap the ions an AC potential is used, however it is not necessary to make the calculations indicated in previous sections for every instant of time. Note that, the system that needs to be solved to find the potential in all space $V(\vec{r})$ is linear. Assume we have done the calculations of the space potential $V(\vec{r}$ for a specific electrodes potential V_0. Then, taking advantage of the system linearity, since the electrodes potential over time is $V_0 \cos(\omega t)$, then the space potential over time is $V(\vec{r}, t) = V(\vec{r}) \cos(\omega t)$.

In order to calculate the electric field acting on an ion, we discretized the space region where we wanted to trap the ions with a grid, computed the potential in the grid points and the electric field too, with a linear approxima-

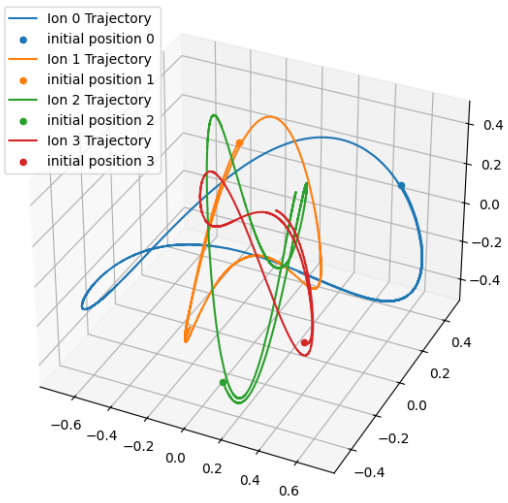

FIG. 7. 4-ions simulation with a potential $0.02V\cos(2\pi\cdot 10^3\cdot t)$, a total time of simulation of 10 s and a step time of 0.5 ms.

tion like *numpy.gradient*. Finally, from the electric field in the grid points, we interpolated it to any point in space with *scipy.interpolate.RegularGridRnterpolator*. Finally, the equation of motion was solved with a central difference method using total time of simulation large enough and a step time of, at most, $\frac{T}{20}$, T being the AC period.

For all simulations, we chose to work with ytterbium ions Yb^+, the electrodes geometry was the one seen previously, and we looked forward to trap the ions in the region $[-1,1]\times[-1,1]\times[-1,1]m$. In addition, the initial positions followed a uniform distribution in the cube $[-0.5,0.5]\times[-0.5,0.5]\times[-0.5,0.5]$. In Figure 7, we can see the ions movement for some specific values of the potential amplitude and frequency. The initial speeds were of the order of $0.5\frac{m}{s}$. Indeed, our configuration is capable of trapping ions.

VII. TRAP DESIGN

Next, we wanted to study the relation that the potential amplitude and frequency must satisfy to trap the ions. Conceptually, if the amplitude is too small or the frequency is too small, we will not be able to control the particles, if the amplitude is too large the ions will go away quickly and if the frequency is too large, the particles will suffer tiny oscillations, but their behavior will be mainly dictated by their initial velocity.

We chose the initial ions velocities to follow a uniform distribution in $[-100,100]\frac{m}{s}$ and ran many simulations for frequencies between 1 kHz and 10 kHz, and amplitudes between 3.1623 V and 1 kV, to see in which conditions the ions stayed within the region. The results can be seen in Figure 8. More or less, log(potential) and log(frequency) follow a linear relation, although the "green region" for which the ions are trapped has some upper and lower limits, and it does not extend to infinity.

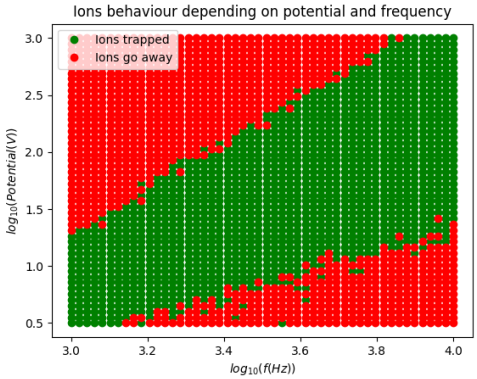

FIG. 8. Ions behavior for different frequencies $\in$ [1kHz, 10k Hz] and electrodes potentials $\in$ [3.1623V, 1kV] for initial speeds of $\sim 100\frac{m}{s}$.

VIII. CONCLUSION

We have simulated and studied the properties of a Paul / quadrupole trap made of a one-sheet hyperboloid electrode and another two-sheets hyperboloid electrode set to potentials with distinct sign. Then, ions trapping has been successfully achieved for multiple ions and for ions with speeds of more than $100\frac{m}{s}$. Lastly, we have concluded that in order to get the ions trapped, the amplitude and the frequency of the AC potential have to fulfill a linear relation in the logarithmic scale.

[1] Richard Carter. The method of moments in electromagnetics, by w.c. gibson. *Contemporary Physics - CONTEMP PHYS*, 51:183–184, 03 2010.

[2] S. Rao, A. Glisson, D. Wilton, and B. Vidula. A simple numerical solution procedure for statics problems involving arbitrary-shaped surfaces. *IEEE Transactions on Antennas and Propagation*, 27(5):604–608, 1979.