

Modeling and Design of a Paul Ion Trap

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The aim of this project is to carry out a series of simulations of a Paul ion trap, also referred to as quadrupole ion trap, which takes advantage of the sinusoidal potential created by hyperbolic electrodes to confine charged particles. The current report includes the description of the discretization technique used to work with the main integral equations, known as Method of Moments (MoM); and the head steps made to get the final results, starting from the calculation of capacitances, the design of the hyperbolic electrodes and the calculation of the potential and electric field, and ending up with the representation of the trajectory of an ion inside the 3D trap, in addition to showing the relation between charge/mass of the particle with the characteristics of the potential.

Keywords: Quadrupole trap, potential, MoM, triangle mesh, trajectory, charge, mass, frequency.

I. INTRODUCTION

The Paul ion trap was named after the physicist Wolfgang Paul's invention, work for which he was rewarded with the Nobel prize in 1989. The trap consists in two hyperbolic electrodes facing each other, and a third one shaped as a hyperbolic ring, halfway between the other two. In those electrodes a sinusoidal potential is applied, such that it prevents ions from escaping.

In this work, we realize a series of computations using Matlab in order to represent the final result consisting of a simulation of a confined ion inside the structure.

We start converting the Poisson's equation for the potential into an integral equation that can be solved numerically. After that, we perform a discretization process using the MoM, that works with lineal operators, to get finally a linear system expressed in matrix form.

Later on, we test our program obtaining the capacitance of two infinite cylinders and of a parallel plate capacitor from the charge calculated. Once checked, we proceed to get the hyperbolic geometry by Delaunay's triangulation, and we compute the charge distribution that allows to get the potential in all space and consequently, the electric field.

Lastly, using classical kinematic formulas and an adequate value of the amplitude and frequency of the AC voltage, we get the confined trajectory, in addition to the relation between the ion's charge and mass, and the harmonic potential.

II. PHYSICAL APPROACH

First of all, we define the problem and the set of equations to be solved. In our case, we are interested in knowing the potential, so we start with Poisson's equation:

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

where $\phi(\vec{r})$ is a scalar potential. Using the appropriate Green's function:

$$G(\vec{r}) = \frac{1}{4\pi\epsilon|\vec{r}|} \quad (2)$$

one ends up with the integral equation

$$\phi(\vec{r}) = \int_S q(\vec{r}') \frac{1}{4\pi\epsilon|\vec{r} - \vec{r}'|} d\vec{r}' \quad (3)$$

and applying the boundary condition $\phi(\vec{r})|_s = V_o$, that is, we know the potential at the surface of the electrodes, the final equation to be solved is

$$V_o = \int_S q(\vec{r}') \frac{1}{4\pi\epsilon|\vec{r} - \vec{r}'|} d\vec{r}'|_s \quad (4)$$

Hence, by employing the Green's function we have limited the problem of finding the potential in all space to finding the charge in the surface.

A. Method of Moments

In order to solve (4), we turned to numerical methods, in particular the MoM, which allows to calculate integrals for a discrete set of points.

The aim of this method in our case is to convert

$\mathcal{L}q(\vec{r}) = V_o(\vec{r})$ (5)
where \mathcal{L} is a linear integral operator and $q(\vec{r})$ the unknown, into a linear system

$$[Z_{mn}][q_n] = [V_o(\vec{r}_m)] \quad (6)$$

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This is done by expanding the charge into a linear combination of pulse basis functions $x_n(\vec{r})$:

$$q_N(\vec{r}) = \sum_{n=1}^N q_n x_n(\vec{r}) \quad (7)$$

so that the residual error at the electrodes surface is

$$R(\vec{r}) = \mathcal{L}q_N(\vec{r}) - V_o(\vec{r}) = \sum_{n=1}^N q_n \mathcal{L}x_n(\vec{r}) - V_o(\vec{r}) \quad (8)$$

and forcing $R(\vec{r}) = 0$ at N points \vec{r}_m we find (6), where

$$Z_{mn} = \mathcal{L}x_n(\vec{r}) \Big|_{\vec{r}=\vec{r}_m} \quad (9)$$

III. PROCEDURE

A. Capacitors

The first step carried out was checking if the linear system works by computing the capacitance of two infinite cylinders and comparing it with the analytical result. But in this case, (4) cannot be used since the 2D Green's function changes and the whole equation becomes

$$V_o = \int_C q(\vec{s}') \frac{-\ln|\vec{s} - \vec{s}'|}{2\pi\epsilon} dl' \Big|_C \quad (10)$$

expressed in cylindrical coordinates and to be evaluated over the contour C .

Having set two circumferences, of the same radius and at distance $2d$ between their centers, at a potential ($V_o/2$) equal in magnitude, but with opposite sign; with the algorithm described in *Section II A*, the charge of a discrete set of points conforming the mentioned circumferences has been calculated.

With the value of the charge known, the numeric capacitance can be calculated using the formula:

$$C = \frac{1}{V} \sum_{n=1}^N h_n q_n \quad (11)$$

where h_n is the separation between two consecutive points. In this case h_n is constant for all the values of n .

For the given capacitor, the capacitance can be analytically obtained as

$$C = \frac{\pi\epsilon}{\text{arccosh}\left(\frac{d}{R}\right)} \quad (12)$$

With a distance $d=2$, a radius $R=1$, a voltage $V_o=1V$, a spaced $h_n=0.0628$ and a total number of points $N=100$, one obtains:

$$\begin{aligned} C_{analytical} &= 2.1088e - 11 \\ C_{numerical} &= 2.1108e - 11 \end{aligned}$$

The error made in the calculation of the capacitance, and therefore of the charge, is of 0.0963%. This acceptable result validates the method implemented.

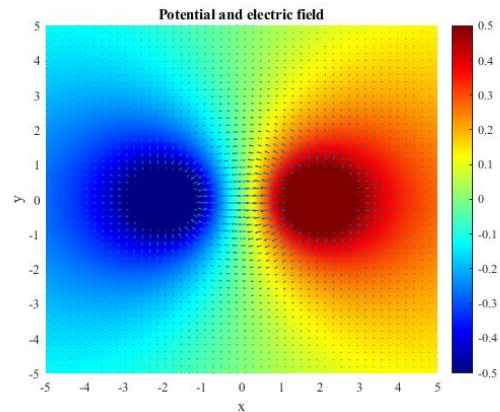


Figure 1: Potential and electric field created by two infinite cylinders at the cross section.

After having tested the code in 2D, we moved to the 3D space and began to work with triangle meshes, starting by a simple parallel plate capacitor. Matlab has its own function that carries out Delaunay triangulation, allowing the discretization of surfaces into triangles, that will play the role of the point charges used previously. Again, we want to compare the analytical capacitance and the approximated one:

$$\begin{aligned} C_{analytical} &= \frac{\epsilon A}{d} = 3.1824e - 09 \\ C_{numerical} &= \frac{1}{V} \sum_{n=1}^{N/2} a_n q_n = 3.3118e - 09 \end{aligned}$$

Having used the plate's surface $A=36$, the separation between plates (setted at $\pm V_o/2$) $d=0.1$, a_n the surface of each triangle (computed in the program) and $N/2=81$ the positive half of the charge vector q_n ; the error found was of 4.0660%. However, it can be reduced increasing N to the detriment of the computing time.

B. Quadrupole

The limiting condition when it comes to the potential is the Laplace equation:

$$\nabla^2 \phi(\vec{r}) = 0 \quad (13)$$

implying that the potential cannot have maxima or minima but only saddle points. However, with an adequate selection of the electrodes one could get a small variation of the potential around those saddle points, making them able to confine different ions, both anions and cations, since they would not get high accelerations. With the hyperbolic electrodes simulated in *Figure 2*, setting at negative potential $-V_o$ the ring and at positive potential $+V_o$ the upper and lower surfaces, one gets the quadrupole potential shown in *Figure 3*, calculated using (6), once the charge (*Figure 2*) is known. The central area is our region of interest.

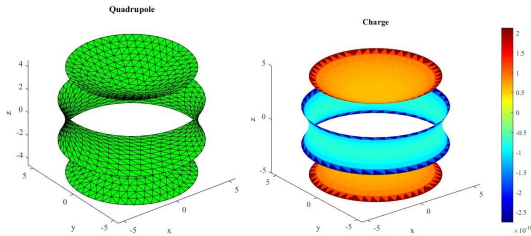


Figure 2: Quadrupole geometry discretized in a triangle mesh (left). Quadrupole charge for a voltage of 1V in the upper and lower electrodes, and -1V in the middle one (right).

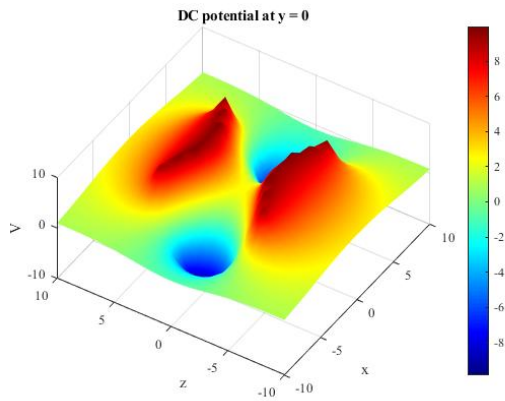


Figure 3: Potential created by the quadrupole in a longitudinal section, showing the saddle point at the center.

One has to be careful when discretizing the surface into a triangular mesh not to create any zero surface triangle. Otherwise it will cause the Z matrix to be singular, and therefore the linear system will not be possible to solve.

C. Trajectory

Once the charge in the electrodes is calculated, using a dense grid of points and interpolation, the potential at any point can be computed, and the electric field is obtained as

$$\vec{E} = -\vec{\nabla}V \quad (14)$$

Then the force is computed as

$$\vec{F} = q\vec{E} \quad (15)$$

and the trajectory is calculated using classic expressions:

$$\vec{F} = m\vec{a} \rightarrow \vec{a} = \frac{q\vec{E}}{m} \quad (16)$$

hence,

$$\vec{v} = v_o + \vec{a} \cdot \delta t \quad (17)$$

and finally

$$\vec{r} = r_o + \vec{v} \cdot \delta t + 0.5 \cdot \vec{a} \cdot \delta t^2 \quad (18)$$

As said before, the hyperbolic geometry of the electrodes gives an almost constant potential at the center (*Figure 4*), making the ions move slowly. However, this condition is not enough to confine them, since at a given moment they would approach the regions with increasing potential and they would escape speeding up. To solve this problem, a harmonic potential $V(t) = V_o \cos(\omega t)$ can be used. The potential frequency f has to be sufficient so the ion cannot escape but not too high so the ion would not be able to move. In other words, we need $T = 1/f \gg \delta t$ (in our particular case, $T = 20\delta t$). Another aspect to take into account is the amplitude V_o , responsible of giving the ion acceleration. Therefore there is a compromise in the selection of both the value of V_o and f when designing the trap.

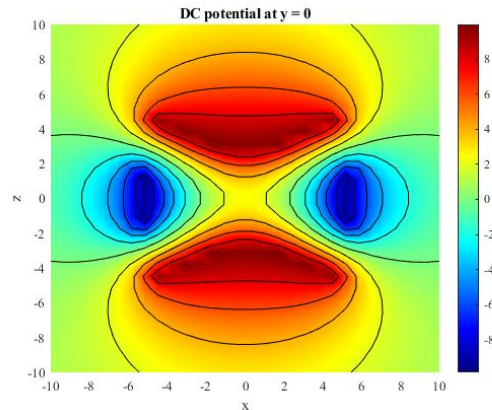


Figure 4: Potential created by the quadrupole in a longitudinal section.

IV. RESULTS

All in all, the trajectory followed by an ion is similar to the one illustrated in *Figure 5*, for Fe^{2+} with $V_o = 10V$ and $f = 900Hz$.

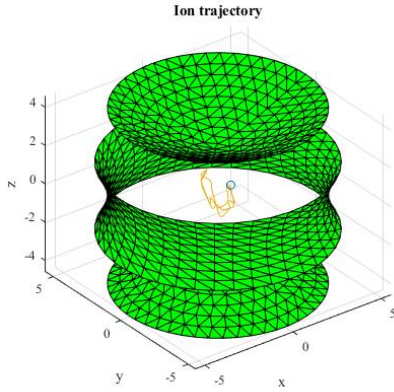


Figure 5: Trajectory of an ion inside the Paul trap computed using a random starting point in the region $x, y, z \in (-1,1)$.

For different ions, hence, for different masses and charges, the frequency and the V_o required vary. When it comes to the mass, increasing mass means less acceleration (16), thus less frequency or more amplitude V_o is needed. However, increasing charge means more acceleration, so one needs more frequency or less voltage. Therefore the ratio q/m is an interesting characteristic to take into account when designing the trap, and as such, *Figure 6* shows how V_o and f behave for different values of q/m . One can observe that the minimum f required increases as a function of m/q following the law $f_{min} = a\sqrt{m/q} + b$, while the voltage goes like $V_{max} = \frac{a}{m/q} + b$. The values represented in *Figure 6* are for cations; nonetheless, the same tendency can be deduced for anions, but with higher frequencies and lower voltages for the same mass; since given the geometry of the trap, there is less route in the vertical axis, and for the first semi-period the upper and lower electrodes are set up to positive potential, meaning that it is easier for negative

charges to gain acceleration and escape.

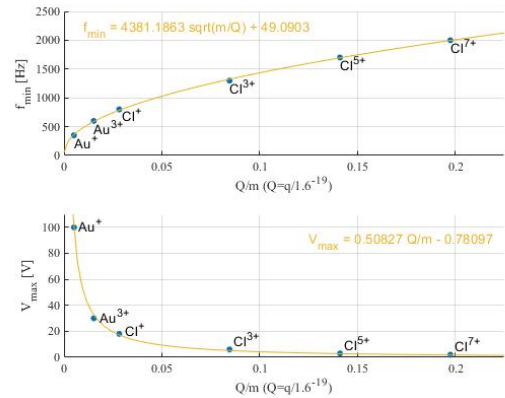


Figure 6: Voltage and frequency required to confine ions with different q/m ratios.

V. CONCLUSIONS

Apart from the satisfactory results of the simulations showing the trapped particles, this project is a first approach to numerical techniques used in physics and engineering in order to solve electrostatic problems. The work offered to us the opportunity not only to learn about the same Paul ion trap and its functioning, but to discover useful tools to solve systems of differential and integral equations numerically, and to discretize three dimensional surfaces into triangle meshes, process that is often used in such kind of problems.

VI. REFERENCES

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