Modelling and designing a Paul ion trap

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(Dated: June 4, 2021)

The present article consists in the modelling an design of a Paul ion trap using the Method of Moments for numerical integration. Firstly, we have developed some preliminary work with simple geometries in two and three dimensions. Then we have designed the geometry of the trap, consisting in two hiperboloid plates which have been discretized, triangulated, and solved by the Method of Moments. The potential in the plates has been set to vary harmonically, since sinusoidal signals have proved to be more effective than triangular and square signals. We have then simulated the confinement of one, two and multiple ions, and we have studied how the chosen frequency and potential affect the effectiveness of the trap. Our simulation code can be found in our Github repo.

I. INTRODUCTION

In 1989, physicist Wolfgang Paul received the Nobel prize together with Hans Dehmelt for creating a device capable of trapping charged particles. This device, known as the *Paul ion trap*, consists of two hyperbolic electrodes charged with oscillating potentials, creating an AC electric field in its interior. The trap has applications in a great number of areas including mass spectropy and quantum computing.

The aim of our paper is to model a Paul ion trap using MatLab, with the help of computational physics techniques such as the Method of Moments (MoM) [1] and the triangulation method of Delaunay [2], and simulate, and to simulate the confinement of several particles.

II. PRELIMINARY WORK

In order to gain insight into electrode simulation using MatLab and to validate the performance of the MoM, we proceed to design and test some capacitors in two and three dimensions. We compute the potential using the MoM and use the finite element method –already implemented in the MatLab function `gradient`– to sketch the electric field. Finally, we compare the derived capacity to the ideal one to check the validity of our results.

A. Two-dimensional geometry design

We start designing a planar and a cylindrical 2D capacitors. From [3], we know that the electrostatics integral equation in two dimensions can be expressed as

$$\frac{-1}{2\pi\varepsilon_0}\int_C q(\boldsymbol{\rho}')\ln(|\boldsymbol{\rho}-\boldsymbol{\rho}'|)\,d\boldsymbol{\rho}'\bigg|_C = V_0(\boldsymbol{\rho})$$

for any closed curve C. To find the charge distribution in each plate, we discretize them as a linear combination of pulse basis functions centered at the sites $\boldsymbol{\rho}_m$, with length h_m. Their respective charges q_m are given by a vector $[q]$, which can be found through the MoM. Indeed, it satisfies the linear system $[Z][q]=[b]$, where the elements of $[Z]$ and $[b]$ are given by

$$Z_{nm} = \begin{cases} -\frac{h_n}{2\pi\varepsilon_0}\ln(|\boldsymbol{\rho}_m-\boldsymbol{\rho}_n|) & \text{if } m\neq n \\ -\frac{h_m}{2\pi\varepsilon_0}\left[\ln\left(\frac{h_m}{2}\right)-1\right] & \text{if } m=n \end{cases}$$

and $b_m = V_0(\boldsymbol{\rho}_m)$, respectively. We proceed to solve this linear system by setting a fixed $V=\pm 0.5\,\mathrm{V}$ on the plates. Once the discrete charge distribution $[q]$ has been found, we can easily find the potential in each point of the plane, and take the gradient to find the electric field. The results of these simulations are plotted in figure 1.

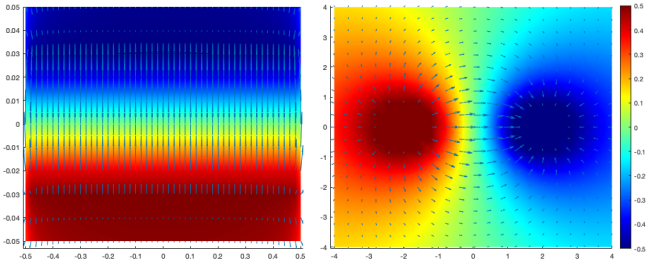

Figure 1. Magnitude of the potential (in V) and direction of the electric field, for the planar (left) and cylindrical (right) capacitors. The same color bar applies to both graphics.

The capacity of both capacitors can be experimentally calculated as $C_{exp} = \frac{1}{\Delta V}\sum h_m q_m$. For the planar capacitor we obtain

$$C_{ideal} = \varepsilon_0\frac{L}{d} \approx 177.08\text{ pF}, \quad C_{exp} = 195.04\text{ pF},$$

which leads to a relative error of $\varepsilon_r = 10,14\%$. However, since the ideal capacity formula refers to an infinite capacitor, we cannot conclude whether the largest source of error is the MoM or the finite geometry approximation. For the cylindrical capacitor we have

$$C_{ideal} = \frac{\pi\varepsilon_0}{\operatorname{acosh}\left(\frac{d}{R}\right)} \approx 21.121\text{ pF}, \quad C_{exp} = 21.148\text{ pF}$$

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In this case, there is no geometry approximation, so all discrepancies are due to the discretization method. But now $\varepsilon_r = 0,13\%$, so we conclude the MoM is a good approximation for this problem.

B. Three-dimensional geometry design

We now want to design a 3D planar capacitor, consisting of two parallel square plates of side $L = 1\,\text{m}$ and a separation of $d = 0.1\,\text{m}$. In the three-dimensional case, the electrostatics integral equation reads (see [3]):

$$\int_S q(\boldsymbol{r}')\frac{1}{4\pi\varepsilon_0|\boldsymbol{r}-\boldsymbol{r}'|}\,d\boldsymbol{r}'\Big|_S = V_0(\boldsymbol{r}).$$

Now the challenge is to discretize the capacitor surfaces. To this end, we use the MatLab function `delaunay`, that given a mesh of points from a surface returns a set of triangles along with their topology matrix, corresponding to a surface triangulation. With the help of the MoM and the function `int_S_1divR` documented in [4] to determine the matrix $[Z]$ of the linear system, we are able to find the charge distribution of the capacitor, as well as the potential and electric field (figure 2). We have set with $V = \pm 0.5\,\text{V}$ on the plates.

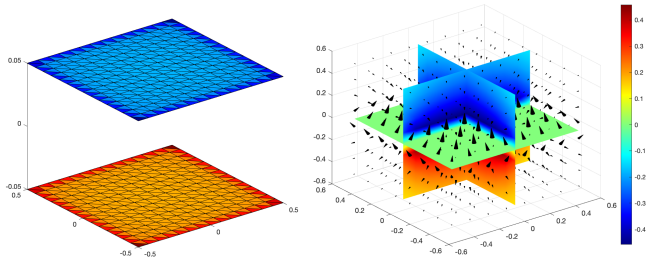

Figure 2. Left: Charged planar plates, triangulated using `delaunay` function. Right: potential along the axes' slices (in V), and electric field displayed using `coneplot` function.

We can now compute the discrepancy between the ideal and experimental capacity of this model:

$$C_{ideal} = \frac{\varepsilon_0 L^2}{d} \approx 88,540\ \text{pF}, \quad C_{exp} = 66,737\ \text{pF},$$

which leads to a relative error of $\varepsilon_r = 24,6\%$. This is a successful result, keeping in mind our conclusions of the 2D case: must of the error must come from the finite geometry approximation.

III. SIMULATION OF A PAUL ION TRAP

A. Geometry design

The Paul ion trap we will design consists in two hyperboloid plates which enclose a region in space for effective ion confinement. One plate consists in a two-sheet hyperboloid along the z axis, given implicitly by

$$2x^2 + 2y^2 - z^2 = -z_0^2,$$

with points taken from the disk $x^2 + y^2 < r_0^2$. The other plate is a one-sheet hyperboloid around the z axis, which is in turn given by

$$x^2 + y^2 - 2z^2 = r_0^2,$$

with points from the ring $r_0^2 < x^2 + y^2 < r_0^2 + 2z_0^2$. We take positive and negative values of z, and fix the geometry parameters to $r_0 = 1\,\text{m}$ and $z_0 = 0.3\,\text{m}$.

We thus proceed to discretize the surface of the plates and solve the MoM as done with the 3D planar capacitor. Once again, we set $V = \pm 0.5\,\text{V}$ in the hyperboloid plates. Figure 3 shows the resulting charge distribution and the potential and electric field it creates.

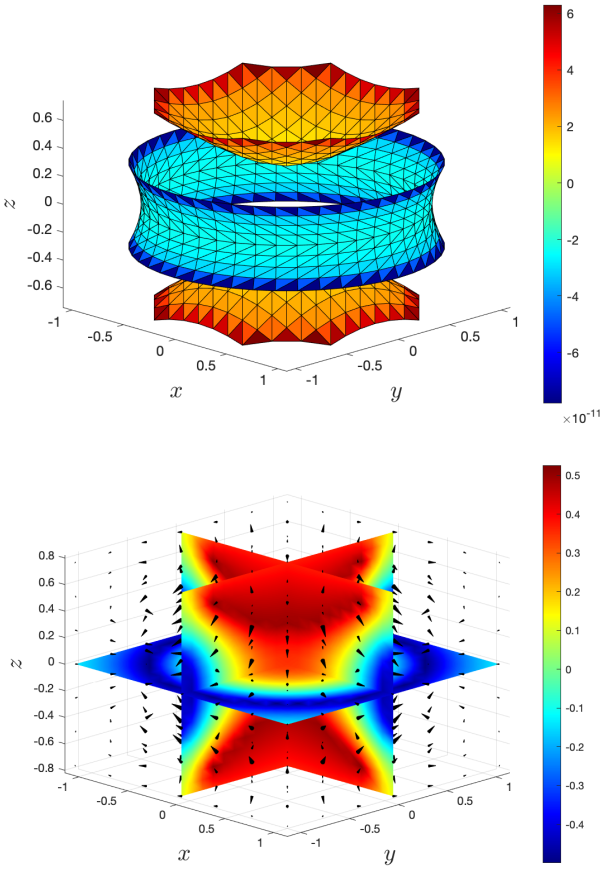

Figure 3. Top: charged hyperboloid plates of our Paul ion trap. The color shows the charge per unit surface on the plates, in units of $10^{-11}\,\text{C/m}^2$. Bottom: potential along the axes' slices (in V) and electric field, flowing from the positively charged plate to the negative one.

B. Single ion with DC potential

The first step towards testing our trap is to study the motion of a positively charged ion when placed at a random position near the center of the system. We fix the mass and the charge of the ion to be $m = 30\,\mathrm{u}$ and $q = +e$, respectively. The trajectory of the ion is obtained using Newton's equations of motion by computing its acceleration from the electric field, and assuming it remains constant for very short periods of time.

However, there are two ways to compute the electric field at the ion's instantaneous position. The most efficient option is to interpolate the electric field plotted in 3, but this would lead to precision errors due to both approximating the gradient of V and its subsequent interpolation. Instead, we choose a less efficient but more precise alternative: using the plate charge distribution to compute the resulting electric field, modelling each triangle in the plates by a point charge. Our implementation has been properly vectorized and has thus proved to be time efficient for our applications.

Our results show the positive ion moves towards the negatively charged plate, as expected. However, we are interested in knowing the average time T it takes for it to escape the trap. Figure 4 shows our results when running the simulation for different plate potentials V.

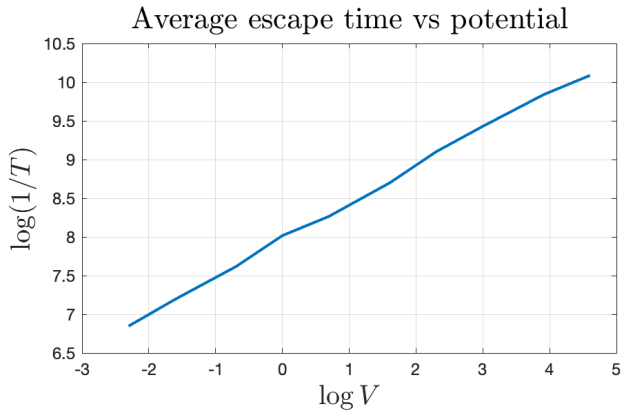

Figure 4. The average escape time T has obtained using 100 trials for each potential V supplied to the hyperbolic plates.

A linear regression using the `polyfit` MatLab function yields a slope of $m \approx 0.4889$ for the plot in figure 4. Moreover, it is reasonable to hypothesise the minimum threshold frequency needed to trap an ion using a periodic signal will be proportional to the inverse average escape time. Thus, we obtain the relation

$$f_{\min} \propto \sqrt{V}, \tag{1}$$

where the constant on proportionality depends on several factors such as the charge to mass ratio q/m and the geometrical parameters r_0 and z_0.

C. Single ion with AC potential

Once the ion trajectories have been tested with a fixed plate potential, these are set to periodically vary in order to perform our first ion confinement. Knowing the charge on the plates $[q]$ is proportional to V, it suffices to compute the charge with a fixed potential and then multiply it by our periodic signal. A logical pattern is observed when varying the frequency: for $f \ll 1/T$, the ion escapes the trap, whilst $f \gg 1/T$ leads to a successful trapping of the particle.

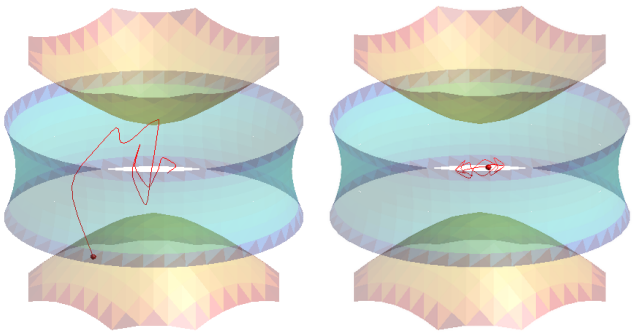

Figure 5. Ion trapping using a sinusoidal signal, at $f = 670\,\mathrm{Hz}$ (unsuccessful) and $f = 680\,\mathrm{Hz}$ (successful).

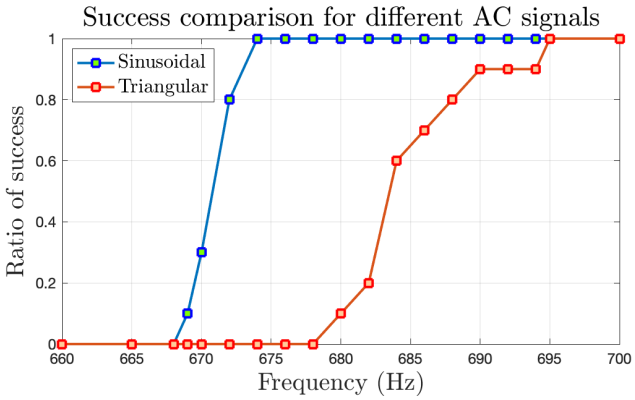

Figure 6. $N = 10$ trials per frequency have been performed. The minimum frequencies for the Paul trap at $V = 0.5\,\mathrm{V}$ are $f = 674\,\mathrm{Hz}$ for the sinusoidal potential and $f = 695\,\mathrm{Hz}$ for the triangular one. Their transition bandwidths are $\sim 5\,\mathrm{Hz}$, $20\,\mathrm{Hz}$ respectively.

Let $f_{\min} \propto \sqrt{V}$ be the threshold frequency at which the ion's trapping is first successful. Ideally $f_{\min}$ should be low, and also well defined (with a small transition bandwidth). We compare these aspects when the potential is varied using a sinusoidal, triangular or square signal. The latter has shown to be the worst at particle trapping, having a very high and undefined threshold frequency compared to the sinusoidal and triangular signals. These in turn show very similar behavior, although

the former is better in both aspects as shown in figure 6.

It is also interesting to mention that the relation $f_{\min} \propto \sqrt{V}$ shows to be extremely precise for the sinusoidal signal. The constant of proportionality can be computed with the data in figure 6, and predictions of the threshold frequency for different potentials are extremely accurate.

D. Increasing the number of ions

A simulation with two identical ions in the trap is performed by taking into account the electrostatic force acting between them. The confinement is shown to be successful above the same threshold frequency (see figure 7), since the interaction between the ions is negligible compared to the force due to the electrodes (with charges of $\sim 10^{-13}\,\mathrm{C} \sim 10^{6}e$). However, if the charge of the ions is increased (or the trap potential is reduced), their mutual interaction should have a greater impact.

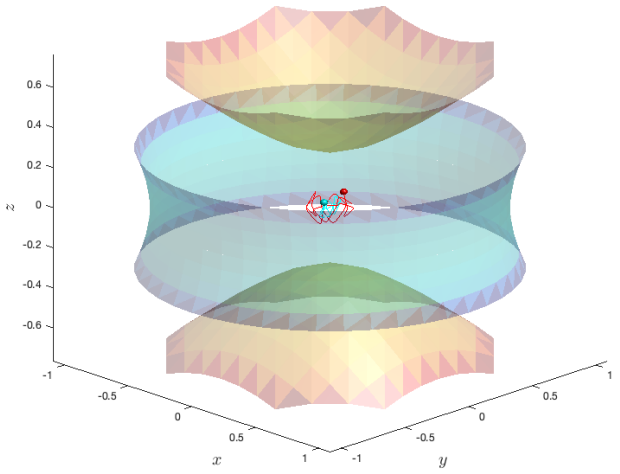

Figure 7. Two ions trapped using a sinusoidal potential, at $f = 672\,\mathrm{Hz}$. The threshold frequency remains the same.

Finally perform simulations with more than two ions in the trap. We are interested in studying the effect of ion interaction without altering the parameters of the single ion simulation, so we proceed to increase the charge of each ion by a certain scale factor factor with respect to the elementary charge $+e$, while reducing the potential on the surfaces by the same factor. This way, the interaction between the electrodes and the ions remains the same, and so does the expected working frequency. Of course, if the ions' charge is increased, so does the likelihood they overcome the confining potential due to the increase in electrostatic forces between them. Figure 8 shows the results for the the maximum charge scale factor for which all the ions are successfully trapped, varying the number of ions up to $N = 200$.

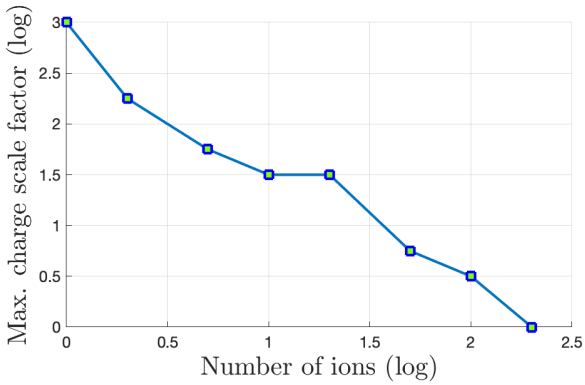

Figure 8. Maximum scale factor of ions charge for which a set of N ions remains confined into the trap, shown for up to $N = 200$ in a $\log - \log$ scale. The case $N = 1$ would admit arbitrarily large scale factors since there is no interaction between ions, but we only tested scale factors up to $k = 1000$.

As we expected, larger the number of trapped ions, the lower the charge they will need to escape it, since the resulting force on each ion is roughly proportional to the number of ions in the trap. The results in 8 have to be interpreted only from a qualitative point of view, since for a large number of particles the main reason why ions leak is due to numerical approximations. In fact, with a large number of ions, there is a non-negligible probability that two ions became so close that in the next time-step they are fired out of the trap.

IV. CONCLUSIONS

We have been able to successfully model and simulate single and multiple ion confinement using a Paul ion charged with hyperbolic plates. Optimal conditions have been achieved through a sinusoidal variation of the plates' potential, leading to a very well defined threshold frequency satisfying $f_{\min} \propto \sqrt{V}$.

Our simulation has been capable of determining the trajectory of more than $N = 200$ trapped ions. However, simulations with large values of N become too slow to compute. Alternative implementations for larger N include a higher level of code vectorization or using a linear interpolation of the field created by the plates.

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[4] S. M. Rao, A. W. Glisson, D. R. Wilton, and B. S. Vidula, Transactions on Antennas and Propagation **27** (1979).