Modelling and designing a Paul ion trap

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A Paul trap or quadrupole ion trap is a device designed to confine ions or charged particles in a given space. It consists of four electrodes that produce electric fields varying in time. The voltage applied to these electrodes varies harmonically with low frequency (quasi-static regime), which simplifies the model. The goal of this project is to numerically simulate in matlab a Paul trap and the motion of the ions trapped in it by discretizing the Poisson equation and applying the method of moments (MoM), first in 2D and then generalized to 3D.

I. MATHEMATICAL BASIS, MOM

The first step is to formulate the electromagnetic equations that rule our system. These are integral equations, that we can discretize using the MoM. This method transforms our equations into a linear system which we can solve to find the potential at every point in space.

We start with Poisson's equation

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

And Green's function that satisfies, in the 3D case

$$\nabla^2 G(\vec{r}) = -\delta(\vec{r}) \quad G = \frac{1}{4\pi\varepsilon|\vec{r}|}$$

And so we obtain an expression for the potential:

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

If we impose that the potential at a given surface must be a certain value (boundary conditions) we arrive to the following integral equation.

$$\int_S q\left(\vec{r}'\right)\frac{1}{4\pi\varepsilon\left|\vec{r}-\vec{r}'\right|}d\vec{r}'\Bigg|_S = V_0$$

In the 2D case, Green's function is

$$G = \frac{-1}{2\pi\varepsilon}\ln\rho$$

And the integral equation we obtain is

$$\frac{-1}{2\pi\varepsilon}\int_C q\left(\vec{\rho}'\right)\ln\left(\left|\vec{\rho}-\vec{\rho}'\right|\right)d\ell'\Bigg|_C = V_0$$

For our simulations we need to discretize the charged surfaces. To do this, we will create a triangles mesh with constant charge in the center of every triangle. Using the function meshgrid we can create a 2-dimensional grid, and then convert it into a 3-dimensional one by computing the z coordinate in function of the x and y ones. By this method we can obtain a vertex matrix, and then a topology matrix by using the delaunay function.

Now the method of moments allows us to transform the integral equation into a linear system. The unknown charge is now discretized and can be expressed as a linear combination of basis functions. The new unknowns will be the coefficients of this combination.

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

The potential then can be approximated by applying L, a linear operator, to this charge:

$$\mathcal{L}q_N(\vec{r}) = \sum_{n=1}^{N} q_n \mathcal{L}x_n(\vec{r}) \approx V_0(\vec{r})$$

To make this approximation as accurate as possible, we set to zero the inner products of the error by introducing a set of weighting functions Wm(r). By imposing

$$(w_{m_n}(\vec{r}), R(\vec{r})) = \langle \mathbf{w}_m(\vec{r}), V_0(\vec{r})\rangle - \sum_{n=1}^{\infty} q_n \langle w_m(\vec{r}), \mathcal{L}x_n(\vec{r})\rangle = 0$$

$$w_m(\vec{r}) = \delta(\vec{\rho}-\vec{\rho}_m)$$

We obtain the following linear system of equations[**1**]:

$$[Z][q] = [b] \begin{matrix} Z_{mn} = \mathcal{L}x_n(\vec{r})|_{\vec{r}=\vec{r}_m} \\ b_m = V_0(\vec{r}_m) \end{matrix}$$

Solving this system we obtain the coefficients q and thus the charge and the potential.

II. SIMULATION IN 2D

We simulated the potential that two circular plates would produce, one at 5V and the other at -5V, separated by a distance of 4 units and with a radius of 1. With this example we tested how the MoM can be used to calculate the potential created by a set of objects. We represented the potential obtained in the following figures:

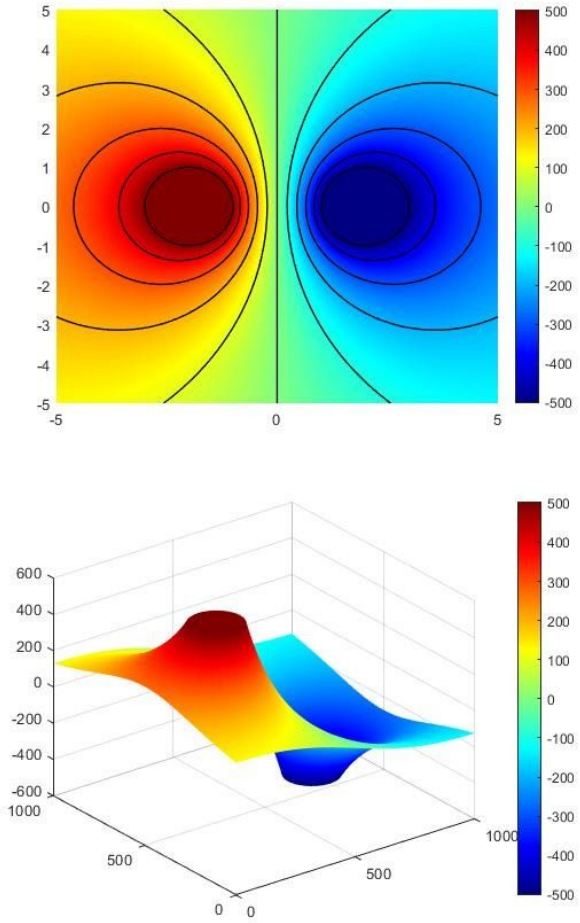

figure 1. Potential due to the circular plates.

The simulation is consistent with the expected result. We also computed the capacitance numerically, with the obtained discrete charges, and confirmed that it is almost equal to the theoretical capacitance (with a relative error of ~0.1%).

$$C = \frac{\pi\varepsilon}{\operatorname{arccosh}\left(\frac{d}{R}\right)} \approx \frac{1}{V}\sum_{n=1}^{N} h_n q_n$$

III. THE ION TRAP

Usually, Paul Ion Traps are designed using hyperbolically shaped poles instead of plane plates, spheres or any other different simpler surfaces. The reason behind this is that hyperboloid-like poles generate almost constant Electric Field at their centers, making the confinement of ions much easier. In fact, hyperboloids are the optimal shape for the design of the poles (it can be analytically proven but it is not the aim of the project).

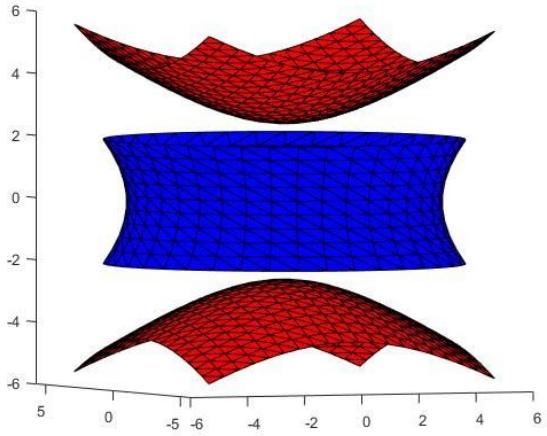

figure 2. Poles distribution of the Ion Trap.

In our case, we used the design shown in figure 1. The vertical poles in red are situated at z_0=+2.5 and z_0=-2.5, the blue pole has a minimum radius from the center r_0=5. With this information we can obtain their corresponding equations, which are used to discretise the surfaces:

$$Eq1. \qquad z = \pm\sqrt{(\tfrac{z_0}{2})^2 + 0.5r^2} \quad \text{(Vertical)}$$

$$Eq2. \qquad r = \sqrt{r_0{}^2 + 2z^2} \quad \text{(Horizontal)}$$

To keep the ions confined in the center, a harmonic potential of the form $V(t) = \sqrt{2}\cdot V_0 \cdot sin(2\pi f \cdot t)$ is applied at the poles. We can change the values of V_0 and f according to the type of ions we need to trap. In general, we would want to use a relatively low frequency in order to consider quasi-static regime. However it has to be taken into account that the lower the frequency is the more likely the ions are to escape, since we are headed to constant voltage. Another important factor to consider is that the applied voltage V_0 must be small enough because if the electric field is strong the particles are pulled to the poles faster than the time it takes to change the polarity.

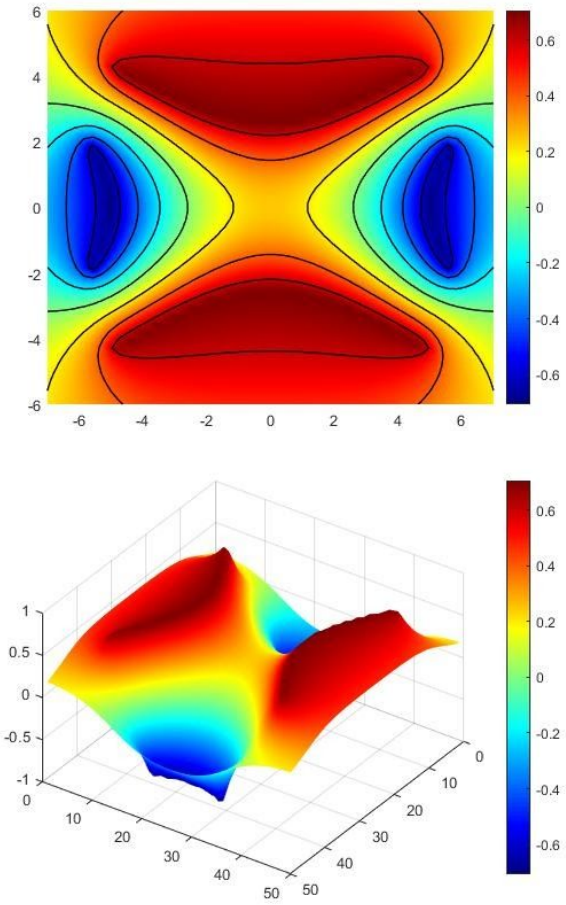

figure 3. Potential at y=0 plane for V(T/4)= $\sqrt{2}$.

For particles with a charge/mass ratio (R_{qm}) of 1, as protons, we found stability when using V_0 = 10 V and $f = 1500\,Hz$. Stability is preserved if lower voltage or higher frequencies are used; on the contrary, decreasing the frequency and raising the potential causes the ions to leave the trap.

It is possible to design a trap for any type of R_{qm} only varying the potential, this is due to the fact that:

$$a = \frac{F}{m} = \frac{qE}{m} = \frac{q}{m}E = R_{qm}(-\nabla V)$$

The potential in every point in space V is directly proportional to the voltage applied to the poles V(t) and consequently to V_0. If we found stability for R_{qm}= 1 and V_0 = 10 V, we need to keep constant the product $R_{qm}V_0$=10 obtaining the final relation:

$$V_0 = \frac{10}{R_{qm}}$$

IV. SIMULATION RESULTS

With the parameters of the trap already chosen, we can run a simulation of the movement of the ions, placing them near the center with zero initial velocity:

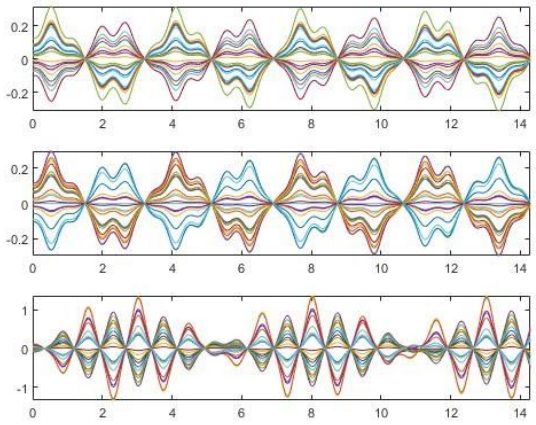

figure 4. x, y and z coordinates of confined ions over time [ms]

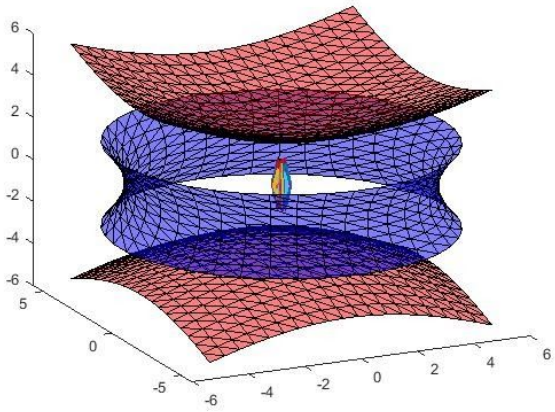

figure 5. Path described by the confined ions

As we see in both figure 4 and figure 5, when using the proper voltage and frequency the ions remain near the center of the trap following periodic movements. However, if the parameters of the trap are wrongly designed, such as an excessive potential or low frequency, we observe the following:

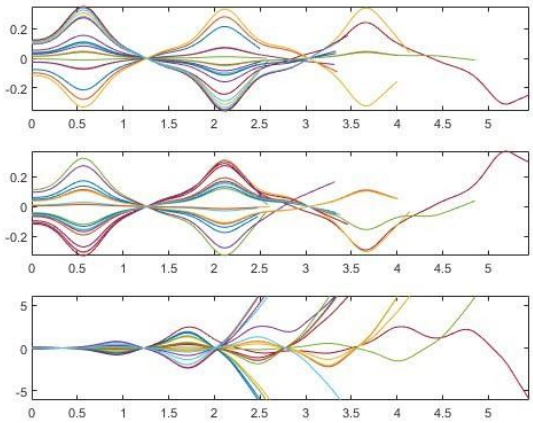

figure 4. x, y and z coordinates of not confined ions over time [ms]

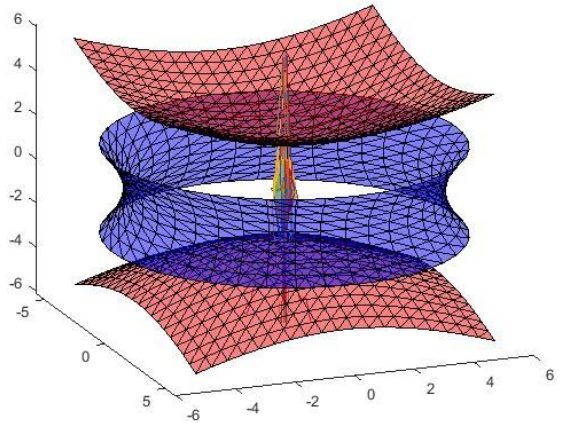

figure 5. Path described by the not confined ions

As seen in both figures 4 and 5, the ions escape the trap and are headed to the poles. In this precise case the used parameters were $V_0 = 12V$ and $f = 1400$ Hz.

V. CONCLUSIONS

With this project we show how one can use programming and numerical methods to understand and work on electromagnetic problems. We have successfully simulated a Paul ion trap, allowing us to freely experiment with the parameters to seek the optimal ones for a real ion trap.

VI. REFERENCES

[**1**] R. F. Harrington, Field Computation by Moment Methods. New York: Macmillan, 1968.

[**2**] Sadasiva M.Rao, Allen W.Glisson, Donald R.Wilton and B. Sarma Vidula, "A Simple Numerical Solution Procedure for Statics Problems Involving Arbitrary-Shaped Surfaces".