Modelling and Design of a Paul Ion Trap

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A Paul ion trap is a device designed to confine charged particles in a small region of uniform, dynamic quadrupole potential. The aim of this project is to simulate numerically the distribution of charges and the potential generated by our electrodes using the method of moments (MoM), and to predict the trajectory of the confined ions when the electrodes are subject to a harmonic potential. Starting with simpler models in 2D and 3D, we provide the optimal design parameters needed for the trap to work, depending on the number and properties of the ions and the quadrupole potential. We also provide different numerical mechanisms aimed at reducing the computational cost of the simulation.

I. INTRODUCTION

If a distribution of electrodes in space is aimed to be used as an ion trap, the potential generated by them must have an almost uniform value in a sufficiently broad region in which the ions will be placed. This will be achieved when considering a symmetrical disposition of 4 electrodes at symmetrically opposite voltage, which will generate a quadrupole-type potential in space consisting in a small almost uniform region which at the same time behaves as a saddle point. If we make the potential vary harmonically with time, with a proper amplitude and frequency, the ions will not have time to reach the valley and they keep turning around inside the trap.

II. THE METHOD OF MOMENTS (MOM)

This is a method which is commonly used to solve Poisson's differential equation in a discretized numerical environment [1]. This equation, which associates the potential in all space created by a certain distribution of charges, will be used in the two directions. First of all, we will fix the potential in the electrodes, which will be discretized by triangularization using *delaunay*'s method, and we will find out the distribution of punctual charges (located at the center of the triangles) generated by our potential. After that, we will use the equation again to compute the potential in all space generated by the former charge distribution, in this case discretizing our region with a simple rectangular mesh.

Poisson's equation reads:

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

where $\phi(\vec{r})$ is the potential in space and $q(\vec{r})$ is the charge density of the object. The Green's function associated with Poisson's in 3D is:

$$G = \frac{1}{4\pi\varepsilon|\vec{r}|} \tag{2}$$

which leads to the following convolution integral:

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

As stated previously, in order to calculate the distribution of charges in the electrodes, we must fix their potential V_0 as a boundary condition: $\phi(\vec{r})\big|_S = V_0$. We finally obtain the integral equation that we will solve with MoM:

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

As we will be testing our method with simpler cases, we also need the expressions for a 2D space:

$$G = \frac{-1}{2\pi\varepsilon} \ln \rho \tag{5}$$

$$V_0 = \frac{-1}{2\pi\varepsilon} \int_S q(\vec{\rho'}) \ln(|\vec{\rho} - \vec{\rho'}|) d\vec{l'}\big|_C \tag{6}$$

The method of moments (MoM) is based on the fact that the integral equation is linear and, therefore, it can be expressed as a linear operator $\mathcal{L}$ acting on the scalar field $q(\vec{r})$. If we expand the scalar field $q(\vec{r})$ in a space of N basis functions $x_n(\vec{r})$ with real coefficients q_n, we can use the linearity of the operator as follows:

$$\mathcal{L}q_N(\vec{r}) = \sum_{n=1}^{N} q_n \mathcal{L}x_n(\vec{r}) \approx V_0(\vec{r}) \tag{7}$$

The best approximation is the one with the sum equal to the potential. A function residual error, which is the potential minus the sum, is multiplied in an inner product by a set of weighting functions $w_m(\vec{r})$, and the result must be 0. The chosen weights are (point-matching):

$$w_m(\vec{r}) = \delta(\vec{\rho} - \vec{\rho_m}) \tag{8}$$

Finally, this results in a linear matrix system:

$$[Z][q] = [b] \Rightarrow Z_{mn} = \mathcal{L}x_n(\vec{r}) \,|_{\vec{r}=\vec{r}_m}, b_m = V_0(\vec{r}_m) \tag{9}$$

For the 2D case, the elements of $[Z]$ can be found by point-matching and one-point integration where $[q]$ will

be the height of each step $h_n = 1$.

$$Z_{mn} = \frac{-h_n}{2\pi\varepsilon} \ln(|\vec{\rho_m} - \vec{\rho_n}|), Z_{mm} = \frac{-h_m}{2\pi\varepsilon} \left[\ln \frac{h_m}{2} - 1 \right] \quad (10)$$

In the case of 3D geometry, a Matlab function `int_S_1divR().m` developed by E. Úbeda (UPC) [2] returns a row of $[Z]$ for a point corresponding to a center of a triangle of the mesh, thus solving the integral

$$\int_{S_{T_n}} \frac{1}{|\vec{r_m} - \vec{r'}|} d\vec{r'} \quad (11)$$

III. SIMPLER MODELS

Prior to the modelling of the trap, the geometry discretization and the MoM methods were tested in 2D and 3D capacitors, for which we have an analytical expression for the capacitance to compare with, remembering that its validity in the parallel case is restricted to $d \ll L$. The numerical capacitance can be calculated as:

$$C = \frac{Q}{V} = \frac{1}{V_0} \sum_{n=1}^{N} h_n q_n \quad (12)$$

A. 2D capacitors: parallel-plate and circular

This model allowed us to validate the implementation of the MoM in a case where the geometry was a simple line of charge.
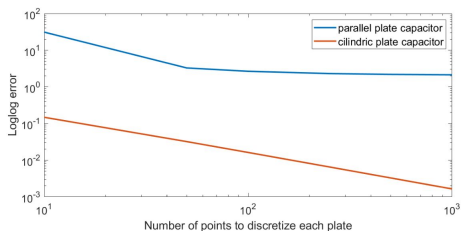

FIG. 1: Loglog error between analytical and numerical capacitance as the number of basis functions N is increased.

It is interesting to observe that for the circular capacitor the error decreases linearly in the logarithmic scale, but for the parallel plate the error becomes stagnant due to the analytical formula being an approximation that would only yield the exact result in an infinitely large parallel plate capacitor.

B. 3D parallel-plate capacitor

This model allowed us to learn how to properly use *delaunay*'s function to discretize a given geometry. In this case, given the plates' uniformity, they were discretized as a rectangular mesh in XY plane, which then we projected at two different Z heights (to account for the 2 plates) where *delaunay* function constructed the topology and vertex matrices corresponding to the triangular mesh.

By using $V_0 = 3$ and a distance between plates of $L/250$, where L is the dimension of the plate, we got $C_{analytical} = 1.6594 \times 10^{-8}F$ while $C_{numerical} = 1.6646 \times 10^{-8}F$. Results were acceptable and the error rate decreased with N until it came to a halt, as in the 2D parallel-plate case.

IV. QUADRUPOLE ION TRAP

A. Discretization of the geometry

In this case, since the electrodes are symmetrical by revolution around the Z axis, we decided to build circumferences of increasing radius on the XY plane and then projecting them on the Z coordinate according to the given hyperbolic equation. The radius of the circles were not arbitrary but they were calculated using a Newton's method imposing the area of the triangles to be equal and then obtain a uniform discretization of the charge.
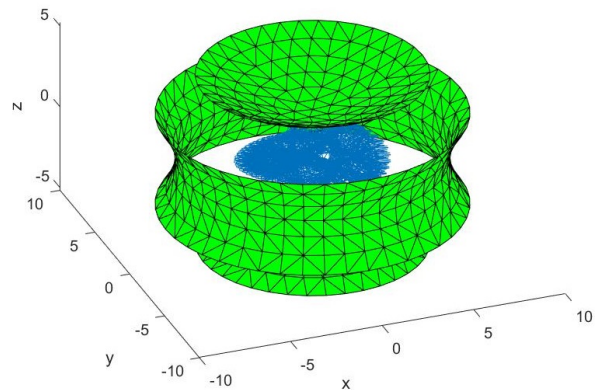

FIG. 2: Geometry of the electrodes and trajectory of a cation Au^{3+} for $T = 10s$. The top/bottom electrodes have their initial height at $z_0 = 3$, and the lateral one is set with a radius of $R_0 = 7$. The trajectory calculation will be addressed later on.

B. Computational cost concerns

Given the three-dimensionality of our problem, the computation of the solution of the integral equation is very costly, since N_s^3 operations must be performed for each of our N charges. This becomes a major issue when calculating the trajectory of the ions, for that we need the value of the electric field at the position of the particle at
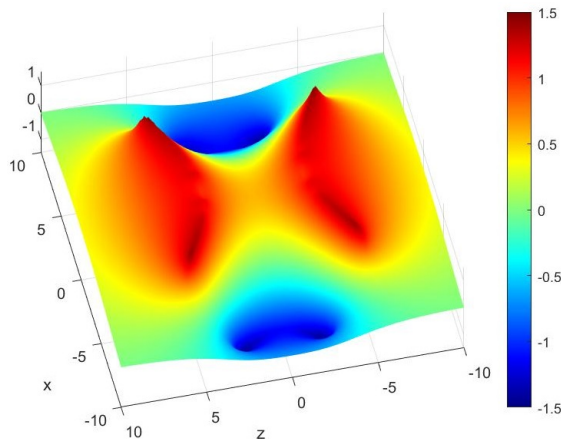
FIG. 3: Potential created by the hyperbolic quadrupole at y=0 plane with $N_s = 100$ and $V_0 = 3$. We can clearly see that the central region constitutes a saddle point with a slightly-varying potential.

every instant of time, being the time steps of the order of 1×10^{-4} second for the UARM approximation to work. The little displacement of the particle from step to step makes it necessary to have a sufficiently fine electric field discretization, which is only possible if the N_s value is unassumingly high, despite the fact that we can reduce our space to that in which we assume the particles are going to move.

Two principal strategies were used to solve this:

(1) The operator that we are discretizing is linear, and in this project we are assuming that any distance d in our parcel satisfies $d \ll \lambda$, which means that any modulation on the voltage in the electrodes will apply immediately in the whole space. In other words, it is possible to obtain the same results by computing the potential in space $\mathbb{V}$ only once, for $V_0 = 1$, and then apply any modulation in magnitude or shape at every instant of time in the moment of calculating the trajectories:

$$\mathbb{V}(t) = V_{mod} \cdot sin(\omega t) \cdot \mathbb{V}_{V_0 = 1}$$

This correction makes computational cost decrease dramatically, and it also helps us to increase N_s: we run the code just once and keep the results for future simulations.

(2) Even though a fine mesh of potential can be calculated and stored in the computer, the kinematics of the particles require of an even more precise value of the field acting on the particle at every instant of time. The solution to this problem is provided by *interp3* function, which approximates the potential in the position of the particle by interpolating the values at the nodes of the mesh. Even though this is a precise method, it turns out to be so costly. Our alternative consists in a weighted average of the field in the 64 nodes (better than 8) that surround our particle at every instant. Then, the modulation can be applied only to the interpolated value, and the method itself is much faster than *interp3* without a

big loss on precision. The results given here, however, correspond to those obtained by the *interp3* method.

C. Trajectories of the particles

With the proper corrections discussed in the previous section, we can calculate the trajectories of multiple ions during a relatively long time window, that we have set to be $T = 10s$, working with a stored potential in a space of 100^3 nodes.

We will work with an UARM approximation using a time step of $\Delta t = 1 \times 10^{-4}$ s. The force acting on the particles is:

$$\vec{F}_{el} = q \cdot \vec{E} \quad \text{with} \quad \vec{E} = -\vec{\nabla} V \tag{13}$$

$$\vec{F}_{int} = \sum_{i,j,i \neq j} \vec{F}_{ij} = \sum_{i,j,i \neq j} k \frac{q^2}{|r_i - r_j|^3} \vec{r}_{ji} \tag{14}$$

And then, the motion of the particle is described by the equation: $\vec{F} = \vec{F}_{el} + \vec{F}_{int} = m \cdot \vec{a}$.

With regard to the particles used in the simulation, we have decided to work only with the Au^{3+} cation, rather than considering the factor q/m as another degree of freedom. The reason for this is that previous projects have gone in this direction, and we find it more useful to explore the necessary conditions that will allow a major number of particles confined. It is in the technological implementations of the Paul trap that we are interested, and these implementations, such as the confinement of qbits in quantum computers [4] or the mass spectroscopy devices [5], require a number of the order of $10 - 10^2$ ions confined.

First of all, we will consider the trajectory described by only one particle with electrodes subject to a given harmonic potential. In this simple case we are only interested in the shape of the position components, as they must show a periodic permanent regime for the ion to be confined. We see however three different frequencies modulating the behaviour of the particle: the frequency of the harmonic potential in the plates, which is reflected in a little jiggling in the trajectories, the frequency of oscillation of the components, which is much smaller than the first and that reflects the symmetry of the problem (X and Y are equal, Z different), and the smallest and most surprising one, corresponding to the modulation of the maximum values of the components when the time interval is sufficiently long. This behaviour has been reproduced for a much longer time interval, and it is consistent with respect to changes of the initial conditions.

Finally, we will proceed to study the limit cases of confinement for a given ω and V_0 using proper random initial conditions for a given number of particles. We are interested in finding the minimum frequencies so that they don't escape. These results, which in fact correspond to the upper-bound approximation of the ω_{min} (there can be a slightly lower available frequencies, but with this value it will never diverge), can be seen in Table 5a.
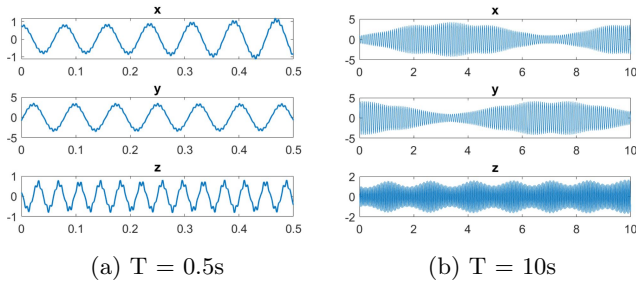
(a) T = 0.5s (b) T = 10s

FIG. 4: Behaviour of the position components of one particle subject to $V_0 = 10$, $w = 1050$. In (a) we see that the shape of the oscillations coincides with the results presented by G. Werth in [3]. In (b) we appreciate the permanent regime accomplished by the particle in our time window.
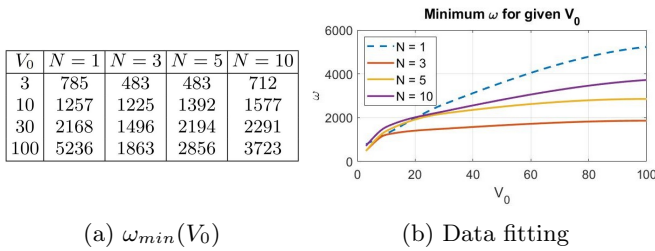

V_0	$N=1$	$N=3$	$N=5$	$N=10$
3	785	483	483	712
10	1257	1225	1392	1577
30	2168	1496	2194	2291
100	5236	1863	2856	3723

(a) $\omega_{min}(V_0)$ (b) Data fitting

FIG. 5: Upper-bound approximation of ω_{min}.

Through an interpolation, the profiles look like in Figure 5b. We observe that higher initial potentials require higher frequencies to confine the particles. Not only that, but these values also increase when there are more particles. This happens because not only the plates interact with the particles, but also the particles with themselves. In this case, for $N = 1$, initial conditions are different to the others and this behavior is not visible.

V. CONCLUSIONS

The first aspect that shall be considered in the conclusions of this project is the validity of the results provided. **In all simulations presented we have considered as initial conditions for position and velocity of the particles random values of the order of the ones which have been shown to display un**der these conditions. That is, we try to make our study independent of absolute time, only considering a certain time window of the particles inside the trap. If we manage to maintain a permanent regime behaviour in our sufficiently long time window, it is reasonable to assume that this behaviour will be maintained for any time window, and therefore that we can assure that the ions will be confined.

The ω_{min} that we provide as a conclusion of this project can be found in Table 5a, and they can be reproduced using our Matlab code for any given parameters, and also for different number and type of ions.

Regarding our first experience in computational electromagnetism, we shall say that this has been an inspiring but demanding project since we have had to reject most of our strategies aimed at solving the many problems that we faced along these five weeks. There were many aspects that could suppose a malfunctioning of the code and therefore lead us to incorrect results, and we have been aware of the importance of optimization and cost reduction for the first time. It has been, however, a great opportunity for learning numerous programming skills, which are of great utility for the computational resolution of physical problems, especially regarding spatial discretization of operators and the scalar and vectorial fields which they operate.
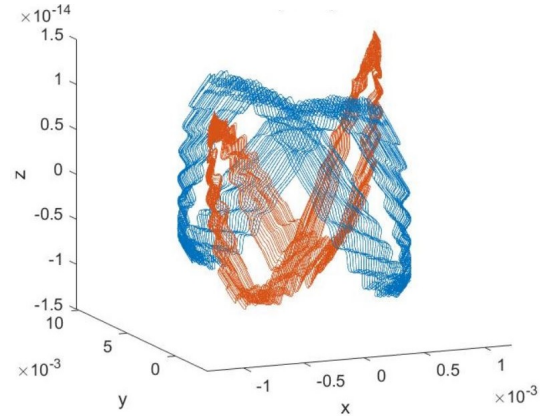

FIG. 6: Trajectory of 2 particles subject to $V_0 = 5$ and $\omega = 1256$ with a simulation time of $T = 1s$. The shapes obtained coincide with those presented by Raymond E. March in [5].

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