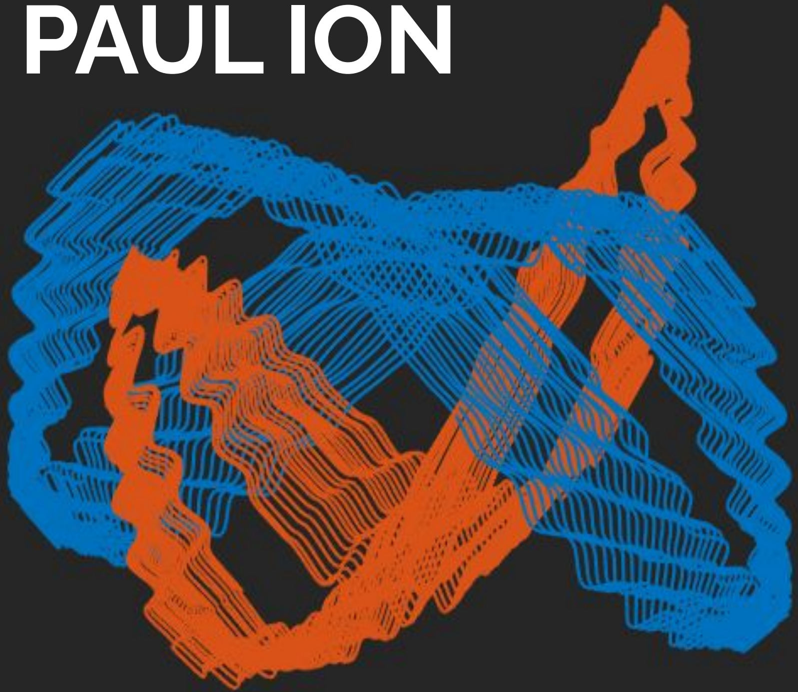
MODELLING AND DESIGN OF A PAUL ION TRAP

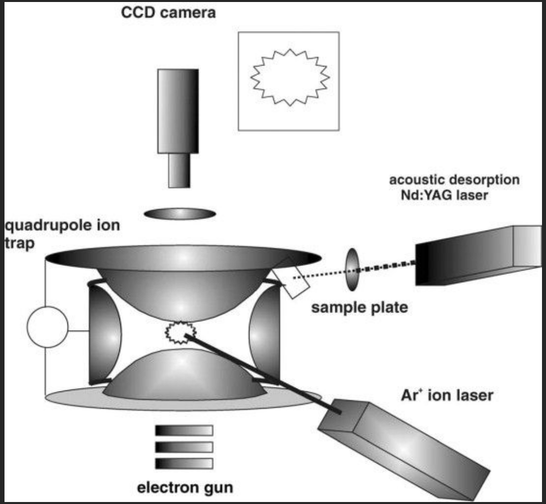


PEF2, 2nd Term, 2020-2021

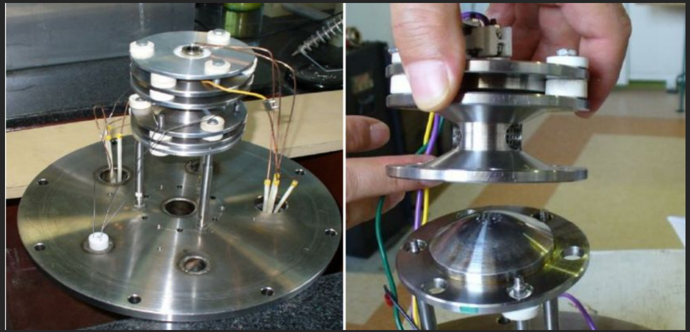
Raúl Adell Segarra, Francesc Xavier Capella Guardià, Víctor Jiménez Rodríguez

INTRODUCTION

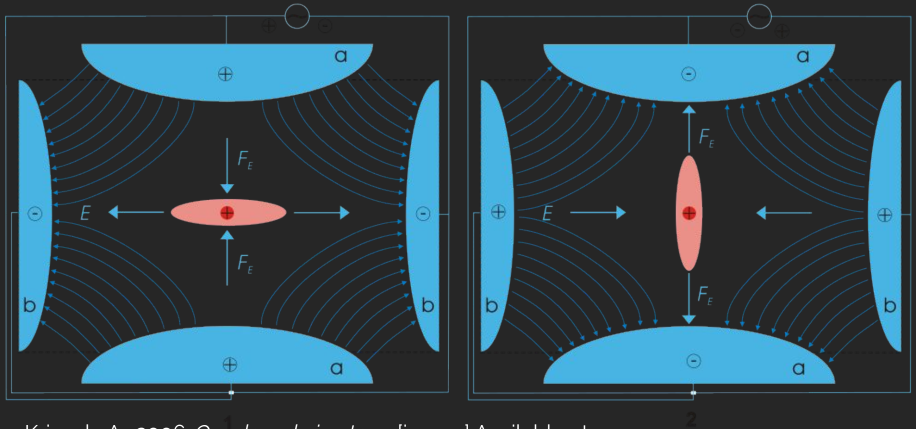
Wolfgang Paul, 1989



Schermann, J., 2008. *Optical detection of particles*. [image] Available at: <https://www.sciencedirect.com/topics/chemistry/paul-trap> [Accessed 19 June 2021].

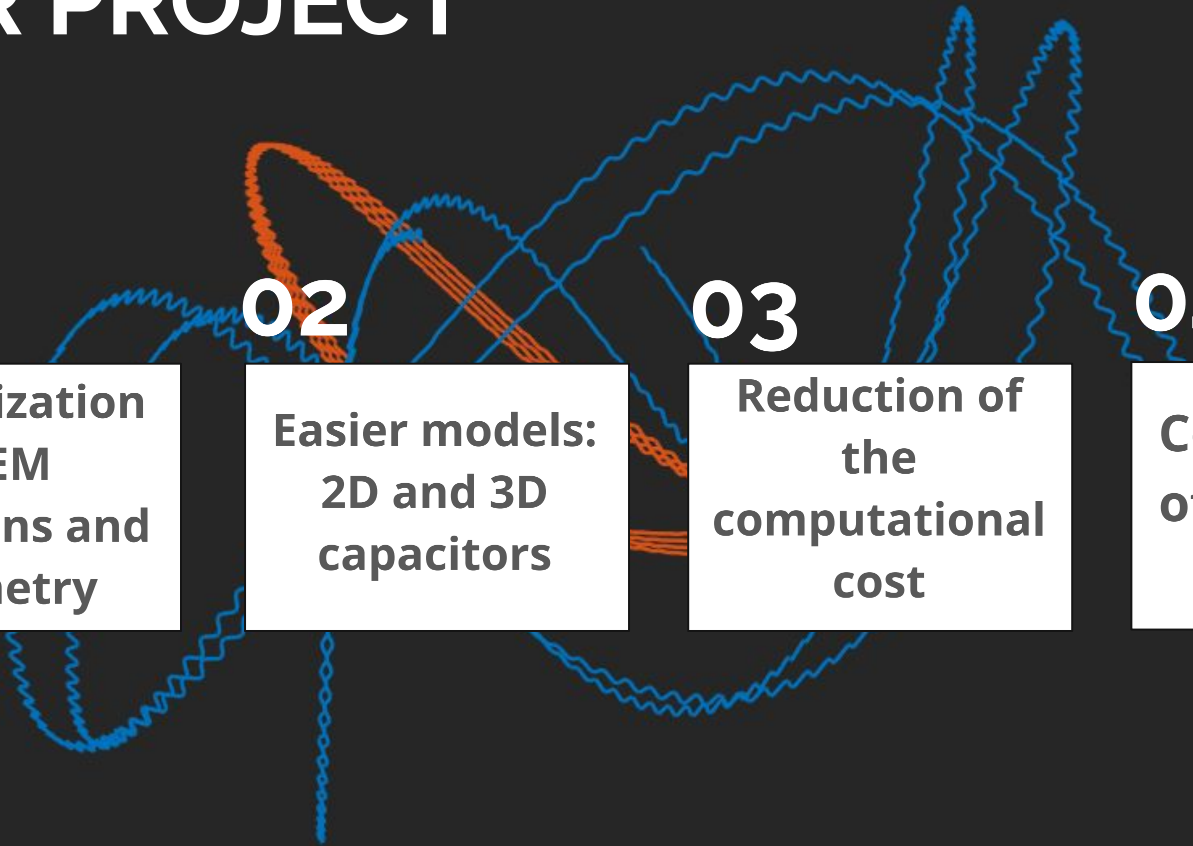


Sadat Kiai, S., 2010. *Paul Ion Trap*. [image] Available at: <https://www.researchgate.net/figure/Photos-of-Paul-ion-trap_fig1_225511033> [Accessed 19 June 2021].



Kriesch, A., 2006. *Quadrupole ion trap*. [image] Available at: <https://de.wikipedia.org/wiki/Benutzer:Akriesch#/media/Datei:Paul-Trap.svg> [Accessed 19 June 2021].

OUR PROJECT



01

Discretization of EM equations and geometry

02

Easier models: 2D and 3D capacitors

03

Reduction of the computational cost

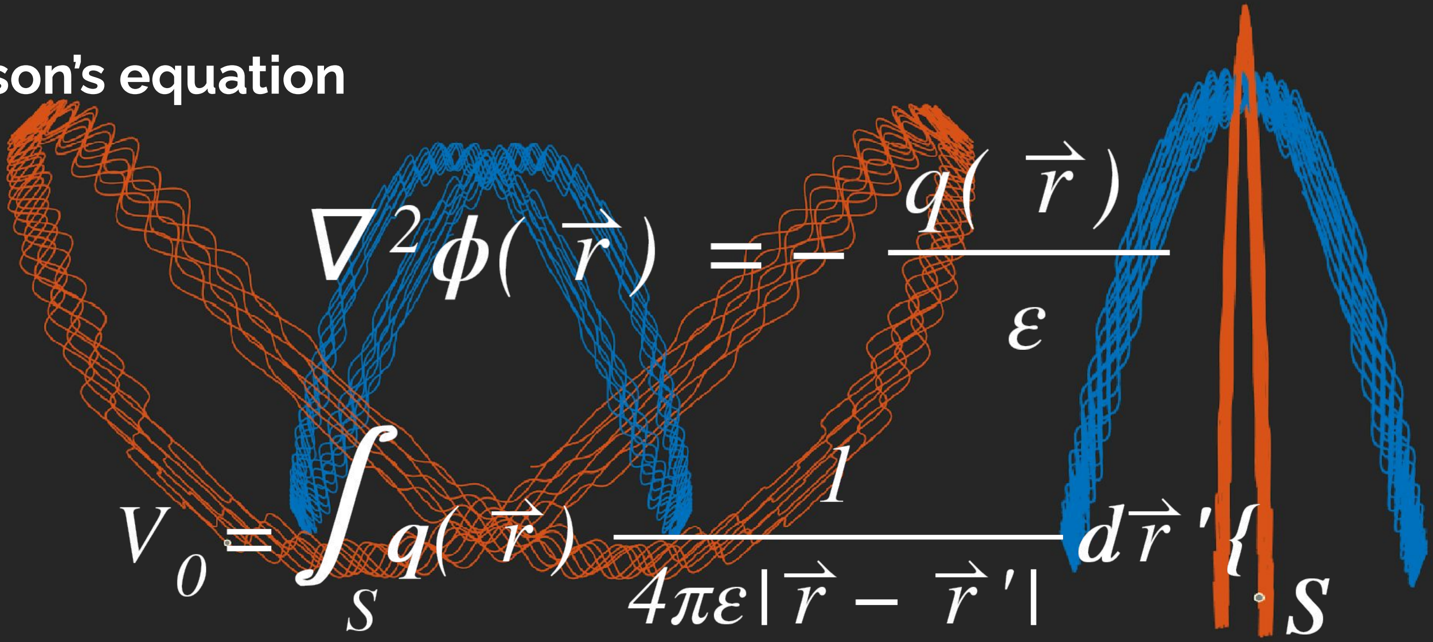
04

Confinement of ions in the trap

w = 3.1416e+03 V_{01}= (7.818, 0.759, 3.997e-14) V_{02}= (-8.195, -1.636,-5.276e-14)

MATHEMATICAL INSIGHT

Poisson's equation



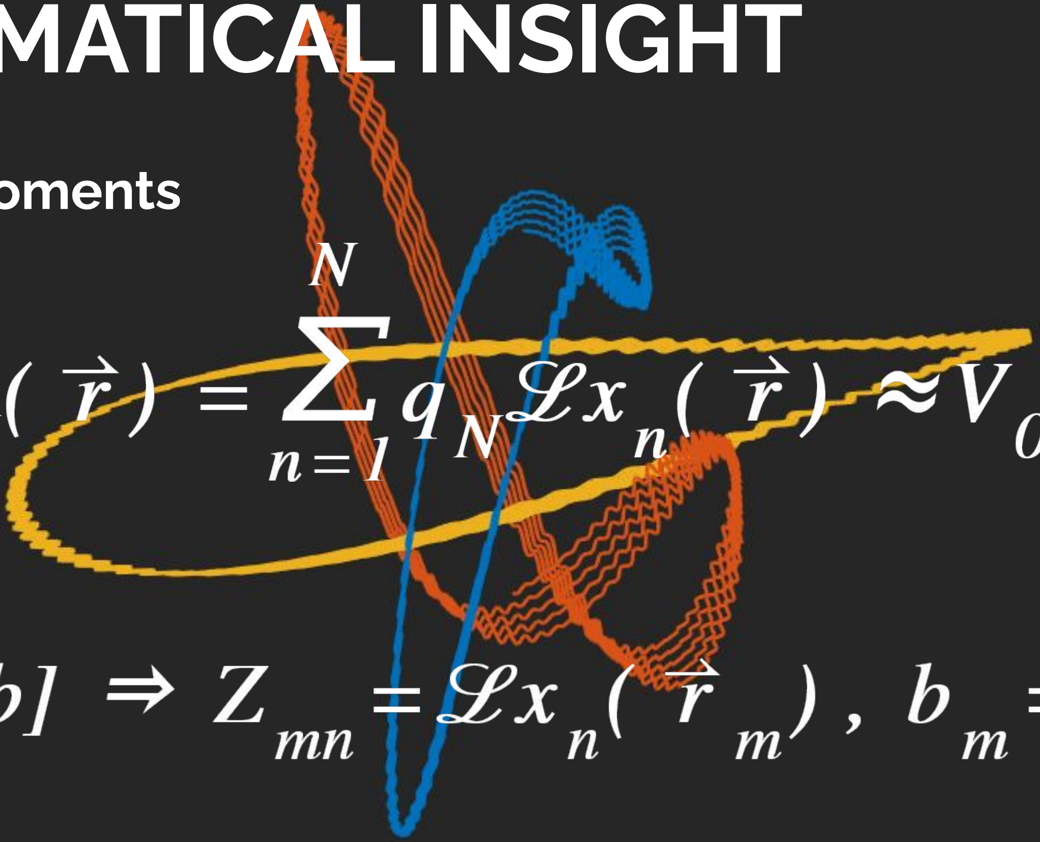
$$\nabla^2 \phi(\vec{r}) = -\frac{q(\vec{r})}{\varepsilon}$$

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

w = 1.7453e+03 V_{01}= (3.897, 1.933, 4.039e-14) V_{02}= (-7.649, -6.902, -1.195e-14)

MATHEMATICAL INSIGHT

Method of Moments



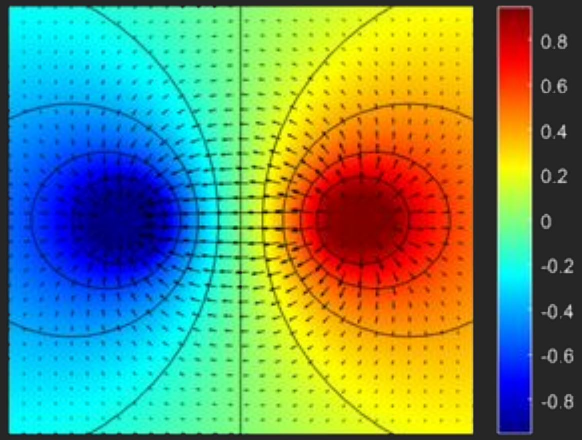
$$\mathscr{L} q_N(\vec{r}) = \sum_{n=1}^{N} q_N \mathscr{L} x_n(\vec{r}) \approx V_0(\vec{r})$$

$$[Z][q] = [b] \;\Rightarrow\; Z_{mn} = \mathscr{L} x_n(\vec{r}_m)\,,\; b_m = V_0(\vec{r}_m)$$

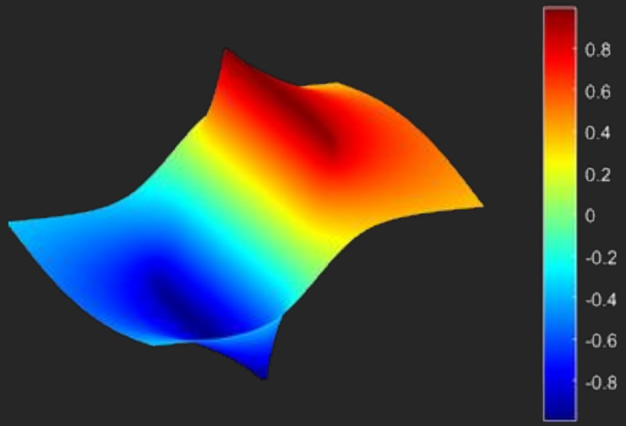
$w = 2.6180e{+}03$ $V_{01} = (2.935, 0.830, 3.012e{-}14)$ $V_{02} = (-1.558, -2.711, -3.414e{-}14)$ $V_{03} = (-6.463, 2.151, -1.848e{-}14)$

GEOMETRIES AND POTENTIALS

Capacitors

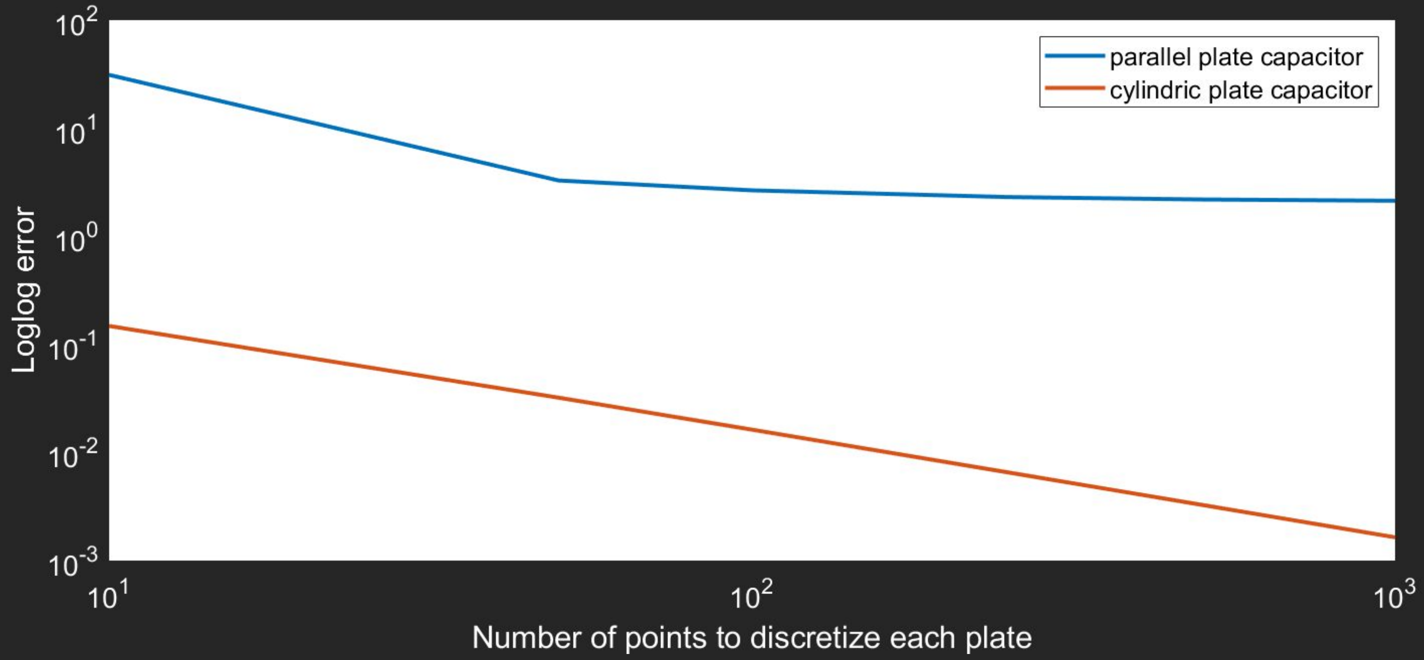


Circular



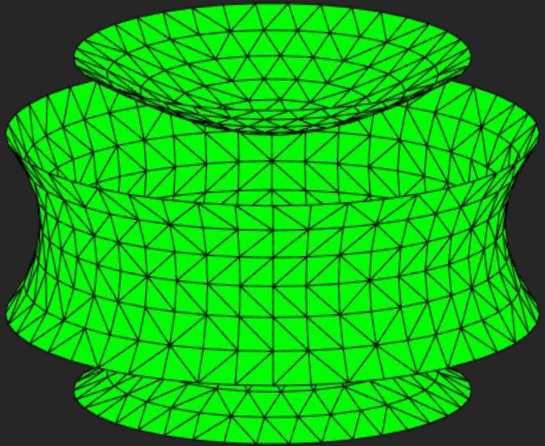
Parallel-plate

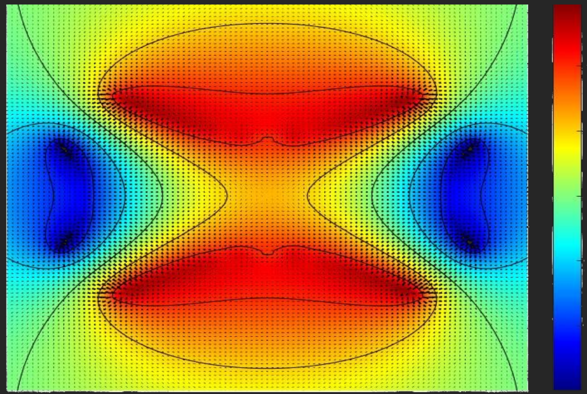
GEOMETRIES AND POTENTIALS

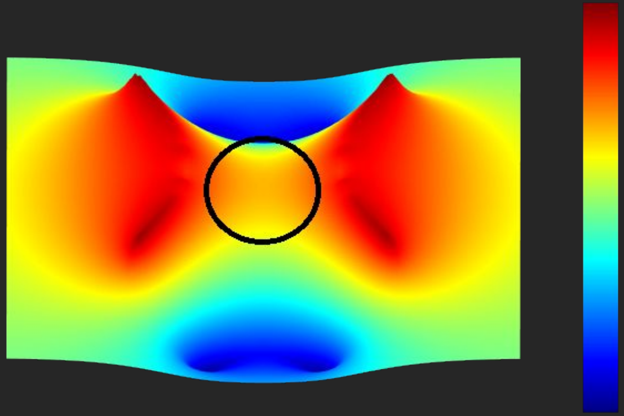


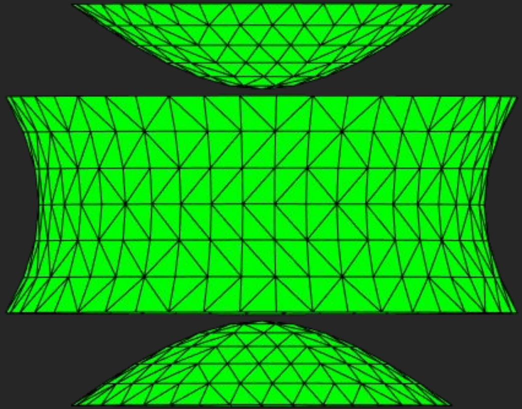
GEOMETRIES AND POTENTIALS

Quadruple trap





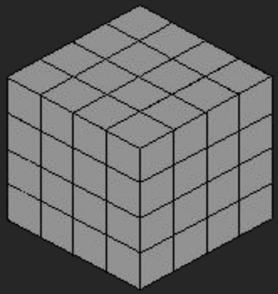




COMPUTATIONAL COST CONCERNS

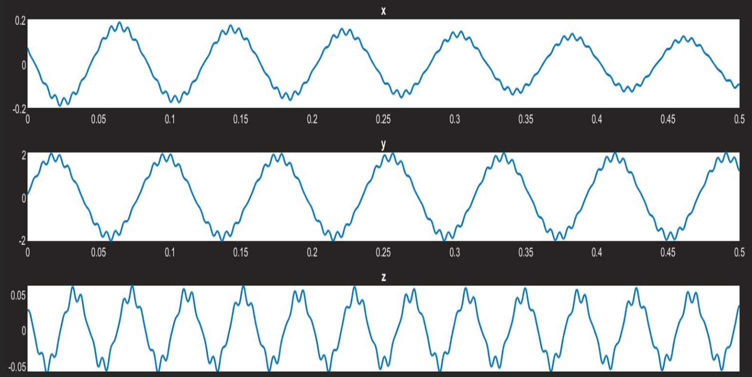
$$\mathbb{V}(t) = V_{mod} \cdot sin(\omega t) \cdot \mathbb{V}_{V_0 = 1}$$

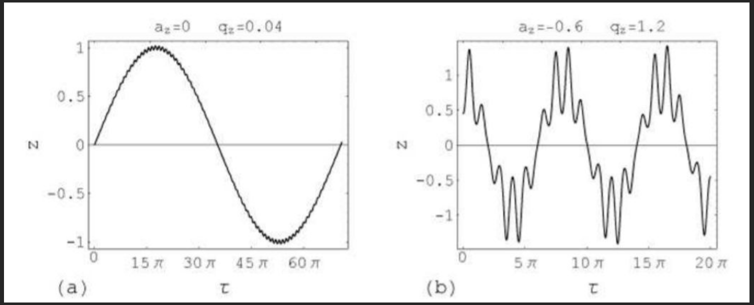
Distribution of potential in all space for V=1



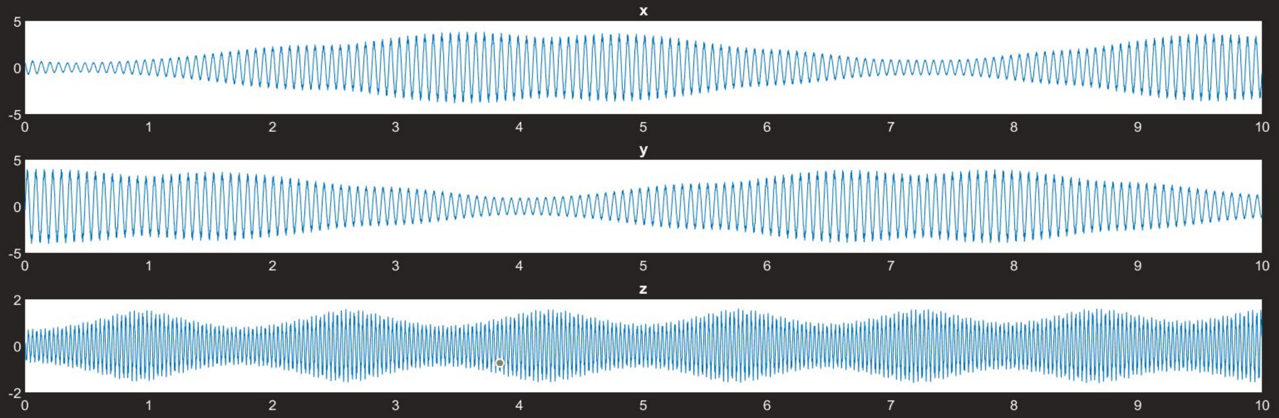
Vertex: grid point
64 nearest neighbours

TRAJECTORIES

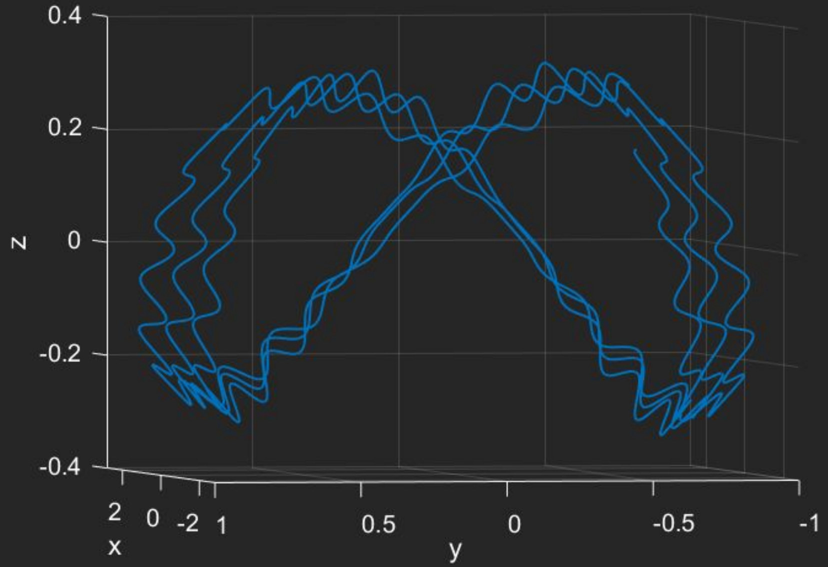




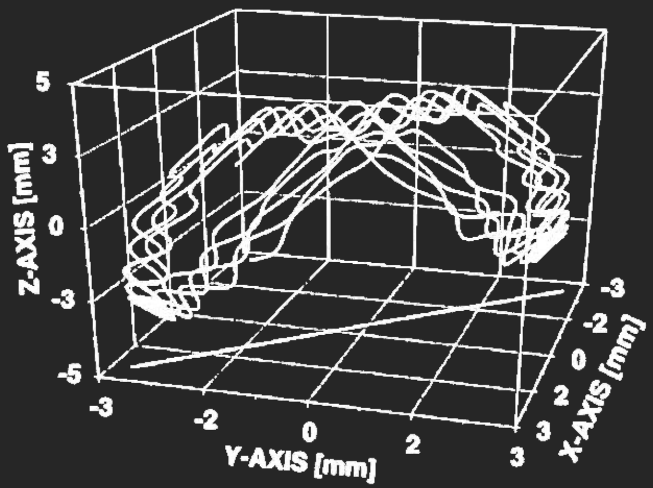
G. Werth. Basics of Ion Traps (page 16)



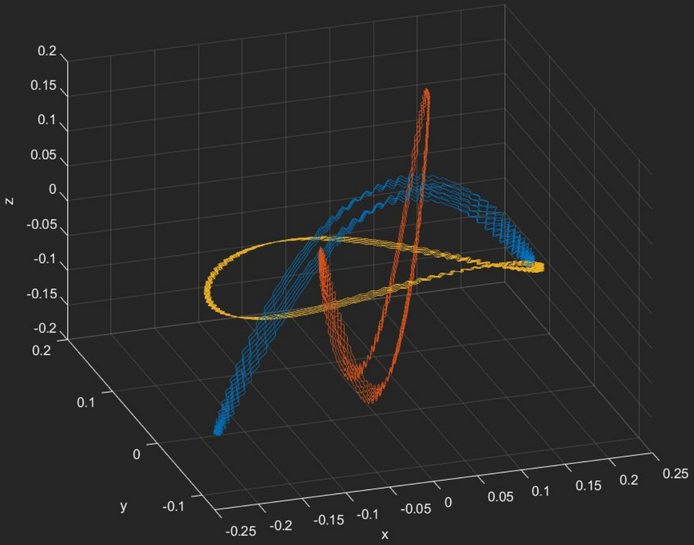
TRAJECTORIES



w=1500 T=0.35s



R.E. March. An Introduction to Quadrupole Ion Trap Mass Spectrometry (page 8)



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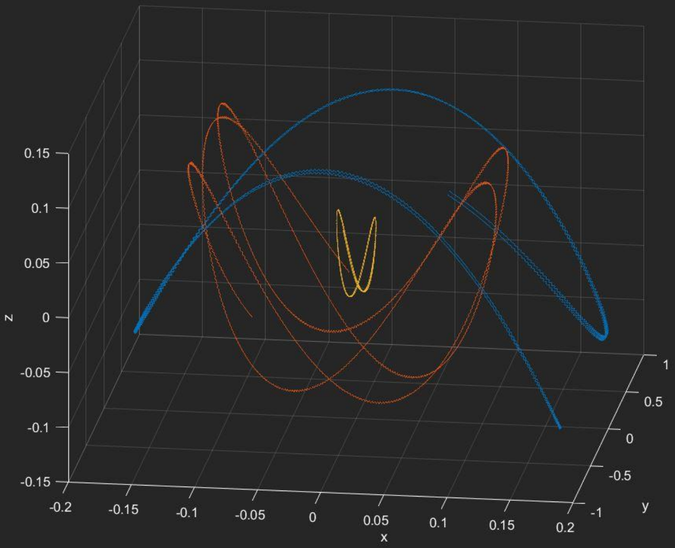
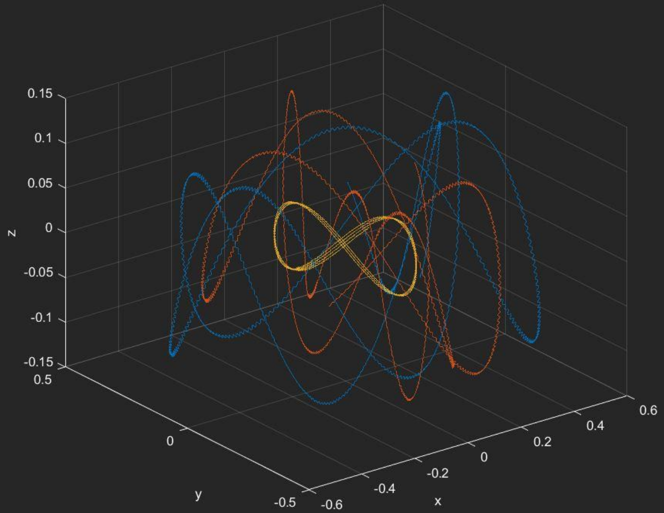
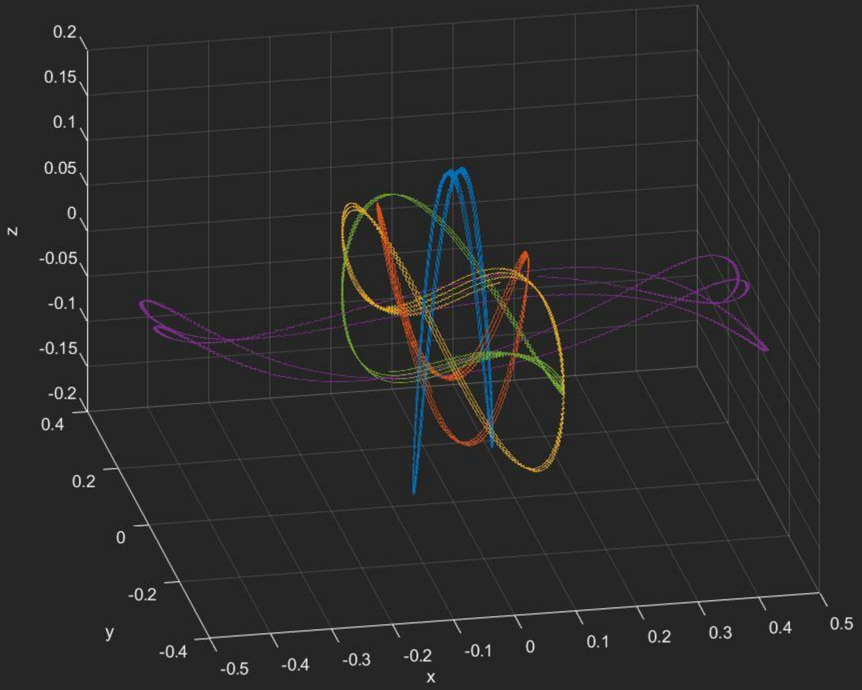
V_{03}= (-6.463, 2.151, -1.848e-14)

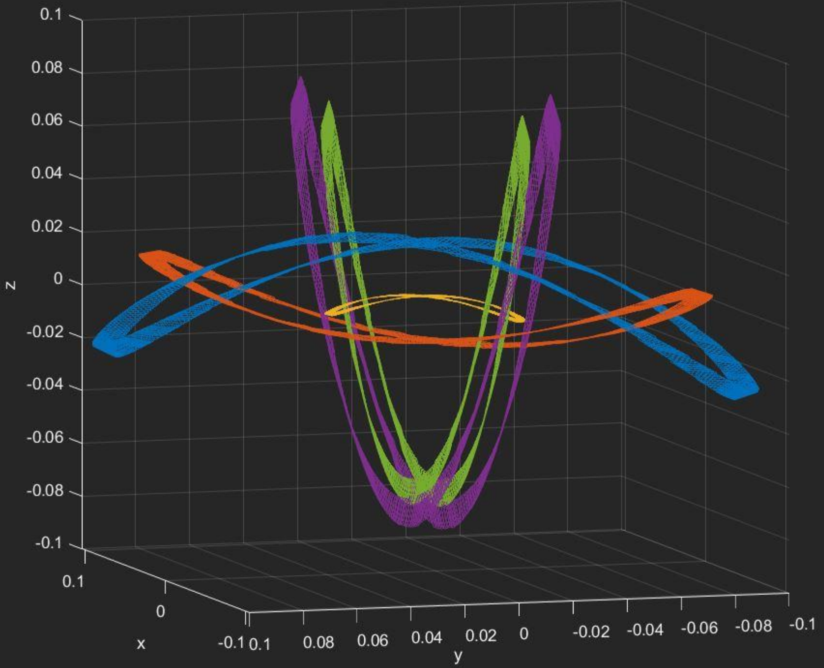


w = 5.2360e+03
V_{01}= (0.969, 7.250, 8.796e-14)
V_{02}= (0.337, -5.528, -6.254e-14)
V_{03}= (-0.376, 1.197, -4.709e-14)

w = 3.9270e+03
V_{01}= (7.599, 4.478, 7.805e-14)
V_{02}= (5.801, -7.327, -2.302e-16)
V_{03}= (-3.080, 4.837, -7.847e-14)







w = 3.9270e+03
V_{01}= (0.246, 0.422, 1.420e-13)
V_{02}= (-0.260, 4.656, -1.457e-13)
V_{03}= (-3.737, 6.890, -8.589e-13)
V_{04}= (3.188, -0.803, -3.088e-15)
V_{05}= (4.994, -3.736, -1.296e-13)

w = 3.1416e+03
V_{01}= (-8.530, -4.976, -3.509e-15)
V_{02}= (2.399, 0.986, 1.839e-15)
V_{03}= (-9.027, -7.558,-4.908e-15)
V_{04}= (3.691, 0.889, 7.802e-15)
V_{05}= (0.964, 1.055, 9.4e-15)

$w = 3.9270e+03$

$V_{01} = (1.345,\ 1.463,\ 7.635e\text{-}13)$

$V_{02} = (-4.863,\ 0.960,\ -2.777e\text{-}14)$

$V_{03} = (-2.121,\ 6.027,\ -4.848e\text{-}13)$

$V_{04} = (4.160,\ -2.086,\ -1.499e\text{-}14)$

$V_{05} = (11.32,\ -1.942,\ -8.848e\text{-}14)$

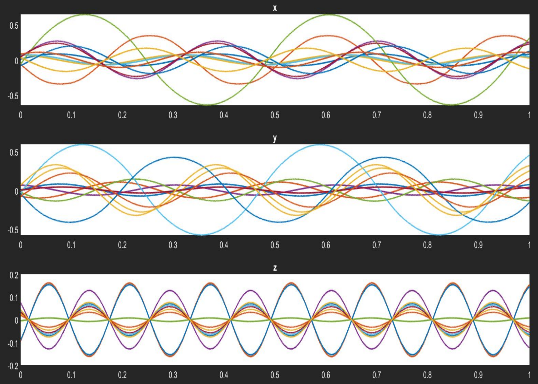
$V_{06} = (-1.578,\ 10.251,\ -7.040e\text{-}13)$

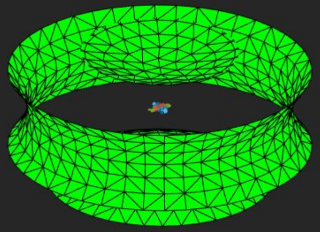
$V_{07} = (3.394,\ 0.810,\ -1.970e\text{-}14)$

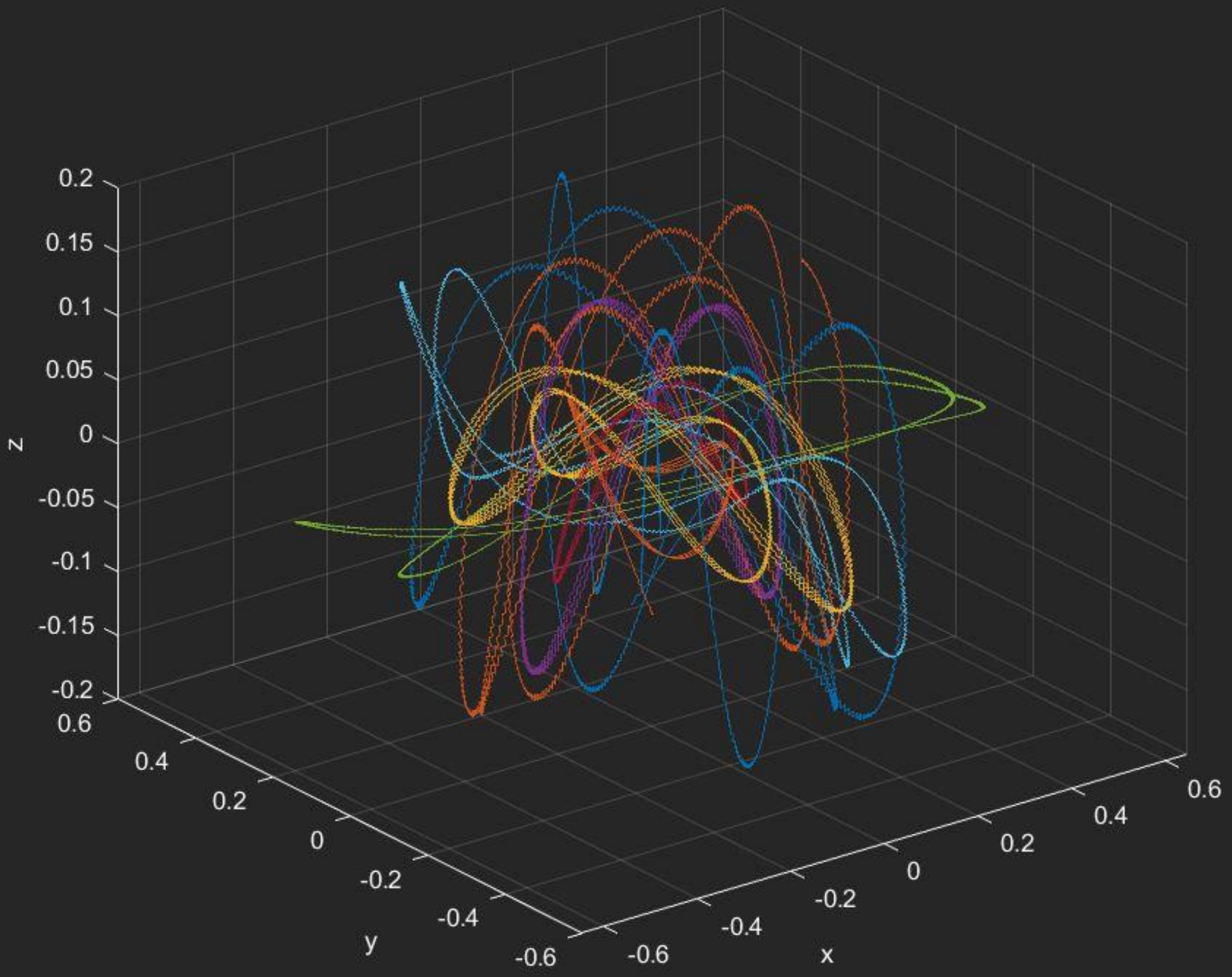
$V_{08} = (5.867,\ -6.152,\ -7.935e\text{-}11)$

$V_{09} = (-0.864,\ 6.323,\ 9.493e\text{-}14)$

$V_{010} = (-4.167,\ 4.613,\ 1.672e\text{-}10)$

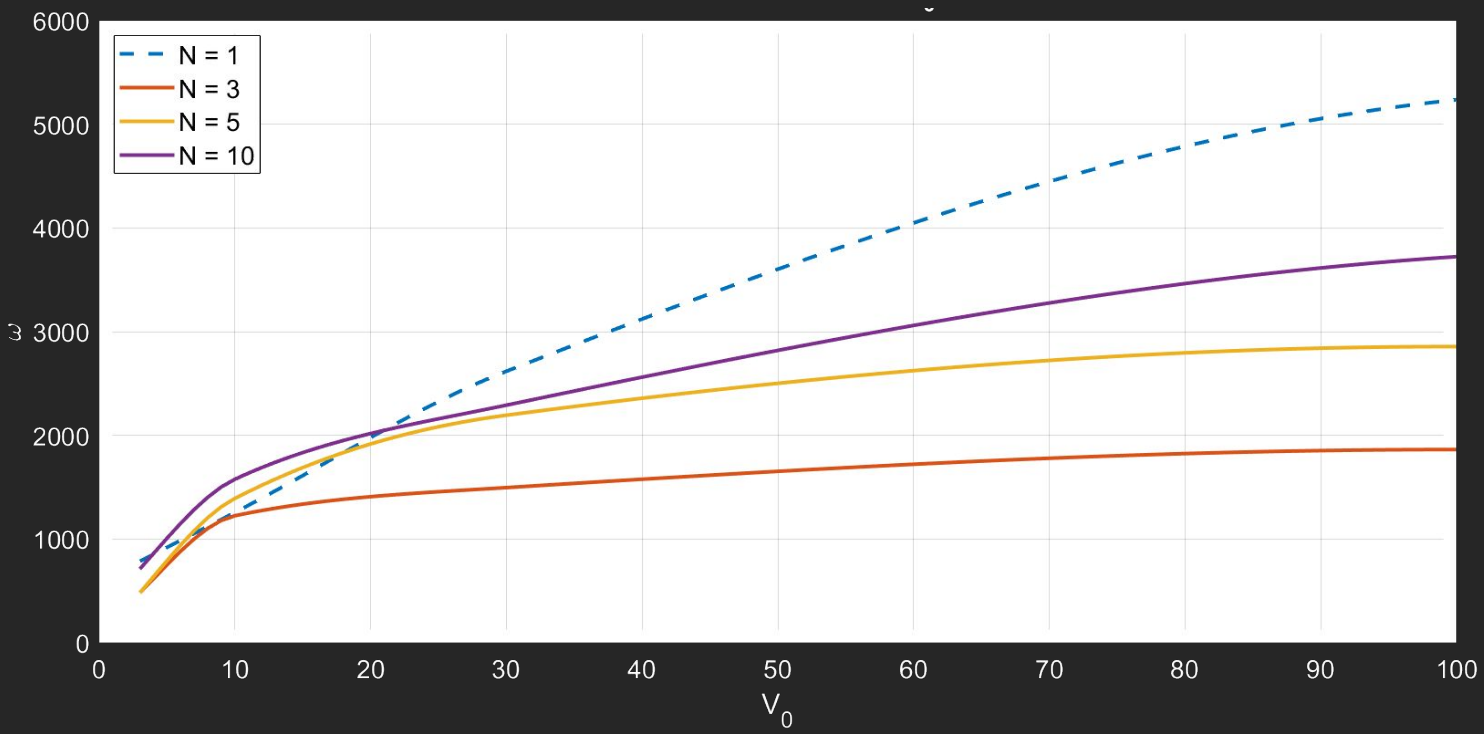






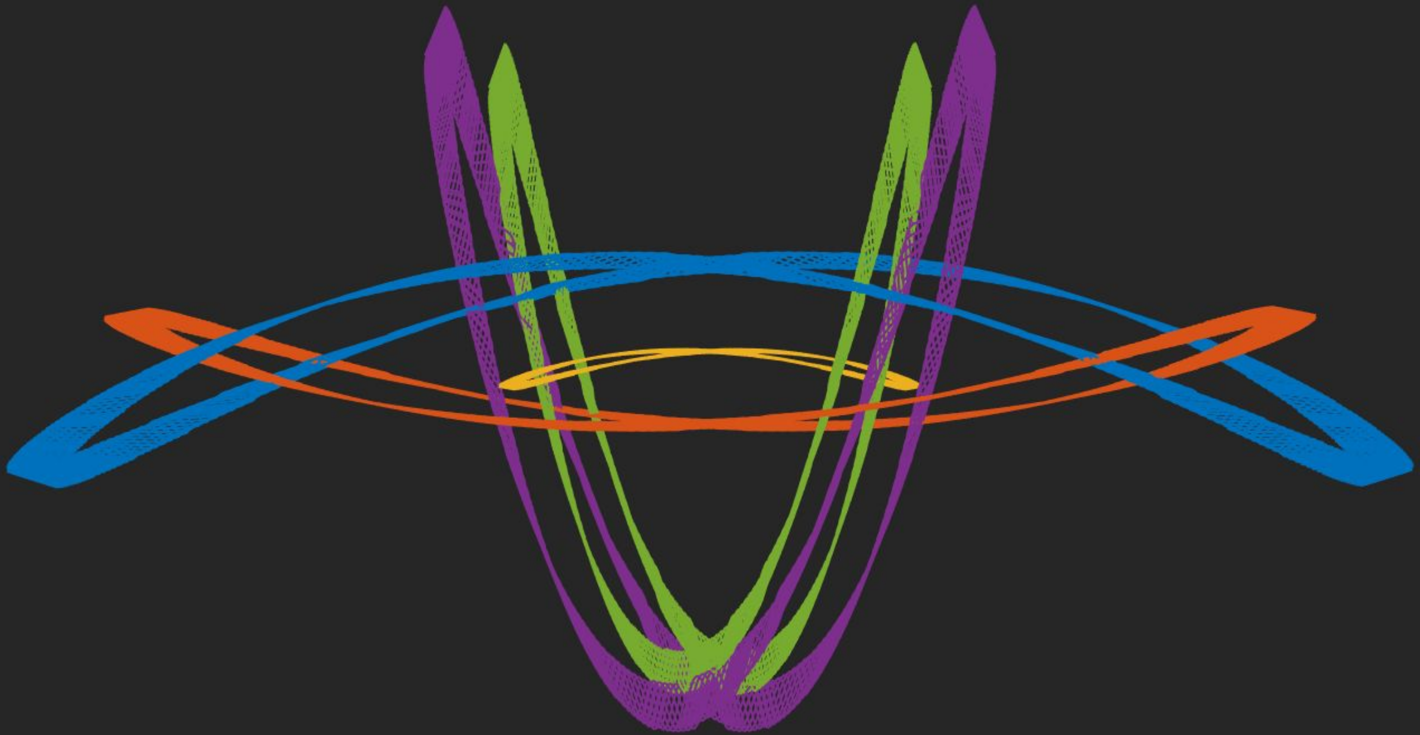
RESULTS OF STUDY

Limit frequencies for different particles



x_0= (1e-3*rand, 1e-3*rand, 1e-14*rand) V_0= (1e-3*rand, 1e-3*rand, 1e-14*rand)

QUESTIONS



$w = 3.1416e+03$ V_{01}= (-8.530, -4.976, -3.509e-15) V_{02}= (2.399, 0.986, 1.839e-15) V_{03}= (-9.027, -7.558,-4.908e-15)
V_{04}= (3.691, 0.889, 7.802e-15) V_{05}= (0.964, 1.055, 9.4e-15)