Simulating Particles in an Ideal Penning Trap

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https://github.uio.no/FYS3150-G2-2023/Project-3
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We have studied the behavior of singly-charged Calcium ions (Ca^+), inside an ideal Penning trap. With a numerical approach, we studied the equations of motion by implementing the forward Euler method FE and the 4th order Runge-Kutta $RK4$. We found that RK4 approximates the solution with smaller relative error than the relative error of FE. In addition, we evaluated the methods by their rate of convergence. We found that RK4 has a higher convergence rate at approx. 4.0, compared to FE at approx. 1.4. For particles interacting we explored angular frequencies, and amplitudes, of the time-dependent potential applied to the particles. We found that angular frequency in the range $\omega_V \in (1.3, 1.4)$ MHz is effective in pushing out particles, even for amplitude $f = 0.1$.

I. INTRODUCTION

We are surrounded by matter, which are made up of elementary particles. In the field of physics we want to understand the properties of these particles, and measure their physical quantities. We want to describe the particles such that we can explain the origin of mass [**?**].

However, to study a particle, it is necessary isolate and contain it over time. The Penning trap is a device, able to confine charged particles for a period of time. This concept was evolved from F. M. Penning's implementation of magnetic fields to a vaccuum gauge, and J. R. Pierce's work with electron beams, and put into practice by Hans Dehmelt. In 1973 Dehmelt and his group of researchers were able to confine a particle and store it over several months [**?**].

In practice, a Penning trap is not easy to obtain, and an experiment would be both time consuming and expensive. A numerical approach, allow us to study the effects of the Penning trap on a charged particle, without the equipment and material cost. With ordinary differential equations (ODE) we can model the movement of particles, confined within a Penning trap.

We will study an ideal Penning trap, where an electrostatic field confines the particle in z-direction, and a magnetic field confines it in the radial direction. We will use numerical methods to model a single particle, and study the particle motion in radial direction. In addition, we will model a system of particles, and study their motion both with and without particle interaction.

II. METHODS

A. Theoretical background

In this experiment we study a particle with a charge q. To do so, we need to consider the forces acting on that particle. These forces are given by the Penning trap's electric field and magnetic field, an illustration can be found in fig. **??**. The electric field $\mathbf{E}$ in our model is related to the electric potential V through

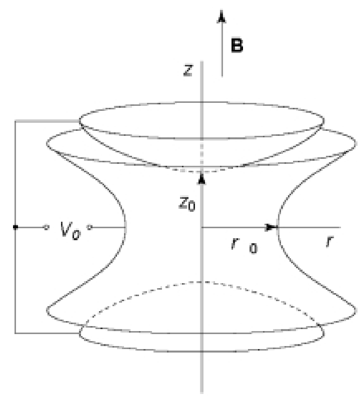

FIG. 1. The basic configuration of a hyperbolic Penning trap [**?**]. Electric potential V_0 is applied to the electrodes in end caps (top and bottom), and in the ring (middle). The magnetic field is denoted as $\mathbf{B}$, the distance from the center to the end caps are denoted as z_0, and the radial distance as r_0.

$$\mathbf{E} = -\nabla V, \tag{1}$$

where we define the electric potential as

$$V(x, y, z) = \frac{V_0}{2d^2}(2z^2 - x^2 - y^2). \tag{2}$$

The characteristic dimension $d = \sqrt{z_0^2 + r_0^2/2}$ determine the scale of the region between the electrodes. The magnetic field is homogeneous and defined as

$$\mathbf{B} = B_0\hat{e}_z = (0, 0, B), \tag{3}$$

where $B_0 > 0$ determines the strength of the field. The electric potential V_0 is applied to the electrodes, where the end caps are positively charged and the ring is negatively charged. The particle is confined by the electric field in the z-direction, however, it is not confined in the radial direction (xy-plane). The magnetic field is necessary to ensure the particle is fully confined in the Penning trap, and will force the particle to move in a circular orbit.

First, we consider Newton's second law (**??**), to determine the position of the particle.

$$m\ddot{\mathbf{r}} = \sum_i \mathbf{F}_i \tag{4}$$

In addition, we introduce the Lorentz force (**??**), which describes the force acting on the particle.

$$\mathbf{F} = q\mathbf{E} + q\mathbf{v} \times \mathbf{B}, \tag{5}$$

where $\ddot{\mathbf{r}} = d^2\mathbf{r}/dt^2$. We combine eq. (**??**) and eq. (**??**) in

$$m\ddot{\mathbf{r}} = (q\mathbf{E} + q\mathbf{v} \times \mathbf{B}), \tag{6}$$

and derive the differential equations in appendix **??**. We can rewrite and simplify these equations as

$$\ddot{x} - \omega_0\dot{y} - \frac{1}{2}\omega_z^2 x = 0, \tag{7}$$

$$\ddot{y} - \omega_0\dot{x} - \frac{1}{2}\omega_z^2 y = 0, \tag{8}$$

$$\ddot{z} + \omega_z^2 z = 0, \tag{9}$$

where

$$\omega_0 \equiv \frac{qB_0}{m}, \quad \omega_z^2 \equiv \frac{2qV_0}{md^2}.$$

We find the general solution for eq. (**??**)

$$z(t) = c_1 e^{i\omega_z t} + c_2 e^{-i\omega_z t}, \tag{10}$$

derived in appendix **??**. Continuing, we will use a Calcium ion with a single positive charge. That is, we assume the charge of the particle is $q > 0$.

Since eq. (**??**) and eq. (**??**) are coupled, we want to rewrite them as a single differential equation. We derive this in appendix **??**, and the resulting equation is given by

$$\ddot{f} + i\omega_0\dot{f} - \frac{1}{2}\omega_z^2 f = 0. \tag{11}$$

Eq. (**??**) has a general solution given by

$$f(t) = A_+ e^{-i(\omega_+ t + \phi_+)} + A_- e^{-i(\omega_- t + \phi_-)}. \tag{12}$$

The amplitude A_+ and A_- are positive, the phases ϕ_+ and ϕ_- are constant, and the angular rate is given by

$$\omega_\pm = \frac{\omega_0 \pm \sqrt{\omega_0^2 - 2\omega_z^2}}{2}. \tag{13}$$

We find the physical coordinates at a given time t using

$$x(t) = \mathrm{Re} f(t), \quad y(t) = \mathrm{Im} f(t),$$

and eq. (**??**). We can rearrange the right hand side of the expression derived in **??**, to find the physical coordinates

$$x(t) = A_+ \cos(\omega_+ t + \phi_+) + A_- \cos(\omega_- t + \phi_-) \tag{14}$$

$$y(t) = -A_+ \sin(\omega_+ t + \phi_+) - A_- \sin(\omega_- t + \phi_-) \tag{15}$$

However, to obtain a bound on the particle's movement in the radial direction, we have to ensure that

$$|f(t)| = \sqrt{(x(t))^2 + (y(t))^2}.$$

Which means we have to put constraint on the values of ω_0 and ω_z^2 in order to find a bounded solution $|f(t)| < \infty$. We derive an expression for this in appendix **??**. Since we have assumed the particle charge $q > 0$, and the mass $m > 0$, the constraints are

$$\frac{q}{m} > \frac{4V_0}{d^2 B_0^2}. \tag{16}$$

When $t \to \infty$, the upper and lower limits are

$$R_+ = A_+ + A_-, \tag{17}$$

$$R_- = |A_+ - A_-|, \tag{18}$$

which we derive in appendix **??**.

In this experiment, we will use the initial conditions for the particle given in table **??**. From eq. (**??**) and the initial conditions, we find the specific solution

$$z(t) = z_0 \cos(\omega_z t)$$

For the particle movement in the radial direction, we find the specific solution using eq. (**??**) with

$$A_+ = \frac{v_0 + \omega_- x0}{\omega_- - \omega_+}, \qquad A_- = -\frac{v_0 + \omega_+ x0}{\omega_- - \omega_+},$$

$$\phi_+ = 0, \qquad \phi_- = 0.$$

We will also consider the numerical simulation of multiple particles, confined in a Penning trap. The particles will experience a repelling force from each other, giving the electric field

$$\mathbf{E} = k_e \sum_{j=1}^{n} q_j \frac{\mathbf{r} - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|^3}. \tag{19}$$

The Coulomb constant k_e value can be found in table **??**.

For multiple particles we have to modify the equations of motion, by adding a term for the force a given particle experience at a given point. When we scale eq. (**??**) by charge and mass, we get a new set of equations of motion

$$\ddot{x}_i - \omega_{0,i}\dot{y}_i - \frac{1}{2}\omega_{z,i}^2 x_i - k_e \frac{q_i}{m_i} \sum_{j \neq i} q_j \frac{x_i - x_j}{|\mathbf{r}_i - \mathbf{r}_j|^3} = 0, \tag{20}$$

$$\ddot{y}_i - \omega_{0,i}\dot{x}_i - \frac{1}{2}\omega_{z,i}^2 y_i - k_e \frac{q_i}{m_i} \sum_{j \neq i} q_j \frac{y_i - y_j}{|\mathbf{r}_i - \mathbf{r}_j|^3} = 0, \tag{21}$$

$$\ddot{z}_i + \omega_{z,i}^2 z_i - k_e \frac{q_i}{m_i} \sum_{j \neq i} q_j \frac{z_i - z_j}{|\mathbf{r}_i - \mathbf{r}_j|^3} = 0, \tag{22}$$

where i and j denote the particle indices. When we include a time-dependence to the applied potential we make a replacement of the initial electric potential

$$V_0 \to V_0(1 + f\cos(\omega_V t)), \tag{23}$$

where f denotes the amplitude and ω_V the angular rate.

B. Algorithms and implementation

When we consider a multi-particle system, we adapt the notation in our derived equations. The force acting on a particle in the Penning trap, which experience particle interaction, can be written as

$$\mathbf{F}_i(t, \mathbf{v}_i, \mathbf{r}_i) = q_i\mathbf{E}(t, \mathbf{r}_i) + q_i\mathbf{v}_i \times \mathbf{B} - \mathbf{E}_p(t, \mathbf{r}_i), \quad (24)$$

where i and j still denotes the particle indices, and $\mathbf{E}_p$ denotes the force exerted on particle i by particle j.

$$\mathbf{E}_p(t, \mathbf{r}_i) = k_e q_i \sum_{j \neq i} q_j \frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|^3}. \quad (25)$$

In addition, we adapt the notation of (**??**), and define the first derivative of the particle position as

$$\frac{d\mathbf{r}_i}{dt} = \dot{\mathbf{r}}_i = \mathbf{v}_i, \quad (26)$$

$$\frac{d\mathbf{v}_i}{dt} = \dot{\mathbf{v}}_i = \frac{\mathbf{F}_i(t, \mathbf{v}_i, \mathbf{r}_i}{m_i}, \quad (27)$$

We first implemented the forward Euler method, using the expression for a coupled system given in appendix **??**. We define the forward Euler algorithm in **??**.

Algorithm 1 Forward Euler method

procedure EVOLVE FORWARD EULER($particles, dt$)
  $N \leftarrow$ Number of particles in *particles*
  $a \leftarrow$ Calculate $\frac{\mathbf{F_i}}{m_i}$ for each particle in *particles*
  for $i = 1, 2, \ldots, N$ **do**
    $particles_i.\mathbf{r} \leftarrow particles_i.\mathbf{r} + dt \cdot particles_i.\mathbf{v}$
    $particles_i.\mathbf{v} \leftarrow particles_i.\mathbf{v} + dt \cdot a_i$

We also implemented the 4th order Runge-Kutta (RK4) method, using the expression given in appendix **??**. We define the RK4 algorithm in **??**. $\mathbf{F}$ does not take any arguments, however, the total force acting on the particle is calculated using the value of position and velocity within *particles*. For a system of particles, the positional value of one particle affects the rest of the particles. We calculated the next step for all particles, updated their values in a copy, and updated the positional value based on the original values. We simulated the movement of particles confined in a Penning trap. All simulations used the initial conditions for particle 1 and 2 given in table **??**.

Algorithm 2 RK4 method

procedure EVOLVE RK4($particles, dt$)
  $N \leftarrow$ Number of particles inside the Penning trap
  $orig\_p \leftarrow$ Copy of particles
  $tmp\_p \leftarrow$ Array of particles of size N
  $\mathbf{k_r} \leftarrow$ 2D array of vectors of size $4 \times N$
  $\mathbf{k_v} \leftarrow$ 2D array of vectors of size $4 \times N$
  for $i = 1, 2, \ldots, N$ **do**
    $\mathbf{k}_{\mathbf{r},1,i} \leftarrow particles_i.\mathbf{v}$
    $\mathbf{k}_{\mathbf{v},1,i} \leftarrow \frac{\mathbf{F}_i}{m_i}$
    $tmp\_p_i.\mathbf{r} \leftarrow orig\_p_i.\mathbf{r} + \frac{dt}{2} \cdot \mathbf{k}_{\mathbf{r},1,i}$
    $tmp\_p_i.\mathbf{v} \leftarrow orig\_p_i.\mathbf{v} + \frac{dt}{2} \cdot \mathbf{k}_{\mathbf{v},1,i}$
  $particles \leftarrow tmp\_p$ ▷ Update particles
  for $i = 1, 2, \ldots, N$ **do**
    $\mathbf{k}_{\mathbf{r},2,i} \leftarrow particles_i.\mathbf{v}$
    $\mathbf{k}_{\mathbf{v},2,i} \leftarrow \frac{\mathbf{F}_i}{m_i}$
    $tmp\_p_i.\mathbf{r} \leftarrow orig\_p_i.\mathbf{r} + \frac{dt}{2} \cdot \mathbf{k}_{\mathbf{r},2,i}$
    $tmp\_p_i.\mathbf{v} \leftarrow orig\_p_i.\mathbf{v} + \frac{dt}{2} \cdot \mathbf{k}_{\mathbf{v},2,i}$
  $particles \leftarrow tmp\_p$ ▷ Update particles
  for $i = 1, 2, \ldots, N$ **do**
    $\mathbf{k}_{\mathbf{r},3,i} \leftarrow particles_i.\mathbf{v}$
    $\mathbf{k}_{\mathbf{v},3,i} \leftarrow \frac{\mathbf{F}_i}{m}$
    $tmp\_p_i.\mathbf{r} \leftarrow orig\_p_i.\mathbf{r} + dt \cdot \mathbf{k}_{\mathbf{r},3,i}$
    $tmp\_p_i.\mathbf{v} \leftarrow orig\_p_i.\mathbf{v} + dt \cdot \mathbf{k}_{\mathbf{v},3,i}$
  $particles \leftarrow tmp\_p$ ▷ Update particles
  for $i = 1, 2, \ldots, N$ **do**
    $\mathbf{k}_{\mathbf{r},4,i} \leftarrow particles_i.\mathbf{v}$
    $\mathbf{k}_{\mathbf{v},4,i} \leftarrow \frac{\mathbf{F}}{m}$
    $tmp\_p_i.\mathbf{r} \leftarrow orig\_p_i.\mathbf{r} + \frac{dt}{6} \cdot (\mathbf{k}_{\mathbf{r},1,i} + 2\mathbf{k}_{\mathbf{r},2,i} + 2\mathbf{k}_{\mathbf{r},3,i} + \mathbf{k}_{\mathbf{r},4,i})$
    $tmp\_p_i.\mathbf{v} \leftarrow orig\_p_i.\mathbf{v} + \frac{dt}{6} \cdot (\mathbf{k}_{\mathbf{v},1,i} + 2\mathbf{k}_{\mathbf{v},2,i} + 2\mathbf{k}_{\mathbf{v},3,i} + \mathbf{k}_{\mathbf{v},4,i})$
  $particles \leftarrow tmp\_p$ ▷ Final update

C. Testing and error analysis

We implemented a test suite to validate our results, details can be found in appendix **??**. To analyze our results, we compared the relative error of the analytical solution with the result from the implemented forward Euler method and RK4 method. We simulated four times using time steps given in table **??**, and estimated the error convergence rate r_{err} for both methods using

$$r_{\text{err}} = \frac{1}{3} \sum_{k=2}^{4} \frac{\log(\Delta_{\max,k}/\Delta_{\max,k-1})}{\log(h_k/h_{k-1})}. \quad (28)$$

The maximum error of a simulation k with a step size h_k is given by

$$\Delta_{\max,k} = \max_i |\mathbf{r}_{i,\text{exact}} - \mathbf{r}_i|,$$

where $\mathbf{r}_{i,\text{exact}}$ is the analytical solution, and $\mathbf{r}_i$ is the computed result.

D. Tools

The numerical methods are implemented in C++, and parallelized using `OpenMP` [?]. In addition, we used the profiler `Scalasca` [?] and `Score-P` [?] event tracking, during development. We used the Python library matplotlib [?] to produce all the plots, and seaborn [?] to set the theme in the figures.

III. RESULTS AND DISCUSSION

The simulations were performed using a constant configuration for the Penning trap, where the values of B_0, V_0, and d can be found in table ??. We also used a constant configuration for the particles, found in table ??. Initial position of particle 1 p_1 was set to $(20, 0, 20)\mu m$ with velocity $(0, 25, 0)\mu m/\mu s$, whereas the position of particle 2 p_2 was set to $(25, 25, 0)\mu m$ with velocity $(0, 40, 5)\mu m/\mu s$.

First, we simulated a single particle for $50\mu s$, approximating the particle's motion using the RK4 method. In addition we compared the result with the analytical solution in figure ??. The approximated solution completely overlap the analytical, suggesting the implemented method is approximating the solution with minimal error. The angular frequency is

$$\omega_z = \sqrt{\frac{2qV_0}{md^2}} = \sqrt{\frac{2 \cdot 1 \cdot 9.65}{40.078}} \approx 0.694 \text{ rad/µs},$$

which result in a period (P) of

$$\text{P} = \frac{2\pi}{|\omega_z|} \approx 9.054\text{µs}.$$

From figure ?? we see that the period, the time it takes for the particle to reach the same position, is close to 9 µs. This is what we would expect given the value of ω_z.

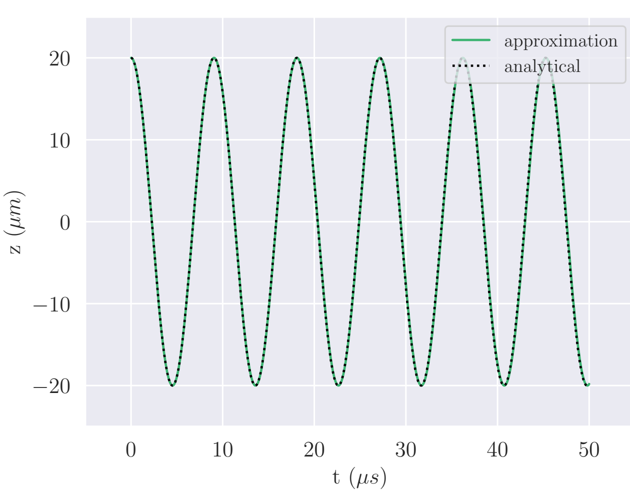

FIG. 2. Movement of a single particle in z-direction. Approximated using the 4th order Runge-Kutta method, compared to the analytical solution $z(t) = z_0 \cos(\omega_z t)$.

To evaluate the implemented methods we simulated the particle using both forward Euler (FE) and RK4, with different time steps given in ??. Again, we simulated the particle movement for 50 µs, and estimated the relative error of each method. The result can be found in figure ??. The relative error of FE is large compared to the relative error of RK4. The error convergence rate for FE is $r_{\text{err}} \approx 1.39652$, and RK4 $r_{\text{err}} \approx 3.99998$, which means RK4 converges faster compared to FE.

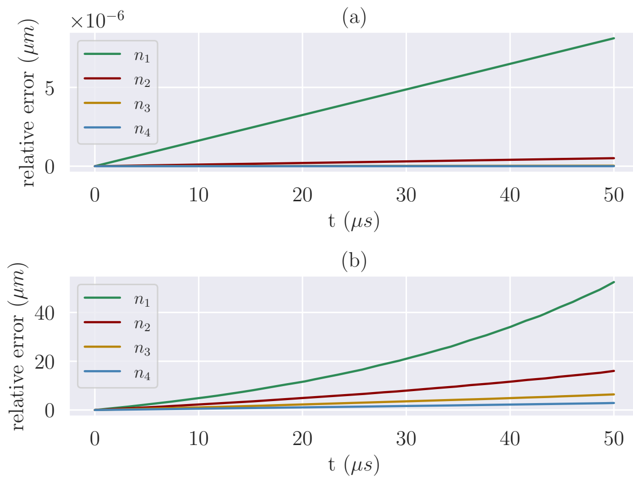

FIG. 3. Relative error measured for 4th order Runge-Kutta *a* and foreward Euler *b*. Important to notice when reading the plot, that the scale of measured relative error differ between the methods.

RK4 is a more complex method, which requires four times the calculations compared to FE. When the simulation is done with $n_4 = 32000$ time steps, the difference in relative error decreases. The cost of calculation exceed the benefit of accuracy. That is, at a large number of time steps we could find a satisfying approximation to the solution using FE, with less calculations.

Next, we simulated the movement of two particles in radial direction. In figure ??, we see the path of both particles without interaction. The starting position of particle 1 p_1 is closer to the center of the Penning trap, than the starting position of p. Both particles move in an orbital path arount the center, however, the starting velocity of each particles determine the minimum and maximum distance a particle moves from the center. We find these values bounds using eq. ?? and eq. ??

$$\begin{aligned} R_+ &= A_+ + A_- \\ &= -12.3232\text{µm} + 32.3232\text{µm} \\ &= 20.00\text{µm}, \end{aligned}$$

and

$$\begin{aligned} R_- &= |A_+ - A_-| \\ &= |-12.3232\text{µm} - 32.3232\text{µm}| \\ &= 44.6464\text{µm}. \end{aligned}$$

The distance is similar that in figure ??. In addition, we can see from ?? that the distance differ between p_1 and p_2. When we study the particle movement in z-direction, in figure **??**, we see a circular movement. Again, the distance the particle moves from the center is determined by its initial conditions.

In figure **??** we see the movement in radial direction, where particle interaction is included. The orbital path is similar to what we see without particle interaction. However, the additional force acting on the particle is affecting it's trajectory. The distance each particle is moving from the center, differs depending on the position. Which is also seen in figure **??**, where we see the trajectory of the particle at a given position. When we study the phase space plot, where particle interaction is included, in figure **??** a similar difference is observed. In figure **??** we see the movement of two particles in both the radial direction and z-direction. The figure include particle movement with and without interaction, where we can observe the change in movement.

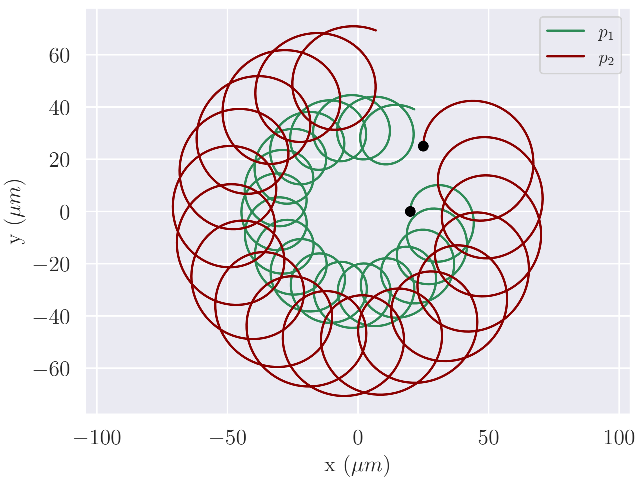

FIG. 4. Path of two particles, p_1 and p_2, without interaction. The black dot marks the starting position of each particle.

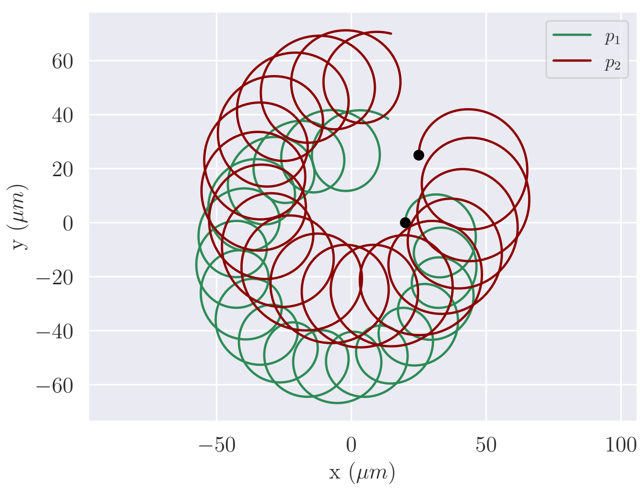

FIG. 5. Path of two particles, p_1 and p_2, with interaction. The black dot marks the starting position of each particle.

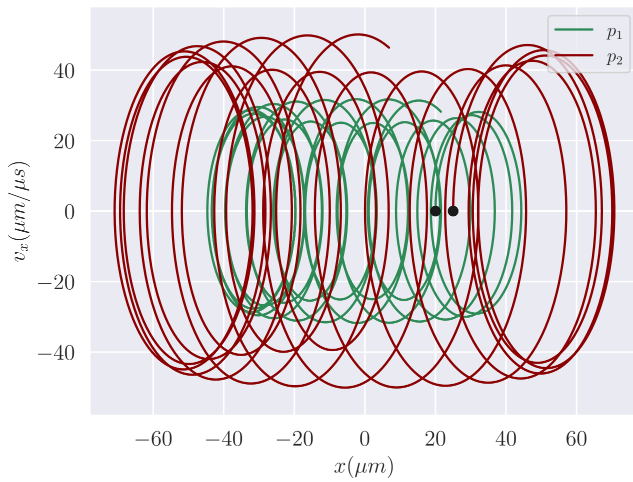

FIG. 6. Particle trajectory at a given position x, without particle interaction. The black dot marks the starting position of each particle.

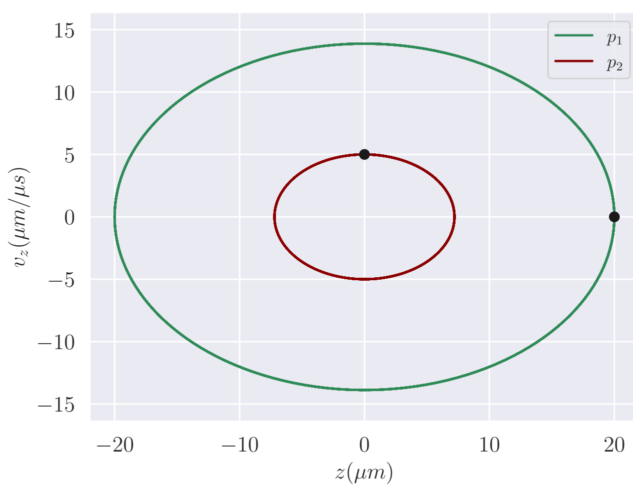

FIG. 7. Particle trajectory at a given position z, without particle interaction. The black dot marks the starting position of each particle.

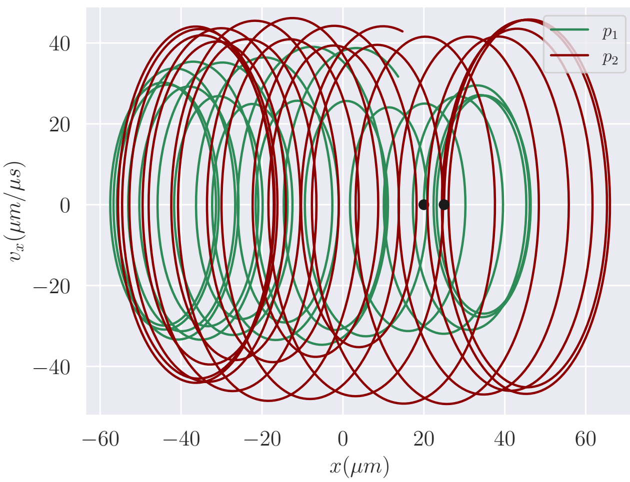

FIG. 8. Particle trajectory at a given position x, with particle interaction. The black dot marks the starting position of each particle.

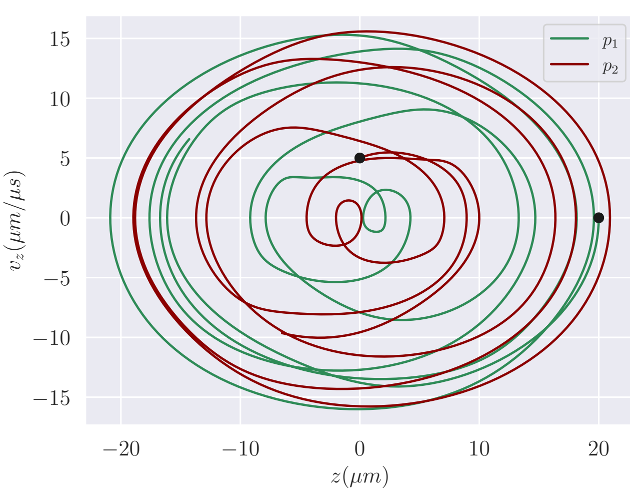

FIG. 9. Particle trajectory at a given position z, with particle interaction. The black dot marks the starting position of each particle.

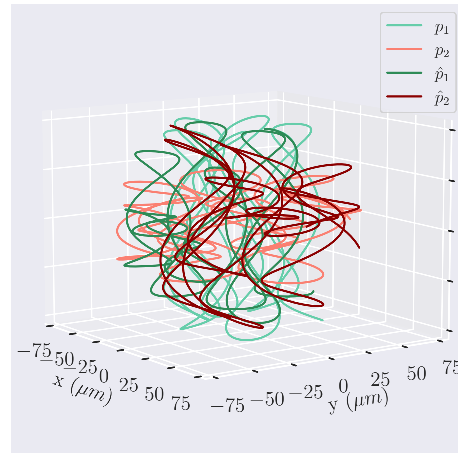

FIG. 10. The movement of particles in a Penning trap. Where p_1 and p_2 is without interaction, $\hat{p}_1$ and $\hat{p}_2$ is without interaction.

Finally, by subjecting the system to a time-dependent field, making the replacement in **??**, we study the fraction of particles left at different amplitudes f. We can see how the different amplitudes lead to loss of particles, at different angular frequencies ω_V in **??**. We study frequencies in the range $\omega_V \in (0.2, 2.5)$ MHz, with steps of 0.02 MHz, and find that angular frequencies in the range $(1.0, 2.5)$ is effective in pushing the particles out of the Penning trap.

We explore the range $\omega_V \in (1.0, 1.7)$ MHz closer in figure **??**, and observe a gradual loss of particles for amplitude $f_1 = 0.1$. Since they are additive, a greater amplitude will result in a larger bound for the particle movement, and particles are easily pushed out. Certain angular frequencies are more effective in pushing particles out of the Penning trap, as we see in figure **??** where $\omega_V \in (1.3, 1.4)$ is also effective for pushing out particles of amplitude $f_1 = 0.1$.

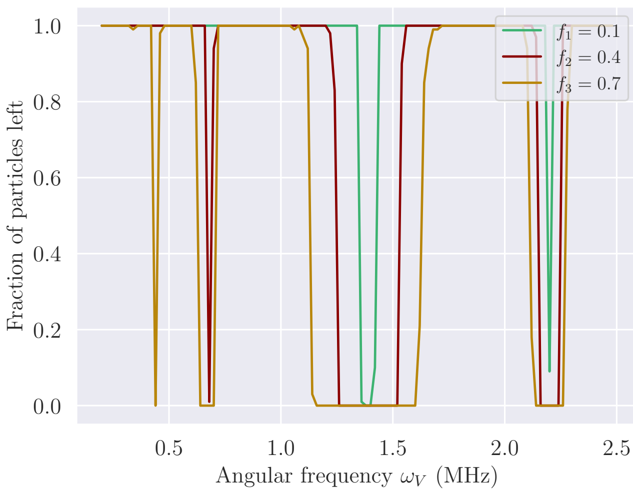

FIG. 11. Exploring the behavior of particles, where the amplitude of time-dependent potential $f = [0.1, 0.4, 0.7]$, for angular frequency $\omega_V \in (0.2, 2.5)$ MHz.

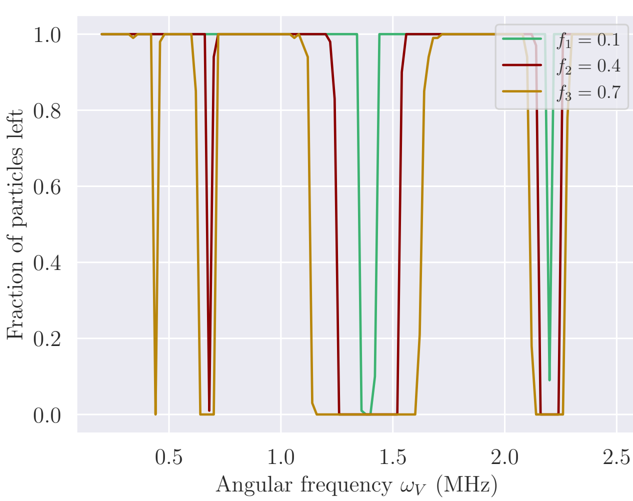

FIG. 12. Exploring the behavior of particles, where the amplitude of time-dependent potential $f = [0.1, 0.4, 0.7]$, for angular frequency $\omega_V \in (1.0, 1.7)$ MHz.

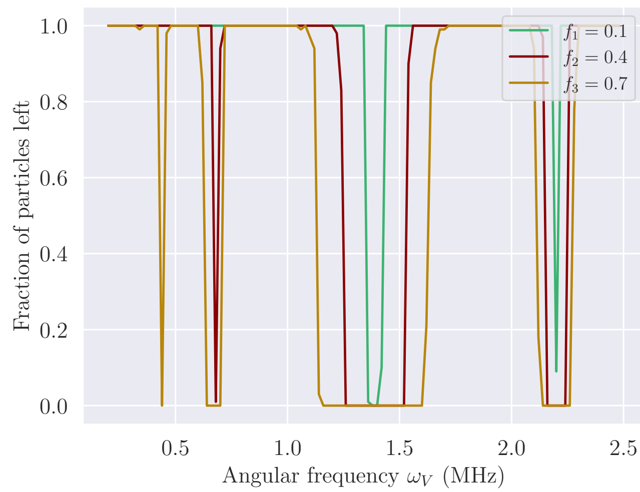

FIG. 13. Exploring the behavior of particles, where the amplitude of time-dependent potential $f = [0.1, 0.4, 0.7]$, for angular frequency $\omega_V \in (1.3, 1.4)$ MHz.

IV. CONCLUSION

We studied the movement of particles confined by an ideal Penning trap, where we used iterative methods to simulate the particle behavior. We included the magnetic and electric field of the Penning trap, in addition to simulating the particles behavior when interaction with other each other. When we introduced the interaction, the movement in both radial direction and z-direction changed. From a circular path, to a more elliptical path, where the particles initial condition determine how it is affecting other particles path.

We also compared iterative methods, with the analytical solution, and found that the forward Euler FE method result in an approximation with a large relative error compared to the relative error of the 4th order Runge-kutta $RK4$ method. In addition, we also found that RK4 has a higher convergence rate at approx. 4.0, compared to FE at approx. 1.4. Which suggest RK4 reach the solution faster than what FE, however, when we increase the number of time steps both methods result in similar relative error. When the number of calculations increase, and the number of time steps is sufficient, FE can be the better choise to conserve computational resources.

When we explored the particles behavior at angular frequencies $\omega_V \in (0.2, 2.5)$ MHz, we found that particles are pushed out of the Penning trap when the amplitude of the applied time-dependent potential increase. The amplitude $f = 0.7$ result in particles being pushed out at most of the range of angular frequencies, whereas an amplitude $f = 0.1$ result in particles being pushed in a more narrow range. Since particles are being pushed out when the amplitude is low, there is likely a resonance frequency at around 1.4 MHz.

Appendix A: Derivation of equations

1. Equations of motion

First, we need to define the velocity of the particle

$$\mathbf{v} \equiv \frac{d\mathbf{r}}{dt} = \left(\frac{dx}{dt}, \frac{dy}{dt}, \frac{dz}{dt}\right).$$

We can rewrite the velocity as $\dot{r} = (\dot{x}, \dot{y}, \dot{z})$, and find the cross product

$$q\mathbf{v} \times \mathbf{B} = q \begin{vmatrix} \hat{e}_x & \hat{e}_y & \hat{e}_z \\ \dot{x} & \dot{y} & \dot{z} \\ 0 & 0 & B_0 \end{vmatrix} = q\big(B_0\dot{y}, -B_0\dot{x}, 0\big).$$

We are considering an ideal Penning traps, where we define the electric potential as

$$V(x, y, z) = \frac{V_0}{2d^2}(2z^2 - x^2 - y^2).$$

The relationship between the electric field $\mathbf{E}$ and the electric potential of the field is given by

$$\begin{aligned} \mathbf{E} &= -\nabla V \\ &= -\left(\frac{dV}{dx}, \frac{dV}{dy} \frac{dV}{dz}\right) \\ &= \frac{V_0}{d^2}\big(x, y, -2z\big). \end{aligned}$$

We can now express the Lorentz force as

$$\begin{aligned} \mathbf{F} &= q\mathbf{E} + q\mathbf{v} \times \mathbf{B} \\ &= \frac{qV_0}{d^2}\big(x, y, -2z\big) + \big(qB_0\dot{y}, -qB_0\dot{x}, 0\big), \end{aligned}$$

and insert it into Newtons equation (**??**). We get

$$\ddot{\mathbf{r}} = \left(\frac{qV_0}{md^2}x, \frac{qV_0}{md^2}y, -\frac{2qV_0}{md^2}z\right) + \left(\frac{qB_0}{m}\dot{y}, -\frac{qB_0}{m}\dot{x}, 0\right),$$

which can be written as

$$\begin{aligned} \ddot{x} &= \frac{qV_0}{md^2}x + \frac{qB_0}{m}\dot{y}, \\ \ddot{y} &= \frac{qV_0}{md^2}y - \frac{qB_0}{m}\dot{x}, \\ \ddot{z} &= -\frac{2qV_0}{md^2}z. \end{aligned}$$

If we define

$$\omega_0 \equiv \frac{qB_0}{m}, \quad \omega_z^2 \equiv \frac{2qV_0}{md^2},$$

the equations of motion can be written as

$$\begin{aligned} \ddot{x} &= \frac{1}{2}\omega_z^2 x + \omega_0\dot{y}, \\ \ddot{y} &= \frac{1}{2}\omega_z^2 y - \omega_0\dot{x}, \\ \ddot{z} &= -\omega_z^2 z. \end{aligned}$$

2. General solution

We consider the characteristic equation of a second order differential equation [**?**],

$$\begin{aligned} r^2 + \omega_z^2 &= 0 \\ r &= \pm\sqrt{-\omega_z^2}. \end{aligned}$$

The characteristic equation has two complex roots

$$r_1 = -i\omega_z, \quad r_2 = i\omega_z,$$

which give us solutions in the general form

$$z = c_1 e^{i\omega_z t} + c_2 e^{-i\omega_z t}.$$

In addition, for a complex number $z = a + ib$, we can define $e^z \equiv e^a(\cos b + i\sin b)$ [**?**]. We can rewrite the general solution as

$$\begin{aligned} c_1 e^{i\omega_z t} + c_2 e^{-i\omega_z t} &= c_1(\cos\omega_z t + i\sin\omega_z t) \\ &\quad + c_2(\cos\omega_z t - i\sin\omega_z t \\ &= E\cos\omega_z t + iF\sin\omega_z t. \end{aligned}$$

3. Complex function

In sec. **??** we found the differential equations for $\ddot{x}$ and $\ddot{y}$. To derive a single differential equation, we introduce the complex function $f(t) = x(t) + iy(t)$, which gives us

$$\begin{aligned} 0 &= \Big(\ddot{x} - \omega_0\dot{y} - \frac{1}{2}\omega_z^2 x\Big) + i\Big(\ddot{y} + \omega_0\dot{x} - \frac{1}{2}\omega_z^2 y\Big) \\ &= \ddot{x} - \omega_0\dot{y} - \frac{1}{2}\omega_z^2 x + i\ddot{y} + i\omega_0\dot{x} - i\frac{1}{2}\omega_z^2 y \\ &= \ddot{x} + i\ddot{y} + i\omega_0\dot{x} - \omega_0\dot{y} - \frac{1}{2}\omega_z^2 x - i\frac{1}{2}\omega_z^2 y. \end{aligned}$$

Using the definition $i = \sqrt{-1}$, we can rewrite

$$i\omega_0\dot{x} + (-1)\omega_0\dot{y} = i\omega_0\dot{x} + i^2\omega_0\dot{y}.$$

This gives us a single differential equation

$$\begin{aligned} 0 &= \ddot{x} + i\ddot{y} + i\omega_0(\dot{x} + i\dot{y}) - \frac{1}{2}\omega_z^2 x - i\frac{1}{2}\omega_z^2 y \\ &= \ddot{f} + i\omega_0\dot{f} - \frac{1}{2}\omega_z^2 f. \end{aligned}$$

4. Physical coordinates

We can rewrite eq. (**??**), as

$$\begin{aligned} f(t) &= A_+ e^{-i(\omega_+ t + \phi_+)} + A_- e^{-i(\omega_- t + \phi_-)} \\ &= A_+(\cos(\omega_+ t + \phi_+) - i\sin(\omega_+ t + \phi_+)) \\ &\quad + A_-(\cos(\omega_- t + \phi_-) - i\sin(\omega_- t + \phi_-)). \end{aligned}$$

5. Upper and lower bounds

To obtain the upper and lower bounds of the particle's distance from the origin, we first find an expression for the second norm defined as $|f(t)| = \sqrt{(x(t))^2 + (y(t))^2}$.

$$\begin{aligned}(x(t))^2 &= \big(A_+ \cos(\omega_+ t + \phi_+) + A_- \cos(\omega_- t + \phi_-)\big)^2 \\ &= A_+^2 \cos^2(\omega_+ t + \phi_+) \\ &\quad + 2A_+A_- \cos(\omega_+ t + \phi_+)\cos(\omega_- t + \phi_-) \\ &\quad + A_-^2 \cos^2(\omega_- t + \phi_-),\end{aligned}$$

$$\begin{aligned}(y(t))^2 &= \big(-A_+ \sin(\omega_+ t + \phi_+) - A_- \sin(\omega_- t + \phi_-)\big)^2 \\ &= A_+^2 \sin^2(\omega_+ t + \phi_+) \\ &\quad + 2A_+A_- \sin(\omega_+ t + \phi_+)\sin(\omega_- t + \phi_-) \\ &\quad + A_-^2 \sin^2(\omega_- t + \phi_-).\end{aligned}$$

We insert these expressions, and find

$$\begin{aligned}|f(t)| &= \sqrt{(x(t))^2 + (y(t))^2} \\ &= \sqrt{A_+^2 + 2A_+A_- \cos^2(\alpha) + A_-^2},\end{aligned}$$

where $\alpha = (\omega_+ - \omega_-)t + (\phi_+ - \phi_-)$. If we set $\alpha = 0$ we get $\cos(0) = 1$, and obtain the upper bound

$$\begin{aligned}R_+ &= \sqrt{A_+^2 + 2A_+A_- + A_-^2} \\ &= \sqrt{(A_+ + A_-)^2} \\ &= A_+ + A_-.\end{aligned}$$

If $\alpha = \pi$ we get $\cos(\pi) = -1$, and find the lower bound

$$\begin{aligned}R_- &= \sqrt{A_+^2 - 2A_+A_- + A_-^2} \\ &= \sqrt{(A_+ - A_-)^2} \\ &= |A_+ - A_-|.\end{aligned}$$

6. Bounded solution

To find a bounded solution, we need to consider the angular rate in eq. (**??**). Specifically the square-root expression

$$\sqrt{\omega_0^2 - 2\omega_z^2}.$$

A bounded solution can be found when this expression is greater than zero. Meaning

$$\omega_0^2 > 2\omega_z^2.$$

We can now use the definition of ω_0 and ω_z^2 to find an expression related to the Penning trap parameters, and the particle properties, to get

$$\begin{aligned}\left(\frac{qB_0}{m}\right)^2 &> 2\frac{2qV_0}{md^2} \\ \frac{q^2B_0^2}{m^2} &> \frac{4qV_0}{md^2}.\end{aligned}$$

Appendix B: Values used in simulation

1. Specific analytical solution

To compare our implementation of the Penning trap and particle, we have to specify initial conditions of the system to compare with the analytical solution. The initial conditions of a particle with a single positive charge, can be found in table **??**.

$\mathbf{r}(0)$	$\dot{\mathbf{r}}(0)$
$x(0) = x_0$	$\dot{x}(0) = 0$
$y(0) = 0$	$\dot{y}(0) = v_0$
$z(0) = z_0$	$\dot{z}(0) = 0$

TABLE I. Initial values of a particle with a single charge q, and mass m, confined in a Penning trap.

Property	Value
B_0	$1.00T = 9.65 \times 10^1 \frac{u}{(\mu s)e}$
V_0	$25.0mV = 2.41 \times 10^6 \frac{u(\mu m)^2}{(\mu s)^2 e}$
d	$500\ \mu m =$

TABLE II. Default configuration of the Penning trap, where the value of T and V can be found in table **??**.

Property	Value	
q	$1.00T$	$9.65 \times 10^1 \frac{u}{(\mu s)e}$
m	$25.0mV$	$2.41 \times 10^6 \frac{u(\mu m)^2}{(\mu s)^2 e}$

TABLE III. Default configuration of the Penning trap, where the value of T and V can be found in table **??**.

n_k	Time steps	Step size
n_1	4000	0.0125
n_2	8000	0.00625
n_3	16000	0.003125
n_4	32000	0.0015625

TABLE IV. Number of steps used in a given simulation k, where the step size corresponds to $h_1 = 50/n_k \mu s$.

2. Numbers and units

Constant	Value	Unit
k_e (Coulomb)	1.38935333×10^5	$\frac{u(\mu m)^3}{(\mu s)^2 e^2}$
T (Tesla)	9.64852558×10^1	$\frac{u}{(\mu s)e}$
V (Volt)	9.64852558×10^7	$\frac{u(\mu m)^2}{(\mu s)^2 e}$

TABLE V. Value of the Coulomb constant (k_e), and the SI units for magnetic field strength (T) and electric potential (V). The base units are given by length in micrometre (μm), time in microseconds (μs), mass in (u), and charge in elementary charge (e).

Appendix C: Algorithm implementation and testing

1. Forward Euler

For a particle i, at time step j, the forward Euler method for a coupled system can be expressed as

$$\mathbf{r}_{i,j+1} = \mathbf{r}_{i,j} + h\frac{d\mathbf{r}_{i,j}}{dt} = \mathbf{r}_{i,j} + h\mathbf{v}_{i,j}$$
$$\mathbf{v}_{i,j+1} = \mathbf{v}_{i,j} + h\frac{\mathbf{v}_{i,j}}{dt} = \mathbf{v}_{i,j} + h\frac{\mathbf{F}(t_j, \mathbf{v}_{i,j}, \mathbf{r}_{i,j})}{m_i},$$

m_i is the mass of the particle, and h is the step length.

2. 4th order Runge-Kutta

For a particle i, at time step j, the 4th order Runge-Kutta method for a coupled system can be expressed as

$$\mathbf{v}_{i,j+1} = \mathbf{v}_{i,j} + \frac{h}{6}(\mathbf{k}_{\mathbf{v},1,i} + 2\mathbf{k}_{\mathbf{v},2,i} + 2\mathbf{k}_{\mathbf{v},3,i} + \mathbf{k}_{\mathbf{v},4,i}),$$
$$\mathbf{r}_{i,j+1} = \mathbf{r}_{i,j} + \frac{h}{6}(\mathbf{k}_{\mathbf{r},1,i} + 2\mathbf{k}_{\mathbf{r},2,i} + 2\mathbf{k}_{\mathbf{r},3,i} + \mathbf{k}_{\mathbf{r},4,i}),$$

where

$$\mathbf{k}_{\mathbf{v},1,i} = \frac{\mathbf{F}_i(t_j, \mathbf{v}_{i,j}, \mathbf{r}_{i,j})}{m_i},$$
$$\mathbf{k}_{\mathbf{r},1,i} = \mathbf{v}_{i,j},$$
$$\mathbf{k}_{\mathbf{v},2,i} = \frac{\mathbf{F}_i(t_j + \frac{h}{2}, \mathbf{v}_{i,j} + h\frac{\mathbf{k}_{\mathbf{v},1,i}}{2}, \mathbf{r}_{i,j} + h\frac{\mathbf{k}_{\mathbf{r},1,i}}{2})}{m_i},$$
$$\mathbf{k}_{\mathbf{r},2,i} = \mathbf{v}_{i,j} + h\frac{\mathbf{k}_{\mathbf{v},1,i}}{2},$$
$$\mathbf{k}_{\mathbf{v},3,i} = \frac{\mathbf{F}_i(t_j + \frac{h}{2}, \mathbf{v}_{i,j} + h\frac{\mathbf{k}_{\mathbf{v},2,i}}{2}, \mathbf{r}_{i,j} + h\frac{\mathbf{k}_{\mathbf{r},2,i}}{2})}{m_i},$$
$$\mathbf{k}_{\mathbf{r},3,i} = \mathbf{v}_{i,j} + h\frac{\mathbf{k}_{\mathbf{v},2,i}}{2},$$
$$\mathbf{k}_{\mathbf{v},4,i} = \frac{\mathbf{F}_i(t_j + h, \mathbf{v}_{i,j} + h\mathbf{k}_{\mathbf{v},3,i}, \mathbf{r}_{i,j} + h\mathbf{k}_{\mathbf{r},3,i})}{m_i}$$
$$\mathbf{k}_{\mathbf{r},4,i} = \mathbf{v}_{i,j} + h\frac{\mathbf{k}_{\mathbf{v},1,i}}{2}.$$

In order to find each $\mathbf{k}_{\mathbf{r},i}$ and $\mathbf{k}_{\mathbf{v},i}$, we need to first compute all $\mathbf{k}_{\mathbf{r},i}$ and $\mathbf{k}_{\mathbf{v},i}$ for all particles, then update the particle values in order to compute $\mathbf{k}_{\mathbf{r},i+1}$ and $\mathbf{k}_{\mathbf{v},i+1}$.

3. Test of implementation

We implemented a test suite, to validate the implementation during code development. In addition, we have implemented functionality to get informative output while testing the code. Further instructions with code can be found in the github repo [**?**].

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