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Numerical Simulation of Alpha Particle Scattering Based on the Symplectic Euler and Heun Methods

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Abstract: This paper constructs a two-dimensional numerical model of α-particle scattering based on Coulomb forces and compares simulations using the Rutherford concentrated-charge model and the Thomson uniform-charge model. The Symplectic Euler method and the Heun prediction-correction algorithm were employed to calculate particle trajectories, scattering angles, and energy changes, which were then validated against theoretical scattering angles. The results show that in the Rutherford model, the scattering angle exhibits an approximately linear relationship with 1/b, with a maximum deflection angle of approximately 160°; in the Thomson model, the overall deflection is weaker, and the scattering angle is generally less than 3 .5°. The Symplectic Euler method exhibits smaller energy fluctuations and superior long-term stability, while the Heun algorithm provides better trajectory fitting accuracy. This study establishes a general simulation framework applicable to charged part icle scattering processes, which can serve as a reference for classical scattering modeling and numerical calculations of conservative systems.

Keywords: Symplectic Euler Method, Heun Method, Coulomb Force Model.

1. Introduction

Numerical simulation of particle motion is a crucial aspect of computational physics, and its key lies in describing complex motion patterns through appropriate models and stable algorithms. When charged particles move in an electric field, their trajectories are influenced by factors such as charge distribution, initial velocity, and interaction range, often exhibiting distinct nonlinear characteristics. Therefore, establishing a reliable algorithmic framework is of great significance for improving simulation accuracy and result stability.

Existing research has primarily focused on the physical models themselves, with insufficient comparison of different numerical integration algorithms in terms of trajectory calculation, energy conservation, and long-term stability. Traditional algorithms are simple to implement but are prone to cumulative errors; while prediction-correction algorithms can improve local accuracy, they may lead to energy drift [1]. Therefore, it is necessary to establish a unified simulation method that balances accuracy and stability.

Taking α-particle scattering as an example, this paper constructs a two-dimensional numerical simulation framework based on Coulomb interactions, integrating the equations of motion, charge distribution models, and integration algorithms. By introducing the Symplectic Euler and Heun algorithms, calculations and comparisons are performed on particle trajectories, scattering angles, and energy variations under the Rutherford and Thomson models. The main contribution of this paper lies in the development of a general algorithmic framework applicable to charged particle scattering processes, which serves as a reference for the numerical simulation of conservative systems and the validation of related models.

2. Methodology

2.1. Construction of Scattering Physical Models Based on Charge Distribution

(1) Rutherford Nuclear Model

In the Rutherford model, the gold nucleus is simplified as a single fixed point charge located at the coordinate origin, with a charge of $q_g = 79 \times 1.6 \times 10^{-19}$ C. Since the mass of the gold nucleus is much larger than that of the incident particle, its motion is neglected, and only the motion of the incident α particle in the electrostatic field is considered [2, 3].

The α particle enters from position $[-x_0, b]$, where b is the impact parameter, with an initial velocity along the positive x-axis of $v_0 = 1.5 \times 10^7$ m/s. The particle has a charge of $q = 2 \times 1.6 \times 10^{-19}$ C and a mass of $m = 6.644 \times 10^{-27}$ kg. The particle trajectory is continuously tracked during the simulation until it leaves the predefined calculation region. Here, $x_0 = 10^{-12}$ m.

(2) Thomson Plum-Pudding Model

To simulate the Thomson "Plum-Pudding" atomic model, the nucleus region is represented as a square with a side length of 200 pm, in which $N \times N$ fixed point charges are uniformly arranged. All point charges together carry the total charge of the nucleus, and each point charge has the same charge.

In this model, the Coulomb force on the α particle is obtained by summing the contributions from all point charges. Since the positive charge is more spread out, the resulting electric field is smoother compared to the Rutherford model, and the particle scattering behavior is therefore different.

2.2. Governing Equations of Particle Motion Based on Coulomb Force

To simplify calculations, the influence of electron motion on the electric field is neglected, and only the electrostatic field generated by fixed positive charges is considered. A test particle with mass m and charge q moves in a two-dimensional plane, in a field containing N fixed point charges with charges q_i and positions $R_i = [x_i, y_i]$.

According to Coulomb's law, the net force on the test particle can be expressed as

$$F = kq\sum_{i=1}^{N}\frac{q_i(r-R_i)}{|r-R_i|^3} \tag{1}$$

Where $k = \frac{1}{4\pi\varepsilon_0}$ is the Coulomb constant, and r is the instantaneous position vector of the test particle.

The particle's motion follows Newton's equations:

$$\frac{dr}{dt} = v, \quad \frac{dv}{dt} = \frac{F}{m} \tag{2}$$

The potential energy of the system is

$$U(r) = kq\sum_{i=1}^{N}\frac{q_i}{|r-R_i|} \tag{3}$$

Thus, the total mechanical energy of the particle is

$$E = \frac{1}{2}mv^2 + U(r) \tag{4}$$

These equations form the basis for the numerical simulation of both atomic models.

2.3. Design of Symplectic Euler and Heun Methods

To calculate particle trajectories and their energy evolution, the Symplectic Euler method and Heun method are used for time integration.

The Symplectic Euler method belongs to symplectic integrators, which are characterized by their ability to preserve the system's symplectic structure over long-term calculations. This ensures that the total energy fluctuates around the true value without significant cumulative drift, making the method especially suitable for long-term numerical simulation of conservative systems [4].

The Heun method is a predictor–corrector type integration method. It first predicts the next state using the Euler method and then applies a correction step to improve accuracy. Compared to first-order integration schemes, the Heun method can describe particle trajectories more accurately, though some energy drift may still occur over long-term calculations [5].

2.4. Simulation Setup

To determine an appropriate time step, multiple steps in the range of $10^{-22} \sim 10^{-20}$ s were tested, and comparisons were made based on trajectory shapes and scattering angle errors. The final choices are a time step of 10^{-21} s for the Rutherford model and 10^{-20} s for the Thomson model. With this setting, the single-step displacement is much smaller than the characteristic scale of the model, balancing computational accuracy and efficiency.

The simulation stops when the particle leaves the calculation region. For the Rutherford model, the termination conditions are $|x| > 10^{-12}$ m or $|y| > 5\times10^{-13}$ m.

For the Thomson model, the termination conditions are $|x| > 2\times10^{-10}$ m or $|y| > 2\times10^{-10}$ m.

To verify the reasonableness of the numerical results, the scattering angle is calculated using the particle's velocity components when it leaves the calculation region:

$$\theta = \arctan\left(\frac{v_{y,\text{final}}}{v_{x,\text{final}}}\right) \tag{5}$$

For Rutherford scattering, the theoretical scattering angle is expressed as

$$\theta_{\text{theory}} = 2\arctan\left(\frac{kq_aq_g}{m_av_0^2b}\right) \tag{6}$$

Where q_a and m_a are the charge and mass of the α particle, respectively. Comparison between numerical and theoretical results is used to assess the accuracy of the integration methods and parameter settings.

3. Numerical Simulation Results and Algorithm Performance Analysis

3.1. Rutherford Scattering Simulation

From Figure 1, particle trajectories vary clearly with the impact parameter b. When b is small, the Coulomb force on the particle is more concentrated, causing a larger deflection. As b increases, the deflection angle gradually decreases. Comparing the two integration methods, the overall trajectory shapes are similar, but the Symplectic Euler method maintains slightly better trajectory stability during long-time integration.

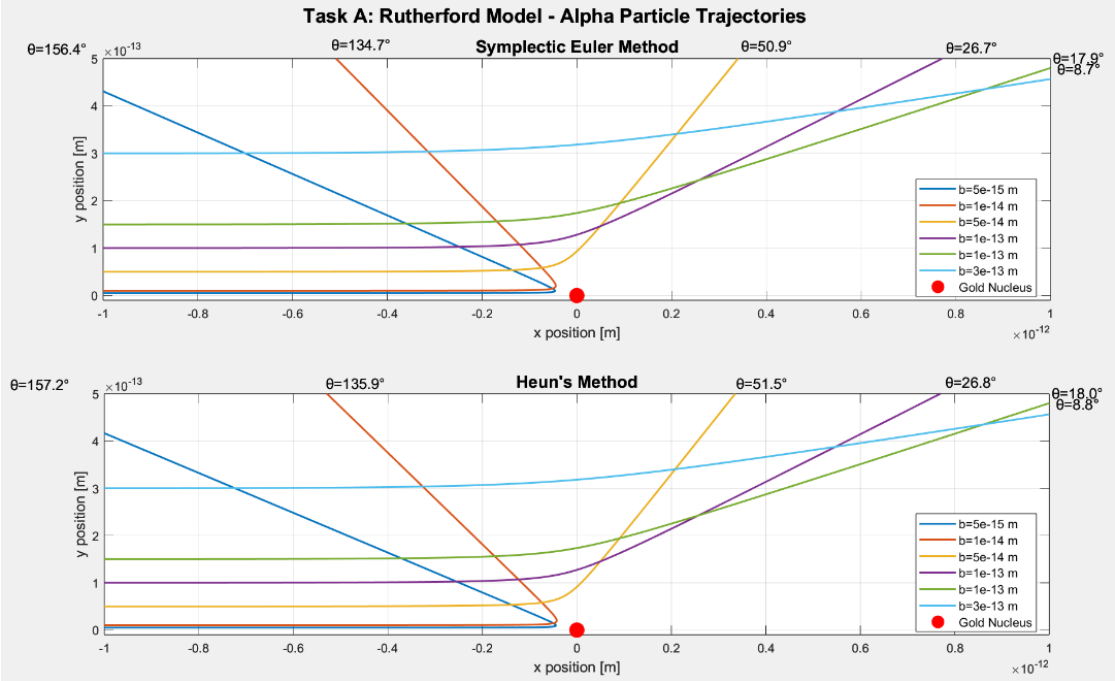

Figure 1. Alpha particle trajectories. Top: Symplectic Euler method. Bottom: Heun's method. Different line colors represent different values of b.

Figure 2 shows the relationship between the scattering angle θ and $1/b$, comparing both integration methods with the theoretical curve. It can be seen that, under the given parameters, the scattering angle is approximately proportional to $1/b$. The numerical results of both methods are very close to the theoretical prediction, indicating that the simulation reproduces the Rutherford scattering behavior well.

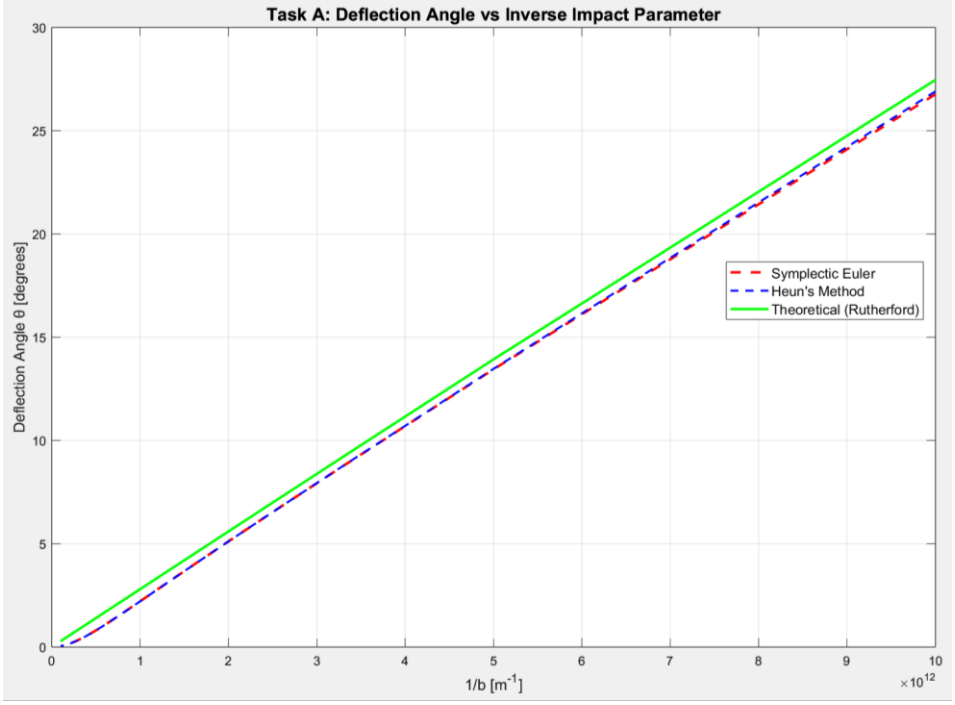

Figure 2. Relationship between the deflection angle and the inverse impact parameter. Green line represents the theoretical deflection angle. Red and blue lines represent the deflection angle under Symplectic Euler and Heun's method, respectively.

Figure 3 shows the energy variation of the system under different integration methods. Compared with the theoretical initial energy, the Symplectic Euler method keeps the total energy fluctuating within a small range, without obvious cumulative drift. The Heun method, however, shows gradually increasing energy drift in long-term simulations. This indicates that the Symplectic Euler method is more reliable for maintaining system energy stability [6].

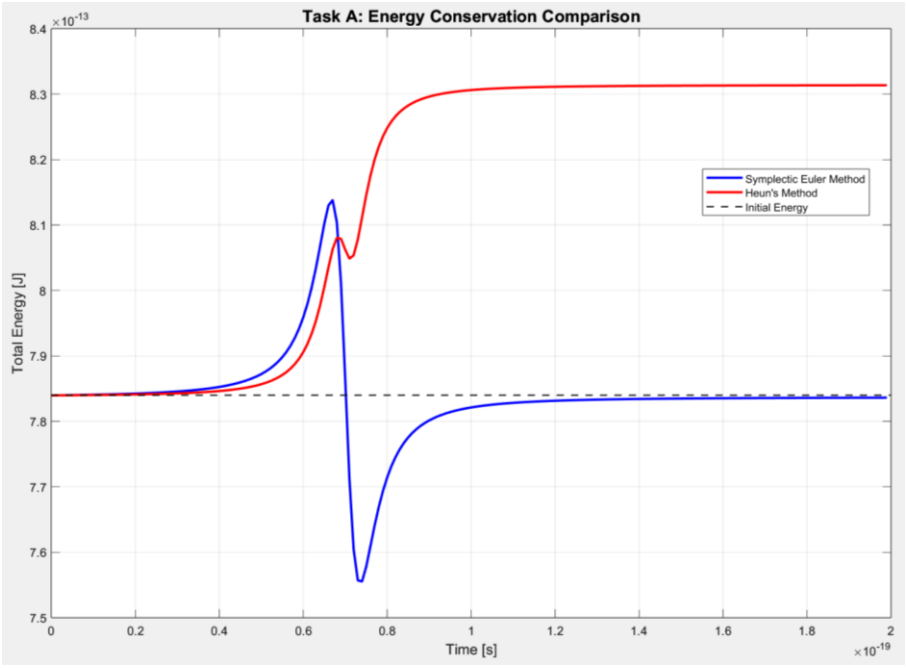

Figure 3. Energy conservation comparison. Black line represents the theoretical initial energy. Blue and red lines represent the total energy of the Symplectic Euler and Heun's method, respectively.

3.2. Thomson Plum-Pudding Simulation

Figure 4 shows the trajectories of α particles in the Thomson "Plum-Pudding" model. Compared with the Rutherford model, the particle deflection is significantly weaker. Even under small impact parameters, large-angle scattering does not occur. This is mainly because the positive charge is distributed across the grid region, making the electric field more spread out and reducing local field gradients, so the repulsive force on the particle is weaker. Overall, particle trajectories remain nearly straight, with only slight deflections when passing through charged regions.

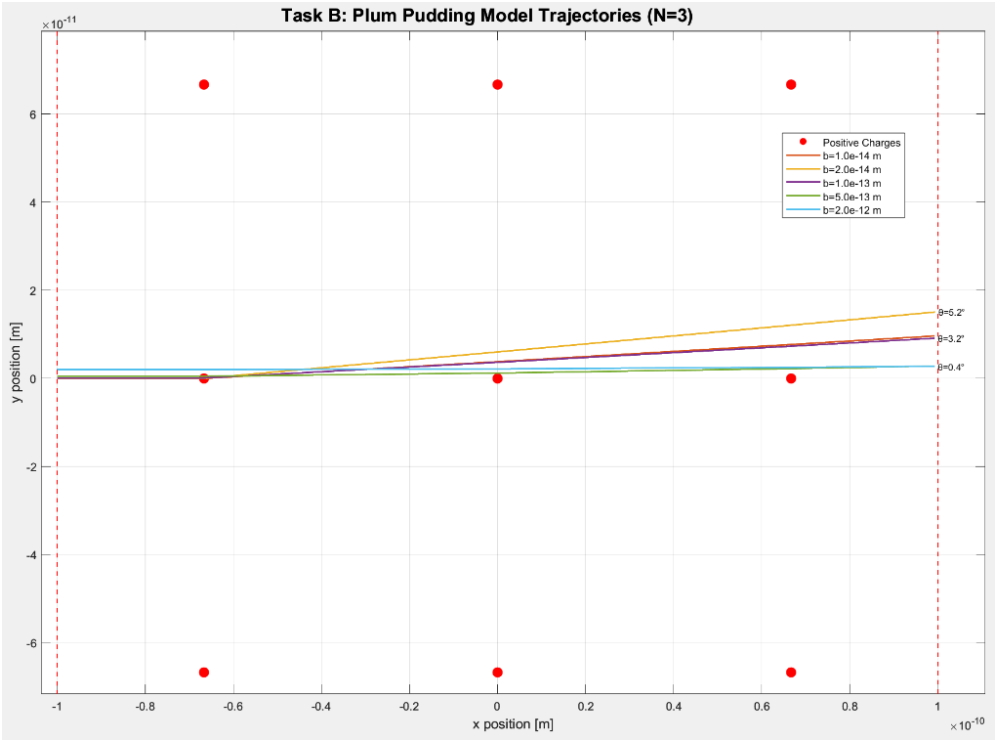

Figure 4. Alpha particle trajectories under the Symplectic Euler method. Different line colors represent different values of b.

Figure 5 shows the relationship between the scattering angle and the impact parameter, comparing results from the two integration methods with $N = 3$. As the impact parameter increases, the particle moves farther from the positive charge region, and the Coulomb force decreases, so the scattering angle continues to decrease.

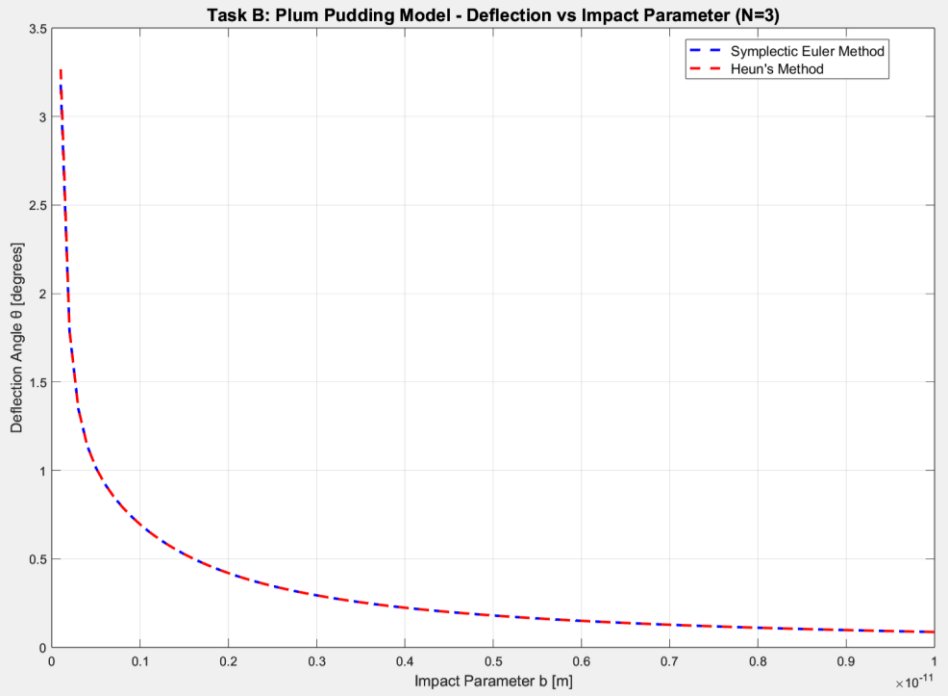

Figure 5. Relationship between the deflection angle and the inverse impact parameter. Blue and red lines represent the deflection angle under the Symplectic Euler and Heun's method, respectively.

The results from the two integration methods nearly overlap, indicating that numerical integration errors are small in this model and the simulation results are stable and consistent. Compared to the Rutherford model, the overall scattering angles are much smaller, further demonstrating that uniformly distributed positive charges produce weaker scattering effects.

Figure 6 shows the electric potential distribution for different grid densities. Overall, the potential field maintains good symmetry around the central region, with peaks near the positions of the positive charges. When $N = 1$, the model degenerates to a single point charge, and its potential distribution is similar to the point charge in the Rutherford model, with steep potential gradients.

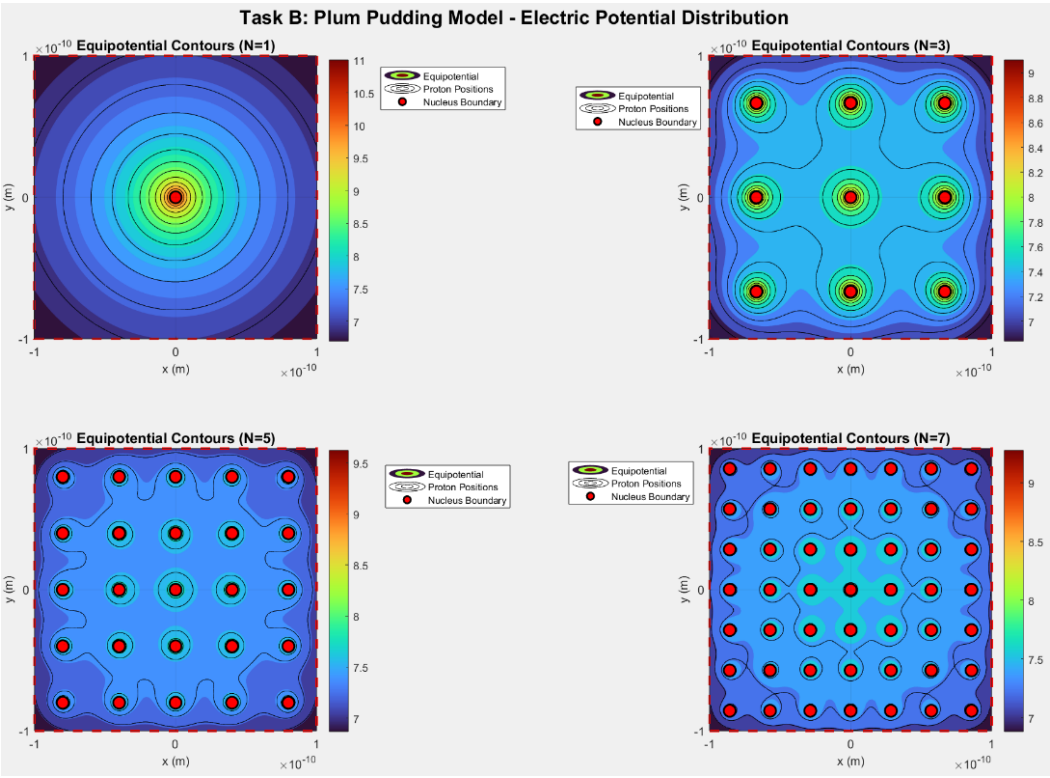

Figure 6. Electric potential distribution

As the grid density increases, the total charge is distributed among more point charges, the local potential peaks decrease, and the potential distribution becomes smoother. Meanwhile, the potential gradients become more uniform, meaning the forces experienced by particles during motion vary less. Therefore, scattering in the Thomson model is generally weak, and large-angle deflections like those observed in Rutherford scattering experiments are unlikely.

3.3. Comparative Analysis

A comparison of the simulation results from the Rutherford model and the Thomson "Plum-Pudding" model shows that the two atomic structure hypotheses lead to very different scattering behaviors.

In the Rutherford model, the positive charge is concentrated near the nucleus, creating a strong electric field in a localized region. When an α particle approaches the nucleus, it experiences significant Coulomb repulsion, resulting in large trajectory deflections. For small impact parameters, scattering can even approach backward reflection. Figures 1 and 2 both show that this model reproduces the large-angle scattering observed in the classical Rutherford scattering experiment.

In contrast, the positive charge in the Thomson model is distributed uniformly throughout the grid region. As the charge becomes more spread out, the local electric field strength is greatly reduced, and the force acting on the particle changes more gradually during its motion. As a result, even for small impact parameters, particle trajectories remain close to straight lines and only undergo limited deflection. Figures 4 and 5 show that the scattering angle remains small throughout the simulation, with no large-angle scattering comparable to that seen in the Rutherford model.

The difference between the two models is also clear from the potential distribution. Figure 6 shows that as the grid density increases, the potential distribution becomes progressively smoother and the electric field gradient continues to decrease. This more uniform field structure further limits particle deflection and is one of the main reasons why the Thomson model cannot account for large-angle scattering.

For the numerical integration methods, both approaches predict particle trajectories and scattering angles with good accuracy, and their results are generally consistent. However, their energy conservation performance differs. As shown in Figure 3, the Symplectic Euler method keeps the total system energy fluctuating around the theoretical value, with no obvious long-term drift. The Heun method, although offering higher local accuracy, shows a gradual deviation of the system energy from its initial value as the integration time increases.

Overall, the Rutherford model is more consistent with the experimentally observed large-angle scattering behavior, whereas the Thomson model produces only weak deflection effects. For numerical calculations, the Symplectic Euler method shows better long-term stability, while the Heun method offers some advantages in trajectory accuracy. Both methods can effectively simulate the scattering process, although their strengths differ depending on the application.

4. Discussion

4.1. Physical Interpretation

In the Rutherford model, the positive charge of the nucleus is highly concentrated, creating a strong electrostatic field. When an α particle approaches the nucleus, it experiences significant repulsion, leading to large-angle deflections at small impact parameters, and even near-backward scattering. This is consistent with classical Rutherford experiment results (see Figure 1). In contrast, in the Thomson "Plum-Pudding" model, the positive charge is distributed uniformly across the grid, resulting in a smoother electric field with smaller local gradients. As a result, the particle deflection remains small during passage, and even with increased impact parameters, large-angle scattering does not occur (see Figures 4 and 5).

4.2. Numerical Performance

The performance of the two integration methods varies slightly across models. The Symplectic Euler method updates positions using the updated velocity, which allows the total system energy to fluctuate slightly around the theoretical value, preventing significant cumulative drift during long-term simulations. Although its local trajectory accuracy is lower than that of the Heun method, its long-term energy stability is clearly better. The Heun method improves trajectory accuracy through its predictor–corrector steps but may still experience energy drift in long-term integration (Figure 3). Overall, Symplectic Euler is more stable for energy conservation, while Heun is preferable in scenarios requiring higher trajectory accuracy.

In the Thomson model, because the electric field is smooth and weaker, energy fluctuations are naturally smaller, yet Symplectic Euler still shows better stability. The Heun method exhibits slight drift, but the impact of long-term drift decreases as the grid density increases. Computational efficiency differences between the two methods are minimal; Symplectic Euler is slightly faster, but the difference is negligible for the scale of this study.

4.3. Sensitivity Analysis

Simulation results are sensitive to the time step. Figures 7 and 8 show that increasing the step from 1×10^{-21} s to 6×10^{-21} s leads to noticeable increases in energy deviation and scattering angle errors. Reducing the time step improves numerical accuracy but increases computation time, and for the precision required in this study, excessively small steps offer limited advantage. In the Rutherford model, the simulation region must be large enough to fully capture the trajectory, while in the Thomson model, the calculation region is determined by the nucleus size (200×200 pm).

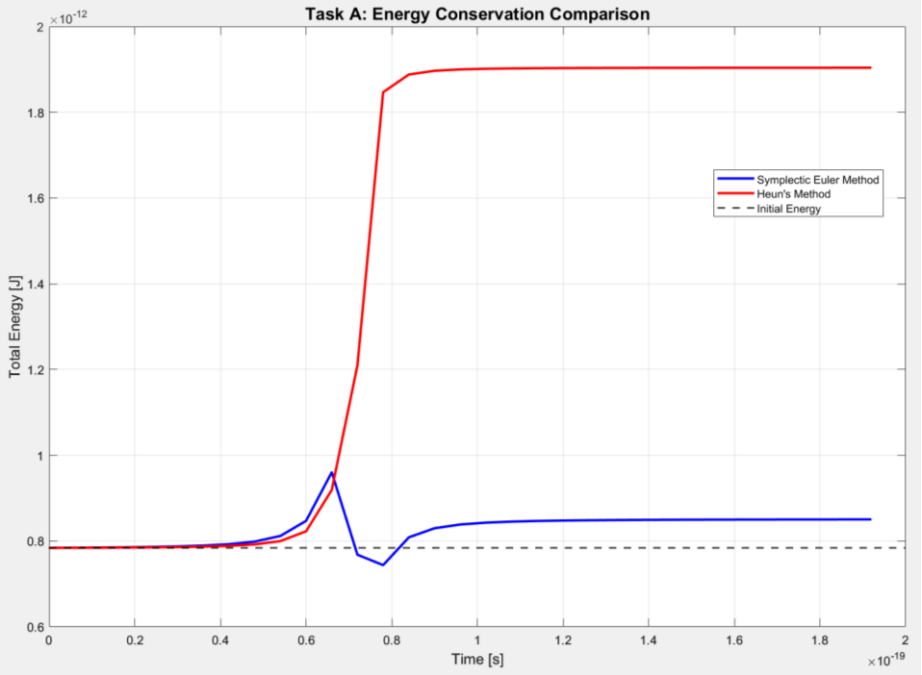

Figure 7. Energy conservation comparison (change the timestep)

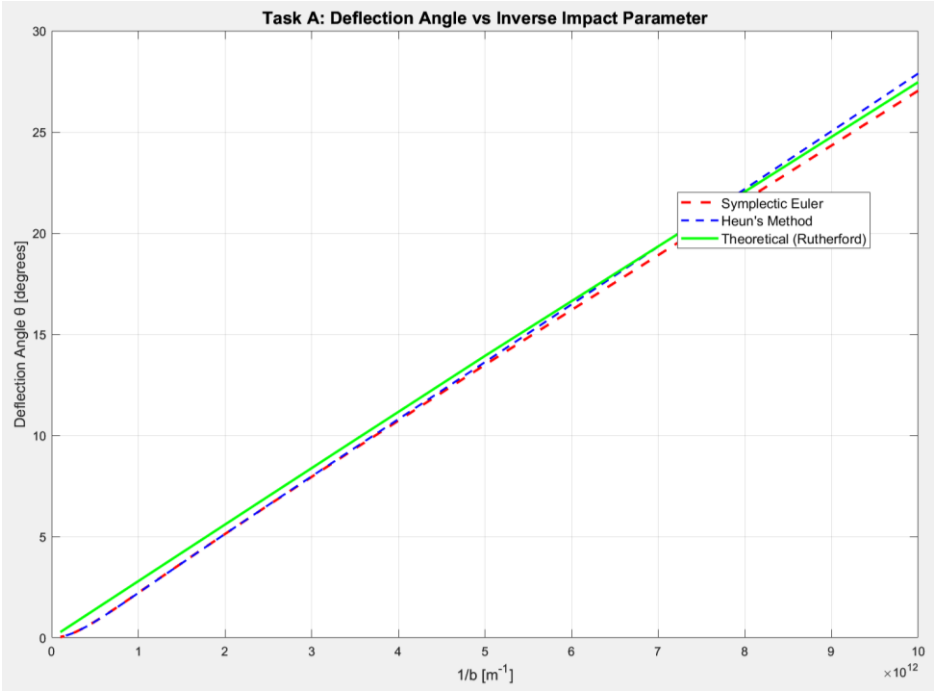

Figure 8. Deflection angle (change the timestep)

5. Conclusions

This paper establishes a numerical model for α-particle scattering based on Coulombic interactions and uses the Symplectic Euler and Heun algorithms to simulate different charge distribution structures. The results show that the Rutherford model produces a large deflection angle of approximately 160°, reflecting the scattering characteristics of a concentrated charge structure; in contrast, the Thomson model yields scattering angles generally below 3.5°, with relatively weak particle trajectory deflection. A comparison of the algorithms reveals that the Symplectic Euler method performs better in terms of energy conservation and long-term stability, while the Heun algorithm has certain advantages in local trajectory calculations. The study demonstrates that a unified numerical simulation framework can effectively analyze particle motion patterns under different models, providing a reference for charged particle scattering calculations and algorithm selection. Future research could be further extended to three-dimensional scenarios and multi-particle interaction processes.

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