NUMERICAL INTEGRATOR FOR COULOMB COLLISIONS

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Abstract

The trajectories of protons interacting through Coulomb forces were computed using a numerical integrator based on Picard's iteration method. This is a variable order, adaptive integrator with dense output. We show different cases by varying some parameters such as the impact parameter, the relative velocity of the protons and the order of the differential algebraic (DA) vector. The accuracy of the trajectories was tested by changing the order of the DA vector while fixing the other parameters. The impact parameter between the protons and the velocity of the incident proton has the most impact on the trajectories. The maximum time step is determined by the radius of convergence of the expansions, while a fixed accuracy is attained by varying the order.

INTRODUCTION

Many physical phenomena involve N bodies (particles) interacting with one another by long range forces which decrease inversely as the square of the distance. Examples include the gravitational interaction among the stars in a galaxy, and the Coulomb forces between charges. Many particle systems have wide range of applications in different areas such as biophysics, chemistry, astrophysics [1], etc.

This work includes the two-body problem, in which two charges interact through Coulomb forces. Coulomb's law describes the force between two point charges by the following equation:

$$\overrightarrow{F} = \frac{1}{4\pi\varepsilon_o}\frac{q_1 q_2 \vec{r}}{|\vec{r}|^3},$$

where $\overrightarrow{F}$ is the force, q is the charge, $\vec{r}$ is the radial distance between the two charges, and ε_o is the permittivity of free space.

It is complicated to solve the N-body problem numerically due to the singularity of very close encounters where $|\vec{r}| \to 0$ (very strong interaction $\overrightarrow{F} \to \infty$), and the requirements of high precision with violently varying time steps that are necessary to reduce errors to acceptable levels.

We consider the interaction between two protons in two dimensions. The first proton is initially at rest, and the second proton is moving horizontally towards the first one with a specific vertical distance between them. According to Coulomb's law, the electrostatic force between two similar charges is repulsive.

The integrator has applications in electron cooling of heavy ion beams, and any other beam dynamics problem where individual collisions need to be resolved.

ALGORITHM

To compute the trajectories of both of the protons, we used a code developed by us via COSY INFINITY [2]. The code is a numerical integrator based on Picard's iteration method (see [3] for details). Picard's method uses the initial conditions of the system and gives a sequence of functions that converge to the solution. This method can compute completely algebraically the Maclaurin polynomial (Taylor series expansion of a function about zero).

In this program, the Maclaurin polynomial of the solution is represented by DA vectors. The DA vector is an array of elements that describe a multi-variable function when given its value and derivatives at a specific point [4]. The integrator order is equivalent to the DA order, and we can vary this order to the one that we want to truncate the Taylor series at. At each time step, the program evaluates the change of the radius between the particles and compares it with the one at the next time step. Whenever the convergence radius is exceeded, the program will display an error message.

The maximum velocity (β_{max}) used for the incident proton is 0.283. Different fractions of this velocity were used as well. The initial horizontal distance between the protons was varied from 10^{-15}-10^{-9} m. The impact parameter (vertical distance between the particles) was varied from 10^{-15}-10^{-11} m. It is possible to use larger distances (horizontal or vertical), but the strong interactions are localized within these distances. Hence, larger distances would result into very small changes in the positions of the protons that would be hard to see.

EXAMPLES

The parameters of the system will be denoted as follows: d = horizontal distance (m), b = vertical distance (m), δt = time interval ($1/c$ s), N = number of time steps, and the DA order was set to be 4 unless specified otherwise.

Example 1

The impact parameter and the moving proton's velocity are fixed at 10^{-15} m and 10% β_{max}, respectively. The other parameters are varied in two instances:

- The parameters are: d = 10^{-15} m, N =10^4, δt = 3.6 × 10^{-17} $1/c$ s. The trajectories are shown in Fig. 1.
- Fig. 2 shows the protons' paths with the parameters: d = 10^{-10} m, N = 5.5 × 10^4, δt = 10^{-13} $1/c$ s.

The resulted trajectories in this example are as one would expect due to the Coulomb's interaction.

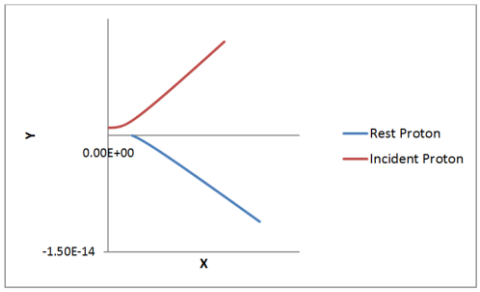

Figure 1: The paths of the protons from Ex. 1 where d = 10^{-15} m and the trajectories are as predicted by the Coulomb interaction.

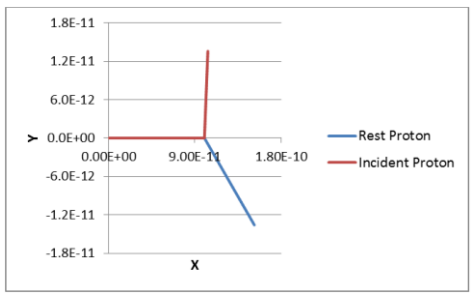

Figure 2: Ex. 1 paths of the protons when d is relatively large (10^{-10} m). The incident proton moves straight horizontally until very close to the rest proton where they start to interact.

Example 2

The horizontal distance is fixed at d = 10^{-12} m and the incident proton has high velocities in the two cases included here:

- The parameters are: b = 10^{-14} m, β = β_{max}, N = 5 × 10^4, δt = 3 ×10^{-16} 1/*c* s. In this case, the rest proton follows a parabolic path for a very short time, and then moves downward (see Fig. 3). This could be a result of the incident proton having a very high velocity such that it knocks the other proton down while its path deviates upward.

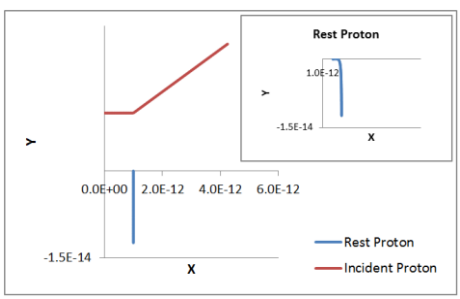

Figure 3: The rest proton moving downward when the moving proton has very high velocity (Ex. 2). The inset shows the parabolic path of the rest proton.

- In this example: b = 10^{-12} m, β = 50% β_{max}, N = 7 × 10^4, δt = 10^{-13} 1/c s. This is one of the cases in which the rest proton exhibited unexpected behavior. It moves downward for a very short interval, and then it starts to recoil and goes backward (as shown in Fig. 4). However, this behavior is very un-noticeable such that it appears like the proton is just going vertically down (as shown in Fig. 5).

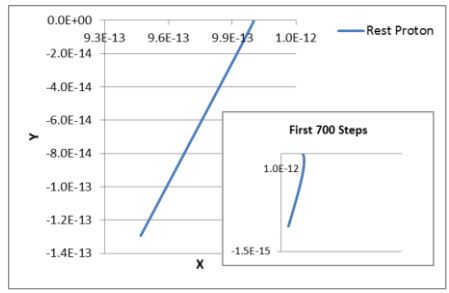

Figure 4: The path of the rest proton going backwards. In the small box, the first 700 steps shows the recoiling.

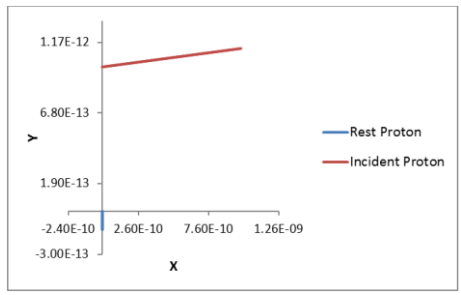

Figure 5: The proton at rest going downward with the un-noticeable recoiling when the moving proton has a relatively high velocity.

ACCURACY TESTS

To check the accuracy of the computed trajectories, we varied the order of the DA vector and the time interval in two ways, as described next.

Fixing the time interval

We used a small δt and different orders of the DA vector. If the trajectory of a low DA order is the same as the trajectory of a higher DA order, then the chosen time interval is sufficiently small to get accurate paths. The other parameters in this example are: d = 10^{-12} m, b = 10^{-13} m, β = 10% β_{max}, N = 6 × 10^4. Fig. 6 shows this accuracy for δt on the order of 10^{-15} 1/*c* s, in which the trajectory with the DA order of 4 is exactly the same as the one with the DA order of 20.

Changing the time interval

We used various time intervals with a specific order of the DA vector. We increased δt until the new trajectory diverges from the accurate one (with small δt) of the same order. We fixed the other parameters at: d = 10^{-12} m, b = 10^{-13} m, β = 10% β_{max}. The number of time steps was changed according to the change of δt.

Since the code we are using tests for errors of the radius of convergence, we include two cases:

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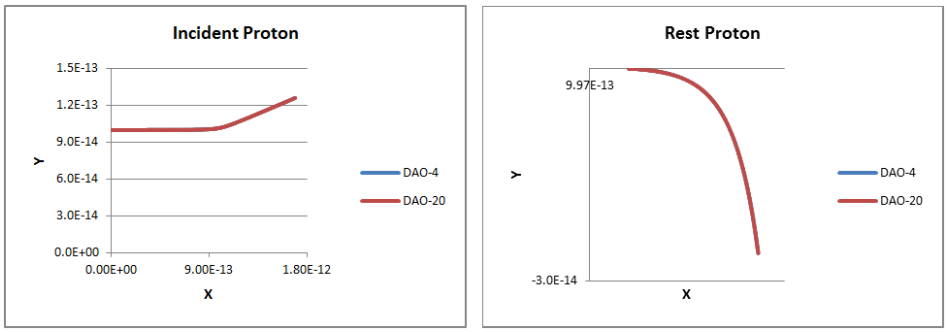

Figure 6: The accuracy test by fixing the time interval and varying the DA order. The paths of the incident proton and the rest proton are illustrated in the left and right pictures, respectively.

- δt is large, but not such that we get errors. Here are two examples with DA order = 4 and 20. In both examples, the trajectory of the moving proton was not affected by changing δt. Therefore, we show only the paths of the rest proton in Fig. 7. For DA order = 4, the paths with large δt start to diverge from the ones with small δt. For DA order = 20, both paths are almost the same.

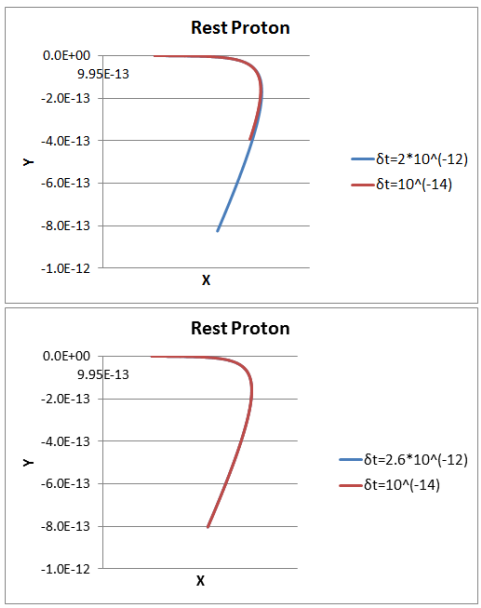

Figure 7: The paths of the rest proton with large δt (in blue), and with small δt (in red). The DA order is 4 in the top box, and 20 in the bottom one.

- Beyond the radius of convergence errors. The resulted trajectories are unphysical and inaccurate. It is hard to explain these results, and the only reason might be the errors of the radius of convergence. Fig. 8 is an example where the DA order is 18.

SUMMARY

Using a numerical integrator based on Picard's iteration method, we computed the trajectories of two protons interacting through the Coulomb force. Our main interest was in close encounters of the protons. We showed different examples by changing different parameters in the problem. The results are in agreement with the theory: to obtain certain accuracy most efficiently, a maximum step size is determined by the region of convergence, and the desired accuracy is achieved by increasing the DA order with the given maximum time step. Also, these results will enable us to automatically adjust the time step adaptively, as needed. More studies are needed to get better understanding of the results. A future work is to apply similar studies for the attracting case (proton-electron interaction).

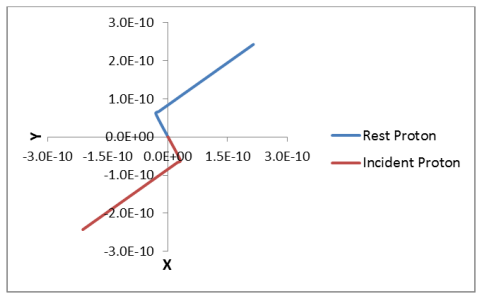

Figure 8: The unphysical results from having large time interval such we get radius of convergence errors.

ACKNOWLEDGMENT

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