Non-relativistic charged particle motion in the electric and magnetic fields using the Runge-Kutta-Nyström method

Indrek Mandre <indrek@mare.ee>
http://www.mare.ee/indrek/

September 29, 2007

1   Problem of particle motion

We intend to numerically simulate the motion of a charged particle in the magnetic and electric fields. Let the position of the particle be $\vec{x}$, its mass m and its charge q. The speed and acceleration of the particle are defined like this:

$$
\begin{aligned}
\vec{x}' &= \vec{v} \\
\vec{v}' &= \vec{a} = \frac{\vec{F}}{m}
\end{aligned}
$$

Lorentz force equation for a charged particle stands

$$
\vec{F} = q\left(\vec{E} + \vec{v}\times\vec{B}\right)
$$

We have here what is called an initial value problem. We have the position and speed of the particle at the initial position and we want to calculate the next position after time $h = \Delta t$, then the next position from that and so on.

2   Runge-Kutta-Nyström method

Lets use the Runge-Kutta-Nyström method to solve the second-order ordinary differential equation intial value problem for particle motion. This is a modification of the fourth-order Runge-Kutta method (RK4). The general problem is given as

$$
y'' = f(y', y, x)
$$

and the formulae as per Bock[1] stand as

---

[1]"The Data Analysis BriefBook", R.K.BOCK, W.KRISCHER, http://rkb.home.cern.ch/rkb/titleA.html

$$
\begin{aligned}
y(x+h) &= y(x) + hy'(x) + \frac{h^2}{6}(K_1 + K_2 + K_3) + O(h^5) \\
y'(x+h) &= y'(x) + \frac{h}{6}(K_1 + 2K_2 + 2K_3 + K_4) + O(h^5) \\
K_j &= f(y'_j, y_j, x_j) \quad \text{for} \quad j = 1,2,3,4 \\
x_1 &= x, \; x_2 = x_3 = x + \frac{h}{2}, \; x_4 = x + h \\
y_1 &= y(x), \; y_2 = y_3 = y(x) + \frac{h}{2}y'(x) + \frac{h^2}{8}K_1 \\
y_4 &= y(x) + hy'(x) + \frac{h^2}{2}K_3 \\
y'_1 &= y'(x), \; y'_2 = y'(x) + \frac{h}{2}K_1, \; y'_3 = y'(x) + \frac{h}{2}K_2 \\
y'_4 &= y'(x) + hK_3
\end{aligned}
$$

3 The solution

The force function depends on two parameters - position and speed - time is not involved:

$$
\vec{F}(\vec{x}, \vec{v}) = q\left(\vec{E}(\vec{x}) + \vec{v} \times \vec{B}(\vec{x})\right)
$$

Lets use index 0 for starting position and 1 for the next position. For better reading I omit the vector signs here. We have:

$$
\begin{aligned}
x_1 &= x_0 + hv_0 + \frac{h^2}{6}(K_1 + K_2 + K_3) \\
v_1 &= v_0 + \frac{h}{6}(K_1 + 2K_2 + 2K_3 + K_4)
\end{aligned}
$$

The coeffcients come out like this:

$$
\begin{aligned}
K_1 &= \frac{1}{m}F(x_0, v_0) \\
K_2 &= \frac{1}{m}F(x_0 + \frac{h}{2}v_0 + \frac{h^2}{8}K_1, \; v_0 + \frac{h}{2}K_1) \\
K_3 &= \frac{1}{m}F(x_0 + \frac{h}{2}v_0 + \frac{h^2}{8}K_1, \; v_0 + \frac{h}{2}K_2) \\
K_4 &= \frac{1}{m}F(x_0 + hv_0 + \frac{h^2}{2}K_3, \; v_0 + hK_3)
\end{aligned}
$$

The fields in K_2 and K_3 are evaluated at the same position. Additionally the position in K_4 is very close to x_1, that means the field value there can be reused at the start of the next step's K_1. This means that we need only two field evaluations per step.

4 Runge-Kutta step size

Runge-Kutta can be used with a variable step size as the current step is always the first and there is no dependance on the previous step distances. Errors will increase in areas where the field changes quickly. So it makes sense to reduce the step size in areas where the field changes quickly and increase it where the field stays the same - in this way we reduce errors but will not do too many unnecessary calculations. Here are some of my ideas on what can be done.

The first idea would be to make sure the covered distance $|v|\Delta t$ is not too great. The field is not likely to change a lot in a short distance. If the distance is greater than a given threshold, divide Δt by 2 and do two steps in those time increments instead of one (and so on).

Another idea would be to calculate the factor

$$\frac{|K_1 - K_2|}{|K_1|}$$

This factor indicates change in the acceleration vector and can be used to dynamically increase or decrease substeps calculated within a timestep.

Figure 1: Here you can see the path of an electron in the cube polywell with a constant timestep. Red indicates the area where relative errors are greatest. It appears the error is greatest when the electron bounces off the magnetic mirror or penetrates it.
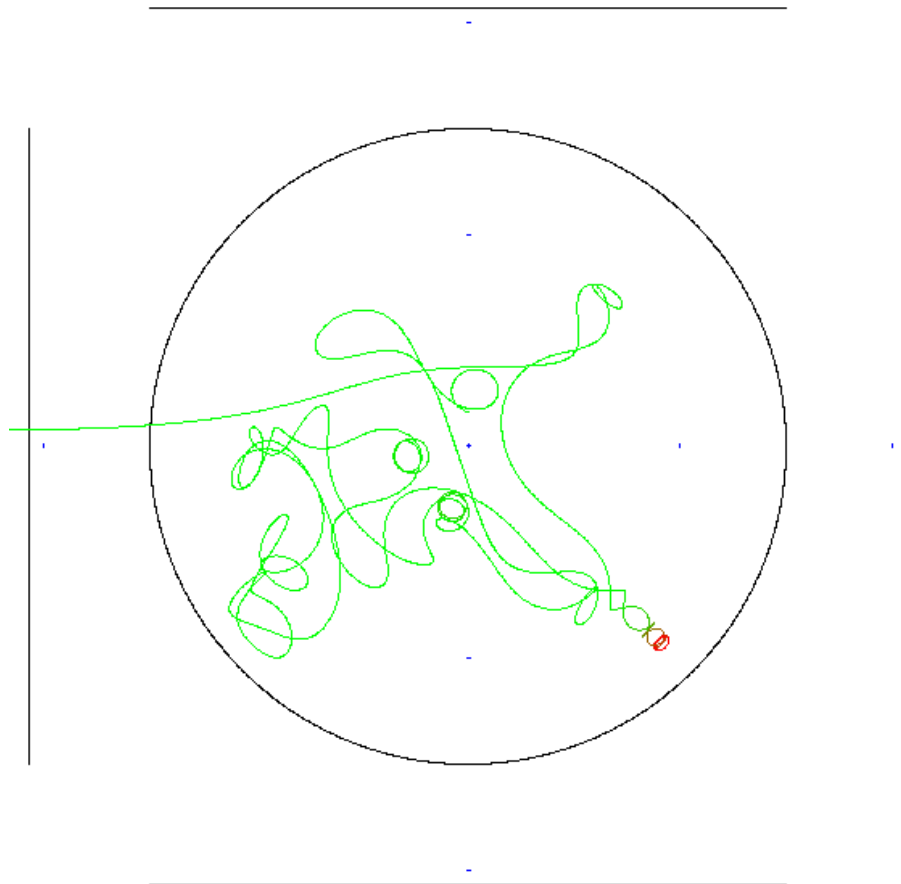
5 Disclaimer

The author of this document is not a physicist nor a mathematician and so is an amateur. The information in this document is provided in the hope it will be useful, but the author takes no responsibility for any errors or problems you may encounter.