TRAJECTORY ACCURACY IMPROVEMENT OF LORENTZ GROUP LIE ALGEBRA MAPPING FOR CHARGED PARTICLE MOTIONS

H.Kawaguchi, Muroran Institute of Technology
27-1, Mizumoto-cho, Muroran 050-8585, Japan

Abstract

The author presented a numerical integrator for charged particle motions, which was based on the Lorentz group Lie algebra, [1][2], and it was shown that the integrator gave us quite precise results in integrating the particle energy and momentum owing to the Lie algebra property. In general, one of difficulties of popular symplectic integrators is that vector potential expression of electromagnetic fields is required in the formulation. This is especially serious in case of particle simulations in 3D magnetic field. The presented integrator shows advantage in this situation too, because it does not include any vector potential expression in the formulation. On the other hand, the Lie algebra property did not guarantee the trajectory accuracy and this sometime caused accuracy degradation on the trajectory calculation. In this paper, a method of trajectory accuracy improvement of the integrator is presented. Beyond this improvement, we can construct quite precise integrator especially for high energy charged particle motions.

1 INTRODUCTION

Owing to remarkable performance progress of computers, we do not need to care about the memory size and CPU time in many situations of computer simulations of physical phenomena. And this trend seems to be continued for the next several years too. In that situation, main interests of computer simulations is accuracy improvement. Especially, quite high accuracy simulations are often required in advanced technologies. The author presented a numerical integrator for charged particle motions, which was based on the Lorentz group Lie algebra. [1][2] To include the Lie algebra property into the numerical integration, quite high accuracy of energy and momentum calculation was achieved. In addition, one of difficulties of popular symplectic integrators is that vector potential expression of electromagnetic fields is required in the formulation. This is especially serious in case of particle simulations in 3D magnetic field. The presented integrator shows advantage in this situation too, because it does not include any vector potential expression in the formulation. On the other hand, the Lie algebra property did not guarantee the trajectory accuracy and this often caused accuracy degradation on the trajectory calculation. In this paper, trajectory accuracy improvement of this integrator based on the Gauss-Legendre interpolation formula is presented. Beyond this improvement, we can construct quite precise integrator especially for high energy charged particle motions.

2 LORENTZ GROUP LIE ALGEBRA MAP OF CHARGED PARTICLE MOTION

In the four dimensional covariant form, the Lorentz force equation of motion is written as follows,

$$mc\frac{du^k(s)}{ds} = e\,F^k{}_j\,u^j(s) \tag{1}$$

where u^k is the four velocity, F_{ik} is the electromagnetic fields tensor, m is particle mass, e is the elementary charge, c is the velocity of light and ds = c d (is the particle proper time). Then it is known that the u^k satisfies the following identity,

$$u^i u_i = 1 \tag{2}$$

This implies that Eq.(1) should have the Lorentz group Lie algebra property which guarantees the Minkowski norm conservation of u^k during the transformation with respect to the parameter s . This Lie algebra property of Eq.(1) is readily confirmed to express the field tensor as follows,

$$F^k{}_j = \left(\frac{\mathbf{E}}{c}\right)\bullet\mathbf{K} - \mathbf{B}\bullet\mathbf{S} \tag{3}$$

where **E** and **B** are electric and magnetic fields, **S** and **K** are so-called “rotational” and “boost” operators, and which are consists of irreducible representation of the Lorentz group Lie algebra.

$$[\mathbf{K}]^k{}_j = \left[\begin{pmatrix}0&1&0&0\\1&0&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix}, \begin{pmatrix}0&0&1&0\\0&0&0&0\\1&0&0&0\\0&0&0&0\end{pmatrix}, \begin{pmatrix}0&0&0&1\\0&0&0&0\\0&0&0&0\\1&0&0&0\end{pmatrix}\right] \tag{4-1}$$

$$[\mathbf{B}]^k{}_j = \left[\begin{pmatrix}0&0&0&0\\0&0&0&0\\0&0&0&-1\\0&0&1&0\end{pmatrix}, \begin{pmatrix}0&0&0&0\\0&0&0&1\\0&0&0&0\\-1&0&0&0\end{pmatrix}, \begin{pmatrix}0&0&0&0\\0&0&-1&0\\0&1&0&0\\0&0&0&0\end{pmatrix}\right] \tag{4-2}$$

In case that the electromagnetic fields are uniform and constant in time, Eq.(1) can be analytically solved as follows,

$$u^k(s) = \exp\left(\frac{e}{mc}F^k{}_j\,s\right)u^j(0) \tag{5}$$

For nonuniform or varying fields, Eq.(5) should be numerically calculated to take the parameter s enough small ds,

$$\begin{aligned} u^k(s+ds) &= \int_0^{ds}\frac{e}{mc}F^k{}_j u^j(s)\,ds \\ &\cong \exp\left(\frac{e}{mc}F^k{}_j\,ds\right)u^j(s) \end{aligned} \tag{6}$$

The physical meaning of the identity (2) is just consistency between the particle energy and momentum,

$$\left(\frac{\mathbf{E}}{c}\right)^2 - \mathbf{p}^2 = m^2c^2 \tag{7}$$

and the Lie algebra property included in Eq.(5) guarantee this important physical property even in discretized form of Eq.(6). In this case, the fields F_{ik} are taken to be constant during the small interval ds, therefore the 4D coordinate $x^k(s)$ is analytically calculated by using the expression of the four velocity $u^k(s)$ as follows,

$$x^k(ds) = x^k(0) + ds\, u^k(0) + \frac{ds^2}{2}\frac{e}{mc}F^k{}_j\, u^j(0) + \frac{ds^3}{3!}(\frac{e}{mc})^2\, F^k{}_l F^l{}_j\, u^j(0) + \cdots\cdots \tag{8}$$

Finally to unify Eqs.(6) and (8), we can express this integrator in the following form of transfer matrix,

$$\begin{bmatrix} x^k(s+ds) \\ u^k(s+ds) \end{bmatrix} = \begin{bmatrix} 1 & \int_0^{ds} \exp\left(\frac{e}{mc}F^k{}_j\, s\right)ds \\ 0 & \exp\left(\frac{e}{mc}F^k{}_j\, ds\right) \end{bmatrix} \begin{bmatrix} x^k(s) \\ u^k(s) \end{bmatrix} \tag{9}$$

On the other hand, the Taylor expansion expression of $x^k(ds)$ around $x^k(0)$ is as follows,

$$\begin{aligned} x^k(ds) &= x^k(0) + ds\,\frac{dx^k(0)}{ds} + \frac{ds^2}{2}\frac{d^2x^k(0)}{ds^2} + \frac{ds^3}{3!}\frac{d^3x^k(0)}{ds^3} + \cdots\cdots \\ &= x^k(0) + ds\, u^k(0) + \frac{ds^2}{2}\frac{e}{mc}F^k{}_j\, u^j(0) + \frac{ds^2}{3!}\left[(\frac{e}{mc})^2\, F^k{}_l F^l{}_j + \frac{e}{mc}\frac{dF^k{}_j}{ds}\right]u^j(0) + \cdots\cdots \end{aligned} \tag{10}$$

therefore in comparison with Eq.(8) one can find that Eq.(9) has at most the second order accuracy in the approximation of $x^k(ds)$. And then accuracy degradation in $x^k(ds)$ is directly connected to accuracy of $u^k(ds)$ too. This means that any improvement of accuracy of $x^k(ds)$ is essential for the formula (9).

3 EVALUATION BY GAUSS-LEGENDRE INTERPOLATION FORMULA

Under the condition that the Lorentz group Lie algebra property should be conserved, unique possibility of accuracy improvement is evaluation of electromagnetic fields **E** and **B** at an appropriate point $x^k(s')$ ($0 < s' < ds$). Mathematically speaking, this appropriate evaluation is just corresponding to appropriate selection of integral parameter as in the mean value theorem,

$$^\exists\xi,\quad \int_a^b \varphi(x)f(x)dx = \varphi(\xi)\int_a^b f(x)dx \tag{11}$$

From this mathematical point of view, we shall here determine the evaluation point of **E** and **B** by using the Gauss-Legendre interpolation formula. In standard Runge-Kutta methods for the Hamilton systems,

$$\frac{d\mathbf{x}}{dt} = \frac{\partial H}{\partial \mathbf{p}} \tag{12-1}$$

$$\frac{d\mathbf{p}}{dt} = -\frac{\partial H}{\partial \mathbf{x}} \tag{12-2}$$

the numerical integration is performed in the following formula, [3]

$$\mathbf{X}_n = \mathbf{X}_{n-1} + \Delta t \sum_s \gamma_s \mathbf{F}(\mathbf{Y}_s) \tag{13-1}$$

$$\mathbf{Y}_k = \mathbf{X}_{n-1} + \Delta t \sum_s \beta_{k\,s} \mathbf{F}(\mathbf{Y}_s) \tag{13-2}$$

where the variable **X** is the canonical coordinates,

$$\mathbf{X}(t) = \begin{bmatrix} \mathbf{x}(t) \\ \mathbf{p}(t) \end{bmatrix} \tag{14}$$

and **G**(**x**,**p**) is the right hand side vectors of Eq.(12),

$$\mathbf{F}(\mathbf{x},\mathbf{p}) = \begin{bmatrix} \dfrac{\partial H}{\partial \mathbf{p}} \\ -\dfrac{\partial H}{\partial \mathbf{x}} \end{bmatrix} \tag{15}$$

Then the concept of the mean value theorem can be introduced to the Lie algebra map in the following form,

$$\begin{bmatrix} x^k(s+ds) \\ u^k(s+ds) \end{bmatrix} = \begin{bmatrix} 1 & \int_0^{ds} \exp\left(\frac{e}{mc}F^k{}_j(Y^i)s\right)ds \\ 0 & \exp\left(\frac{e}{mc}F^k{}_j(Y^i)ds\right) \end{bmatrix} \begin{bmatrix} x^k(s) \\ u^k(s) \end{bmatrix} \tag{16}$$

(where Y_i denotes the right hand side of Eq.(13-2)), that is, the value Y_i is adopted as the evaluation point of the electromagnetic fields **E** and **B**. The Gauss-Legendre formula which belongs to series of the (implicit) Runge-Kutta schemes is known as a kind of symplectic integrator too, which is reason why we adopt this formula for implementation of (13-2).

4 NUMERICAL TEST

A numerical test for the improved Lie algebra map (16) is given here. The numerical test is performed for charged particle motion (with initial velocity v/c = 0.999999) in a magnetic mirror profile. (Fig.1) Then the fifth order Gauss-Legendre formula (Table 1) [3] is applied. As we predicted, the trajectory calculation based on the formula (16) shows same order accuracy as the standard Gauss-Legendre type of implicit Runge-Kutta method. In Fig.2 and Fig.3, comparison of velocity and the Minkowski norm (2) between the Lie algebra map and the Runge-Kutta method are shown.

Table 1 Fifth order Gauss-Legendre Formula

β_{ks}	$\frac{5}{36}$	$\frac{10-3\sqrt{15}}{45}$	$\frac{25-6\sqrt{15}}{180}$
	$\frac{10+3\sqrt{15}}{72}$	$\frac{2}{9}$	$\frac{10-3\sqrt{15}}{72}$
	$\frac{25+6\sqrt{15}}{180}$	$\frac{10+3\sqrt{15}}{45}$	$\frac{5}{36}$
γ_s	$\frac{5}{18}$	$\frac{4}{9}$	$\frac{5}{18}$

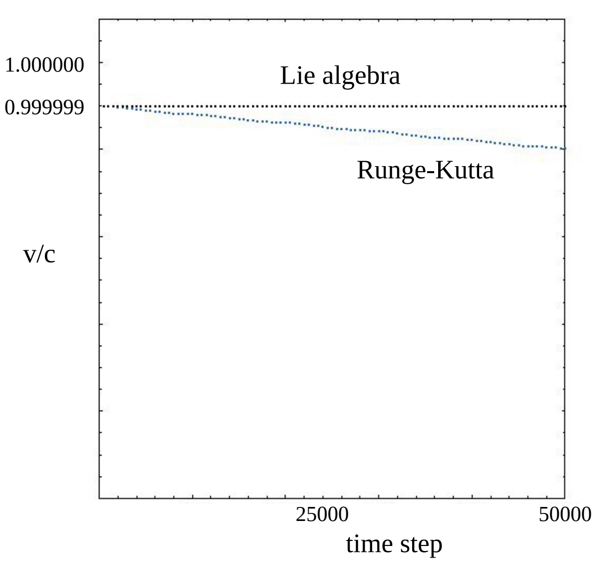

Fig.2 Particle velocity evolution

5 SUMMARY

In this paper, a trajectory accuracy improvement of the Lorentz group Lie algebra mapping based on the Gauss-Legendre interpolation formula has been presented. And a numerical test shows us this improvement effectively give us good accuracy solution for the charged particle simulation for both of particle velocity and trajectory.

REFERENCES

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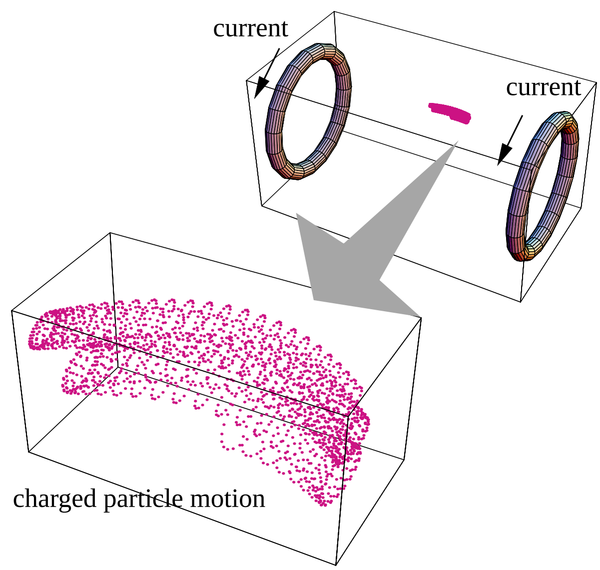

Fig.1 Particle motion in magnetic mirror frofile

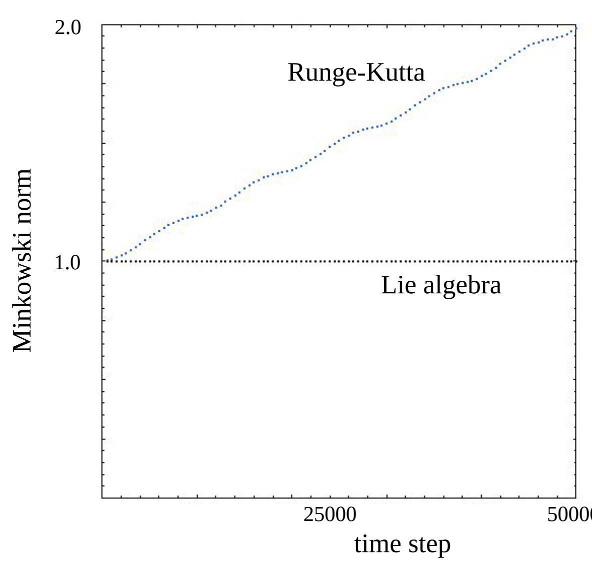

Fig.3 Minkowski norm evolution