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Application of Lie Algebra in Constructing Volume-Preserving Algorithms for Charged Particles Dynamics

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Abstract. Volume-preserving algorithms (VPAs) for the charged particles dynamics is preferred because of their long-term accuracy and conservativeness for phase space volume. Lie algebra and the Baker-Campbell-Hausdorff (BCH) formula can be used as a fundamental theoretical tool to construct VPAs. Using the Lie algebra structure of vector fields, we split the volume-preserving vector field for charged particle dynamics into three volume-preserving parts (sub-algebras), and find the corresponding Lie subgroups. Proper combinations of these subgroups generate volume preserving, second order approximations of the original solution group, and thus second order VPAs. The developed VPAs also show their significant effectiveness in conserving phase-space volume exactly and bounding energy error over long-term simulations.

AMS subject classifications: 17B81, 22E70, 70H33, 70H40

Key words: Lie algebra, Lie group, volume-preserving algorithm, charged particles dynamics.

1 Introduction

Dynamics of non-relativistic and relativistic charged particles arises commonly in plasma physics, accelerator physics, space physics, and many other subfields of physics [1–4, 8,

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10–12, 16–18]. Because charged particle dynamics in a general electromagnetic field preserves phase space volume, it is desirable to construct corresponding volume-preserving algorithms for numerical integrations [5, 15]. Volume-preserving algorithms have been successfully constructed and their superior advantages in terms of long-term accuracy and conservative properties have been demonstrated [9, 14, 19]. It is well-known that vector fields of a dynamical system on a given manifold have the structure of Lie algebra. An important method to construct VPAs is based on the splitting technique applied to the Lie algebra [6,7]. In this method, the original vector field for the dynamics in phase space is split into several parts, such that for each part the system can be solved exactly or a VPA can be easily found [13]. Combining all the sub-algorithms in a proper way, we can obtain a desired VPA for the original system. The procedure to construct VPAs can be executed in three steps:

1) To split the original vector field into several sub-vector fields;

2) To find corresponding Lie groups of the Lie algebra generated by the each sub-vector field;

3) To combine Lie subgroups to obtain a desired VPA for the original system.

Many different VPAs can be constructed following the above three steps, because there are different degrees of freedom in every step. In the first step, a given vector fields can be split in different ways. In the second step, we can choose either the exact solution or an approximate solution which is volume-preserving. In the third step, different composition methods can be used to generate algorithms with different orders and symmetry properties. The order of a VPA is determined by order of the approximation to the original one-parameter Lie group according to the BCH formula.

In this paper, we construct VPAs for non-relativistic and relativistic dynamics of charged particles using the method of Lie algebra by splitting the vector field in phase space into three parts: the force-free part, the electrical part, and the magnetic part. For each sub-vector field the corresponding Lie subgroup can be solved exactly or approximately by the Cayley transformation. Desired VPAs can be constructed symmetrically using the Strang composition method. Applying the developed VPAs to calculate the ware-pinch effect in tokamak, we demonstrate the long-term accuracy and significance of the VPA compared with RK4 method.

The paper is organized as follows. Some basic facts about splitting methods in the view of Lie algebra and Lie group are introduced in Section 2. In Section 3, we apply the theory of Lie algebra to construct VPAs for non-relativistic charged particles dynamics, and VPAs for relativistic dynamics are given in Section 4. Numerical experiments are also provided to demonstrate the effectiveness of VPAs compared with RK4 in Section 5.

2 Lie algebra and its application in splitting methods

For an initial value problem

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$$\begin{cases} \dot{\mathbf{y}} = f(\mathbf{y}), \quad \mathbf{y} \in \mathbb{R}^n, \\ \mathbf{y}(t_0) = \mathbf{y}_0, \end{cases} \tag{2.1}$$

the vector field $f(\mathbf{y})$ can be represented by a differential operator (Lie derivative)

$$X_f = \sum_{i=1}^{n} f_i \frac{\partial}{\partial y_i},$$

and the ordinary differential equation can be written as $\dot{\mathbf{y}} = X_f(\mathbf{y})$. Given arbitrary differentiable function $F: \mathbb{R}^n \longrightarrow \mathbb{R}^m$, we have $X_f F(\mathbf{y}) = F'(\mathbf{y}) f(\mathbf{y})$. The vector field X_f defined above generates a Lie algebra with the normal Lie bracket

$$[X_f, X_g](F) = X_f X_g(F) - X_g X_f(F). \tag{2.2}$$

The one-parameter Lie group $\exp(tX_f)$ generated by X_f is a solution of the ordinary differential equation (2.1) according to the following well-known theorem.

Theorem 2.1. *Denoting $\varphi_t(\mathbf{y}_0)$ be the solution of the initial value problem Eq. (2.1) and X_f be the corresponding Lie derivative, for arbitrary differentiable function $F: \mathbb{R}^n \longrightarrow \mathbb{R}^m$, we have*

$$F(\varphi_t(\mathbf{y}_0)) = \exp(tX_f) F(\mathbf{y}_0). \tag{2.3}$$

If the Lie algebra can be represented by skew-symmetric matrices $so(n) := \{A \in \mathbb{R}^{n\times n},\ A = -A^T\}$, the corresponding Lie group can also be constructed using Cayley transformation, i.e.,

$$Q = Cay(A) = (I - A)^{-1}(I + A), \tag{2.4}$$

which maps the space of skew-symmetric matrices onto the space of special orthogonal matrices, $SO(n) := \{Q \in \mathbb{R}^{n\times n},\ QQ^T = I,\ \det Q = 1\}$. Similar to the exponential map, the Cayley transformation is also a local diffeomorphism in a neighbourhood of $A = 0$. As the second-order *Padé* approximation of the exponential map, i.e.,

$$Cay\left(\frac{tA}{2}\right) = \exp(tA) + \mathcal{O}(t^3), \tag{2.5}$$

the Cayley transformation is widely applicable in constructing volume-preserving algorithms.

Splitting technique is often used as an important and practical way to construct volume-preserving algorithms for source-free systems. Profit from expressing ordinary differential equation using Lie algebra and the Cayley transformation, the method of constructing VPAs by splitting technique can be well explained as follows. Here, we use exponential transformation as an example. If the vector field of Eq. (2.1) is split into two parts $X_f = X_{f_1} + X_{f_2}$, the corresponding subsystems are

$$\dot{\mathbf{y}} = X_{f_1}\mathbf{y} = f_1(\mathbf{y}), \quad \dot{\mathbf{y}} = X_{f_2}\mathbf{y} = f_2(\mathbf{y}). \tag{2.6}$$

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According to Theorem 2.1, the exact solution flows of subsystems can be expressed using one-parameter Lie groups as

$$\varphi_t^1 = \exp(tX_{f_1})Id(\mathbf{y}_0), \quad \varphi_t^2 = \exp(tX_{f_2})Id(\mathbf{y}_0). \tag{2.7}$$

We can combine the Lie groups in a proper way to obtain desired algorithms. Usually, the Lie groups are noncommutative, and different composition methods lead to different approximations. The order of the composite methods can be determined by the well-known BCH formula,

$$\exp(tX_{f_1})\exp(tX_{f_2}) = \exp\left(t(X_{f_1}+X_{f_2})+\frac{t^2}{2}[X_{f_1},X_{f_2}]+\mathcal{O}(t^3)\right), \tag{2.8}$$

where $[\ ,\ ]$ is the Lie bracket. Different composition methods of Lie subgroups create approximations to original Lie group at different orders, for example,

$$\begin{aligned} &\exp(tX_f) = \exp(tX_{f_1})\exp(tX_{f_2})+\mathcal{O}(t),\\ &\exp(tX_f) = \exp\left(\frac{t}{2}X_{f_1}\right)\exp(tX_{f_2})\exp\left(\frac{t}{2}X_{f_1}\right)+\mathcal{O}(t^2). \end{aligned} \tag{2.9}$$

3 Boris method for non-relativistic dynamics

The non-relativistic dynamics of charged particle associated with the Lorentz force can be written as

$$\begin{cases} \dfrac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v}, \\ \dfrac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \dfrac{q}{m}\left(\mathbf{E}(\mathbf{x})+\dfrac{\mathbf{v}\times\mathbf{B}(\mathbf{x})}{c}\right), \end{cases} \tag{3.1}$$

where $\mathbf{x}$ and $\mathbf{v}$ denote position and velocity, c is the speed of light in vacuum, q and m are the electric charge and mass of the particle, and $\mathbf{E}$ and $\mathbf{B}$ are the electric and magnetic field respectively. The non-relativistic dynamics Eq. (3.1) of charged particles can be written as

$$\begin{pmatrix} \dot{\mathbf{x}} \\ \dot{\mathbf{v}} \end{pmatrix} = X_{fn}\begin{pmatrix} \mathbf{x} \\ \mathbf{v} \end{pmatrix}, \tag{3.2}$$

where the Lie derivative can be presented as

$$X_{fn} = \mathbf{v}\cdot\frac{\partial}{\partial\mathbf{x}}+\left(\frac{q}{m}\left(\mathbf{E}(\mathbf{x})+\frac{\mathbf{v}\times\mathbf{B}(\mathbf{x})}{c}\right)\right)\cdot\frac{\partial}{\partial\mathbf{v}}. \tag{3.3}$$

It's straightforward to show that in the phase space $\mathbf{z}\equiv(\mathbf{x},\mathbf{v})$, the divergence of the vector field $\mathbf{F}(\mathbf{z})$ on the right-hand side (RHS) of Eq. (3.1) vanishes

$$\nabla_{\mathbf{z}}\cdot X_{fn} = \nabla_{\mathbf{x}}\cdot\mathbf{v}+\nabla_{\mathbf{v}}\cdot\frac{q}{m}\left(\mathbf{E}(\mathbf{x})+\frac{\mathbf{v}\times\mathbf{B}(\mathbf{x})}{c}\right) = 0, \tag{3.4}$$

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i.e., the system is source-free or volume-preserving. According to Theorem 2.1, the solution flow of the dynamics φ_t is one-parameter subgroup of the Lie algebra generated by X_{fn}

$$\varphi_t(\mathbf{x},\mathbf{v}) = \exp(tX_{fn})Id(\mathbf{x}_0,\mathbf{v}_0). \tag{3.5}$$

The corresponding VPAs can be constructed step by step for non-relativistic dynamics following the above introduced procedure. One of the de facto standard and popular numerical algorithms for the source-free dynamics is Boris method. It has been discovered that the Boris algorithm is a volume-preserving algorithm, so that it's capable of integrating particles' dynamics accurately for an arbitrarily large number of time-steps. We now show that it can be derived as a combined approximation to the Lie group through the splitting method described above.

First, we split the vector field X_{fn} into three parts,

$$X_{vn} = \mathbf{v}\cdot\frac{\partial}{\partial\mathbf{x}}, \quad X_{En} = \frac{q}{m}\mathbf{E}(\mathbf{x})\cdot\frac{\partial}{\partial\mathbf{v}}, \quad X_{Bn} = \frac{q}{m}\frac{\mathbf{v}\times\mathbf{B}(\mathbf{x})}{c}\cdot\frac{\partial}{\partial\mathbf{v}}. \tag{3.6}$$

The corresponding subsystems S_1, S_2, and S_3 are

$$S_1 := \begin{cases} \dfrac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v}, \\ \dfrac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = 0, \end{cases} \quad S_2 := \begin{cases} \dfrac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = 0, \\ \dfrac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \dfrac{q}{m}\mathbf{E}(\mathbf{x}), \end{cases} \quad S_3 := \begin{cases} \dfrac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = 0, \\ \dfrac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \dfrac{q}{m}(\mathbf{v}\times\mathbf{B}(\mathbf{x})), \end{cases} \tag{3.7}$$

all of which are source-free. The one-parameter subgroups generated by X_{vn}, X_{En} and X_{Bn} all can be computed exactly, i.e.,

$$\begin{aligned} \varphi_t^1 &= \exp(tX_{vn})(\mathbf{x}_0,\mathbf{v}_0) = \begin{cases} \mathbf{x}(t) = \mathbf{x}_0 + t\mathbf{v}(t), \\ \mathbf{v}(t) = \mathbf{v}_0, \end{cases} \\ \varphi_t^2 &= \exp(tX_{En})(\mathbf{x}_0,\mathbf{v}_0) = \begin{cases} \mathbf{x}(t) = \mathbf{x}_0, \\ \mathbf{v}(t) = \mathbf{v}_0 + \dfrac{tq}{m}\mathbf{E}(\mathbf{x}), \end{cases} \\ \varphi_t^3 &= \exp(tX_{Bn})(\mathbf{x}_0,\mathbf{v}_0) = \begin{cases} \mathbf{x}(t) = \mathbf{x}_0, \\ \mathbf{v}(t) = \exp(t\hat{B}(\mathbf{x_0}))\mathbf{v_0}, \end{cases} \end{aligned} \tag{3.8}$$

where $\mathbf{v}\times\mathbf{B}(\mathbf{x}) = \hat{B}(\mathbf{x})\mathbf{v}$, and

$$\hat{B}(\mathbf{x}) = \begin{pmatrix} 0 & B_3(\mathbf{x}) & -B_2(\mathbf{x}) \\ -B_3(\mathbf{x}) & 0 & B_1(\mathbf{x}) \\ B_2(\mathbf{x}) & -B_1(\mathbf{x}) & 0 \end{pmatrix} \tag{3.9}$$

is a skew-symmetric matrix. Thus volume-preserving integrators for the three subsystems are

$$\varphi^1(\Delta t): \begin{cases} \mathbf{x}_{k+1} = \mathbf{x}_k + \Delta t\mathbf{v}_k, \\ \mathbf{v}_{k+1} = \mathbf{v}_k, \end{cases} \quad \varphi^2(\Delta t): \begin{cases} \mathbf{x}_{k+1} = \mathbf{x}_k, \\ \mathbf{v}_{k+1} = \mathbf{v}_k + \dfrac{q}{m}\Delta t\mathbf{E}_k, \end{cases} \tag{3.10}$$

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$$\varphi^3(\Delta t):\begin{cases}\mathbf{x}_{k+1}=\mathbf{x}_k,\\ \mathbf{v}_{k+1}=\exp(\Delta t\hat{B}_k)\mathbf{v}_k,\end{cases} \tag{3.11}$$

where $\mathbf{E}_k=\mathbf{E}(\mathbf{x_k})$ and $\hat{B}_k=\hat{B}(\mathbf{x_k})$. Now we combine the Lie subgroups to form an approximation to $\exp(tX_{fr})$. We choose the well-know Strang composition to construct the one-step map $\Phi(\Delta t)$,

$$\Phi(\Delta t)=\varphi^1(\Delta t/2)\circ\varphi^2(\Delta t/2)\circ\varphi^3(\Delta t)\circ\varphi^2(\Delta t/2)\circ\varphi^1(\Delta t/2). \tag{3.12}$$

The resulting VPA in Eq. (3.12) can be explicitly written as

$$\Phi(\Delta t):\begin{cases}\mathbf{x}_{k+\frac{1}{2}}=\mathbf{x}_k+\dfrac{\Delta t}{2}\mathbf{v}_k,\\ \mathbf{v}^-=\mathbf{v}_k+\dfrac{q}{m}\dfrac{\Delta t}{2}\mathbf{E}_{k+\frac{1}{2}},\\ \mathbf{v}^+=\exp(\Delta t\hat{B}_{k+\frac{1}{2}})\mathbf{v}^-,\\ \mathbf{v}_{k+1}=\mathbf{v}^++\dfrac{q}{m}\dfrac{\Delta t}{2}\mathbf{E}_{k+\frac{1}{2}},\\ \mathbf{x}_{k+1}=\mathbf{x}_{k+\frac{1}{2}}+\dfrac{\Delta t}{2}\mathbf{v}_{k+1}.\end{cases} \tag{3.13}$$

According to the BCH formula,

$$\begin{aligned}&\exp\left(\frac{\Delta t}{2}X_{vn}\right)\exp\left(\frac{\Delta t}{2}X_{En}\right)\exp(\Delta tX_{Bn})\exp\left(\frac{\Delta t}{2}X_{En}\right)\exp\left(\frac{\Delta t}{2}X_{vn}\right)\\ =&\exp(\Delta tX_{fn})+\mathcal{O}(\Delta t^2),\end{aligned} \tag{3.14}$$

which indicates that the Strang composition is of second order accuracy.

4 VPA for relativistic dynamics

The relativistic dynamics of charged particle dynamics is

$$\begin{cases}\dfrac{\mathrm{d}\mathbf{x}}{\mathrm{d}t}=\dfrac{\mathbf{p}}{\sqrt{m_0^2+\mathbf{p}^2/c^2}},\\ \dfrac{\mathrm{d}\mathbf{p}}{\mathrm{d}t}=q\left(\mathbf{E}(\mathbf{x})+\dfrac{\mathbf{p}}{\sqrt{m_0^2+\mathbf{p}^2/c^2}}\times\mathbf{B}(\mathbf{x})\right),\end{cases} \tag{4.1}$$

where $\mathbf{x}$ and $\mathbf{p}$ denote position and momentum vector, c is the speed of light in vacuum. As in the non-relativistic case, the vector field on the right-hand side (RHS) of Eq. (4.1) is

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source-free,

$$\nabla_{\mathbf{z}}\cdot\mathbf{F}=\nabla_{\mathbf{x}}\cdot\frac{\mathbf{p}}{\sqrt{m_0^2+\mathbf{p}^2/c^2}}+\nabla_{\mathbf{p}}\cdot q\left(\mathbf{E}(\mathbf{x})+\frac{\mathbf{p}}{\sqrt{m_0^2+\mathbf{p}^2/c^2}}\times\mathbf{B}(\mathbf{x})\right)=0. \tag{4.2}$$

The solution flow of the dynamics is one-parameter Lie group of X_{fr}

$$\varphi_t(\mathbf{x},\mathbf{p})=\exp(tX_{fr})Id(\mathbf{x}_0,\mathbf{p}_0). \tag{4.3}$$

To construct VPAs for relativistic dynamics with time-independent electromagnetic field dynamics, we split the vector field X_{fr} into three parts,

$$\begin{aligned}&X_{pr}=\left(\frac{\mathbf{p}}{\sqrt{m_0^2+\mathbf{p}^2/c^2}}\right)\cdot\frac{\partial}{\partial\mathbf{x}},\quad X_{Er}=q(\mathbf{E}(\mathbf{x}))\cdot\frac{\partial}{\partial\mathbf{p}},\\&X_{Br}=q\left(\frac{\mathbf{p}}{\sqrt{m_0^2+\mathbf{p}^2/c^2}}\times\mathbf{B}(\mathbf{x})\right)\cdot\frac{\partial}{\partial\mathbf{p}}.\end{aligned} \tag{4.4}$$

The original system depicted by Eq. (4.1) are split into three subsystems S_1, S_2, and S_3,

$$S_1:=\begin{cases}\dfrac{\mathrm{d}\mathbf{x}}{\mathrm{d}t}=\dfrac{\mathbf{p}}{\sqrt{m_0^2+\mathbf{p}^2/c^2}},\\[2ex]\dfrac{\mathrm{d}\mathbf{p}}{\mathrm{d}t}=0,\end{cases}\qquad S_2:=\begin{cases}\dfrac{\mathrm{d}\mathbf{x}}{\mathrm{d}t}=0,\\[2ex]\dfrac{\mathrm{d}\mathbf{p}}{\mathrm{d}t}=q\mathbf{E}(\mathbf{x}),\end{cases} \tag{4.5}$$

$$S_3:=\begin{cases}\dfrac{\mathrm{d}\mathbf{x}}{\mathrm{d}t}=0,\\[2ex]\dfrac{\mathrm{d}\mathbf{p}}{\mathrm{d}t}=q\left(\dfrac{\mathbf{p}}{\sqrt{m_0^2+\mathbf{p}^2/c^2}}\times\mathbf{B}(\mathbf{x})\right).\end{cases} \tag{4.6}$$

Again, all the subsystems are source-free. For the vector fields X_{pr} and X_{Er}, their corresponding Lie groups can be computed exactly,

$$\begin{aligned}&\varphi_t^1(\mathbf{x}_0,\mathbf{p}_0)=\exp(tX_{pr})(\mathbf{x}_0,\mathbf{p}_0)=\begin{cases}\mathbf{x}(t)=\mathbf{x}_0+t\dfrac{\mathbf{p}_0}{\sqrt{m_0^2+\mathbf{p}_0^2/c^2}},\\[2ex]\mathbf{p}(t)=\mathbf{p}_0,\end{cases}\\&\varphi_t^2(\mathbf{x}_0,\mathbf{p}_0)=\exp(tX_{Er})(\mathbf{x}_0,\mathbf{p}_0)=\begin{cases}\mathbf{x}(t)=\mathbf{x}_0,\\\mathbf{p}(t)=\mathbf{p}_0+qt\mathbf{E}(\mathbf{x}_0).\end{cases}\end{aligned} \tag{4.7}$$

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For the subsystem S_3 of vector field X_{Br}, $\mathbf{p}^2$ is an invariant and the third vector field X'_{Br} can be represented as

$$X'_{Br}=q\left(\frac{\mathbf{p}}{\sqrt{m_0^2+\mathbf{p}_0^2/c^2}}\times\mathbf{B}(\mathbf{x})\right)\cdot\frac{\partial}{\partial\mathbf{p}}. \tag{4.8}$$

Therefore, subsystem S_3 is equivalent to

$$S'_3:=\begin{cases}\dfrac{\mathrm{d}\mathbf{x}}{\mathrm{d}t}=0,\\[2ex] \dfrac{\mathrm{d}\mathbf{p}}{\mathrm{d}t}=q\left(\dfrac{\mathbf{p}}{\sqrt{m_0^2+\mathbf{p_0}^2/c^2}}\times\mathbf{B}(\mathbf{x})\right).\end{cases} \tag{4.9}$$

whose exact solution is

$$\varphi_t^3(\mathbf{x}_0,\mathbf{p}_0)=\exp(tX_{Br})(\mathbf{x}_0,\mathbf{p}_0)=\begin{cases}\mathbf{x}(t)=\mathbf{x}_0,\\[2ex] \mathbf{p}(t)=\exp\left(\dfrac{tq}{\sqrt{m_0^2+\mathbf{p_0}^2/c^2}}\hat{B}(\mathbf{x})\right)\mathbf{p}_0.\end{cases} \tag{4.10}$$

Here, $\mathbf{p}\times\mathbf{B}(\mathbf{x})=\hat{\mathbf{B}}(\mathbf{x})\mathbf{p}$ with $\hat{B}(\mathbf{x})$ being a skew-symmetric matrix. The special Lie subalgebra generated by X'_{Br} is identity map when acting on $\mathbf{x}$, and is $so(n)$ when acting on $\mathbf{p}$. Then we can also generate its Lie group by Cayley transformation

$$\phi_t^3(\mathbf{x}_0,\mathbf{p}_0)=Cay\left(\frac{tX_{Br}}{2}\right)(\mathbf{x}_0,\mathbf{p}_0)=\begin{cases}\mathbf{x}(t)=\mathbf{x}_0,\\[2ex] \mathbf{p}(t)=Cay\left(\dfrac{tq}{2\sqrt{m_0^2+\mathbf{p_0}^2/c^2}}\hat{B}(\mathbf{x})\right)\mathbf{p}_0.\end{cases} \tag{4.11}$$

The second equation for $\mathbf{p}(t)$ can be rewritten as

$$\mathbf{p}(t)=\left(I-a\hat{B}_0\right)^{-1}\left(I+a\hat{B}_0\right)\mathbf{p}_0=\mathrm{Cay}(\mathrm{a}\hat{\mathrm{B}}_0)\mathbf{p}_0, \tag{4.12}$$

where $\hat{B}_0=\hat{B}(\mathbf{x}_0)$ and

$$a=\frac{tq}{2\sqrt{m_0^2+(\mathbf{p}_0)^2/c^2}}. \tag{4.13}$$

To carry out the Cayley transformation efficiently in the application of the algorithm, the troublesome inverse operation of $I-a\hat{B}_0$ can be avoided after manipulation. Deducing from Eq. (4.12), $\mathbf{p}(t)$ can be explicitly expressed by $\mathbf{p}_0$ as

$$\mathbf{p}(t)=\left(I+\frac{2a}{1+a^2|\mathbf{B}_0|^2}\hat{B}_0+\frac{2a^2}{1+a^2|\mathbf{B}_0|^2}\hat{B}_0^2\right)\mathbf{p}_0\,. \tag{4.14}$$

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So far, we have computed exactly the one parameter Lie groups for X_{pr}, X_{Er} and X_{Br}. For X_{Br}, an approximate solution can be computed by the Cayley transformation. To combine the Lie subgroups to form an approximation for $\exp(tX_{fr})$, we use the Strang composition again:

$$\Phi^1(\Delta t)=\exp\left(\frac{\Delta t}{2}X_{pr}\right)\exp\left(\frac{\Delta t}{2}X_{Er}\right)\exp(\Delta t X_{Br})\exp\left(\frac{\Delta t}{2}X_{Er}\right)\exp\left(\frac{\Delta t}{2}X_{pr}\right)(\mathbf{x}_0,\mathbf{p}_0). \tag{4.15}$$

Explicitly, the resulting VPA is

$$\Phi^1(\Delta t):\begin{cases}\mathbf{x}_{k+\frac{1}{2}}=\mathbf{x}_k+\dfrac{\Delta t}{2}\dfrac{\mathbf{p}_k}{\sqrt{m_0^2+\mathbf{p}_k^2/c^2}},\\ \mathbf{p}^-=\mathbf{p}_k+q\dfrac{\Delta t}{2}\mathbf{E}_k,\\ \mathbf{p}^+=\exp\left(\dfrac{\Delta t q}{\sqrt{m_0^2+(\mathbf{p}^-)^2/c^2}}\hat{B}_k\right)\mathbf{p}^-,\\ \mathbf{p}_{k+1}=\mathbf{p}^++q\dfrac{\Delta t}{2}\mathbf{E}_k,\\ \mathbf{x}_{k+1}=\mathbf{x}_{k+\frac{1}{2}}+\dfrac{\Delta t}{2}\dfrac{\mathbf{p}_{k+1}}{\sqrt{m_0^2+\mathbf{p}_{k+1}^2/c^2}}.\end{cases} \tag{4.16}$$

If choosing the Cayley transformation instead of $\exp(tX_{Br})$, we have

$$\Phi^2(\Delta t)=\exp\left(\frac{\Delta t}{2}X_{pr}\right)\exp\left(\frac{\Delta t}{2}X_{Er}\right)Cay\left(\frac{\Delta t}{2}X_{Br}\right)\exp\left(\frac{\Delta t}{2}X_{Er}\right)\exp\left(\frac{\Delta t}{2}X_{pr}\right)(\mathbf{x}_0,\mathbf{p}_0), \tag{4.17}$$

and the resulting VPA is

$$\Phi^2(\Delta t):\begin{cases}\mathbf{x}_{k+\frac{1}{2}}=\mathbf{x}_k+\dfrac{\Delta t}{2}\dfrac{\mathbf{p}_k}{\sqrt{m_0^2+\mathbf{p}_k^2/c^2}},\\ \mathbf{p}^-=\mathbf{p}_k+q\dfrac{\Delta t}{2}\mathbf{E}_k,\\ \mathbf{p}^+=Cay\left(\dfrac{\Delta t q}{2\sqrt{m_0^2+(\mathbf{p}^-)^2/c^2}}\hat{B}_k\right)\mathbf{p}^-,\\ \mathbf{p}_{k+1}=\mathbf{p}^++q\dfrac{\Delta t}{2}\mathbf{E}_k,\\ \mathbf{x}_{k+1}=\mathbf{x}_{k+\frac{1}{2}}+\dfrac{\Delta t}{2}\dfrac{\mathbf{p}_{k+1}}{\sqrt{m_0^2+\mathbf{p}_{k+1}^2/c^2}}.\end{cases} \tag{4.18}$$

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According to the BCH formula, the VPAs given by Eq. (4.16) and Eq. (4.18) are both of second order. For the one step evolution $(\mathbf{x}_k,\mathbf{p}_k)\to(\mathbf{x}_{k+1},\mathbf{p}_{k+1})$, we can verify that indeed

$$\det\begin{pmatrix} \dfrac{\partial \mathbf{x}_{k+1}}{\partial \mathbf{x}_k} & \dfrac{\partial \mathbf{x}_{k+1}}{\partial \mathbf{p}_k} \\ \dfrac{\partial \mathbf{p}_{k+1}}{\partial \mathbf{x}_k} & \dfrac{\partial \mathbf{p}_{k+1}}{\partial \mathbf{p}_k} \end{pmatrix}=1, \tag{4.19}$$

which is another way to state that the algorithms conserve the phase space volume. Meanwhile, the fact that $\Phi(\Delta t)^{-1}=\Phi(-\Delta t)$ guarantees the algorithm is symmetric with respect to time, which is also the group property of the exact solution flow of the original system.

5 Numerical experiments

To demonstrate the effectiveness of the volume-preserving algorithms developed in Section 4, we apply the algorithms given by Eqs. (4.16) and (4.18) respectively as well as RK4, for comparison, to calculate the ware-pinch effect in tokamak. The electric field and magnetic field are given by

$$\mathbf{B}=-\frac{B_0R_0}{R}\mathbf{e}_\xi-\frac{B_0\sqrt{(R-R_0)^2+z^2}}{qR}\mathbf{e}_\theta,$$
$$\mathbf{E}=E_l\frac{R_0}{R}\mathbf{e}_\xi.$$

Here we use the cylindrical coordinate system (R,ξ,z). The unit vectors $\mathbf{e}_\xi$ and $\mathbf{e}_\theta$ are along the toroidal and poloidal directions respectively, R_0 is the major radius, and q denotes safety factor. The loop electric field and toroidal magnetic field at the torus axis are denoted as E_l and B_0. The time-step of simulation is set as $\Delta t=2.84\times10^{-12}$s. The initial position is $R=1.8$m, $\xi=z=0$, and the initial momentum is set as $p_x=5\mathrm{m}_0\mathrm{c}$, $p_y=1\mathrm{m}_0\mathrm{c}$, $p_z=0$. The electric field is $E_l=2V/m$, and the magnetic field is set as $B_0=2T$.

The ware-pinch effect provides a inward drift of banana orbit if there exists a loop electric field. The velocity of ware-pinch drift can be approximately estimated by $v_{ware}=E_l/B_\theta$. Fig. 1 depicts the ware-pinch effect calculated by the volume-preserving algorithms in this article (see Fig. 1 (a) and (c)). The result of 4th-order Runge-Kutta method is also provided in Fig. 1 (e). The relative error of energy of these three algorithms are plotted in Fig. 1 (b), (d), (f). It is readily to see that the volume-preserving algorithms have long-term energy stability. The RK4 method, however, causes the loss of perpendicular momentum and the numerical energy dissipation. Therefore, the banana orbit transforms to a circle one after only 8×10^5 steps. It is obviously shown that the long-term accuracy and conservativeness of the VPAs enable precise simulations of the long-term dynamics of relativistic particles.

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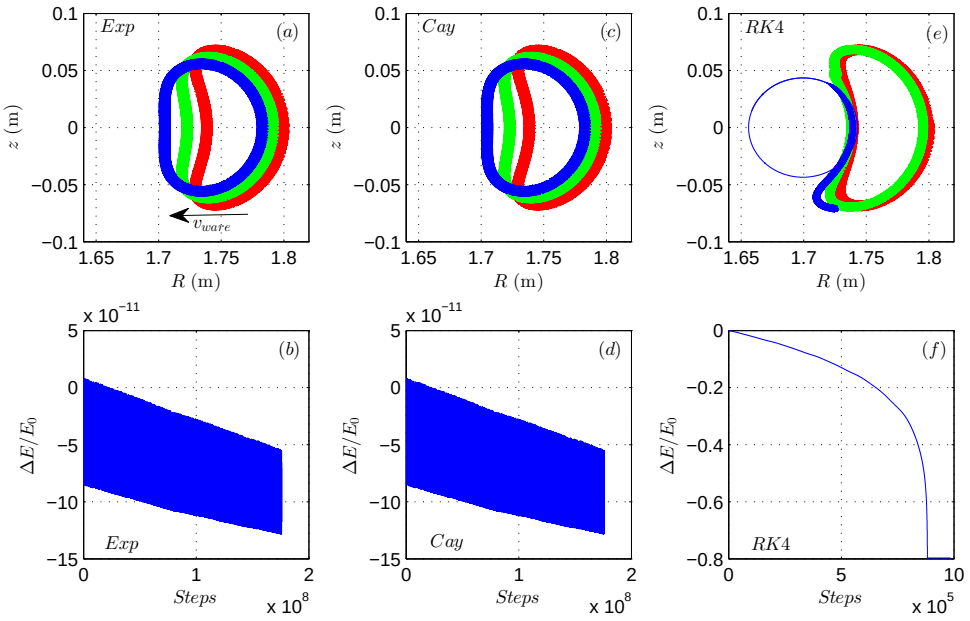


Figure 1: The ware-pinch effect simulated by volume-preserving algorithms and 4th-order Runge-Kutta algorithm. (a) and (b) show the ware-pinch drift orbit and the evolution of relative energy error using the algorithm given by Eq. (4.16); (c) and (d) depict the drift orbit and evolution of the relative energy error using the algorithm given by Eq. (4.18); the results of RK4 are shown in (e) and (f).

6 Conclusion

We have demonstrated the application of Lie algebra in constructing volume-preserving algorithms for non-relativistic and relativistic dynamics of charged particles. Orders of VPAs can be clearly determined from the BCH formula. In the future, we will construct more VPAs using this approach by exploring the degrees of freedom in splitting, combination, and solutions of subsystems. In particular, we will focus on high order VPAs with desired symmetry properties.

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