Variational Symplectic Integrator for Long-Time Simulations of the Guiding-Center Motion of Charged Particles in General Magnetic Fields

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A variational symplectic integrator for the guiding-center motion of charged particles in general magnetic fields is developed for long-time simulation studies of magnetized plasmas. Instead of discretizing the differential equations of the guiding-center motion, the action of the guiding-center motion is discretized and minimized to obtain the iteration rules for advancing the dynamics. The variational symplectic integrator conserves exactly a discrete Lagrangian symplectic structure, and has better numerical properties over long integration time, compared with standard integrators, such as the standard and variable time-step fourth order Runge-Kutta methods.

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For applications of magnetized plasmas, the guiding-center motion of charged particles is the physical process that underlies the collective dynamics of the plasmas. For most simulation studies, the elementary equations of simulated particles are those of the guiding-center dynamics. Because of the multiscale length nature of magnetized plasmas, it is often necessary to carry out simulations in a time scale much larger than that of the guiding-center motion. For example, in simulation studies of plasma transport physics in a tokamak geometry, the simulation time is typically much larger than the transit time of the guiding centers of ions and electrons along the toroidal direction. It is desirable to use numerical integrators with good global conservative properties over long integration time in these simulation studies. Standard integrators, such as the fourth order Runge-Kutta method, only guarantee the error to be small in each time step. The errors at different time-steps often accumulate coherently, and result in a large error over a large number of time steps. A well-known numerical integrator with global conservation property is the symplectic integrator for Hamiltonian systems with canonical structure [1–5]. The symplectic integrator for canonical Hamiltonian system conserves the canonical symplectic structure exactly, and guarantees that the energy error is bounded by a small number for all the time steps.

However, the guiding-center dynamics in general magnetic field does not possess a (global) canonical symplectic structure, and the conventional symplectic integrator does not apply. Recently, Marsden and West [6] developed the method of variational symplectic integrator for dynamic systems with a well-defined Lagrangian, and the variational symplectic integrator conserves exactly a noncanonical symplectic structure. In this Letter, we develop the variational symplectic integrator for the guiding-center dynamics from the guiding-center Lagrangian and demonstrate its superior numerical properties compared with the standard fourth order Runge-Kutta methods.

The Lagrangian for the guiding-center motion first derived by Littlejohn [7] is

$$L(\mathbf{x}, \dot{\mathbf{x}}, u, \dot{u}) = [\mathbf{A}(\mathbf{x}) + u\mathbf{b}(\mathbf{x})] \cdot \dot{\mathbf{x}} - \left[\mu B(\mathbf{x}) + \tfrac{1}{2}u^2 + \phi(\mathbf{x})\right], \tag{1}$$

where we have normalized $\mathbf{A}$ by cm/e and ϕ by m/e. Here $\mathbf{x}$ and u are the position and parallel velocity of the guiding center, and μ is the conserved magnetic moment. The electromagnetic field is assumed to be time-independent in Eq. (1). The Lagrangian for general time-dependent electromagnetic field can be found in Refs. [8,9]. In the present study, we will focus on the case of time-independent field and use it to demonstrate the basic technique. The Euler-Lagrangian equations of L with respect to $\mathbf{x}$ and u give the guiding-center motion equations

$$\frac{d\mathbf{x}}{dt} = \frac{\mathbf{B}^\dagger}{B_{||}^\dagger} u - \frac{\mathbf{b} \times \mathbf{E}^\dagger}{\mathbf{b} \cdot \mathbf{B}^\dagger}, \tag{2}$$

$$\frac{du}{dt} = \frac{\mathbf{B}^\dagger \cdot \mathbf{E}^\dagger}{B_{||}^\dagger}, \tag{3}$$

$$\mathbf{B}^\dagger \equiv \nabla \times \mathbf{A}^\dagger, \qquad \mathbf{A}^\dagger = \mathbf{A}(\mathbf{x}) + u\mathbf{b}(\mathbf{x}),$$
$$B_{||}^\dagger \equiv \mathbf{B}^\dagger \cdot \mathbf{b}, \qquad \mathbf{E}^\dagger \equiv \mathbf{E} - \mu \nabla B.$$

The details of the calculation of the Euler-Lagrangian equations are outlined in Ref. [7]. While the gradient drift can be easily identified in Eq. (2), the whereabouts of the curvature drift is not obvious. We note that the curvature drift is actually hidden inside the term $\mathbf{B}^\dagger / B_{||}^\dagger$. From the viewpoint of variational principle, the dynamics of the

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guiding center according to Eqs. (2) and (3) minimizes the action

$$A = \int_0^{t_1} L(\mathbf{x}, \dot{\mathbf{x}}, u, \dot{u})dt. \tag{4}$$

To simulate particle's guiding-center motion, the conventional method is to numerically solve the guiding-center motion Eqs. (2) and (3) by adopting one of the standard methods for numerical integration of differential equations. Here, we take a different approach. Instead of discretizing the differential equation Eqs. (2) and (3), the idea of variational symplectic integrator is to start from the variational principle. We first discretize the action A, and then minimize the discretized action to obtain the iteration rules for advancing the guiding center's position and parallel velocity. Following Ref. [6], we discretize the action on a uniform time grid $t = [0, h, 2h, \ldots, (N-1)h, Nh = t_1]$ as

$$A \approx A_d = \sum_{k=0}^{N-1} hL_d(k, k+1), \tag{5}$$

where $\Delta t = h$ is the length of the time-step and

$$L_d(k, k+1) \equiv L_d(\mathbf{x}_k, u_k, \mathbf{x}_{k+1}, u_{k+1})$$

is the discretized Lagrangian on the time interval $t = [kh, (k+1)h]$. $L_d(k, k+1)$ is constructed from the values of $(\mathbf{x}, u)$ at $t = kh$ and $t = (k+1)h$, denoted by $(\mathbf{x}_k, u_k)$ and $(\mathbf{x}_{k+1}, u_{k+1})$. In the present study, we select the following expression for L_d as a first order approximation to the L given by Eq. (1)

$$L_d(k, k+1) \equiv \frac{[\mathbf{A}^\dagger(k+1) + \mathbf{A}^\dagger(k)]}{2} \cdot \frac{[\mathbf{x}_{k+1} - \mathbf{x}_k]}{h} - \frac{u_k u_{k+1}}{2} - \mu B(k) - \phi(k), \tag{6}$$

where $\mathbf{A}^\dagger(k) \equiv \mathbf{A}^\dagger(\mathbf{x}_k, u_k)$, $B(k) \equiv B(\mathbf{x}_k)$, and $\phi(k) \equiv \phi(\mathbf{x}_k)$. To obtain the iteration rules for the dynamics, we assume $(\delta\mathbf{x}_0, \delta u_0) = (\delta\mathbf{x}_N, \delta u_N) = (0, 0)$, and minimize the action A_d with respect to arbitrary variation $(\delta\mathbf{x}_k, \delta u_k)$ $(0 < k < N)$. Since A_d depends on $(\mathbf{x}_k, u_k)$ only through $L_d(k-1, k)$ and $L_d(k, k+1)$, the necessary conditions for minimum with respect to $(\mathbf{x}_k, u_k)$ are

$$\frac{\partial}{\partial x_k^j}[L_d(k-1,k) + L_d(k,k+1)] = 0, \quad (j = 1, 2, 3), \tag{7}$$

$$\frac{\partial}{\partial u_k}[L_d(k-1, k) + L_d(k, k+1)] = 0. \tag{8}$$

Here x_k^j is the jth $(j = 1, 2, 3)$ component of $\mathbf{x}_k$. Equations (7) and (8) can be viewed as the discretized Euler-Lagrangian equations. Substituting the expression of L_d from Eq. (6), Eqs. (7) and (8) become

$$\frac{1}{2h}A^{\dagger i}_{,j}(k)(x^i_{k+1} - x^i_{k-1}) - \frac{1}{2h}[A^{\dagger j}(k+1) - A^{\dagger j}(k-1)] = \mu B_{,j}(k) + \phi_{,j}(k), \qquad (j = 1, 2, 3), \tag{9}$$

$$\frac{1}{2h}b^i(k)(x^i_{k+1} - x^i_{k-1}) = \frac{u_{k+1} + u_{k-1}}{2}, \tag{10}$$

where subscript ", j" denotes d/dx^j, and summation over repeated index is assumed. Equations (9) and (10) form an implicit system for $(\mathbf{x}_{k+1}, u_{k+1})$ from $(\mathbf{x}_k, u_k)$ and $(\mathbf{x}_{k-1}, u_{k-1})$, and give the iteration rules for the dynamics on the discrete time grid.

The most important feature of this algorithm is the conservation of a noncanonical symplectic structure Ω_d associated with L_d. To see how Ω_d is defined, we note that $L_d(k, k+1)$ can be viewed as a function of $(\mathbf{x}_k, u_k)$ and $(\mathbf{x}_{k+1}, u_{k+1})$. This allows us to define the following two one-forms

$$\theta^+(k, k+1) \equiv \frac{\partial}{\partial \mathbf{x}_{k+1}} L_d(k, k+1) \cdot d\mathbf{x}_{k+1} + \frac{\partial}{\partial u_{k+1}} L_d(k, k+1) du_{k+1},$$

$$\theta^+(k, k+1) \equiv -\frac{\partial}{\partial \mathbf{x}_k} L_d(k, k+1) \cdot d\mathbf{x}_k - \frac{\partial}{\partial u_k} L_d(k, k+1) du_k,$$

which form a partition of the exterior derivative of $L_d(k, k+1)$, i.e.,

$$dL_d(k, k+1) = \theta^+(k, k+1) - \theta^-(k, k+1). \tag{11}$$

We define the discrete Lagrangian symplectic structure Ω_d as

$$\Omega_d(k, k+1) \equiv d\theta^+ = d\theta^-. \tag{12}$$

In Eq. (12) we have used the fact that $d\theta^+ = d\theta^-$, which is an obvious consequence of Eq. (11). Note that $\Omega_d(k, k+1)$ is a closed two-form on the space of $(\mathbf{x}_k, u_k, \mathbf{x}_{k+1}, u_{k+1})$. Now, taking the exterior derivative of A_d defined in Eq. (5), and utilizing Eqs. (7) and (8), we have

$$dA_d = \theta^+(N-1, N) - \theta^-(0, 1).$$

Taking one more exterior derivative leads to

$$\Omega_d(0, 1) = \Omega_d(N-1, N). \tag{13}$$

What Eq. (13) implies is that the Lagrangian symplectic structure Ω_d is conserved, when the system is advanced from $t = 0$ to $t = t_1 = Nh$ according to the iteration rules given by Eqs. (9) and (10). We note that there are different ways to select the first order discretization in Eq. (6). For example, we can replace the last two terms in Eq. (6) by $[-\mu B(k) - \mu B(k+1) - \phi(k) - \phi(k+1)]/2$, which results in the same iteration rules as Eqs. (9) and (10).

The implicit system (9) and (10) can be solved by using the semi-explicit-Newton's method. We first linearize the implicit terms

$$[A^{\dagger j}(k+1) - A^{\dagger j}(k-1)] \approx A^{\dagger j}_{,i}(k)(x^i_{k+1} - x^i_{k-1}) + b^j(k)(u_{k+1} - u_{k-1}),$$

and turn the system into an explicit one

$$\frac{1}{2h}[A^{\dagger i}_{,j}(k) - A^{\dagger j}_{,i}(k)](x^i_{k+1} - x^i_{k-1}) - \frac{b^j(k)}{2h}\left[2u_{k-1} - \frac{b^i(k)}{h}(x^i_{k+1} - x^i_{k-1})\right] = \mu B_{,j}(k) + \phi_{,j}(k), \tag{14}$$

$$\frac{1}{2h} b^i(k)(x^i_{k+1} - x^i_{k-1}) = \frac{u_{k+1} + u_{k-1}}{2}. \tag{15}$$

It is of course trivial to solve the explicit system (14) and (15), the solution of which will be used as an initial guess for solving the implicit system (9) and (10) using the Newton's method.

We note that for Hamiltonian systems with canonical symplectic structure, symplectic algorithms can be constructed to be explicit. Since the guiding-center dynamics does not have a canonical symplectic structure, our approach is to start from the variational principle to construct a symplectic integrator, which turns out to be implicit. It is not clear to us whether it can be constructed to be explicit, which is clearly a future research topic. Of course, there is additional overhead associated with the implicit nature of the variational symplectic algorithm. However, since there is a good explicit approximation to the implicit system, the root searching algorithm starting from the solution of the explicit system quickly converges in several iterations for practical applications. Because the discretized Lagrangian in Eq. (6) is a first order approximation to the continuous L over one grid, the accuracy of the current algorithm is of the first order. The order of accuracy can be improved if we discretize L over multiple grids. For example, a second order scheme can be constructed if L is discretized over two grids. Of course, this will bring extra computation overhead. The design and tradeoff studies for high order schemes are apparently another interesting topic for future

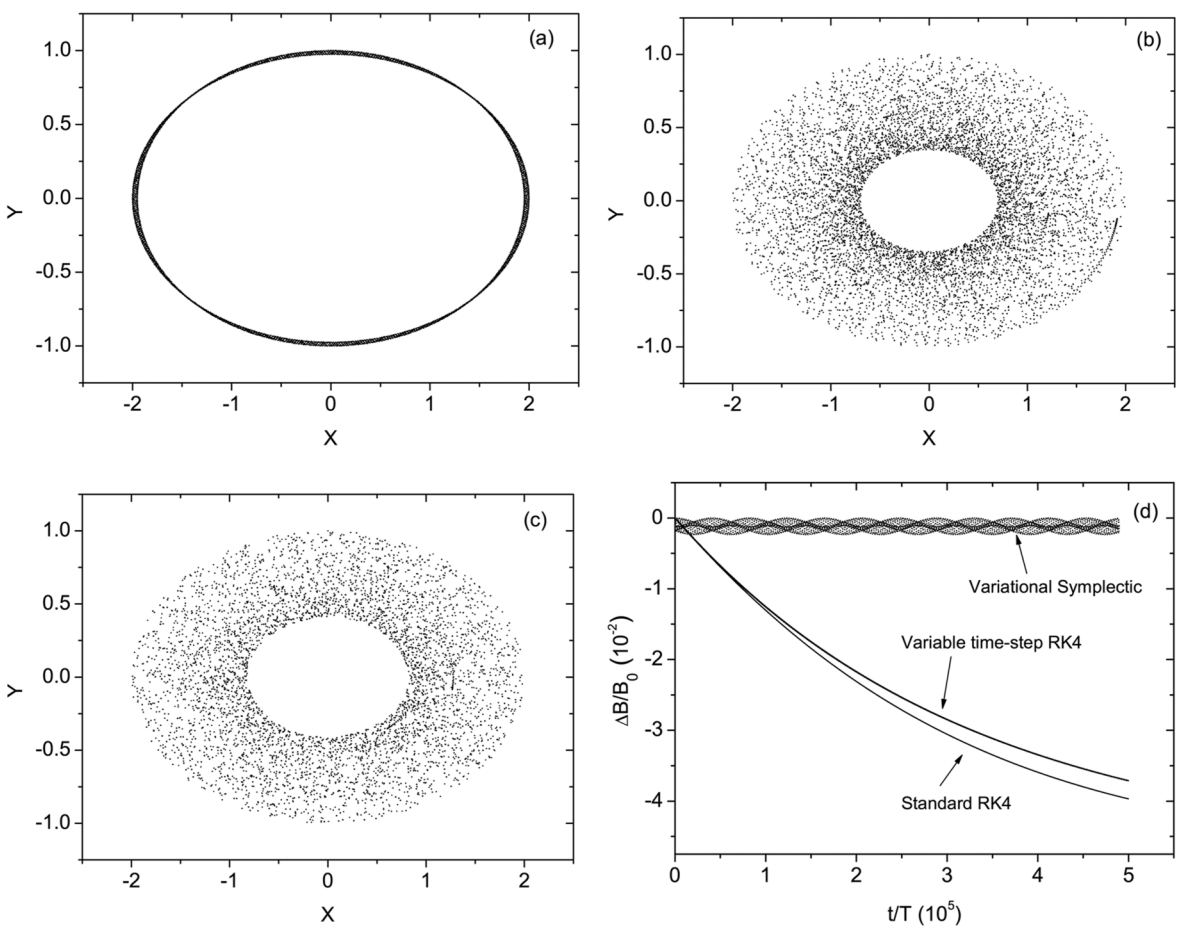

FIG. 1. Guiding-center orbits numerically obtained by using the variational symplectic method (a), standard fourth order Runge-Kutta method (b), and variable time-step fourth order Runge-Kutta method (c). The exact orbit is the ellipse of $x^2/4 + y^2 = 1$. The integration time is 5×10^5 periods of the closed orbit. Deviation $\Delta B/B_0$ as a function of time from the exact orbit for the three methods (d).

research. Compared with other methods, symplectic algorithms can achieve better results with low order schemes because the local errors in symplectic algorithms do not accumulate coherently over the entire integration domain. The energy error is globally bounded. The algorithm presented is expressed in terms of potentials $\mathbf{A}$ and ϕ. This is natural because the governing equation system of the collective dynamics of guiding centers is the gyrokinetic equation system, and the fields, especially the perturbed fields, in contemporary gyrokinetic equations are expressed in terms of potentials $\mathbf{A}$ and ϕ. Therefore it is actually more convenient to advance particles using the potentials. For equilibrium fields, the vector potential can be easily constructed for most magnetic systems, such as those in tokamaks and stellerators. Furthermore, the equilibrium vector potential only needs to be set up once initially with the grid before the dynamic simulation begins. The computation overhead induced is minimum.

Let us give a numerical example of the variational symplectic integrator developed. Consider a 2D, weakly inhomogeneous magnetic field

$$\mathbf{B} = B(x, y)\hat{\mathbf{z}}, \qquad B(x, y) = 1 + 0.05\left(\frac{x^2}{4} + y^2\right).$$

In this ideal geometry designed for the purpose of testing, the guiding-center drift motion forms a closed orbit in the $x - y$ plane,

$$\frac{x^2}{4} + y^2 = \text{const.}$$

The dynamics of u and z is trivial and decoupled from the transverse motion. Shown in Fig. 1(a) is a guiding-center orbit numerically obtained by using the variational symplectic method, and Figs. 1(b) and 1(c) are the same orbit obtained by the standard and variable time-step fourth order Runge-Kutta methods. The total integration time is $5 \times 10^5 T$, where T is the period of the guiding-center periodic motion. The initial position for the guiding center is at $(x_0, y_0) = (0, 1)$, and the exact orbit is the ellipse of $x^2/4 + y^2 = 1$. The time step for the variational symplectic method and the standard fourth order Runge-Kutta method is $\Delta t = 0.02T$. The time-step for the variational time-step fourth order Runge-Kutta method is varied to keep the stepping error $\varepsilon < \varepsilon_0 = 1.1 \times 10^{-5}$, where ε_0 is the initial stepping error corresponding to the initial time step $\Delta t = 0.02T$. Here, the stepping error is calculated by the usual step doubling method. The averaged time-step for the variable time-step fourth order Runge-Kutta method over the entire integration time is $0.0195T$. For each step of the variational symplectic integrator, two Newton iterations are employed for root searching, which requires three evaluations of force. The numbers of force evaluations per step for the standard and variable time-step fourth order Runge-Kutta methods are 4 and 5.5. Therefore, the ratio between the numbers of force evaluations for the three methods is 1:1.3:1.88, with the variational symplectic integrator having the smallest number of force evaluations and the variable time-step fourth order Runge-Kutta method the largest. Plotted in Fig. 1(d) is the normalized deviation from the closed orbit $\Delta B/B_0$ as a function of time for the three integrators. Here $\Delta B \equiv B(x, y) - B_0$ and $B_0 \equiv B(x_0, y_0)$. Clearly demonstrated in the figures is the fact that for the variational symplectic integrator, the deviation from the exact orbit is bounded for all time, whereas for the standard and variable time-step fourth order Runge-Kutta methods, the orbits drift away slowly from the exact orbit in the longer time scale, even though for the integration time comparable to T, the Runge-Kutta methods give an accurate result. The superiority of the variational symplectic integrator over longer integration time can be attributed to the fact that it conserves exactly the discrete symplectic structure Ω_d.

In conclusion, starting from the variational principle for the guiding-center dynamics, we have constructed a variational symplectic integrator for a long-time simulation study of magnetized plasmas. The variational symplectic integrator conserves exactly a discrete Lagrangian symplectic structure, and has better numerical properties over long integration time, compared with standard integrators, such as the fourth order Runge-Kutta methods. We would like to point out that if the integration time is not very long, the advantage of the variational symplectic integrator developed is not prominent. Therefore, what we wish to accomplish is to provide another optional integrator for guiding-center dynamics, with emphasis on the global conservative properties over long integration time, which could benefit long-time simulation studies for magnetized plasmas.

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