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Abstract

In this paper, a long-time accurate explicit integrators is developed to simulate the motion of charged particle in general magnetic field based on variational symplectic integrator. It is proved mathematically that the new integrator is explicit scheme and conserves volume in phase space. In rectangular coordinate system, the new integrator is just Boris Integrator. In guiding center system of three independent position coordinates where variational symplectic integrator is unstable, the new integrator bounds the energy error in a very narrow regime and conserves the accuracy of numerical orbit of charged particles in long-time scale.

In plasma system including magnetic field, where the time scale of the development of mesoscale or macroscale collective phenomena such as transport and wave instability induced by wave-particle interaction is much larger than that of charged particles gyrating around magnetic field, the long-time accurate integrators are needed to carry out a long-time scale to simulate those collective phenomena accurately. For strongly magnetized plasma system, such as tokamak plasma[1, 2] and space plasma[3–5], the gyrating motion around magnetic field can be reduced to get the guiding center version of the orbit[6–8], which makes the simulation of orbit become much easer. Therefore, finding a long-time accurate integrators for guiding center system is especially important for the simulation of long-time motion of strongly magnetized charged particles.

As well-known, classical four-order Runge-Kutta algorithm is of high accuracy in single time-step, but accumulates error coherently in long time scale[1, 9]. Boris integrator (BI)[10, 11] and variational symplectic integrator (VSI)[12–14] have global bound on errors of energy and the shape of orbit of charged particles moving in magnetic field in rectangular coordinate system, so they can be effective in long time simulation in such systems. For guiding center system, VSI was shown to have good performance in long-time two dimensional position coordinate simulation[9], and it was thought to be a good integrator to simulate guiding center motion, since guiding center system is just a non-canonical structure dynamics system and VSI can applies on such system [1, 12], while standard symplectic integrator can't [13, 14]. However, our numerical tests reveal that VSI becomes serious instable in guiding center system of three independent position coordinates. Besides, BI can't be applied neither in guiding center system since it specializes in the motion of charged particle in rectangular coordinate system without guiding enter approximation. So far, no algorithm has been shown to be effective in long-time simulation in guiding center system of three independent position coordinates. In this paper, a new algorithm is put forward based on VSI to consistently apply on rectangular coordinate magnetic system and guiding center system of three independent position coordinates. A new method will be adopted to prove that the new integrators conserve the volume in phase space, and for rectangular coordinate magnetic system the new algorithm is just BI, while guiding center system, the new algorithm globally bounds the error of energy in a very narrow regime and preserves the accuracy of numerical orbit in long time scale. Therefore, the new algorithm is effective in long time simulation of guiding center system.

We first introduce the VSI which conserves a symplectic differential 2-form[12]. For a system of Lagrangian L, VSI is to minimize the discretized version of action $A=\int_0^{t_1} Ldt$, which is $A_d = h\sum\limits_{k=0}^{n-1} L_d(k,k+1)$ where h is the time-step size, to get the iterative rule given by the discrete Euler-Lagrangian equations(DEL)

$$\frac{dL_d(k-1,k)}{dx_k^i}+\frac{dL_d(k,k+1)}{dx_k^i}=0. \tag{1}$$

Taking rectangular coordinate system as an example, its Lagrangian is $L = \mathbf{v}^2/2 - (\phi - \mathbf{v}\cdot\mathbf{A})$ with natural unit system adopted, where ϕ is electric potential and $\mathbf{A}$ is vector potential. For rectangular coordinate system, $L_d(k,k+1) = (\mathbf{x}_{k+1}-\mathbf{x}_k)^2/2h^2 - \left[\phi_{k+1/2} - (\mathbf{x}_{k+1}-\mathbf{x}_k)\,\mathbf{A}_{k+1/2}/h\right]$, where $v_k = (x_k - x_{k-1})/h$ and the subscript $'k \pm 1/2'$ denotes the values of functions at the point $(\mathbf{x}_{k\pm1}+\mathbf{x}_k)/2$. The implicit iterative rule given by DEL is

$$\begin{array}{l}\left(x_{k+1}^i + x_{k-1}^i - 2x_k^i\right)/h^2 - \phi_{k+1/2,i}/2 - \phi_{k-1/2,i}/2 + A_{k+1/2}^i/h \\ -A_{k-1/2}^i/h - \frac{(x_{k+1}^j - x_k^j)}{2h}A_{k+1/2,i}^j - \frac{(x_k^j - x_{k-1}^j)}{2h}A_{k-1/2,j}^i = 0\end{array} \tag{2}$$

where $i = 1,2,3$ for three dimensional position coordinate system. Now Taylor expanding functions of subscript $'k \pm 1/2'$ at location $\mathbf{x}_k$ to get $\phi_{k+1/2,i}/2 + \phi_{k-1/2,i}/2 = \phi_{k,i} + O(h)$ and $A_{k+1/2}^i/h - A_{k-1/2}^i/h - (x_{k+1}^j - x_k^j)A_{k+1/2,i}^j/2h - (x_k^j - x_{k-1}^j)A_{k-1/2,j}^i/2h = \delta_{il}\left[A_{k,l}^i - A_{k,i}^l\right](x_{k+1}^l - x_{k-1}^l)/2h + O(h)$ where δ_{ij} equals one if $i=j$ or else equals zero. Then getting rid of the $O(h)$ part in Eq.(2), it reaches

$$\left(x_{k+1}^i + x_{k-1}^i - 2x_k^i\right)/h^2 - \phi_{k,i} + \left(A_{k,j}^i - A_{k,i}^j\right)(x_{k+1}^j - x_{k-1}^j)/2h = 0. \tag{3}$$

If taking back $v_k = (x_k - x_{k-1})/h$ and defining $B_k^m \equiv \varepsilon_{mij}\left(A_{k,i}^j - A_{k,j}^i\right)$, $E_k^i \equiv \phi_{k,i}$ where ε_{mij} is antisymmetric three order tensor, Eq.(3) can be reformulated to be $\mathbf{v}^- = \mathbf{v}_k + h\mathbf{E_k}/2$, $\left(\mathbf{v}^+ - \mathbf{v}^-\right)/h = \left(\mathbf{v}^+ + \mathbf{v}^-\right)\times\mathbf{B}_k/2$, $\mathbf{v}_{k+1} = \mathbf{v}^+ + h\mathbf{E_k}/2$, which are just the traditional discrete schemes of BI[11].

In Ref.[10], the property of BI to conserve volume in phase space was proved based on the theory of Cayley transformation. In this paper, a new method is adopted to prove this property and will be used on the new integrators of guiding center system. To begin, explicitly multiply Eq.(3) by $h^2dx_k^i$ for each i and add them together, then exteriorly differentiate the result to get

$$\begin{array}{l}dx_{k+1}^i\wedge dx_k^i + dx_{k-1}^i\wedge dx_k^i + h\left(A_{k,j}^i - A_{k,i}^j\right)\left(dx_{k+1}^j\wedge dx_k^i - dx_{k-1}^j\wedge dx_k^i\right)/2 \\ +h\left(A_{k,jl}^i - A_{k,il}^j\right)\left(x_{k+1}^j - x_{k-1}^j\right)dx_k^l\wedge dx_k^i/2 - h^2\phi_{k,ij}dx_k^j\wedge dx_k^i = 0\end{array} \tag{4}$$

where repeated index means summing of all indexes and so does that in the rest of this paper, and $\wedge$ is exterior production symbol. The left of Eq.(4) is combination of differential 2-form. Note that 2-form like $dx \wedge dy$ is antisymmetric [15], thus $h^2\phi_{k,ij}dx_k^j \wedge dx_k^i = 0$. Now reformulate Eq.(4) to be the form of **left** = **right**, where

$$\begin{aligned}\mathbf{left} = {} & dx_{k-1}^i \wedge dx_k^i - \tfrac{h}{2}\left(A_{k,j}^i - A_{k,i}^j\right) dx_{k-1}^j \wedge dx_k^i \\ & + \tfrac{h}{2}\left(A_{k,jl}^i - A_{k,il}^j\right)\left(x_{k+1}^j - x_{k-1}^j\right) dx_k^l \wedge dx_k^i,\end{aligned} \tag{5}$$

$$\mathbf{right} = dx_k^i \wedge dx_{k+1}^i - \frac{h}{2}\left(A_{k,j}^i - A_{k,i}^j\right) dx_k^j \wedge dx_{k+1}^i. \tag{6}$$

For phase space of six dimensions, we exteriorly multiply **left** and **right** by themselves respectively three times to get

$$\mathbf{left} \wedge \mathbf{left} \wedge \mathbf{left} = \mathbf{right} \wedge \mathbf{right} \wedge \mathbf{right}. \tag{7}$$

Terms appearing in both sides of Eq.(7) are differential 6-forms. There are three components of differential 2-forms comprised by **left** in Eq.(5). In the left of Eq.(7), once any one of the three **left**s in the production provide a term like $dx_k^l \wedge dx_k^i$ among the three components given in Eq.(5) to produce a differential 6-form, this production should equal zero, since dx_k^l or dx_k^i in $dx_k^l \wedge dx_k^i$ repeats in the other two 2-forms given by the rest two **left**, and differential forms containing repeated micro-element like $dx \wedge dx$ equal zero[15]. Also differential 6-forms, which are the cross exterior production between components $dx_{k-1}^i \wedge dx_k^i$ and $dx_{k-1}^j \wedge dx_k^i$ in **left**, equal zero, because repeated dx_{k-1}^i or dx_k^i appears in this differential 6-forms. To calculate the self production of component $dx_{k-1}^j \wedge dx_k^i$ in **left**, we first divide terms of this component into two groups $dx_{k-1}^1 \wedge dx_k^2, dx_{k-1}^2 \wedge dx_k^3, dx_{k-1}^3 \wedge dx_k^1$ and $dx_{k-1}^2 \wedge dx_k^1, dx_{k-1}^3 \wedge dx_k^2, dx_{k-1}^1 \wedge dx_k^3$. It's easy to prove that for each differential 6-form resulted from the exterior production of differential 2-forms within one group, there exists one differential 6-form coming from the exterior production of the other group to cancel it. On the other hand, 6-form coming form the cross exterior production between the two groups equals zero, since repeated dx_{k-1}^i or dx_k^i appears for a special i based on the chosen 2-forms for production. Therefore, the self exterior production of $dx_{k-1}^j \wedge dx_k^i$ equals zero. Eventually, the rest non zero part of the left side of Eq.(7) is the self production of component $dx_{k-1}^i \wedge dx_k^i$ given in Eq.(5), which is

$$\mathbf{left} \wedge \mathbf{left} \wedge \mathbf{left} = 3dx_{k-1}^1 \wedge dx_{k-1}^2 \wedge dx_{k-1}^3 \wedge dx_k^1 \wedge dx_k^2 \wedge dx_k^3. \tag{8}$$

It can be proved that $\mathbf{right} \wedge \mathbf{right} \wedge \mathbf{right} = 3dx_k^1 \wedge dx_k^2 \wedge dx_k^3 \wedge dx_{k+1}^1 \wedge dx_{k+1}^2 \wedge dx_{k+1}^3$ in the same way. Therefore, there stands the identity $dx_{k-1}^1 \wedge dx_{k-1}^2 \wedge dx_{k-1}^n \wedge dx_k^1 \wedge dx_k^2 \wedge dx_k^n =$

$dx_k^1\wedge dx_k^2\wedge dx_k^3\wedge dx_{k+1}^1\wedge dx_{k+1}^2\wedge dx_{k+1}^3$. Taking back $v_k^i=(x_k^i-x_{k-1}^i)/h, v_{k+1}^i=(x_{k+1}^i-x_k^i)/h$ in this identity, the conservation law of phase-space volume by BI is derived

$$dx_k^1\wedge dx_k^2\wedge dx_k^3\wedge dv_k^1\wedge dv_k^2\wedge dv_k^3=dx_{k+1}^1\wedge dx_{k+1}^2\wedge dx_{k+1}^3\wedge dv_{k+1}^1\wedge dv_{k+1}^3\wedge dv_{k+1}^3 \quad (9)$$

where both sides of Eq.(9) are micro element of volume in discrete phase space at k and $k+1$ moment.

Up to now, we complete the prove of BI to conserve phase-space volume. The numerical example which shows the superiority of long-time simulation of BI can be found in Ref.[10]. We now turn to apply this procedure to guiding center system to get the new algorithm. The guiding center Lagrangian is $L_g(\mathbf{x},\dot{\mathbf{x}},u,\dot{u})=\mathbf{A}^\dagger\cdot\dot{\mathbf{x}}-[\mu B(\mathbf{x})+u^2/2+\phi(\mathbf{x})],\mathbf{A}^\dagger=\mathbf{A}(\mathbf{x})+u\mathbf{b}(\mathbf{x})$, which is given in Ref.([7]), where constant μ is magnetic moment, u is parallel velocity along magnetic field. The discretized version of L_g is $L_{gd}(k,k+1)=\mathbf{A}^\dagger{}_{k+1/2}\cdot(\mathbf{x}_{k+1}-\mathbf{x}_k)/h-\left[\mu B_{k+1/2}+(u_k+u_{k+1})^2/8+\phi_{k+1/2}\right]$. Adopting the same method of Taylor expanding functions in DEL at time moment k, and getting rid of terms of order equal to or higher than $O(h)$, then we get the new explicit iterative rule for $x_i, i=1,2,3$ and u

$$M_k^{ij}\left(x_{k+1}^j-x_{k-1}^j\right)+\frac{(u_{k-1}-u_{k+1})}{2h}b_k^i-2\mu B_{k,i}-2\phi_{k,i}=0, \quad (10)$$

$$\frac{u_{k+1}-u_{k-1}}{2}+u_k-\frac{1}{2h}b_k^i\left(x_{k+1}^i-x_{k-1}^i\right)=0. \quad (11)$$

In Eq.(10), $M_k^{ij}=\varepsilon_{ijm}B_k^m+u_kb_{k,i}^j-u_kb_{k,j}^i$, B_k^m is the m-th component of the magnetic field and b_i is the i-th component of unit vector of magnetic field. The method used to prove BI conserving volume of phase space is adopted to prove the new integrator given by Eqs.(10,11) of the same conservative property. Multiply Eq.(10) by dx_k^i for each i and Eq.(11) by du_k, and sum all equations together to get a new equation, then exteriorly differentiate the new equation to get a identity constituted by differential 2-forms like Eq.(4). Moving 2-forms containing subscript $k+1$ to the right of this identity, and using $\mathbf{left}_g$ and $\mathbf{right}_g$ to denote the left and right side of this identity, then as Eq.(7), we exteriorly multiply $\mathbf{left}_g$ and $\mathbf{right}_g$ four times by themselves to get a identity $\mathbf{left}_g\wedge\mathbf{left}_g\wedge\mathbf{left}_g\wedge\mathbf{left}_g=\mathbf{right}_g\wedge\mathbf{right}_g\wedge\mathbf{right}_g\wedge\mathbf{right}_g$. As haven been discussed in BI case, 2-forms like $dx_k^j\wedge dx_k^i$ and $dx_k^j\wedge du_k$ make the productions equal zero. After getting rid of these terms, we obtain the effective $\mathbf{left}_{ge}$ and $\mathbf{right}_{ge}$

$$\mathbf{left}_{ge}=M_k^{ij}dx_{k-1}^j\wedge dx_k^i-\frac{1}{2h}b_k^idu_{k-1}\wedge dx_k^i-\frac{1}{2h}du_{k-1}\wedge du_k-\frac{1}{2h}b_k^idx_{k-1}^i\wedge du_k, \quad (12)$$

$$\mathbf{right}_{ge} = M_k^{ij} dx_{k+1}^j \wedge dx_k^i - \frac{1}{2h} b_k^i du_{k+1} \wedge dx_k^i + \frac{1}{2h} du_{k+1} \wedge du_k - \frac{1}{2h} b_k^i dx_{k+1}^i \wedge du_k. \quad (13)$$

Based on Eq.(12), we reach $\mathbf{left}_g \wedge \mathbf{left}_g \wedge \mathbf{left}_g \wedge \mathbf{left}_g = M dx_{k-1}^1 \wedge dx_{k-1}^2 \wedge dx_{k-1}^3 \wedge dx_k^1 \wedge dx_k^2 \wedge dx_k^3 \wedge du_{k-1} \wedge du_k$ and $M = -b_1^2 M_{23}^2 - b_2^2 M_{13}^2 - b_3^2 M_{12}^2 - b_1 b_2 M_{23} M_{13} + b_1 b_3 M_{12} M_{13} - b_1 b_2 M_{13} M_{23} - b_2 b_3 M_{12} M_{13} + b_3 b_1 M_{23} M_{12} - b_3 b_2 M_{12} M_{13}$, which can be checked not to equal zero. The exterior production of $\mathbf{right}_{ge}$ is the exterior production of $\mathbf{left}_{ge}$ through replacing $k-1$ and k by k and $k+1$, respectively. At last we get the conservation law of discrete phase space volume through replacing x_k by $(v_k - v_{k-1})/h$

$$\begin{aligned} & dv_{k-1}^1 \wedge dv_{k-1}^2 \wedge dv_{k-1}^3 \wedge dv_k^1 \wedge dv_k^2 \wedge dv_k^3 \wedge du_{k-1} \wedge du_k \\ &= dv_k^1 \wedge dv_k^2 \wedge dv_k^3 \wedge dv_{k+1}^1 \wedge dv_{k+1}^2 \wedge dv_{k+1}^3 \wedge du_k \wedge du_{k+1}. \end{aligned} \quad (14)$$

We now proceed to exemplify the long-time good performance of this new integrator in guiding center system by simulating the banana orbit of trapped particle. We consider a 3D tokamak model with circular concentric flux surfaces. In toroidal coordinate system (r, θ, ξ) which are radial, poloidal and toloidal coordinates, the magnetic field of this model is chosen to be $\mathbf{B} = \frac{B_0 r}{qR}\mathbf{e}_\theta + \frac{B_0 R_0}{R}\mathbf{e}_\xi$ where B_0, R_0, q are characteristic magnetic field, the major radius of the center of the poloidal cross section and safety factor, respectively. The corresponding vector potential $\mathbf{A}$ is chosen to be $\mathbf{A} = A_r \mathbf{e}_r + A_\theta \mathbf{e}_\theta + A_\xi \mathbf{e}_\xi$ and $A_r = \frac{B_0 R_0 r \sin\theta\cos\theta}{2R} - \ln\left(\frac{R}{R_0}\right)\frac{R_0 B_0}{2}\sin\theta$, $A_\theta = -\ln\left(\frac{R}{R_0}\right)\frac{R_0 B_0}{2}\cos\theta - \frac{B_0 R_0 r \sin^2\theta}{2R}$ and $A_\xi = \frac{B_0 r^2}{2Rq}$. The guiding center Lagrangian is

$$L_g = p_r \dot{r} + p_\theta \dot{\theta} + p_\xi \dot{\xi} - H, \quad (15)$$

$$p_r = -\ln\left(\frac{R}{R_0}\right)\frac{R_0 B_0}{2}\sin\theta + \frac{B_0 R_0 r}{2R}\sin\theta\cos\theta, \quad (16)$$

$$p_\theta = -\ln\left(\frac{R}{R_0}\right)\frac{R_0 B_0 r}{2}\cos\theta - \frac{B_0 R_0 r}{2R}\sin\theta\cos\theta + \frac{ur^2}{\sqrt{r^2 + R_0^2 q^2}}, \quad (17)$$

$$p_\xi = \left(\frac{B_0 r^2}{2Rq} + \frac{R_0 q u}{\sqrt{r^2 + R_0^2 q^2}}\right) R, \quad (18)$$

$$H = \frac{\mu B_0}{Rq}\sqrt{r^2 + R_0^2 q^2} + \frac{u^2}{2}. \quad (19)$$

The comparison between VSI and the new algorithm is carried out. Physical quantities are normalized by the minor radius a, the characteristic magnetic field B_0 and the bounce frequency of trapped electrons $qR_0/\varepsilon^{1/2}v$. The initial condition is $r_0 = 1, R_0 = 4, \phi_0 = 0, \xi_0 = 0, q = 2$ and $v_\parallel / v_\perp = 0.1$. The time-step size is chosen to make 300 steps complete a banana orbit. Plotted in Fig.(1) is the comparison between the normalized numerical energy of the new integrator and VSI. The first figure in Fig.(1) shows that the new integrator bounds the error of energy in a very narrow strip, while that of VSI becomes serious instable with time number increasing. The comparison between orbits of the two algorithms is carried out by comparing the banana orbits within the poloidal cross section. The comparison between the two figures in Fig.(2) reveals that the numerical error of orbit of VSI accumulates coherently that the orbit becomes serious instable with time number increasing, whiles that given by the new integrator shown in Fig.(3) keeps the correctness during $2e + 5$ time steps, which means that the new integrator can keep the correct orbit in long-time scale.

It's necessary to point out that there is no guarantee that the error of phase of a periodic motion numerically calculated is bounded for all time. Volume-preserving algorithms and symplectic algorithms only bound the energy error for all time, but for most cases don't bound other invariants of the dynamics, such as angular momentum for a system with angular symmetry. However, for systems with periodic orbits, such as the banana orbit of trapped particles, the phase error of the new algorithms such as BI in rectangular coordinate system and that in guiding center system, will grow with time linearly, which indicates an error in the frequency of the periodic motion. But our numerical calculations show that the error in frequency is always systematic rather than random, which suggests that an algorithmic correction is possible.

In summary, we put forward a new method to get algorithms of explicit schemes which conserves volume in phase space based on VSI in rectangular coordinate system and guiding center system, and numerical example shows this new algorithm in guiding center system has global bound on the error of energy and orbit. Our method based on VSI can be adopted in other dynamics system to create a explicit scheme conserving volume in phase space, which is usually of faster speed than implicit scheme. Besides, the way in our method to prove whether the iterative scheme conserves volume can be used to other explicit schemes.

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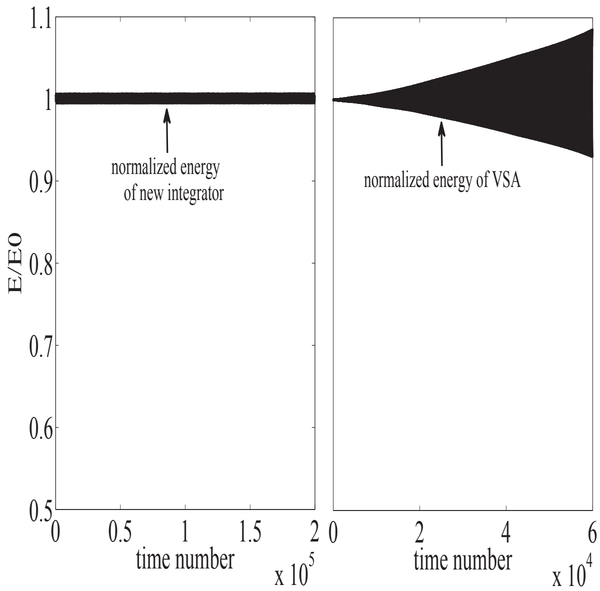

FIG. 1. The comparison of normalized numerical energy between VSI and the new integrator.

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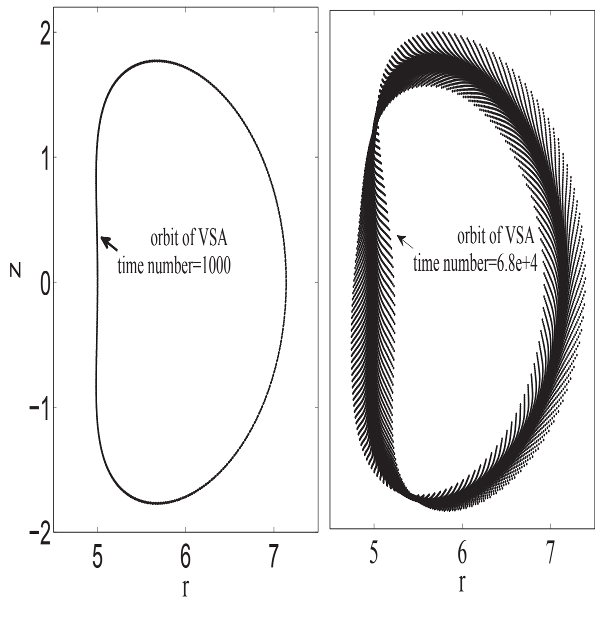

FIG. 2. The orbits of VSI in the first 1000 steps and in 6.8e+4 time steps.

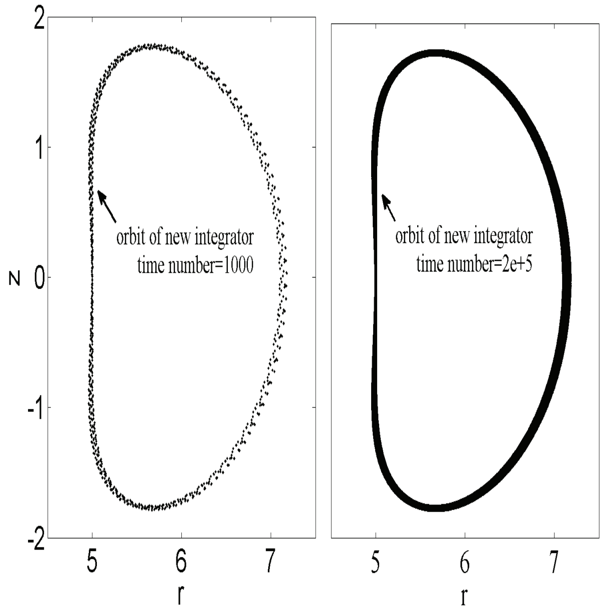

FIG. 3. The orbits of the new integrator in the first 1000 steps and in 2e+5 time steps.