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PRESERVATION OF THE INVARIANTS OF LOTKA-VOLTERRA EQUATIONS BY ITERATED DEFERRED CORRECTION METHODS

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Abstract. In this paper we apply Kahan's nonstandard discretization to three dimensional Lotka-Volterra equations in bi-Hamiltonian form. The periodicity of the solutions and all polynomial and non-polynomial invariants are well preserved in long-term integration. Applying classical deferred correction method, we show that the invariants are preserved with increasing accuracy as a results of more accurate numerical solutions. Substantial speedups over the Kahan's method are achieved at each run with deferred correction method.

Keywords: Lotka-Volterra equations, conserved quantities, Kahan's method, iterated deferred correction.

AMS Subject Classification: 65P10, 65L12

1. Introduction

In the last two decades, many structure preserving geometric integrators are developed to preserve symplectic structure, energy and other invariants, phase space volume, reversing symmetries, dissipation approximately or exactly (up to the round-off errors) [1, 2] of dynamical systems. These are symplectic and variational integrators for Hamiltonian systems [1, 3], integral preserving methods [2] and discrete gradient methods [4]. For special classes of ordinary differential equations (ODEs), there exist non-standard discretization methods [5, 6] which preserve the conserved quantities and other features approximately or exactly. Among them Kahan's method, also known as Hirota-Kimura method, applied to ODEs with quadratic vector fields, preserves the integrals or conserved quantities of many Hamiltonian and integrable systems [7, 8, 9, 10, 11, 12]. It was introduced by W. Kahan as "unconventional" discretization method [5] for quadratic vector fields and applied to a scalar Riccati equation and a two-dimensional Lotka-Volterra system [13].

The Lotka-Volterra systems (LVSs) are first order ODEs with quadratic vector fields, initially designed as an ecological predator-prey model. They occur in epidemiology, in laser physics [14], in evolutionary game theory [15] and as spatial discretization of the Korteweg de Vries equation [13, 16]. Most of the two and three dimensional LVSs have periodic solutions and possess polynomial and non-polynomial integrals. They can be

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written as Poisson systems in bi-Hamiltonian form [17] and Nambu systems [18]. Many numerical methods are applied to LVSs which preserve the integrals, periodic solution, attractors and so on [6, 19, 20, 21, 22, 23].

For Hamiltonian systems, higher order accuracy for integrals can be achieved by composing symplectic integrators in time [24, 25, 26, 27]. Starting with a basic method, arbitrary orders of accuracy can be obtained by applying the composition to a lower order symplectic method recursively. Another class of numerical methods designed for the construction of high-order approximations to the solution of differential equations are the deferred correction methods. A numerical solution of an initial-value problem (IVP) for ODEs is computed by a low order method and then subsequently refined by solving the IVP constructed by the error between the numerical and continuous solutions. Under suitable assumptions, this process can be repeated to produce solutions with an arbitrarily high order of accuracy. Deferred correction methods have been extensively applied to IVPs such as, classical deferred correction (CDC) methods [28, 29], spectral deferred correction methods [28, 30] and integral deferred correction methods [31]. Most of the deferred correction methods are based on implicit, semi-implicit Euler methods and mid-point rule. There are also other Deferred correction methods based on higher order time integrators like Mono-Implicit Runge-Kutta methods [32]. Among them the spectral deferred correction methods are most efficient ones as an iterative scheme for computing a higher-order solutions at Gauss-Lobatto collocation points.

In this paper, two three dimensional (3D) LVSs in bi-Hamiltonian form are solved by the CDC method based on Kahan's method. We show that the periodicity of the solutions and integrals are preserved in long term integration. At each correction step, more accurate solutions are obtained and the integrals are preserved more accurately. Iterated deferred correction methods are more efficient than the composition methods, because at the correction step the same grid is used. Therefore substantial speedups can be obtained by the CDC methods over the basic method, i.e. Kahan's method. To the best of our knowledge, the deferred correction methods are used first time to preserve the conserved quantities of dynamical systems with higher accuracy.

The paper is organized as follows. In Section 2, we present two 3D LVSs in bi-Hamiltonian form. In Section 3, we give a short description of Kahan's method applied to ODEs with a quadratic vector field. Algorithm for the CDC methods is discussed and given in Section 4. Numerical results for Kahan's method with CDC methods and composition methods are compared in Section 5. The paper ends with some conclusions in Section 6.

2. Lotka-Volterra systems

The LVSs are systems of first order ODEs in the following form [33, 34]

$$\dot{u}_i = u_i(r_i + \sum_j \alpha_{ij} u_j), \quad i = 1, \dots, m, \tag{1}$$

where $\mathbf{u} := (u_1, \dots u_m)^T$ is the m-dimensional state vector and $\dot{u}_i = du_i/dt$ denotes the derivative with respect to time. In ecology, u_i describe the densities of each species and r_i are the intrinsic growth or decay rates. The interaction between the species is specified by the coefficient matrix $A = (\alpha_{ij})$, $i, j = 1, \dots, m$. All variables in (1) are real and the densities u_i are positive. There are no closed solutions of LVSs when $m \geq 2$, they have to be integrated numerically [1, 6].

2.1. **Bi-Hamiltonian 3D Lotka-Volterra systems.** Many 3D LVSs can be written in the following bi-Hamiltonian form

$$\dot{\mathbf{u}} = J_1 \nabla H_2 = J_2 \nabla H_1, \tag{2}$$

where $J_1 = J_1(\mathbf{u})$ and $J_2 = J_2(\mathbf{u})$ (possibly constant) are the skew-symmetric Poisson matrices satisfying the Jacobi identity. There exists two independent integrals H_1 and H_2, associated with J_1 and J_2 such that H_2 is the Casimir for one Poisson structure while H_1 is the Casimir for the other [35]. Bi-Hamiltonian systems are completely integrable [17]. 3D LVSs can also be written as Nambu systems [18], as generalization of Hamiltonian systems with multiple Hamiltonians. Nambu form of (2) is given as

$$\dot{\mathbf{u}} = \nabla H_1 \times \nabla H_2.$$

Vector fields of Nambu systems are divergence free and the flow is volume preserving.

A well known 3D LVS possessing bi-Hamiltonian structure is [36, 21, 37]

$$\begin{aligned} \dot{u}_1 &= u_1(cu_2 + u_3 + \lambda), \\ \dot{u}_2 &= u_2(u_1 + au_3 + \mu), \\ \dot{u}_3 &= u_3(bu_1 + u_2 + \nu), \end{aligned} \tag{3}$$

where $\lambda, \mu, \nu > 0$, and with $abc = -1$ and $\nu = \mu b - \lambda ab$. The skew-symmetric Poisson matrices and Hamiltonians then are given by

$$J_1 = \begin{pmatrix} 0 & cu_1u_2 & bcu_1u_3 \\ -cu_1u_2 & 0 & -u_2u_3 \\ -bcu_1u_3 & u_2u_3 & 0 \end{pmatrix},$$

$$J_2 = \begin{pmatrix} 0 & cu_1u_2(au_3+\mu) & cu_1u_3(u_2+\nu) \\ -cu_1u_2(au_3+\mu) & 0 & u_1u_2u_3 \\ -cu_1u_3(u_2+\nu) & -u_1u_2u_3 & 0 \end{pmatrix},$$

$$H_1 = ab\ln u_1 - b\ln u_2 + \ln u_3,\ H_2 = abu_1 + u_2 - au_3 + \nu \ln u_2 - \mu \ln u_3.$$

H_1 and H_2 are Casimirs of J_1 and J_2, respectively, i.e. $J_1\nabla H_1 = 0$ and $J_2 \nabla H_2 = 0$.

Another example of 3D LVS is the reversible 3D LVS with the circulant coefficient matrix A [38]

$$\begin{aligned} \dot{u}_1 &= u_1(u_2 - u_3), \\ \dot{u}_2 &= u_2(u_3 - u_1), \\ \dot{u}_3 &= u_3(u_1 - u_2). \end{aligned} \tag{4}$$

It has a game-theoretical interpretation [15] and possesses bi-Hamiltonian form with the Poisson matrices

$$J_1 = \begin{pmatrix} 0 & -1 & 1 \\ 1 & 0 & -1 \\ -1 & 1 & 0 \end{pmatrix}, \quad J_2 = \begin{pmatrix} 0 & u_1u_2 & -u_1u_3 \\ -u_1u_2 & 0 & u_2u_3 \\ u_1u_3 & -u_2u_3 & 0 \end{pmatrix},$$

and with the linear Hamiltonian $H_1 = u_1+u_2+u_3$ and the cubic Hamiltonian $H_2 = u_1u_2u_3$. It is reversible with respect to $\rho = diag(-1,-1,-1)$, $\rho J_i(\mathbf{u}) = -J_i(\rho\mathbf{u})$, $i = 1, 2$. It can also be written as Nambu system. The flow generated by (4) is source free, i.e. the volume is preserved. The linear integral H_1 represents the volume. The n-dimensional extension of (4) as integrable discretization of the Korteweg de Vries equation was integrated with a Poisson structure preserving integrator in [16]. Necessary and sufficient conditions for conservation laws of n-dimensional LVSs (1) including the two Poisson systems are derived in [34].

3. Kahan's method

The LVS (1) is an autonomous and quadratic ODE system in the following form

$$\dot{\mathbf{u}} = f(\mathbf{u}) := Q(\mathbf{u}) + B\mathbf{u}, \tag{5}$$

with the quadratic vector field $(Q(\mathbf{u}))_i = u_i \sum_j \alpha_{ij} u_j$ and the diagonal matrix $B = diag(r_1, \ldots, r_m)$. In the system (5), the unknown solution vector is $\mathbf{u} = (u_1, \ldots, u_m)^T$, and it is prescribed the vector of initial conditions $\mathbf{u}(t_0) = (u_1(t_0), \ldots, u_m(t_0))^T$.

For the ODE system (5), Kahan introduced in 1993 the "unconventional" discretization as [5]

$$\frac{\mathbf{u}_{n+1} - \mathbf{u}_n}{\Delta t} = Q(\mathbf{u}_n, \mathbf{u}_{n+1}) + \frac{1}{2} B(\mathbf{u}_n + \mathbf{u}_{n+1}),$$

where Δt is the step size of the integration, $\mathbf{u}_{n+1}$ and $\mathbf{u}_n$ are the approximations at the time instances t_{n+1} and t_n, respectively. The symmetric bilinear form $Q(\cdot, \cdot)$ is obtained by the polarization of the quadratic vector field $Q(\cdot)$ [39]

$$Q(\mathbf{u}_n, \mathbf{u}_{n+1}) = \frac{1}{2} \left(Q(\mathbf{u}_n + \mathbf{u}_{n+1}) - Q(\mathbf{u}_n) - Q(\mathbf{u}_{n+1}) \right).$$

The Kahan's method is second order and time-reversal [13]:

$$\frac{\mathbf{u}_{n+1} - \mathbf{u}_n}{\Delta t} = \left(I - \frac{\Delta t}{2} f'(\mathbf{u}_n) \right)^{-1} f(\mathbf{u}_n),$$
$$\frac{\mathbf{u}_{n+1} - \mathbf{u}_n}{\Delta t} = \left(I + \frac{\Delta t}{2} f'(\mathbf{u}_{n+1}) \right)^{-1} f(\mathbf{u}_{n+1}),$$

where $I \in \mathbb{R}^{m \times m}$ is the identity matrix and f' denotes the Jacobian of f. Moreover, Kahan's method is linearly implicit and it coincides with a certain Rosenbrock method on quadratic vector fields, i.e. $\mathbf{u}_{n+1}$ can be computed by solving a single linear system

$$\left(I - \frac{\Delta t}{2} f'(\mathbf{u}_n) \right) \tilde{\mathbf{u}} = \Delta t f(\mathbf{u}_n), \qquad \mathbf{u}_{n+1} = \mathbf{u}_n + \tilde{\mathbf{u}}. \tag{6}$$

Symplectic integrators like the implicit mid-point rule [1], energy preserving average vector field method [22] and conservative methods [40] require at each time step more than one Newton iteration to solve nonlinear implicit equations to preserve the integrals accurately. Due to the linearly implicit nature, Kahan's method is a very efficient structure preserving integrator for ODEs with quadratic vector fields. Applied to linear differential equations Kahan's method is equivalent to the implicit-mid-point or trapezoidal rule [13]. Therefore it is A-stable like the implicit-mid-point and trapezoidal rule without any time step restriction.

Kahan's method is also a Runge-Kutta method, with negative weights, restricted to quadratic vector fields [41]:

$$\frac{\mathbf{u}_{n+1} - \mathbf{u}_n}{\Delta t} = -\frac{1}{2} f(\mathbf{u}_n) + 2 f\left(\frac{\mathbf{u}_{n+1} + \mathbf{u}_n}{2} \right) - \frac{1}{2} f(\mathbf{u}_{n+1}).$$

Kahan's method was independently rediscovered by Hirota and Kimura [42, 9], which preserves the integrability for a large number of integrable quadratic vector fields like Euler top, Lagrange top [9, 10, 12] Suslov and Ishii systems, Nambu systems, Riccati systems, and the first Painlevé equation [41, 39]. Kahan's method is generalized in [39] to cubic and higher degree polynomial vector fields.

4. Iterative deferred correction method

In this section, we apply the CDC method [28, 29] to the ODE system (5) with quadratic vector field, related to the LVSs (1). For a given time interval $[0, T]$, we subdivide it into J equidistant intervals $[t_j, t_{j+1}]$, $j = 0, 1, \ldots, J-1$:

$$0 = t_0 < t_1 < \cdots < t_j < \cdots < t_J = T, \quad t_{j+1} - t_j = \Delta t,$$

on which we define the approximate solutions by $\mathbf{u}_j \approx \mathbf{u}(t_j)$, $j = 1, \ldots, J$, and for $j = 0$ we use the initial condition, $\mathbf{u}_0 = \mathbf{u}(0)$. Further, each interval $[t_j, t_{j+1}]$ is subdivided into $n-1$ equidistant intervals forming n nodes including the end points t_j and t_{j+1} as

$$t_j = t_{j,1} < t_{j,2} < \cdots < t_{j,i} < \cdots < t_{j,n} = t_{j+1},$$

and we define the approximate solutions on these nodes by $\mathbf{u}_{j,i} \approx \mathbf{u}(t_{j,i})$, $i = 1, \ldots, n$, given that $\mathbf{u}_{j,1} = \mathbf{u}_j$. The CDC method, on each subinterval $[t_j, t_{j+1}]$, starts by solving the ODE system (5) for the solutions at the nodes $\{t_{j,i}\}_{i=1}^{n}$, with a method of order p_0. Then, the approximate solutions of the ODE system (5) on the interval $[t_j, t_{j+1}]$ are defined by $\mathbf{U}_j^{[0]} := (\mathbf{u}_{j,1}^{[0]}, \ldots, \mathbf{u}_{j,n}^{[0]})$, and satisfy that

$$\mathbf{u}_{j,i}^{[0]} = \mathbf{u}(t_{j,i}) + \mathcal{O}((\Delta t)^{p_0}), \quad i = 1, \ldots, n.$$

We apply here the second order Kahan's method described in Section 3 as the basic method, so $p_0 = 2$. After, it follows the correction procedure. At the s-th correction step, the CDC method computes an improved (corrected) solution $\mathbf{U}_j^{[s]} := (\mathbf{u}_{j,1}^{[s]}, \ldots, \mathbf{u}_{j,n}^{[s]})$ of the following error system

$$\begin{aligned} &\frac{d}{dt}\mathbf{e}_j^{[s-1]}(t, \mathbf{U}_j^{[s-1]}(t)) = f\left(\mathbf{e}_j^{[s-1]}(t, \mathbf{U}_j^{[s-1]}(t)) + \mathbf{U}_j^{[s-1]}(t)\right) - \frac{d}{dt}\mathbf{U}_j^{[s-1]}(t), \\ &\mathbf{e}_j^{[s-1]}(t_j, \mathbf{U}_j^{[s-1]}(t_j)) = 0, \end{aligned} \tag{7}$$

by a method of order p_s. In (7), $\mathbf{e}_j^{[s]}(t, \mathbf{U}_j^{[s]}(t))$ denotes the error function on the s-th iteration step given by

$$\mathbf{e}_j^{[s]}(t, \mathbf{U}_j^{[s]}(t)) = \mathbf{u}(t) - \mathbf{U}_j^{[s]}(t), \quad t \in [t_j, t_{j+1}]. \tag{8}$$

The differences between the deferred correction methods are based on the formation of an error system; on the continuous level they are equivalent. In the CDC method, the error system (7) is used, which is obtained by the differentiation of the error equation (8) with respect to the time variable t. The function $\mathbf{U}_j^{[s]}(t)$ stands for the continuous approximation of the discrete solutions $\mathbf{U}_j^{[s]} = (\mathbf{u}_{j,1}^{[s]}, \ldots, \mathbf{u}_{j,n}^{[s]})$. Here, we construct the continuous approximation $\mathbf{U}_j^{[s]}(t)$ based on the Lagrange interpolation as

$$\mathbf{U}_j^{[s]}(t) = \sum_{k=1}^{n} l_k(t) \cdot \mathbf{u}_{j,k}^{[s]}, \quad l_k(t) = \prod_{i \neq k} \frac{t - t_{j,i}}{t_{j,k} - t_{j,i}},$$

where $l_k(t)$ are the Lagrange basis functions.

The error system (7) is a non-autonomous and non-quadratic ODE due the occurrence of the time dependent terms $\mathbf{U}_j^{[s-1]}(t)$ and their derivatives. On the other hand, the Kahan's method is applicable to quadratic ODEs [5, 39]. For this reason, in the correction steps, we use mid-point rule which is a second order integrator like the Kahan's method.

Algorithm 1 Classical deferred correction method

Input: Correction number S, partition $\{[t_j, t_{j+1}]\}_{j=1}^{J}$ of the time interval $[0, T]$, initial solution $\mathbf{u}_0 := \mathbf{u}(0)$
Output: The approximate solutions $\{\mathbf{u}_1, \ldots, \mathbf{u}_J\}$

```
for j = 0, 1, ..., J − 1 do
    Set u_{j,1} := u_j
    Solve the ODE system (5) for U_j^[0] = (u_{j,1}^[0], ..., u_{j,n}^[0]) on the nodes {t_{j,i}}_{i=1}^n, using Kahan's method
    for s = 1, 2, ..., S do
        Form the continuous solution U_j^[s−1](t) using discrete set U_j^[s−1]
        Solve the error system (7) for E_j^[s−1] = (e_{j,1}^[s−1], ..., e_{j,n}^[s−1]) on the nodes {t_{j,i}}_{i=1}^n, using mid-point rule
        Update the solution vector as U_j^[s] = U_j^[s−1] + E_j^[s−1]
    end for
    Set the solution u_{j+1} := u_{j,n}^[S]
end for
```

After, defining the vector of error approximations $\mathbf{E}_j^{[s]} := (\mathbf{e}_{j,1}^{[s]}, \ldots, \mathbf{e}_{j,n}^{[s]})$ where $\mathbf{e}_{j,i}^{[s]}$ are the discrete solutions of the error system (7) on the nodes $\{t_{j,i}\}$, we obtain the corrected numerical approximations through the update formula

$$\mathbf{U}_j^{[s]} = \mathbf{U}_j^{[s-1]} + \mathbf{E}_j^{[s-1]}.$$

An outline of the CDC method can be found in Algorithm 1.

Expected order of accuracy of the CDC methods for uniformly spaced nodes is given by $\min\{P_S, n-1\}$, where $P_S = \sum_{s=0}^{S} p_s$, S is the number of corrections and n is the number of nodes used in each interval $[t_j, t_{j+1}]$ [28, 29]. Since we use Kahan's method and mid-point method, both of which are second order methods, we have $p_s = 2$ for all $s = 0, 1, \ldots, S$, and then the expected order of accuracy becomes $\min\{2S + 2, n - 1\}$. According to this fact, we set $n = 2S+3$ in the simulations to obtain the expected order of accuracy as $n-1$. When non-uniform nodes like Gauss–Lobatto, Gauss–Legendre, and Chebyshev nodes are used, for CDC methods the accuracy improves with more corrections although the order of accuracy stagnates at two [29]. When a low order Lagrange interpolation is used on small intervals $[t_j, t_{j+1}]$, the CDC method can produce accurate results on uniform nodes, as it will be shown in the next Section. In case of computational cost, Kahan's method without CDC method requires solution of linear system (6) on J time iterations, whereas it is needed, in total, solution of $J(n-1)(S+1)$ linear systems. However, CDC method can reduce the computational cost especially for small S, since larger time step-sizes results in the same level of accuracy with CDC method.

5. Numerical results

In this section, we present numerical results for the Lotka-Volterra systems described in Section 2 solving by Kahan's method, and demonstrate the performance of the CDC method. In all examples, we give the results of the runs using Kahan's method with a small time step-size without CDC method, and the ones with the CDC method using Kahan's method for the ODE system (5) and the mid-point rule for the error system (7), with a larger time step-size. Hamiltonian errors $H(0) - H(t)$ are plotted over t. We set $S = 1$ and accordingly $n = 2S + 3 = 5$ in the CDC procedure.

The L^2-error for a Hamiltonian $H(t)$, and the L^2-error between the exact solution $\mathbf{u}_{exact}(t)$ and the numerical solution $\mathbf{u}$ are measured using the following norms

$$L^2(H) = \left(\Delta t \sum_{i=1}^{J} [H(t_i) - H(0)]^2 \right)^{1/2}, \quad L^2(\mathbf{u}) = \left(\Delta t \sum_{i=1}^{J} [\mathbf{u}_i - \mathbf{u}_{ref}(t_i)]^2 \right)^{1/2},$$

where an highly accurate reference solution $\mathbf{u}_{ref}(t)$ is obtained by MATLAB's *ode45* solver in which we set the relative and the absolute tolerances as 10^{-13}. The order of accuracy is calculated as

$$\text{order} = \frac{1}{\log 2} \log \left(\frac{\text{Err}_{\Delta t_i}}{\text{Err}_{\Delta t_{i+1}}} \right),$$

where $\text{Err}_{\Delta t_i}$ and $\text{Err}_{\Delta t_{i+1}}$ stand for the L^2-error of an Hamiltonian or the solution, obtained by the consecutive step sizes Δt_i and $\Delta t_{i+1} = \Delta t_i/2$, respectively.

5.1. **Bi-Hamiltonian LVS.** We consider the 3D LVS (3) on the interval $[0, 100]$, with the parameter values $(a, b, c, \lambda, \mu, \nu) = (-1, -1, -1, 0, 1, -1)$ [21]. The initial condition is taken as $(u_1(0), u_2(0), u_3(0))^T = (1, 1.9, 0.5)^T$.

We show that Kahan's method preserves the periodicity of the solutions and the Hamiltonians in Figure 1. It was proved in [19] that Kahan's method preserves the periodicity of LVSs (1). The average vector field method, which preserves the Poisson structure, was also applied to LVSs (1) in [22]. It was shown there that the first Hamiltonian H_1 of (3) is preserved, but the Casimir H_2 shows a drift in long term integration.

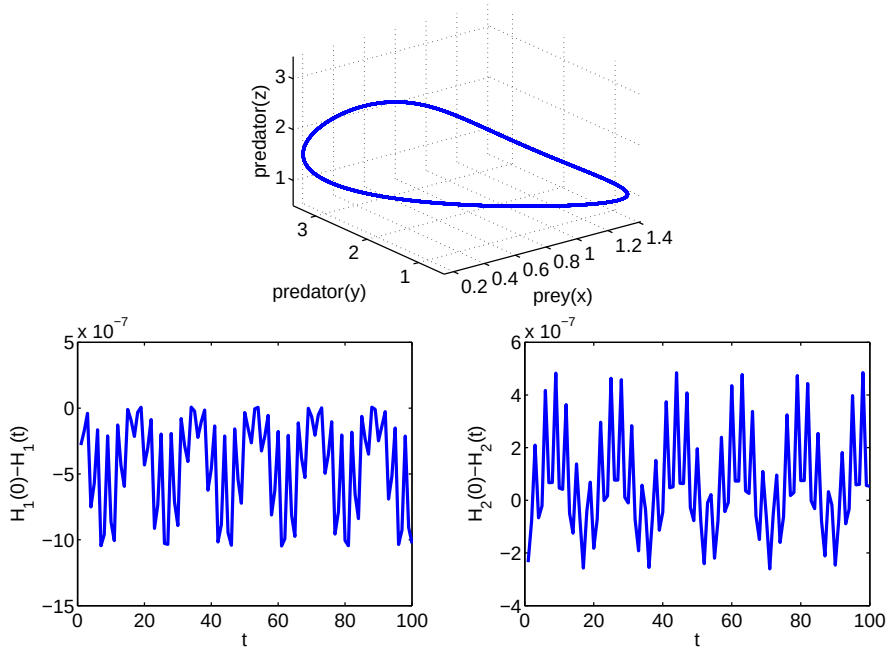

FIGURE 1. Example 5.1 without CDC: (Top) Periodic solutions; (Bottom) errors of Hamiltonians H_1 (left) and H_2 (right) from the initials: $\Delta t = 0.001$

When the CDC method is applied with $S = 1$, $n = 2S+3 = 5$ and with the use of larger time step-size $\Delta t = 0.01$, the periodicity of the solutions and Hamiltonians H_1 and H_2 are preserved in Figure 2. Compared with the numerical results in Figure 1, it turns out that the use of CDC method is not only provides more accurate preservation but also is more

efficient in terms of the time step size. In Figure 2, a slow drift in the preservation of the Hamiltonians is observed. When composition methods are applied to Kahan's method, a comparatively more rapid Hamiltonian drift is observed [41].

In Figure 3, we give the L^2-errors and convergence orders of the solutions, Hamiltonians H_1 and H_2 for different correction number S related with the number of nodes $n = 2S+3$. When the errors reach about 10^{-10} level, the computations are stopped. With increasing number of correction step S, larger time steps are used to attain a prescribed order, which demonstrates the computational efficiency of CDC methods.

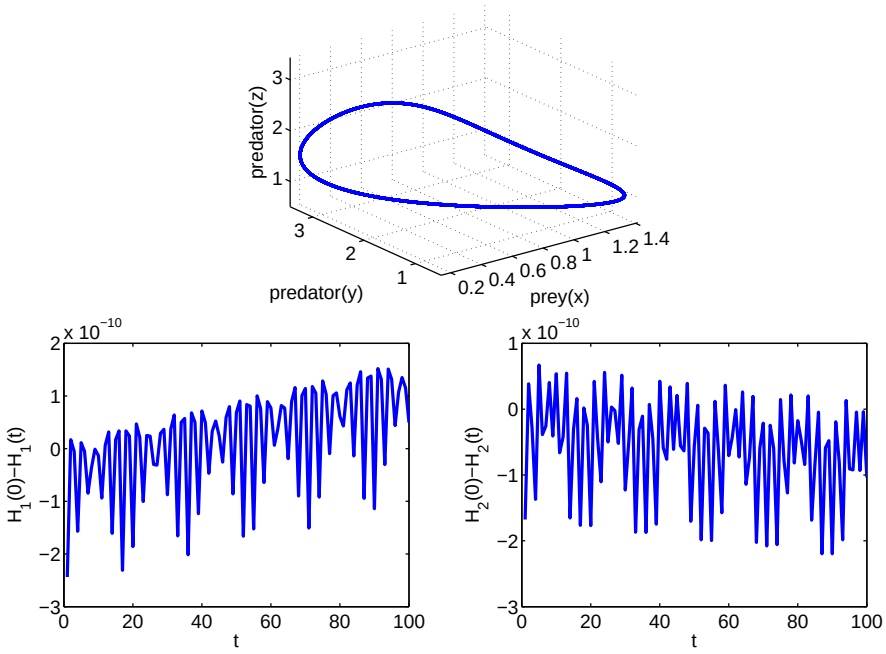

FIGURE 2. Example 5.1 with CDC: (Top) Periodic solutions; (Bottom) errors of Hamiltonians H_1 (left) and H_2 (right) from the initials: $\Delta t = 0.01$, $S = 1$, $n = 5$

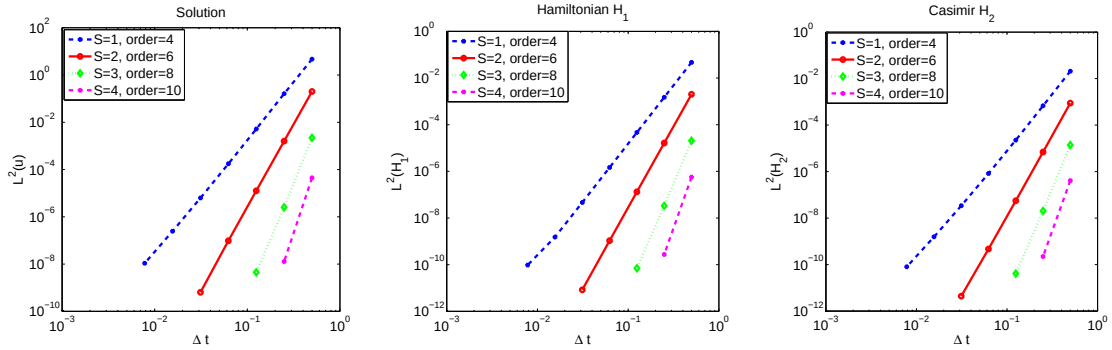

FIGURE 3. Example 5.1 with CDC: L^2-errors and convergence orders for the solution (left), Hamiltonians H_1 (right) and H_2 (right), with the choice $n = 2S + 3$

TABLE 1. Example 5.1: Convergence rates

S/n	5	6	7	8	9	10	11	12	13
1	**4.48**	4.53	4.65	4.47	4.75	4.72	4.83	4.76	5.21
2	4.51	6.99	**6.78**	7.07	6.82	6.85	6.79	6.68	6.69
3	4.84	6.95	6.76	8.89	**8.53**	10.73	10.39	9.80	11.24
4	4.84	7.02	6.76	8.89	9.29	11.02	**11.03**	11.81	11.47
5	4.52	7.02	6.76	8.89	8.46	11.02	11.28	11.85	**12.77**

For varying correction number S and node number n, the convergence orders are presented in Table 1 for the preservation of the Hamiltonian H_1. The results for the Hamiltonian H_2 and solutions are similar. The bold-red labeled order in each row corresponds to the setting $n = 2S+3$, and they agree with the expected orders of accuracy. On the other hand, we give the efficiency results in Table 2, where we arrange for each value of S the time-step size to be used in the CDC method so that the error for the Hamiltonian H_1 is about the same level of accuracy (about 10^{-6}) with the one obtained by solutions without the CDC method using a small time-step size $\Delta t = 0.001$. We see from the speed-up in Table 2 that by the use of CDC method, the computational efficiency is gained with the same level of accuracy, which is calculated as the ratio of the Wall Clock time required for the run without CDC method over the Wall Clock time required for the one with the CDC method.

TABLE 2. Example 5.1: Speed-ups over the system without CDC, $n = 2S+3$ is taken in CDC scheme

	S	$L^2(H_1)$	Δt	Wall Clock (Sec.)	Speed-Up
Without CDC	-	1.05e-06	0.001	10.57	-
With CDC	1	2.77e-06	0.04	1.20	8.8
	2	1.53e-06	0.15	0.69	15.4
	3	1.11e-06	0.31	0.66	16.9
	4	1.81e-06	0.40	0.65	14.3
	5	1.67e-06	0.60	0.70	15.1

5.2. **Reversible LVS.** We consider the reversible LVS (4) on the interval $[0, 100]$, and with the initial conditions $(u_1(0), u_2(0), u_3(0))^T = (0.3, 0.3, 0.4)^T$ [21].

Kahan's method preserves again the periodicity of the reversible LVS (4), Figure 4, top. The reversible LVS (4) was solved in [40] using a conservative multiplier method. It was shown that the linear Hamiltonian H_1 is preserved with an accuracy 10^{-15} and the cubic Hamiltonian H_2 with an accuracy 10^{-14}. Kahan's method also preserves the linear Hamiltonian H_1 and cubic Hamiltonian H_2 accurately in Figure 4, bottom.

Preservation of the periodicity of the solutions and the Hamiltonians in the case of CDC method are presented in Figure 5, which are obtained by using a much more larger step size. Again, similar convergence orders are attained in Figure 6.

6. CONCLUSIONS

We have shown that the Hamiltonians of 3D LVSs can be preserved with a high accuracy, when we use CDC methods based on the Kahan's discretization for quadratic vector fields. In a future work, the integral and spectral correction methods using Gauss-Lobatto collocation points will be applied.

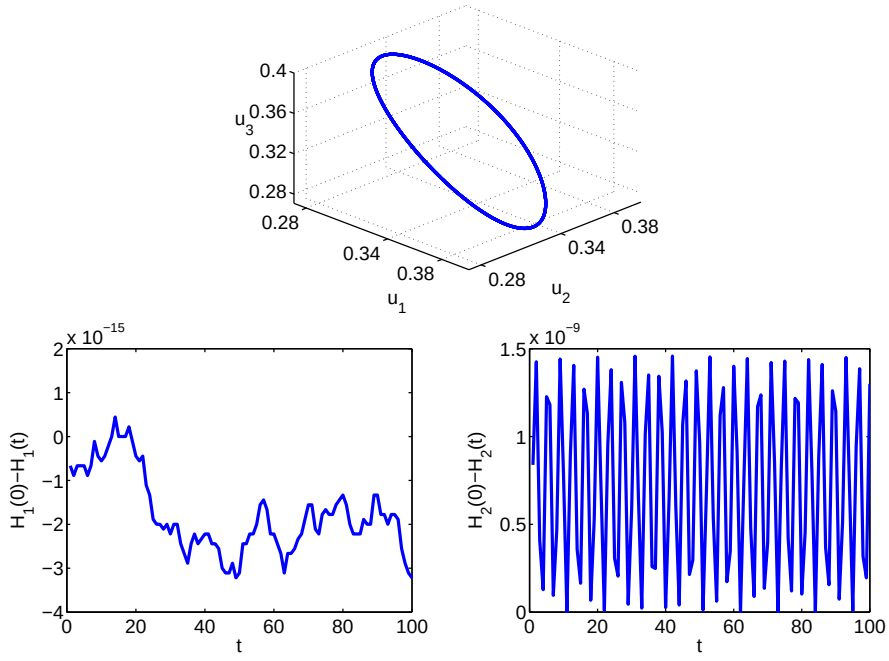

FIGURE 4. Example 5.2 without CDC: (Top) Periodic solutions; (Bottom) errors of Hamiltonians H_1 (left) and H_2 (right) from the initials: $\Delta t = 0.01$

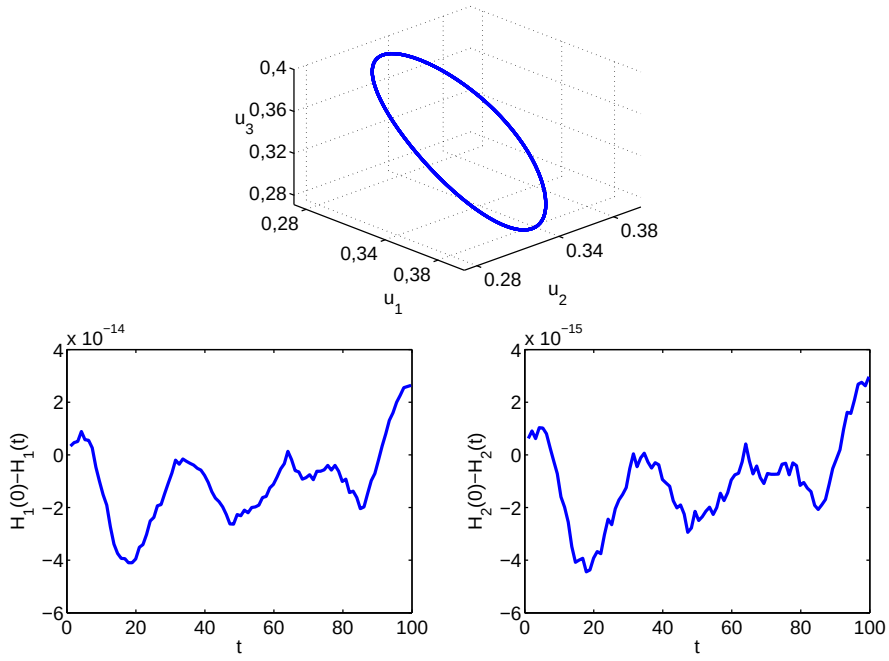

FIGURE 5. Example 5.2 with CDC: (Top) Periodic solutions; (Bottom) errors of Hamiltonians H_1 (left) and H_2 (right) from the initials: $\Delta t = 0.15$, $S = 2$, $n = 7$

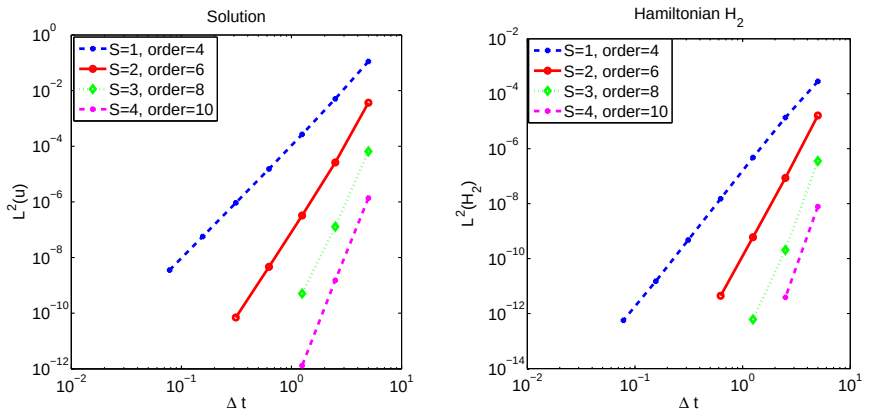

FIGURE 6. Example 5.2 with CDC: L^2-errors and convergence orders for the solution (left) and Hamiltonian H_2 (right), with the choice $n = 2S + 3$

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